

Synthesis of 1-(*para*-methoxyphenyl)tetrazolyl-Substituted 1,2,3,4-Tetrahydroisoquinolines and Their Transformations Involving Activated Alkynes

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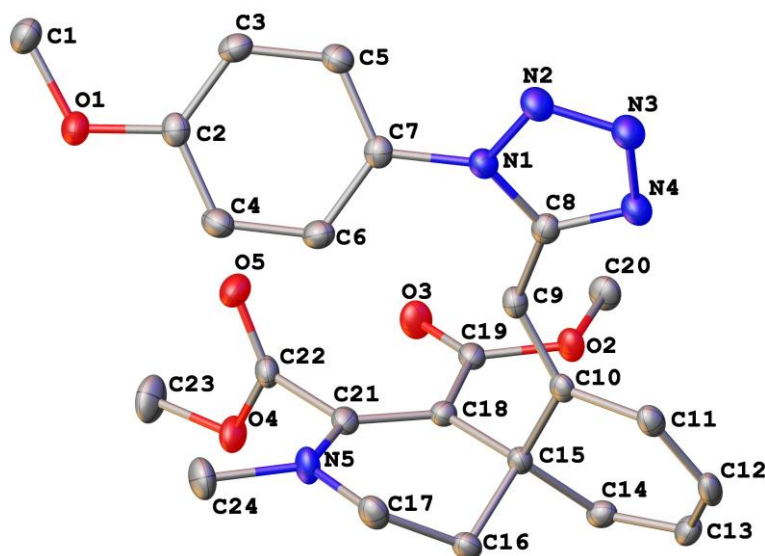


Figure S1. The X-ray crystal diffraction of compound 3 (deposit CCDC 1848342).

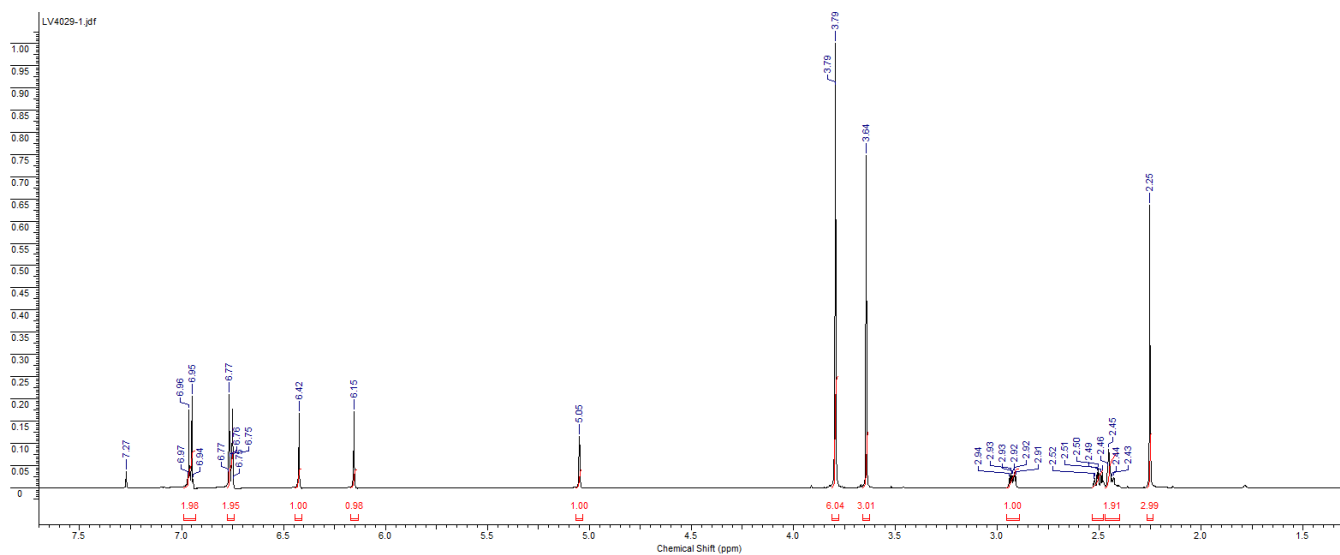
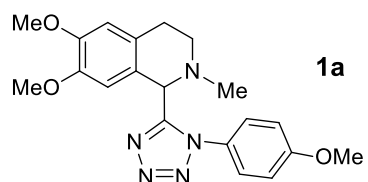


Figure S2. ¹H NMR spectrum of 6,7-dimethoxy-1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinoline **1a**.

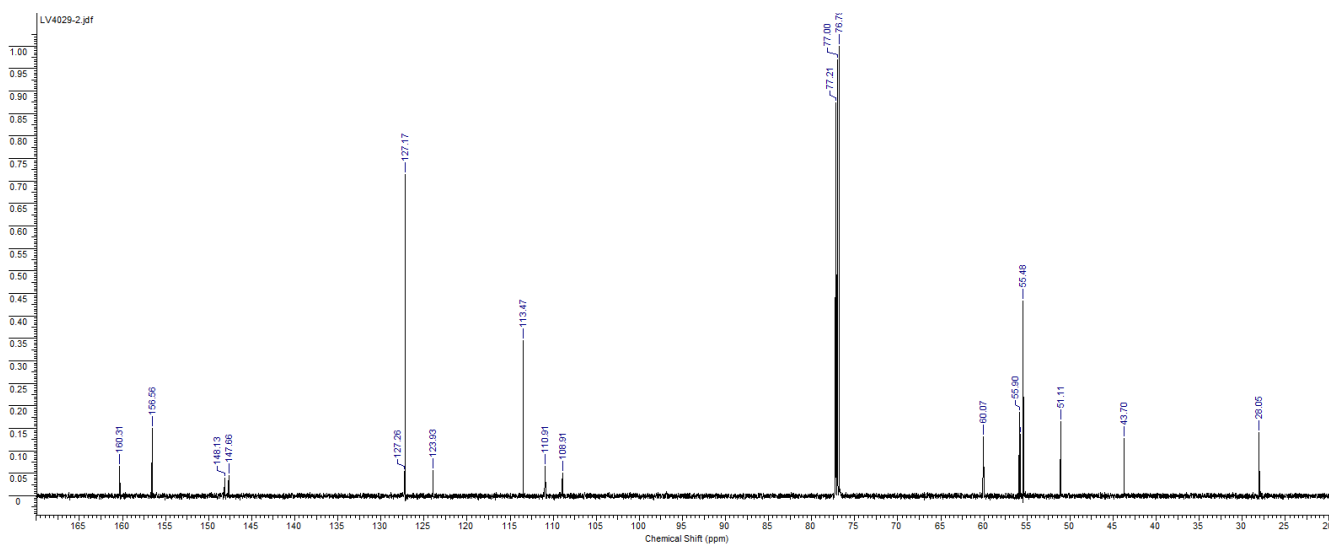


Figure S3. ¹³C NMR spectrum of 6,7-dimethoxy-1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinoline **1a**.

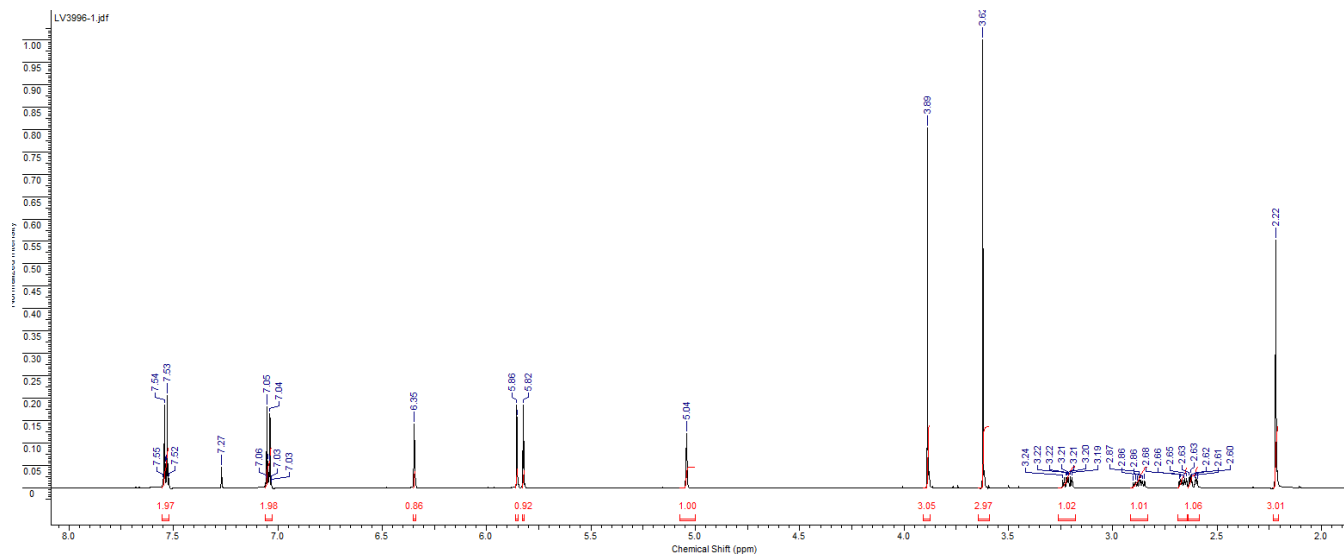
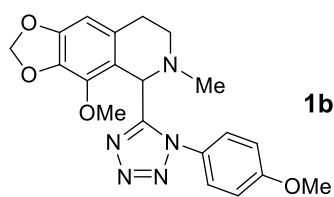


Figure S4. ^1H NMR spectrum of 4-methoxy-5-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-6-methyl-5,6,7,8-tetrahydro[1,3]dioxolo[4,5-*g*]isoquinoline **1b**.

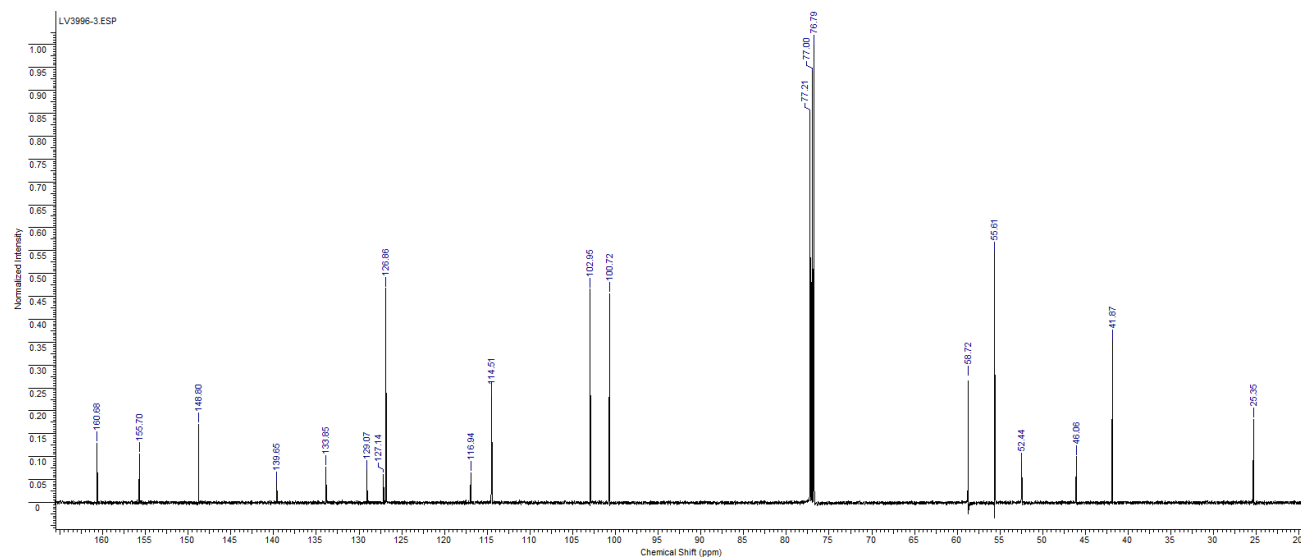


Figure S5. ^{13}C NMR spectrum of 4-methoxy-5-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-6-methyl-5,6,7,8-tetrahydro[1,3]dioxolo[4,5-*g*]isoquinoline **1b**.

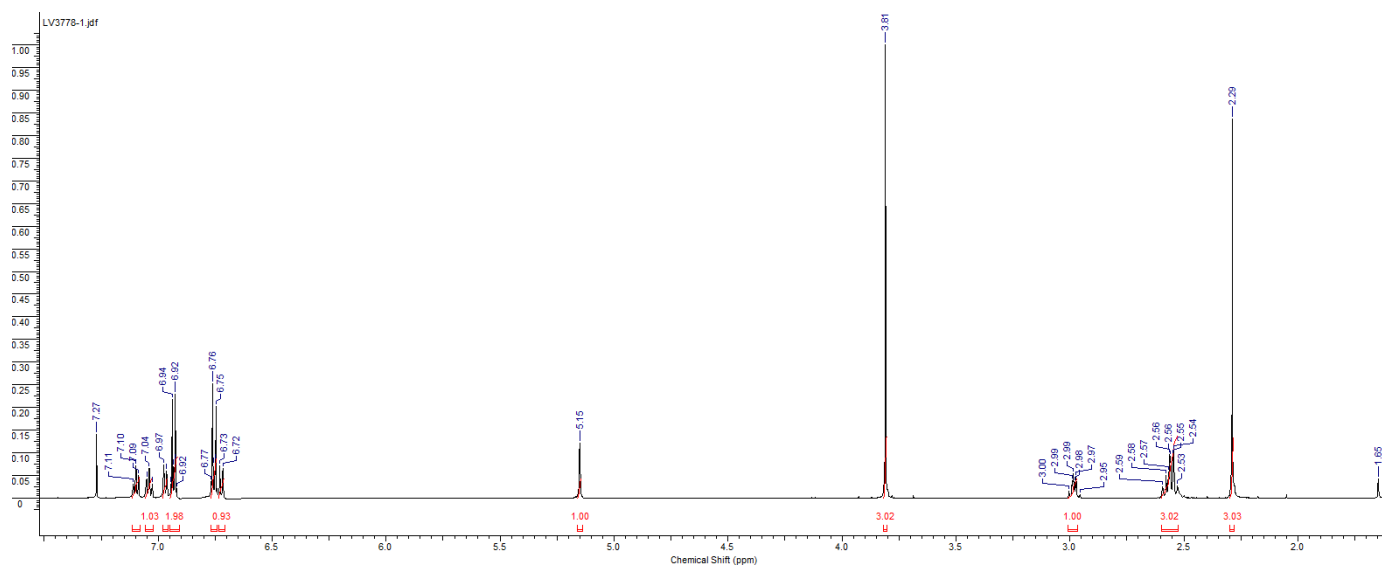
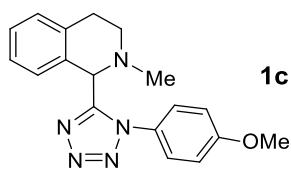


Figure S6. ^1H NMR spectrum of 1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinoline **1c**.

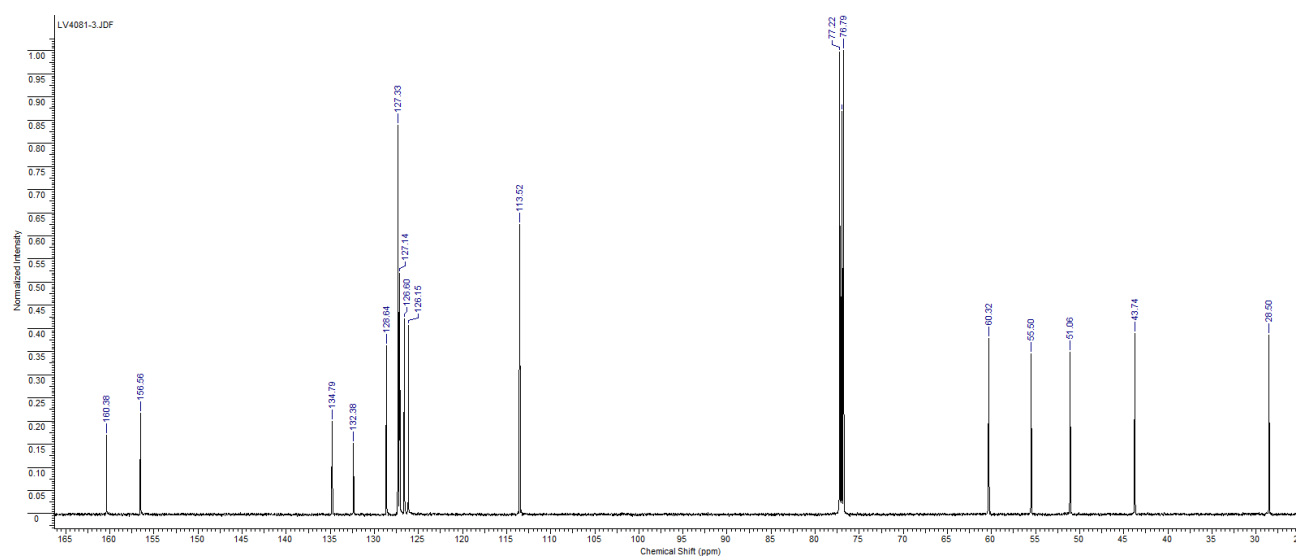


Figure S7. ^{13}C NMR spectrum of 1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinoline **1c**.

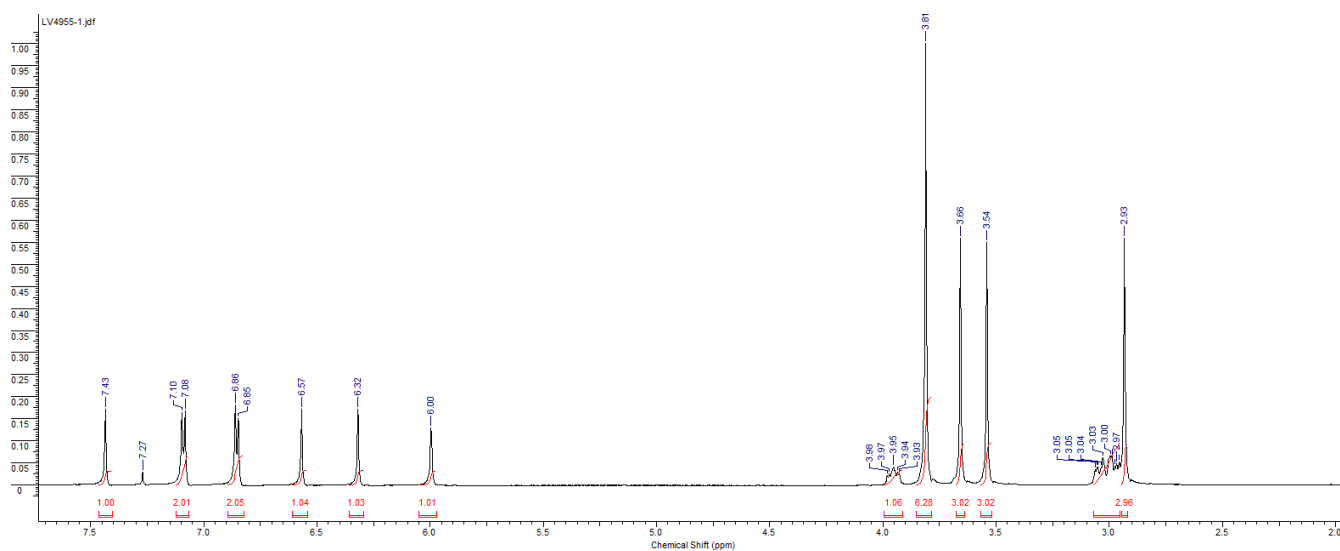
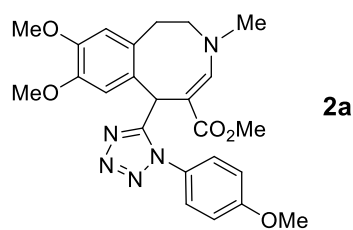


Figure S8. ¹H NMR spectrum of methyl (4E)-8,9-dimethoxy-6-[1-(4-methoxyphenyl)-1H-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-5-carboxylate **2a**.

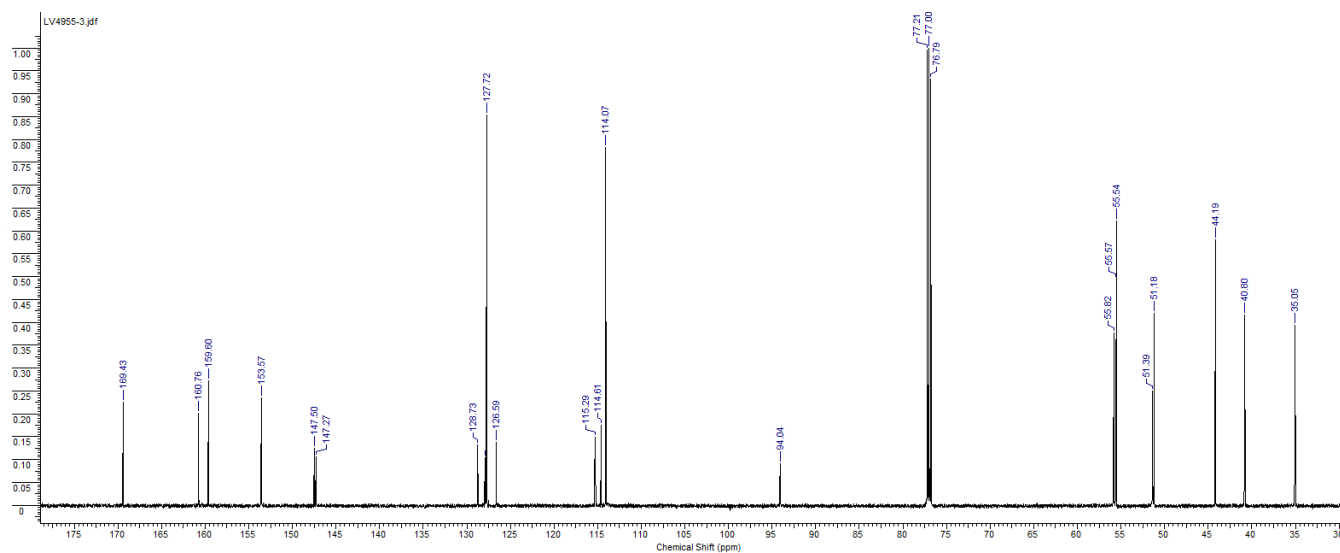


Figure S9. ¹³C NMR spectrum of methyl (4E)-8,9-dimethoxy-6-[1-(4-methoxyphenyl)-1H-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-5-carboxylate **2a**.

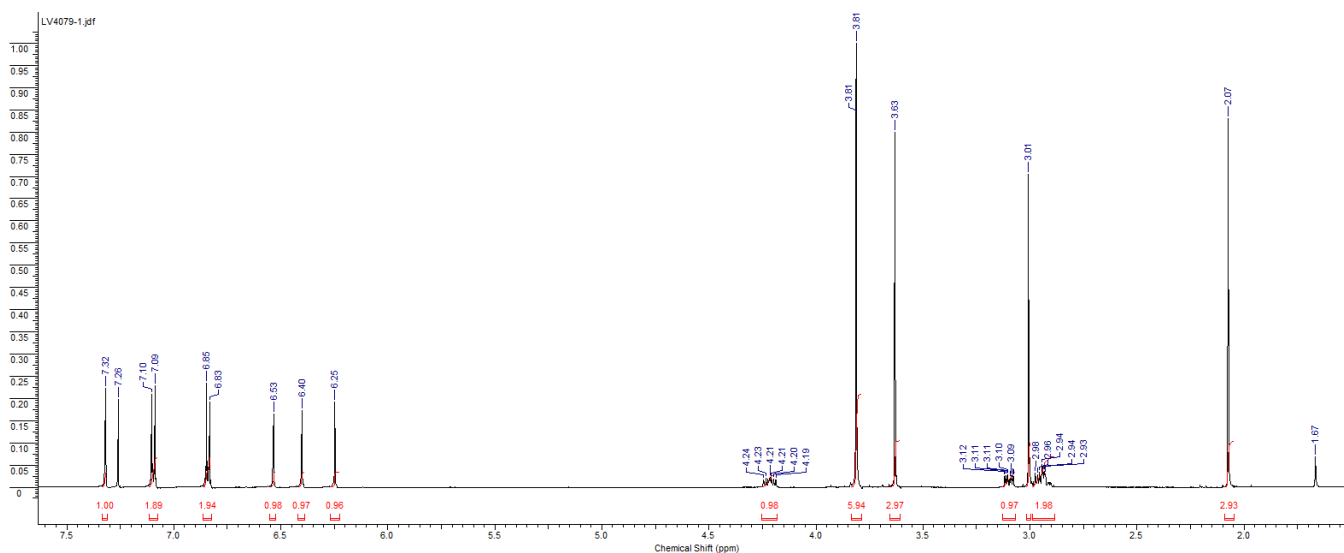
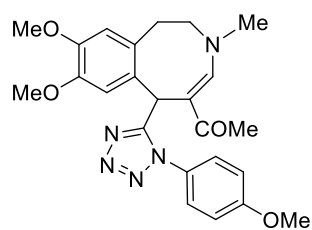


Figure S10. ^1H NMR spectrum of 1-((4E)-8,9-dimethoxy-6-[1-(4-methoxyphenyl)-1H-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocine-5-yl)-ethanone **2b**.

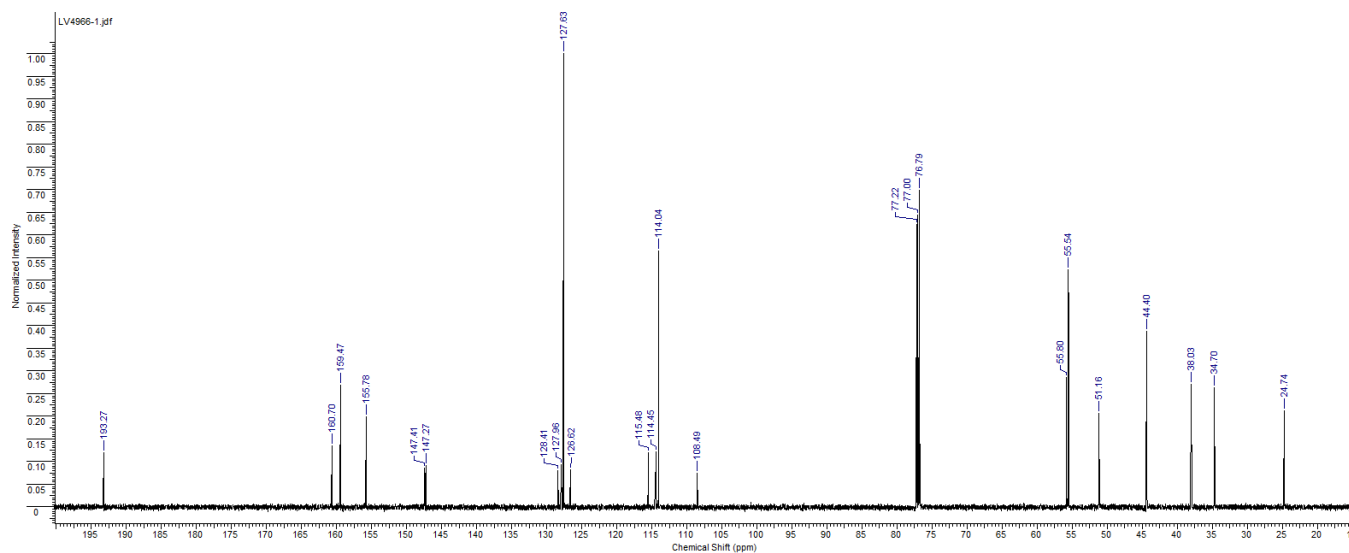


Figure S11. ^{13}C NMR spectrum of 1-((4E)-8,9-dimethoxy-6-[1-(4-methoxyphenyl)-1H-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocine-5-yl)-ethanone **2b**.

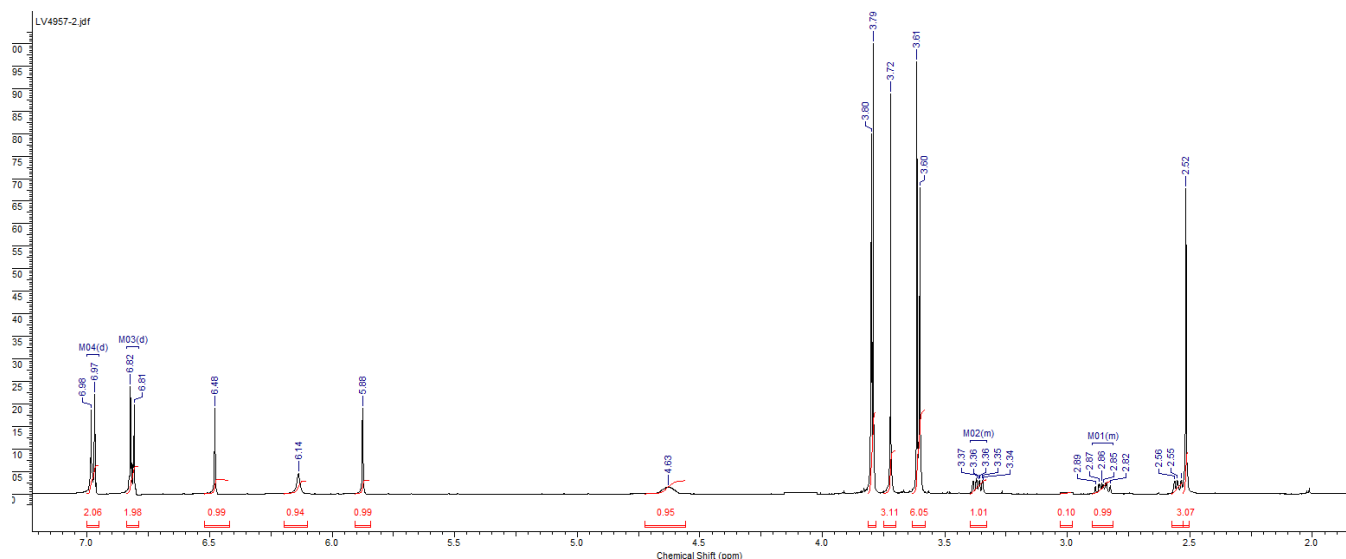
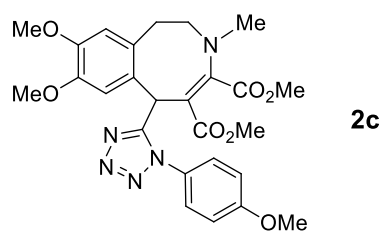


Figure S12. ¹H NMR spectrum of dimethyl (4E)-8,9-dimethoxy-6-[1-(4-methoxyphenyl)-1H-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-4,5-dicarboxylate **2c**.

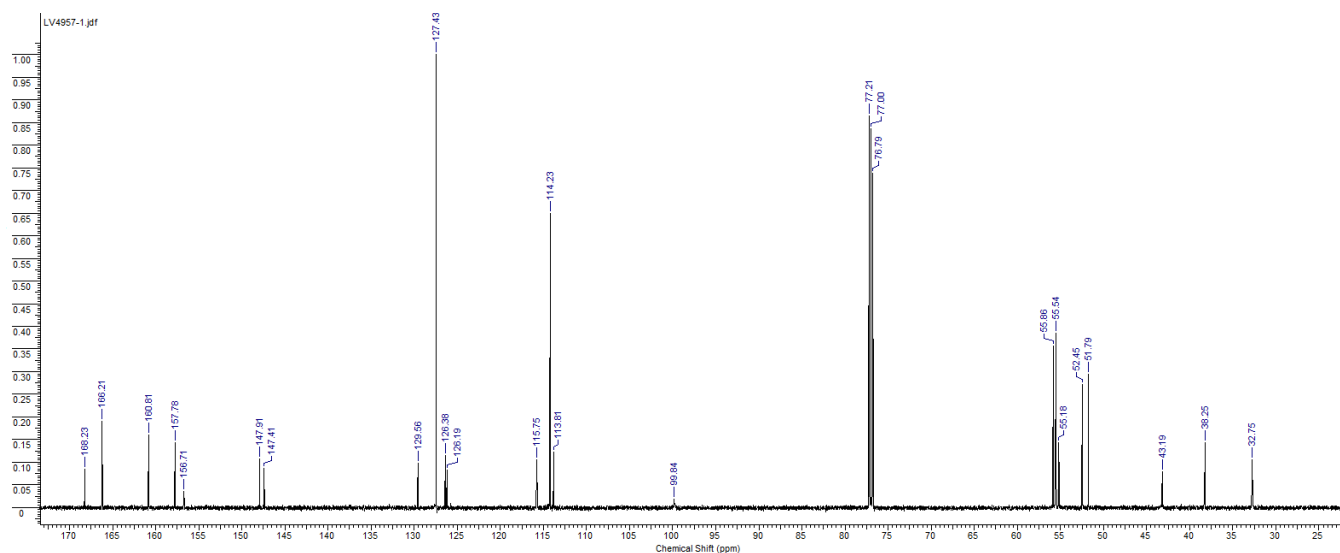


Figure S13. ¹³C NMR spectrum of dimethyl (4E)-8,9-dimethoxy-6-[1-(4-methoxyphenyl)-1H-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-4,5-dicarboxylate **2c**.

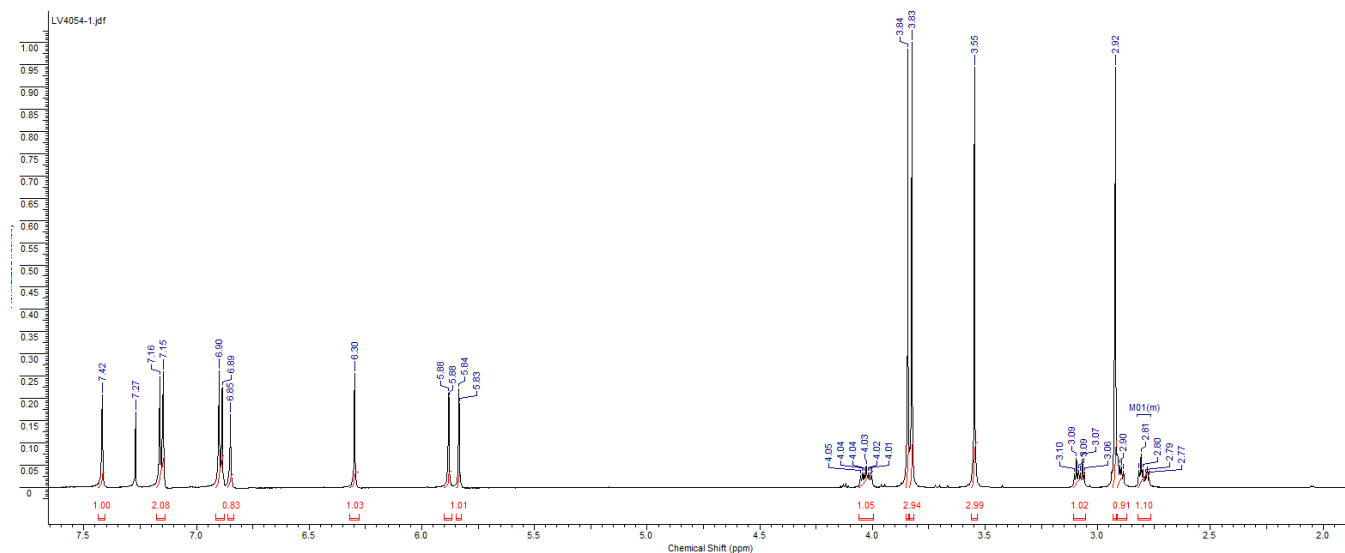
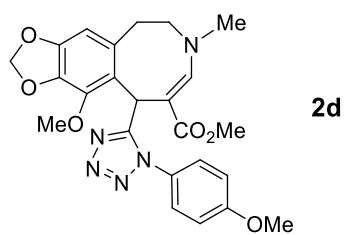


Figure S14. ^1H NMR spectrum of methyl (8*E*)-10-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-7,11-dimethyl-5,6,7,10-tetrahydro[1,3]dioxolo[4,5-*i*][3]benzazocine-9-carboxylate **2d**.

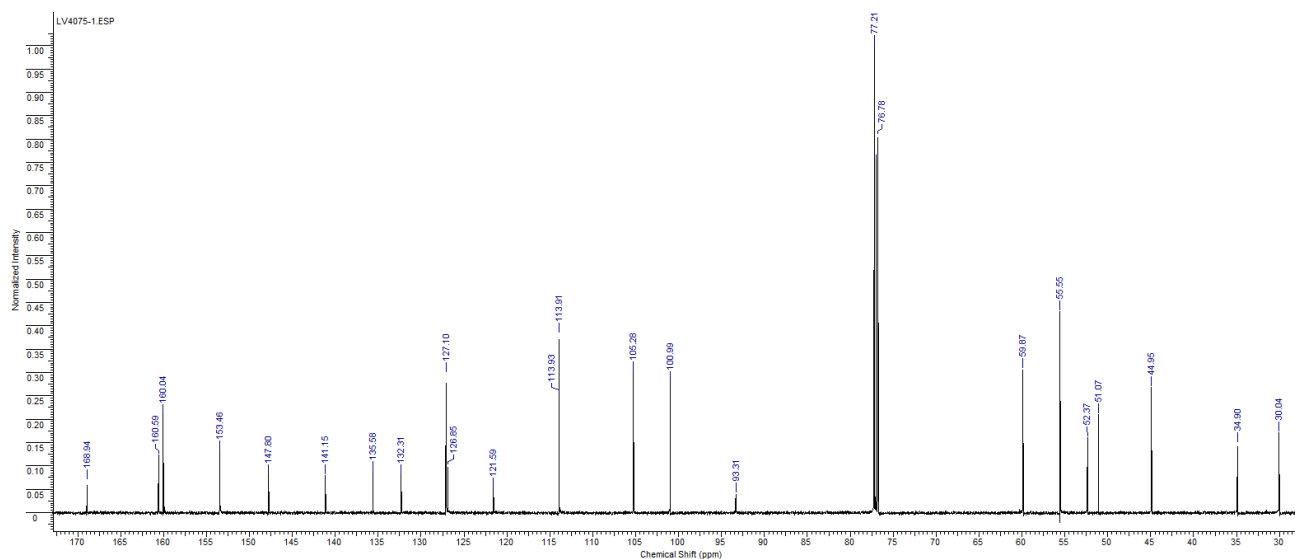


Figure S15. ^{13}C NMR spectrum of methyl (8*E*)-10-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-7,11-dimethyl-5,6,7,10-tetrahydro[1,3]dioxolo[4,5-*i*][3]benzazocine-9-carboxylate **2d**.

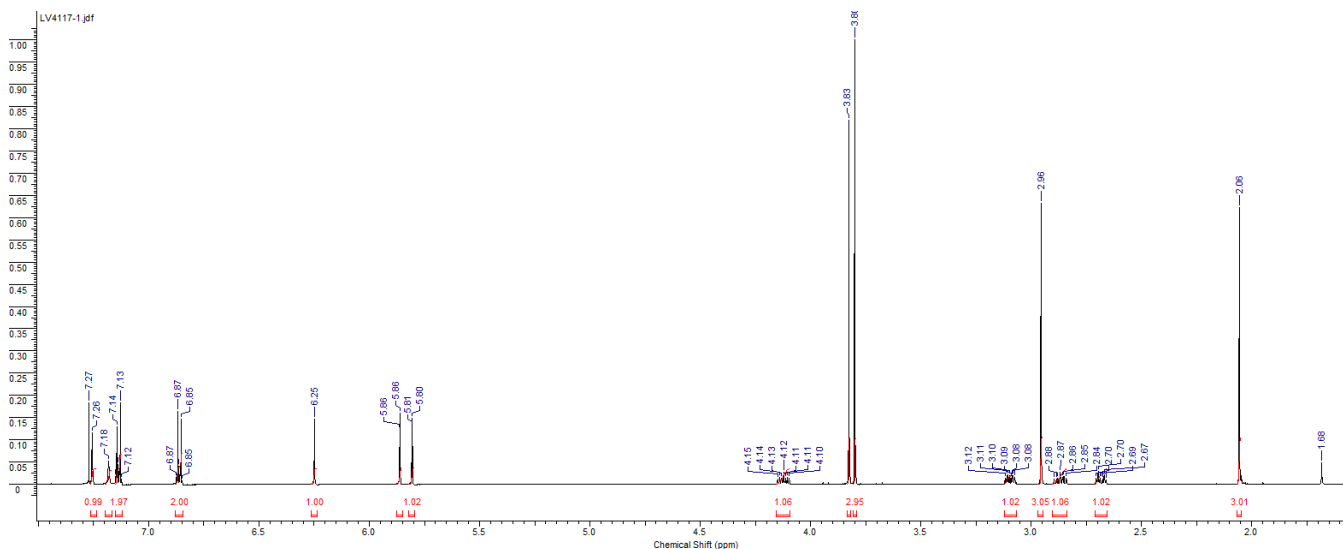
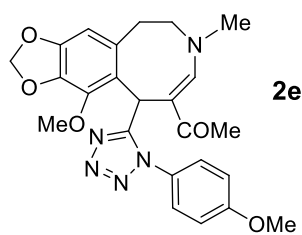


Figure S16. ^1H NMR spectrum of 1-{(8*E*)-11-methoxy-10-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-7-methyl-5,6,7,10-tetrahydro[1,3]dioxolo[4,5-*i*][3]benzazocin-9-yl} ethanone **2e**.

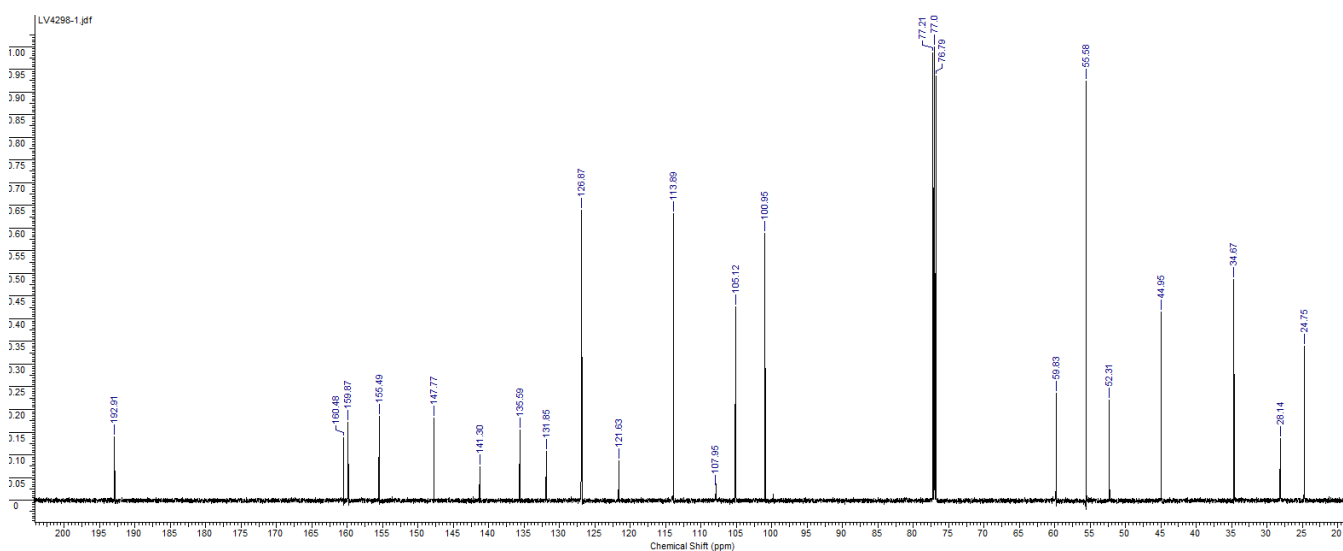


Figure S17. ^{13}C NMR spectrum of 1-{(8*E*)-11-methoxy-10-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-7-methyl-5,6,7,10-tetrahydro[1,3]dioxolo[4,5-*i*][3]benzazocin-9-yl} ethanone **2e**.

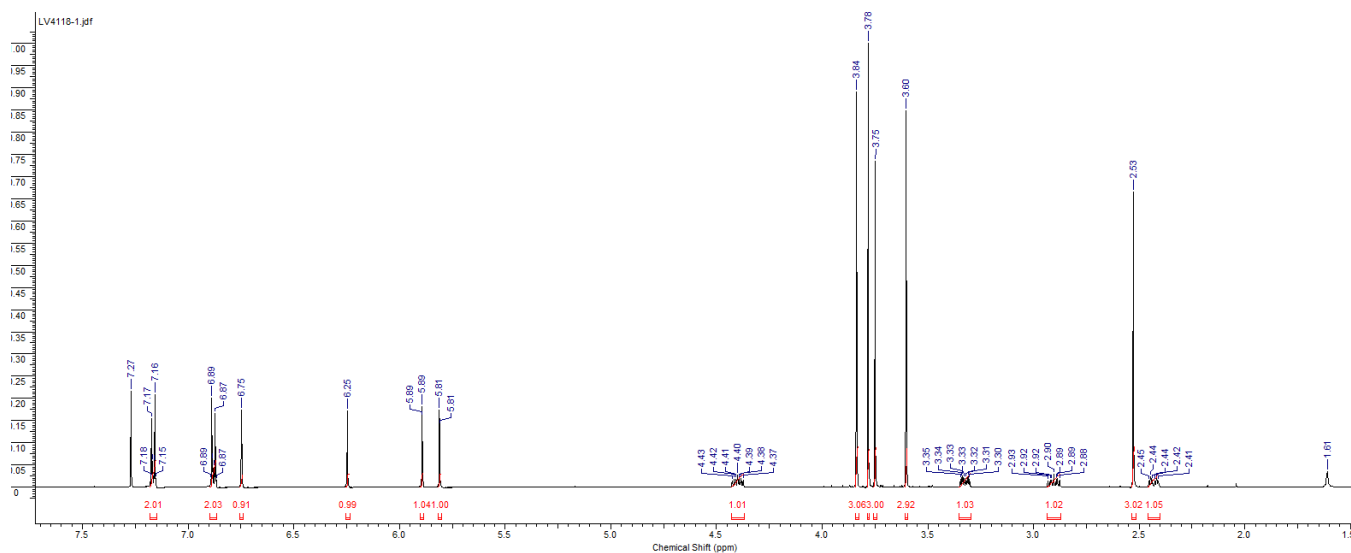
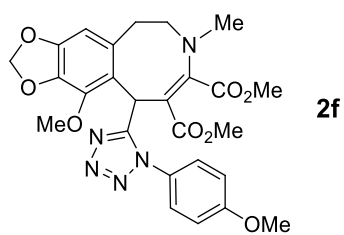


Figure S18. ^1H NMR spectrum of dimethyl (8*E*)-11-methoxy-10-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-7-methyl-5,6,7,10-tetrahydro[1,3]dioxolo[4,5-*i*][3]benzazocin-8,9-dicarboxylate **2f**.

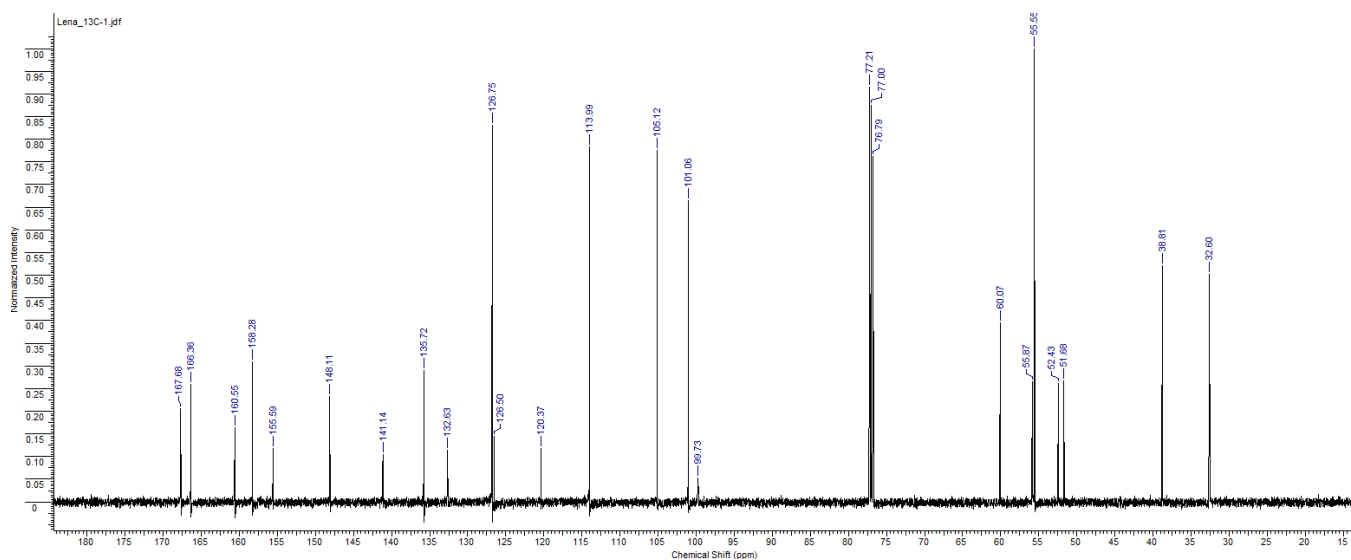


Figure S19. ^{13}C NMR spectrum of dimethyl (8*E*)-11-methoxy-10-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-7-methyl-5,6,7,10-tetrahydro[1,3]dioxolo[4,5-*i*][3]benzazocin-8,9-dicarboxylate **2f**.

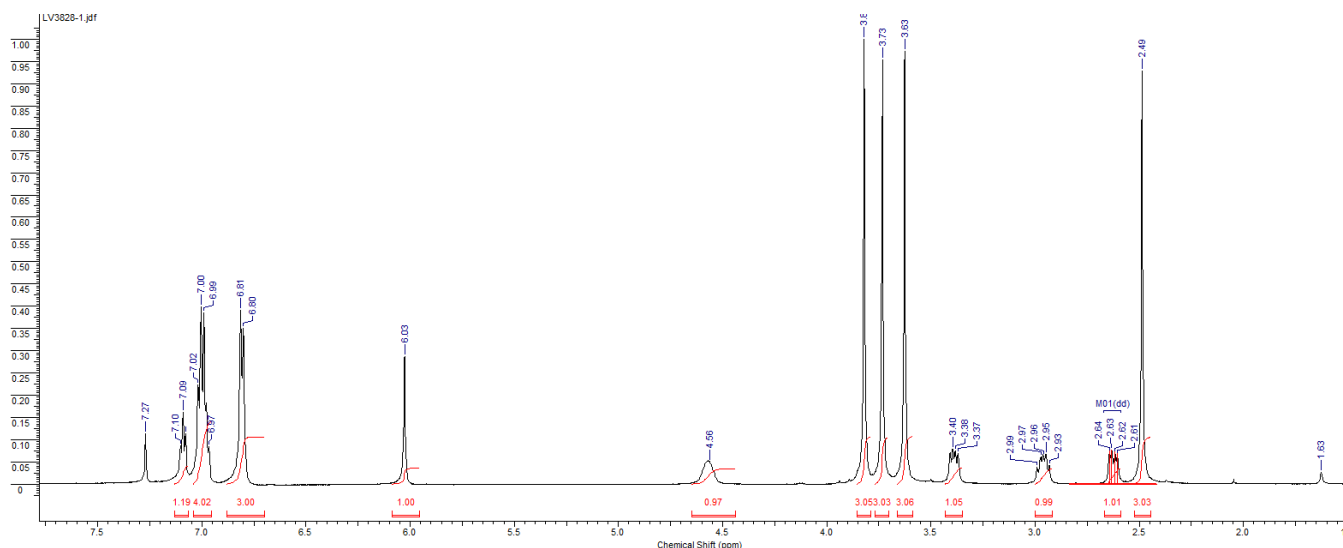
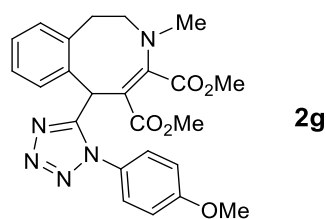


Figure S20. ^1H NMR spectrum of dimethyl 6-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-4,5-dicarboxylate **2g**.

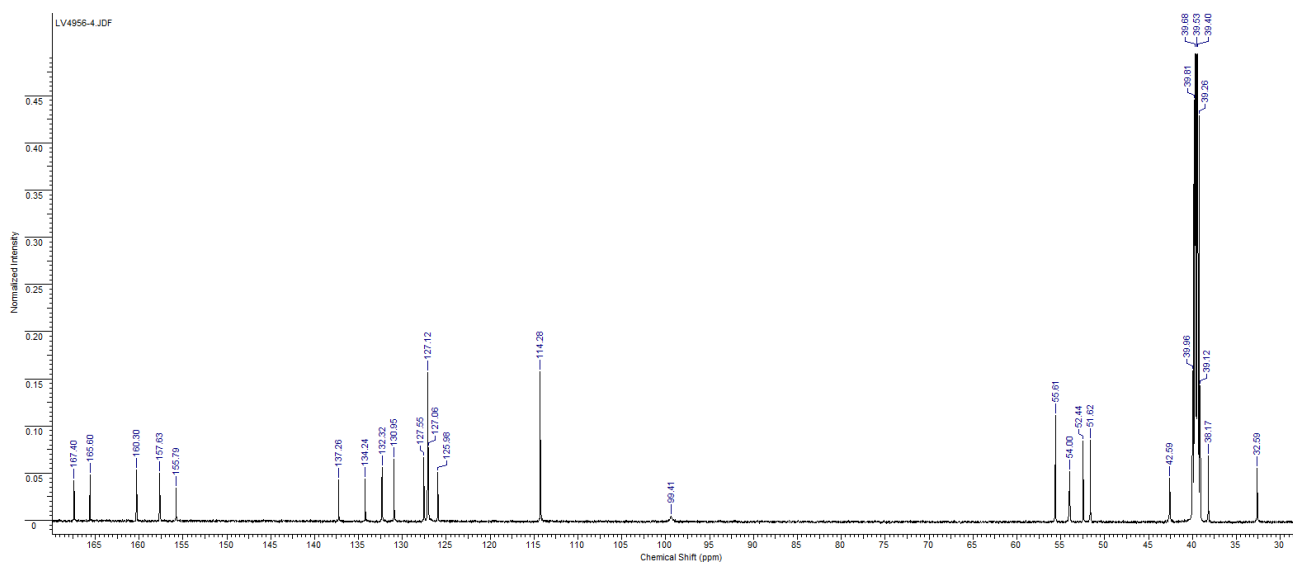


Figure S21. ^{13}C NMR spectrum of dimethyl 6-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-4,5-dicarboxylate **2g**.

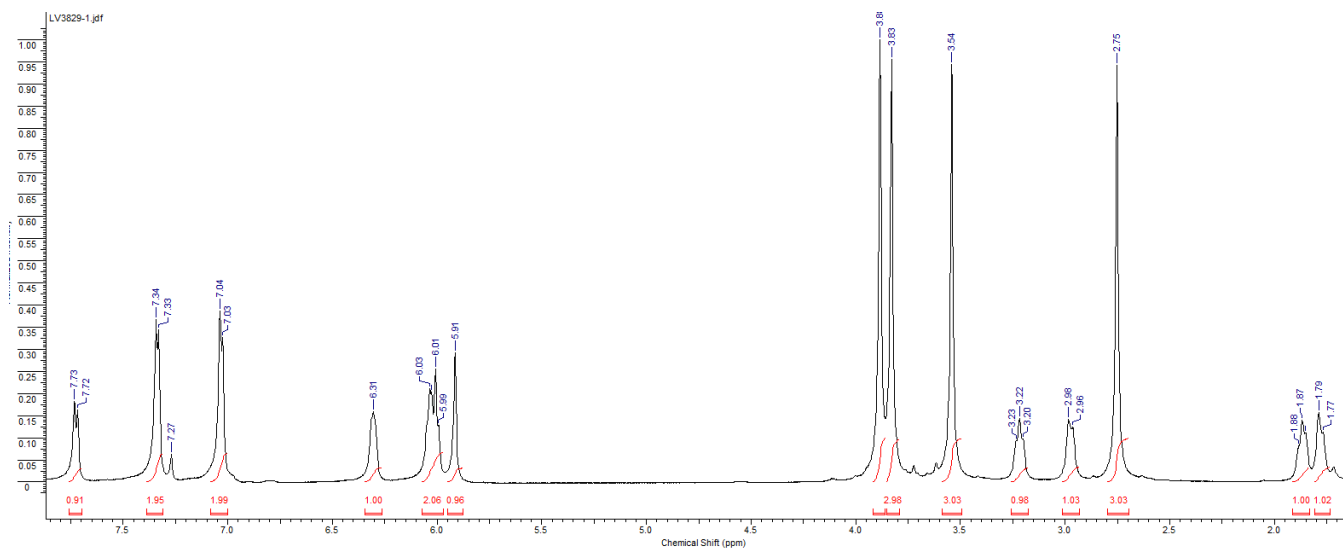
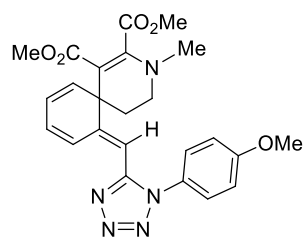


Figure S22. ^1H NMR spectrum of dimethyl (11*E*)-11-{[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]methylidene}-3-methyl-3-azaspiro[5.5]undeca-1,7,9-triene-1,2-dicarboxylate **3**.

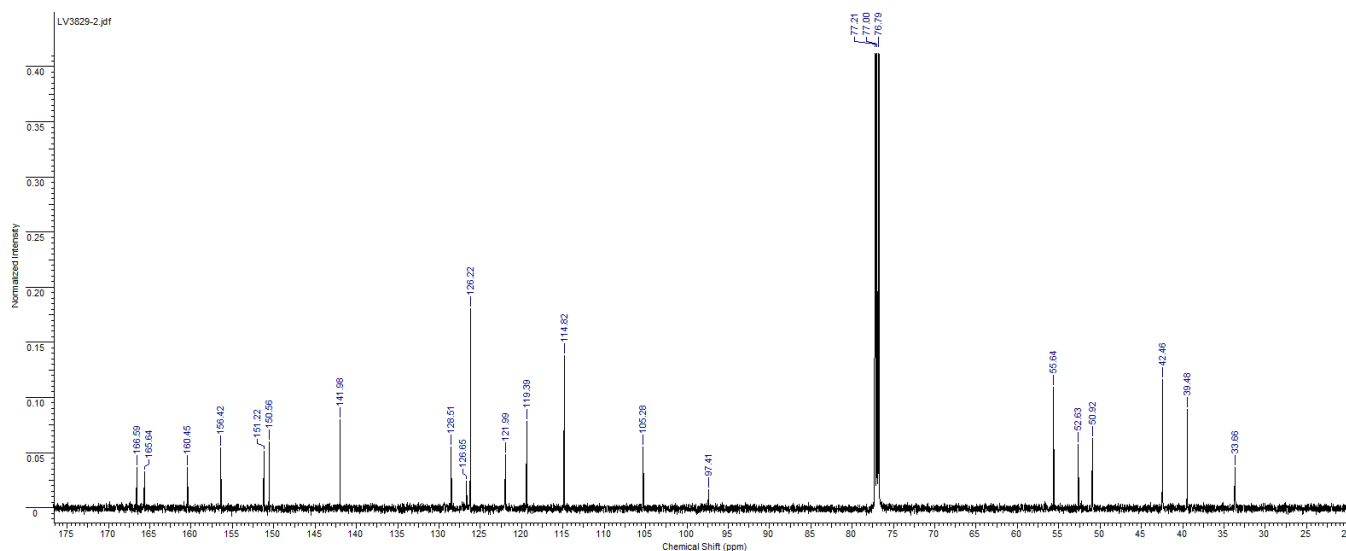


Figure S23. ^{13}C NMR spectrum of dimethyl (11*E*)-11-{[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]methylidene}-3-methyl-3-azaspiro[5.5]undeca-1,7,9-triene-1,2-dicarboxylate **3**.

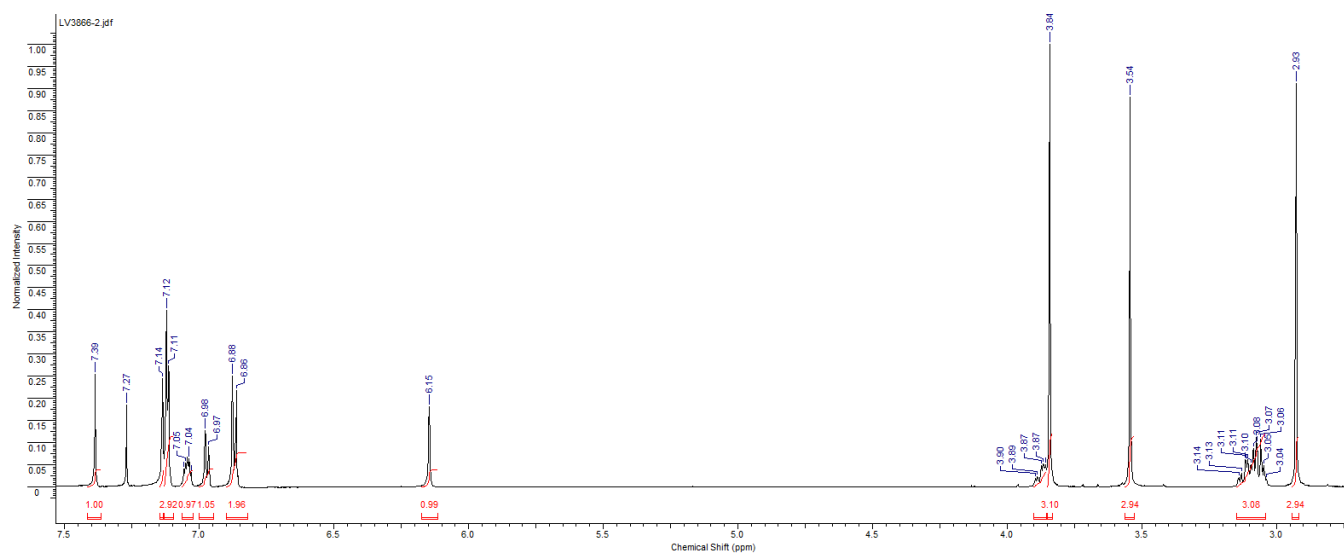
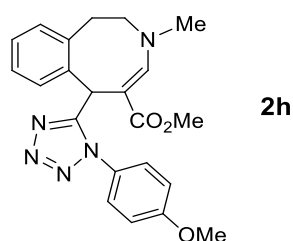


Figure S24. ^1H NMR spectrum of methyl (4*E*)-6-[1-(4-methoxyphenyl) -1*H*-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-5-carboxylate **2h**.

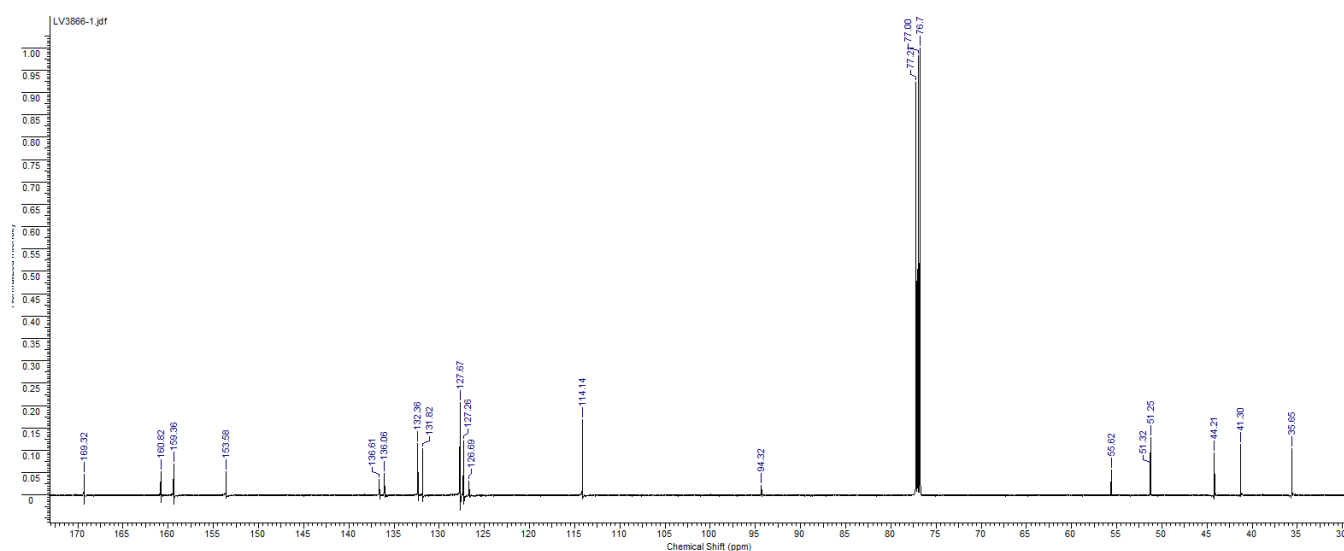


Figure S25. ^{13}C NMR spectrum of methyl (4*E*)-6-[1-(4-methoxyphenyl) -1*H*-tetrazol-5-yl]-3-methyl-1,2,3,6-tetrahydro-3-benzazocin-5-carboxylate **2h**.

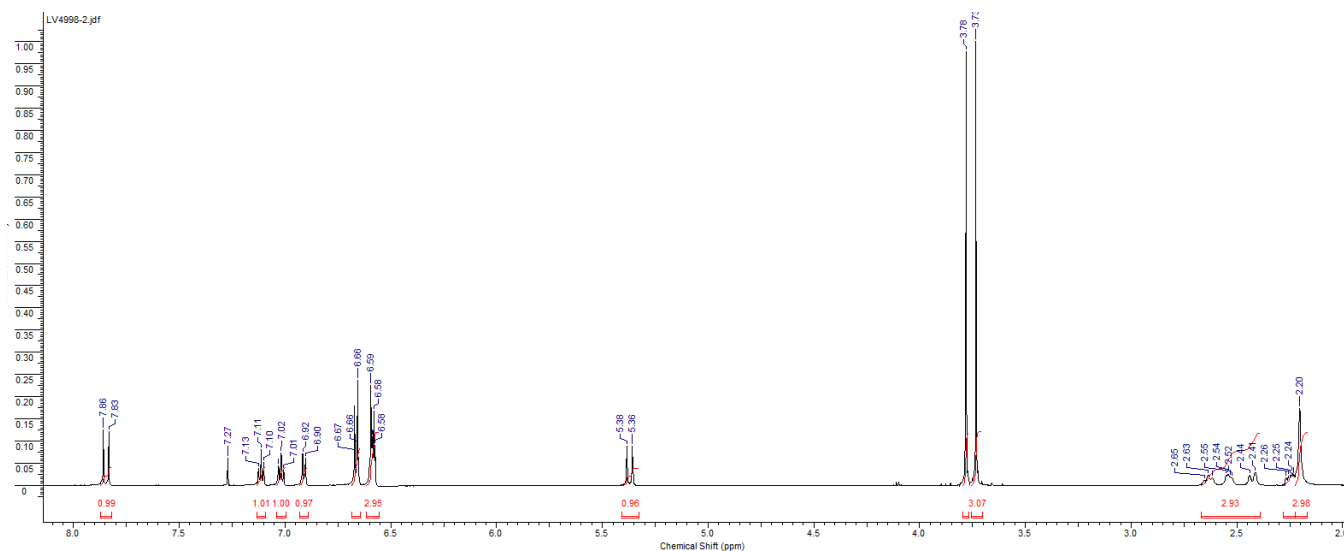
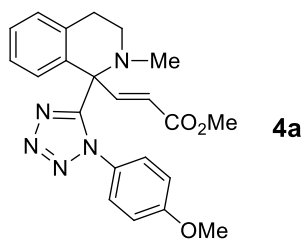


Figure S26. ^1H NMR spectrum of methyl (2*E*)-3-{1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl}prop-2-enoate **4a**.

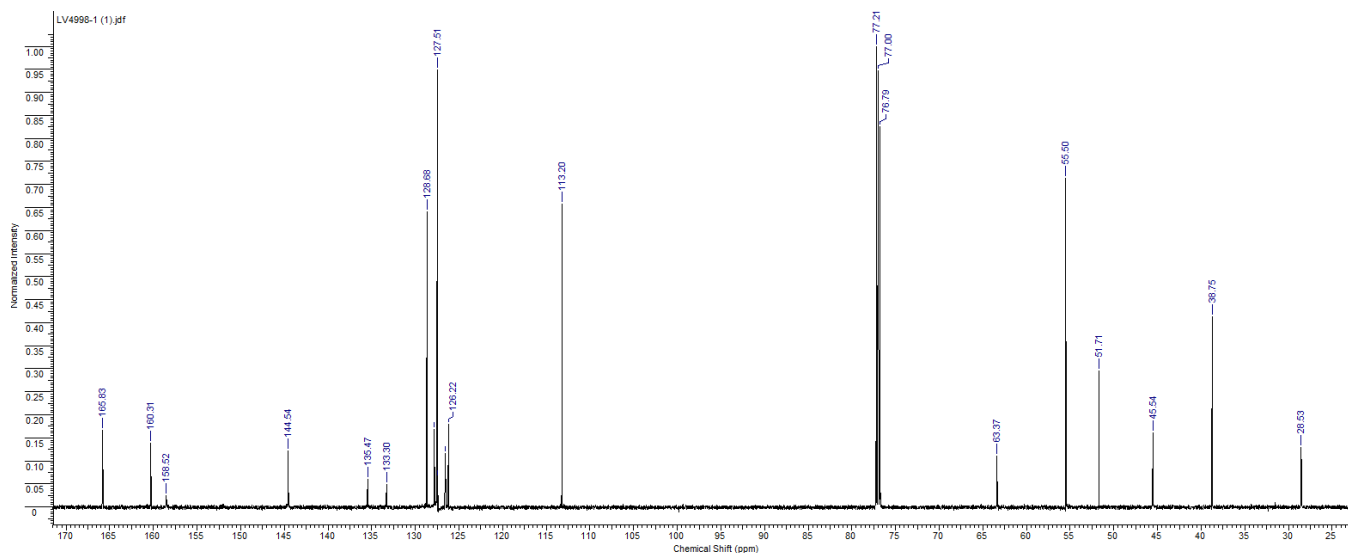


Figure S27. ^{13}C NMR spectrum of methyl (2*E*)-3-{1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl}prop-2-enoate **4a**.

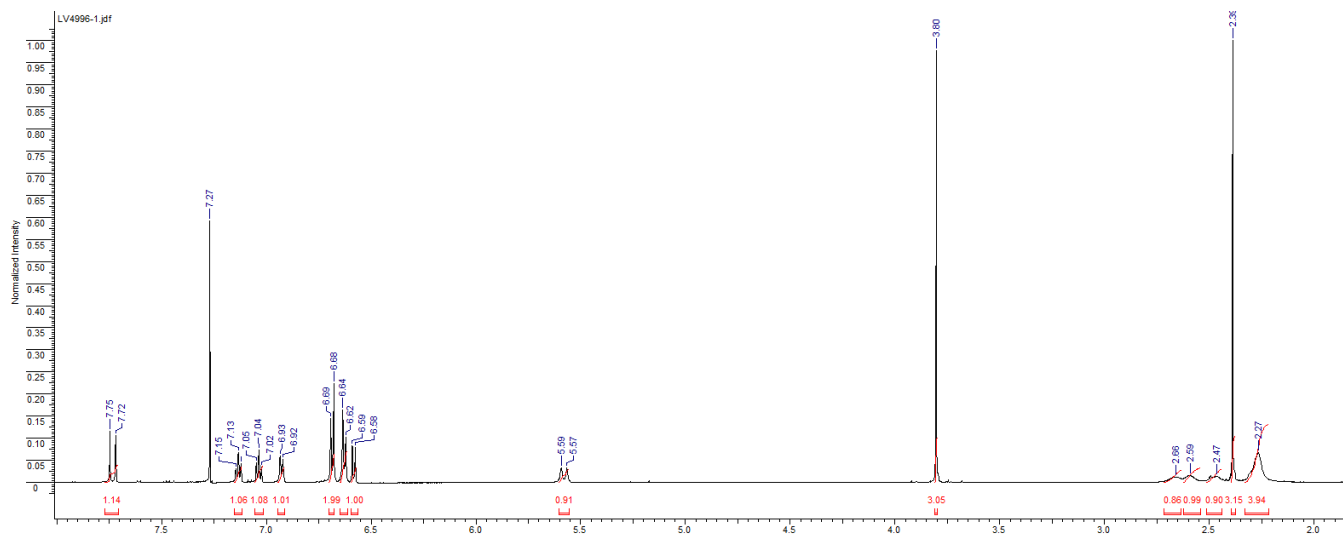
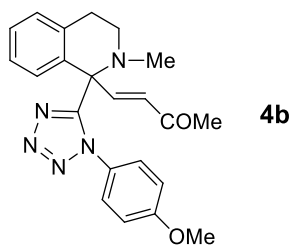


Figure S28. ^1H NMR spectrum of (3*E*)-4-{1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl}but-3-ene-2-one **4b**.

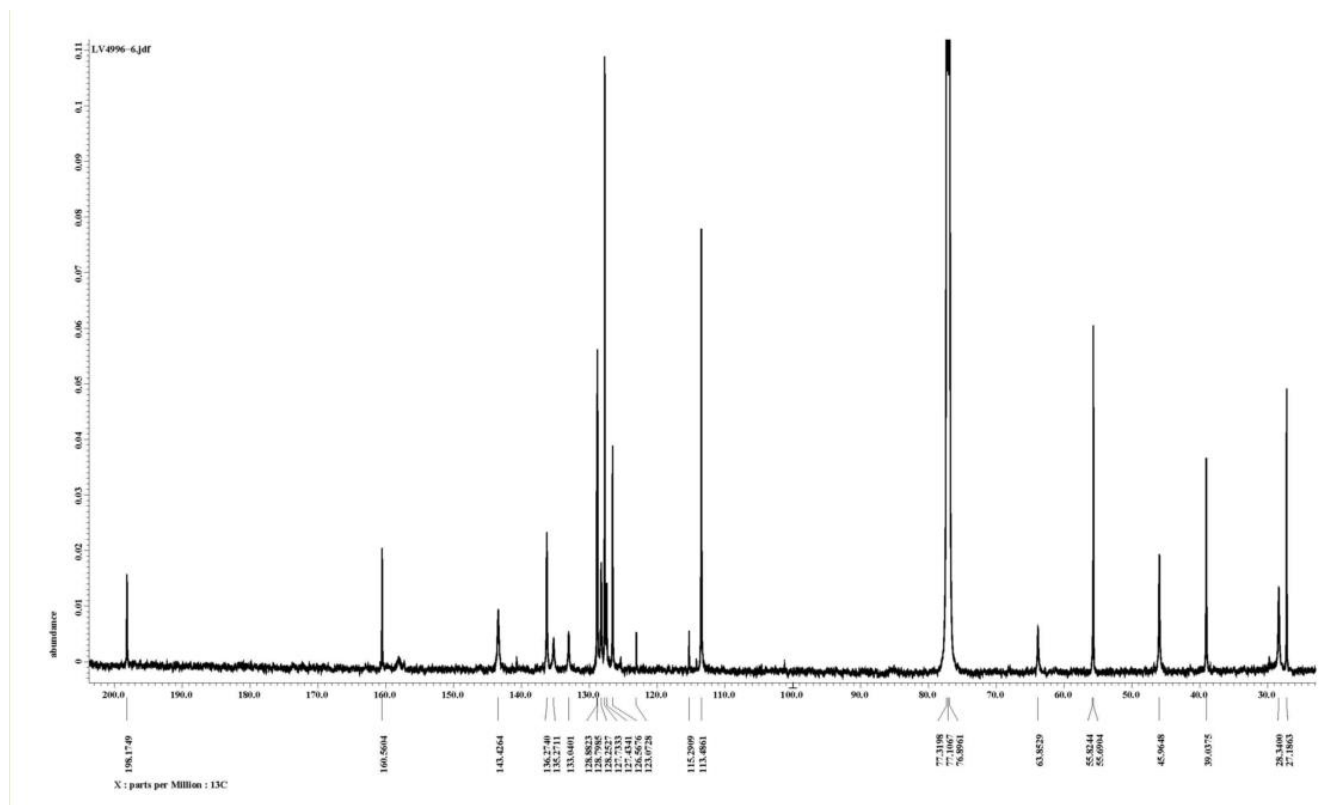


Figure S29. ^{13}C NMR spectrum of (3*E*)-4-{1-[1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl]-2-methyl-1,2,3,4-tetrahydroisoquinolin-1-yl}but-3-ene-2-one **4b**.