

SUPPLEMENTARY MATERIAL

**Microwave-assisted synthesis, molecular docking studies of
1,2,3- Triazole based carbazole derivatives as antimicrobial,
antioxidant, anticancer agents**

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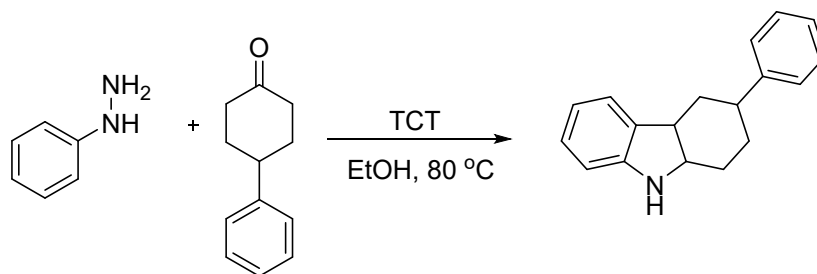
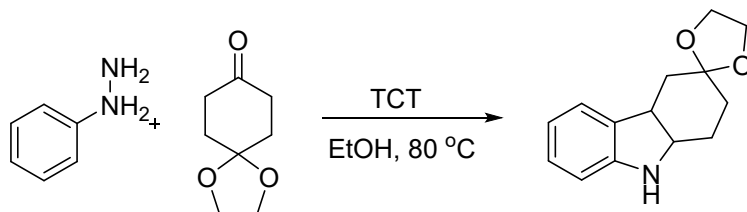
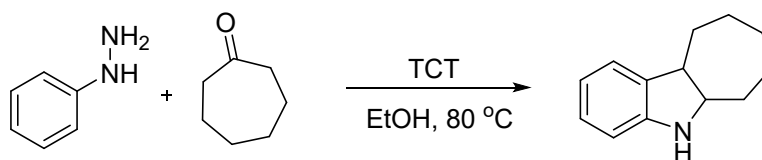
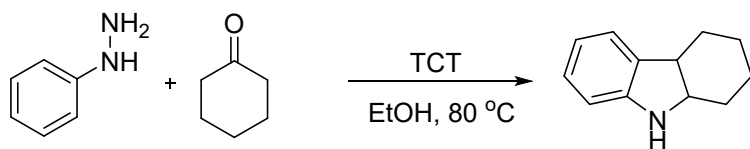
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1. Representation of synthesis of compound **1(a-d)** p2-p2
2. Spectral copies of the intermediates and target compounds **4(a-uz)**..... p3-p8

Representation of synthesis of compound **1** & **2(n)**



Copies of ^1H NMR, ^{13}C NMR, MASS and IR of synthesized compounds:

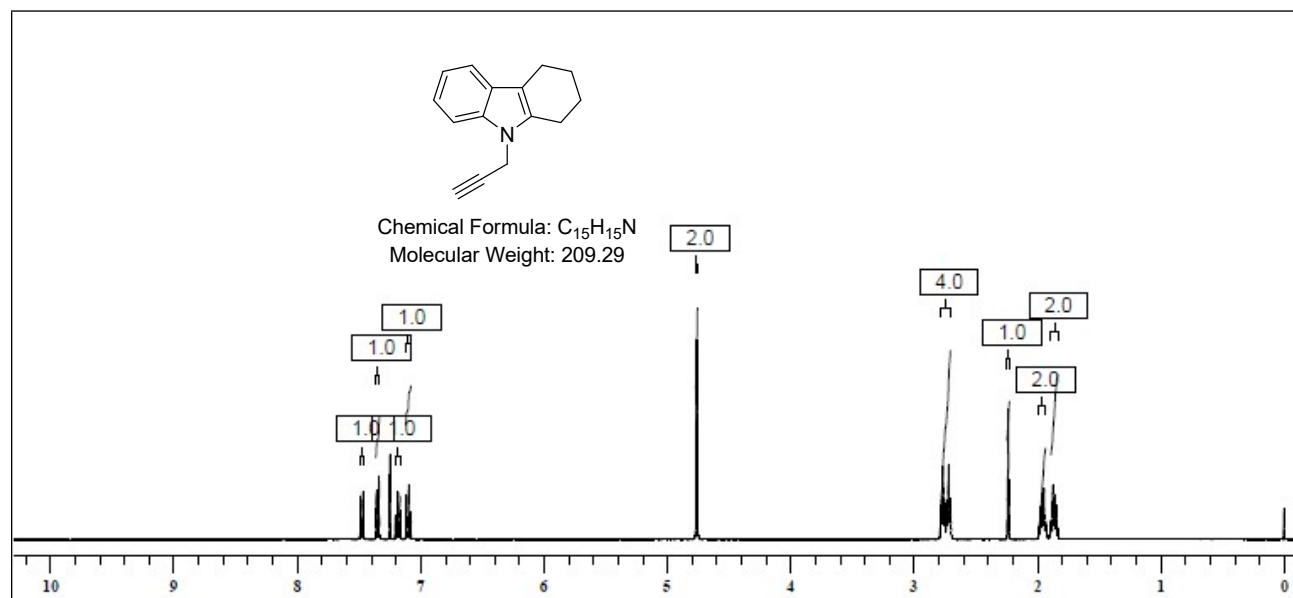


Figure S1: ^1H NMR (400 MHz, CDCl_3) spectrum of 9-(prop-2-yn-1-yl)-2,3,4,9-tetrahydro-1H-fluorene **2**

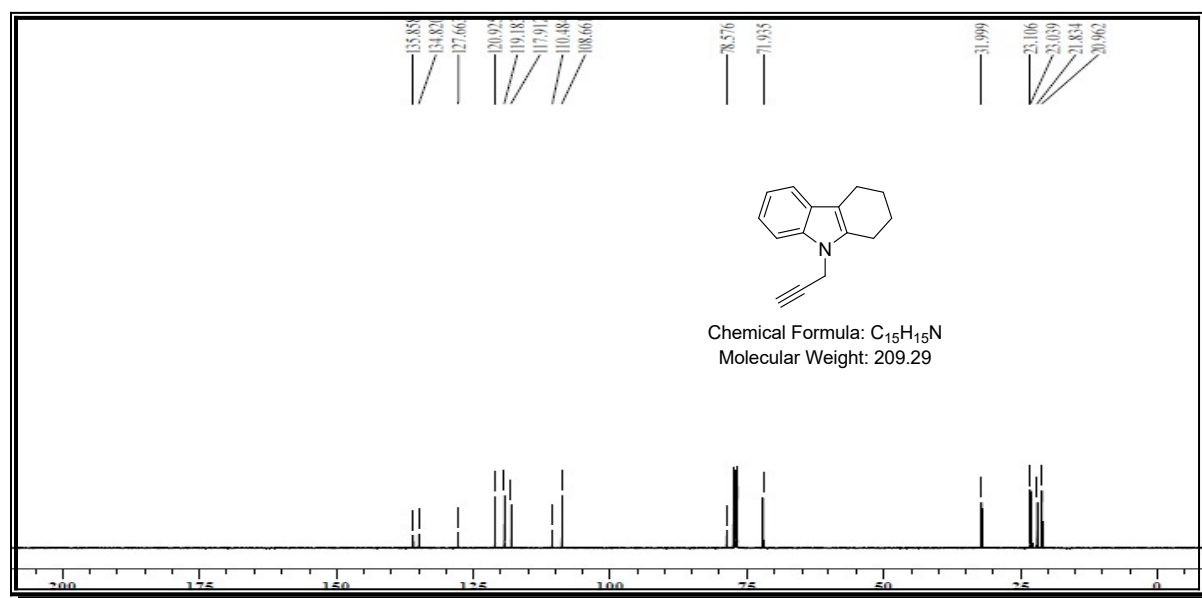


Figure S2: ^{13}C NMR (100 MHz, CDCl_3) spectrum of 9-(prop-2-yn-1-yl)-2,3,4,9-tetrahydro-1H-fluorene **2**

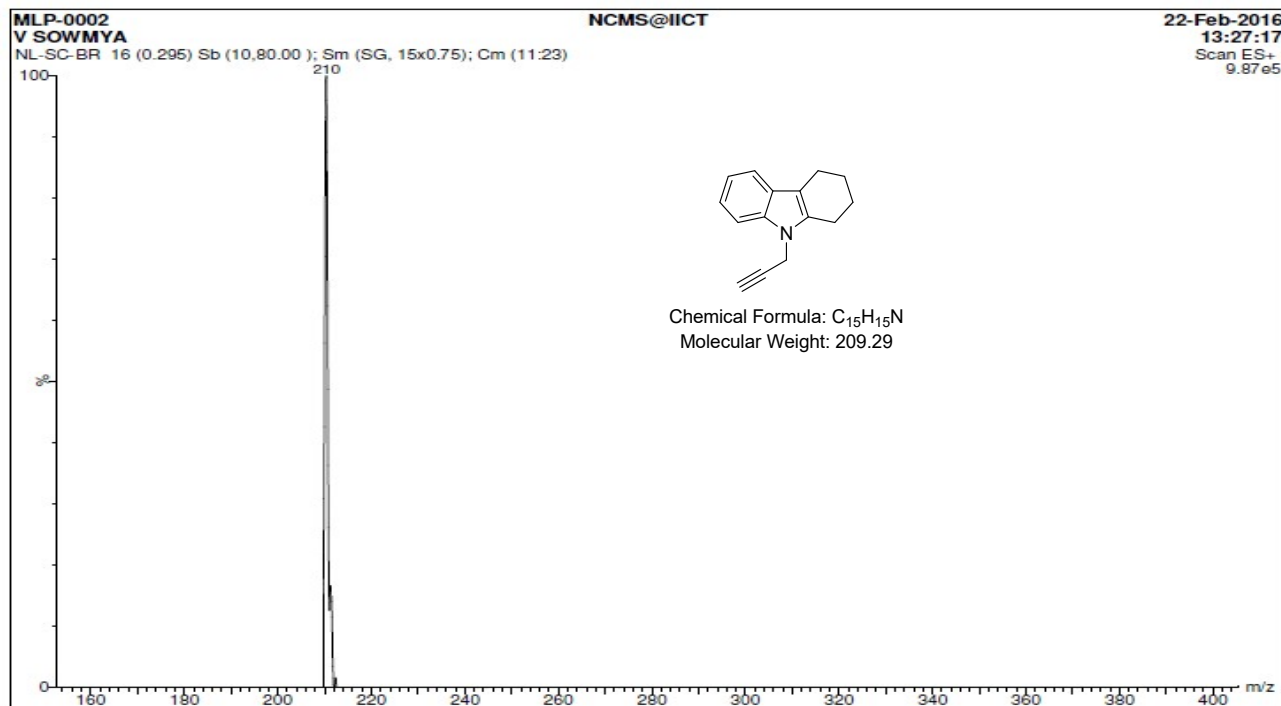


Figure S3: Mass (ES⁺) spectrum of compound 9-(prop-2-yn-1-yl)-2,3,4,9-tetrahydro-1H-fluorene
2

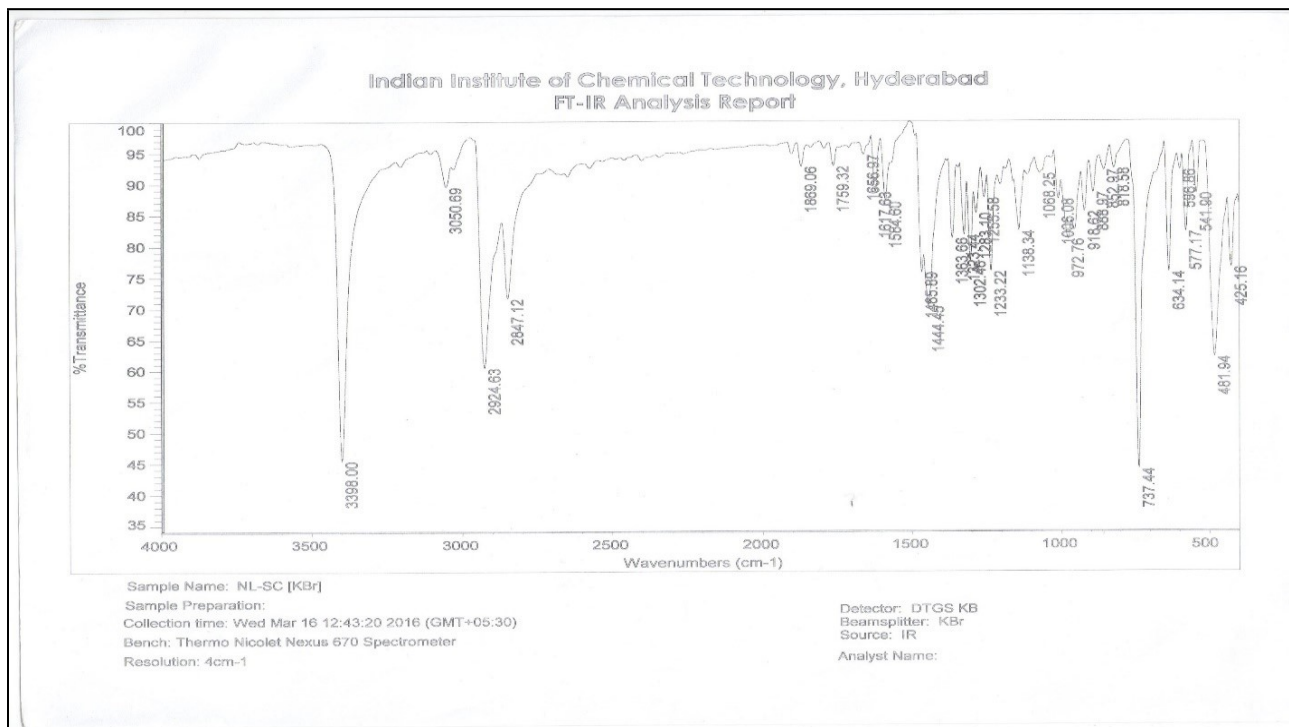


Figure S4: IR (KBr, cm^{-1}) spectrum of compound 9-(prop-2-yn-1-yl)-2,3,4,9-tetrahydro-1*H*-fluorene **2**

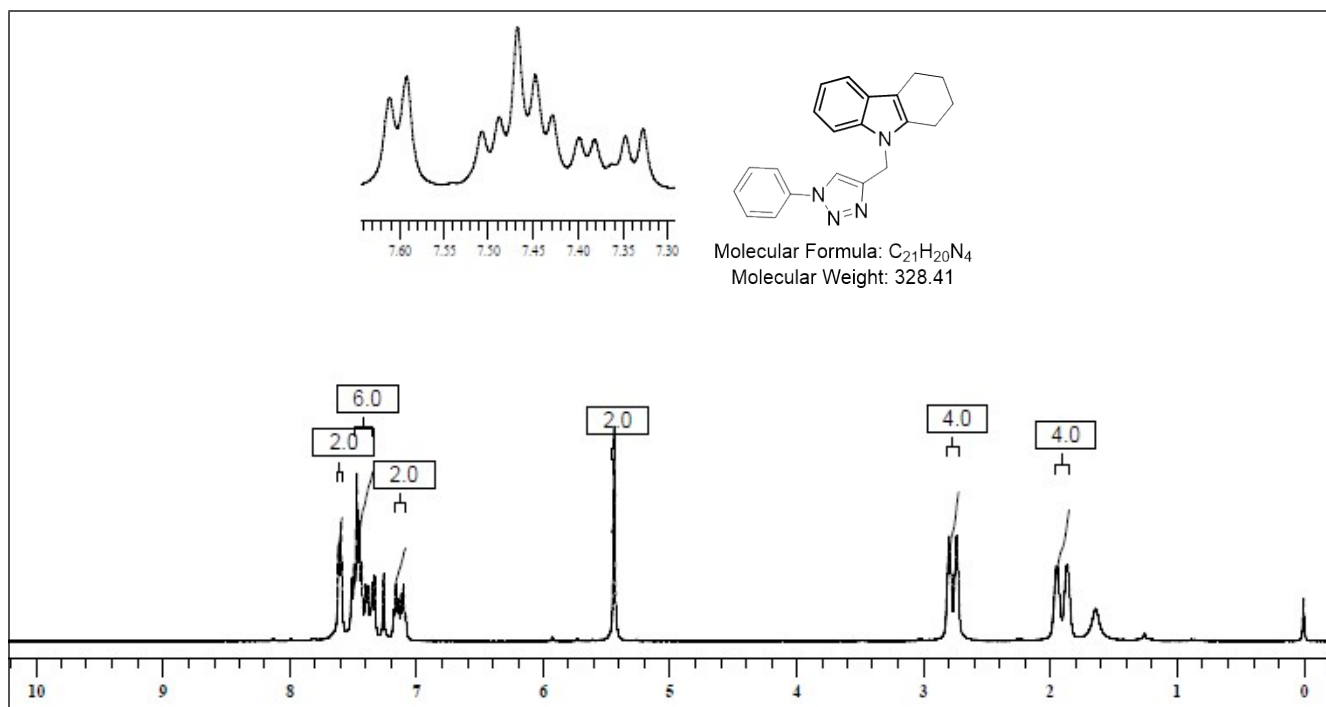


Figure S5: ^1H NMR (400 MHz, CDCl_3) spectrum of 9-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4a**)

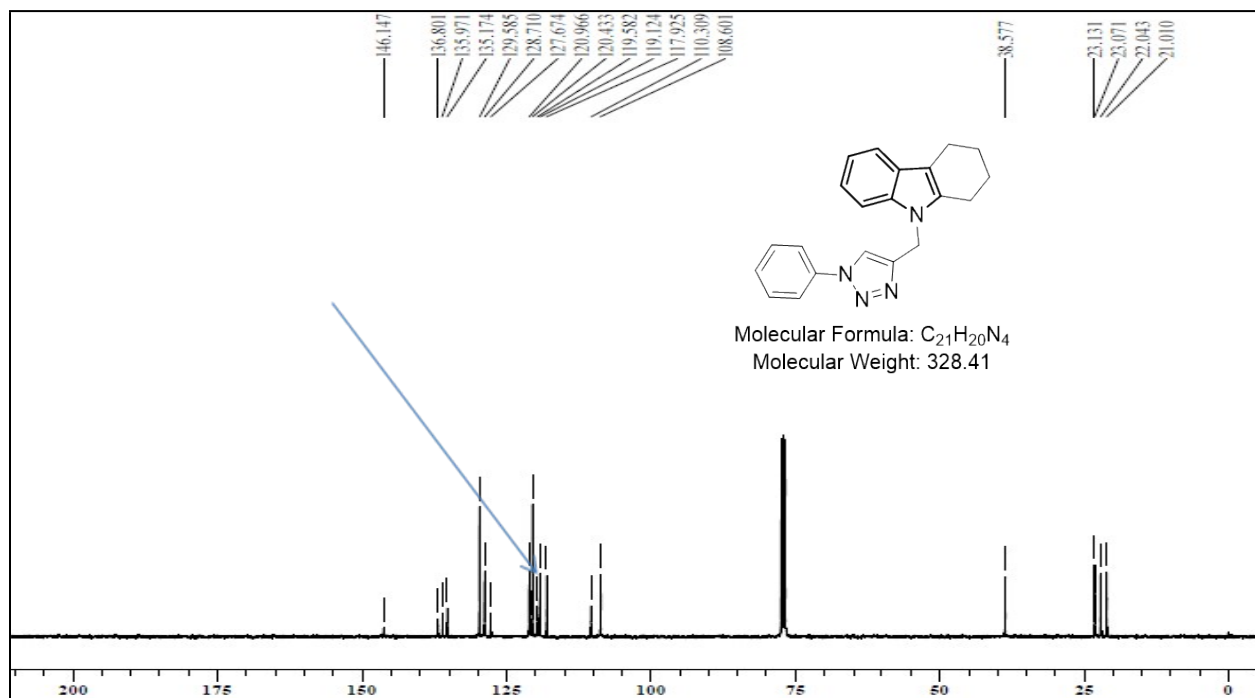


Figure S6: ^{13}C NMR (100 MHz, CDCl_3) spectrum of 9-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4a**)

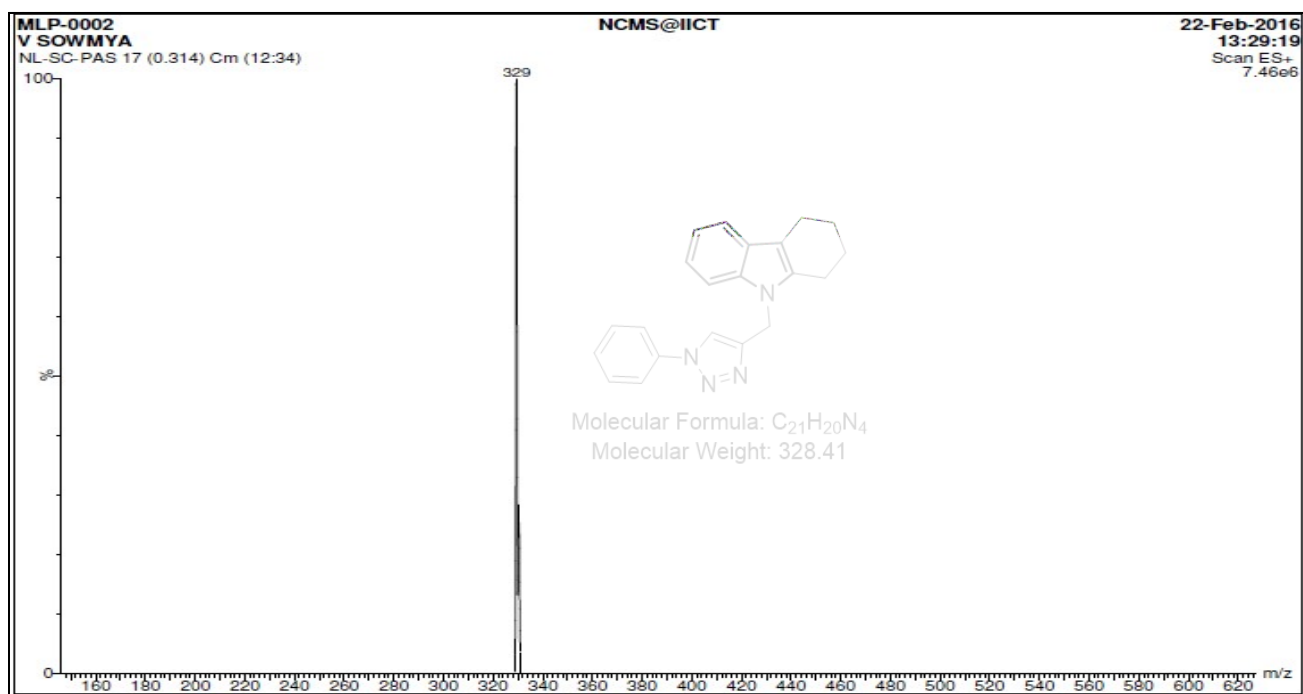


Figure S7: Mass (ES⁺) spectrum of compound 9-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4a**)

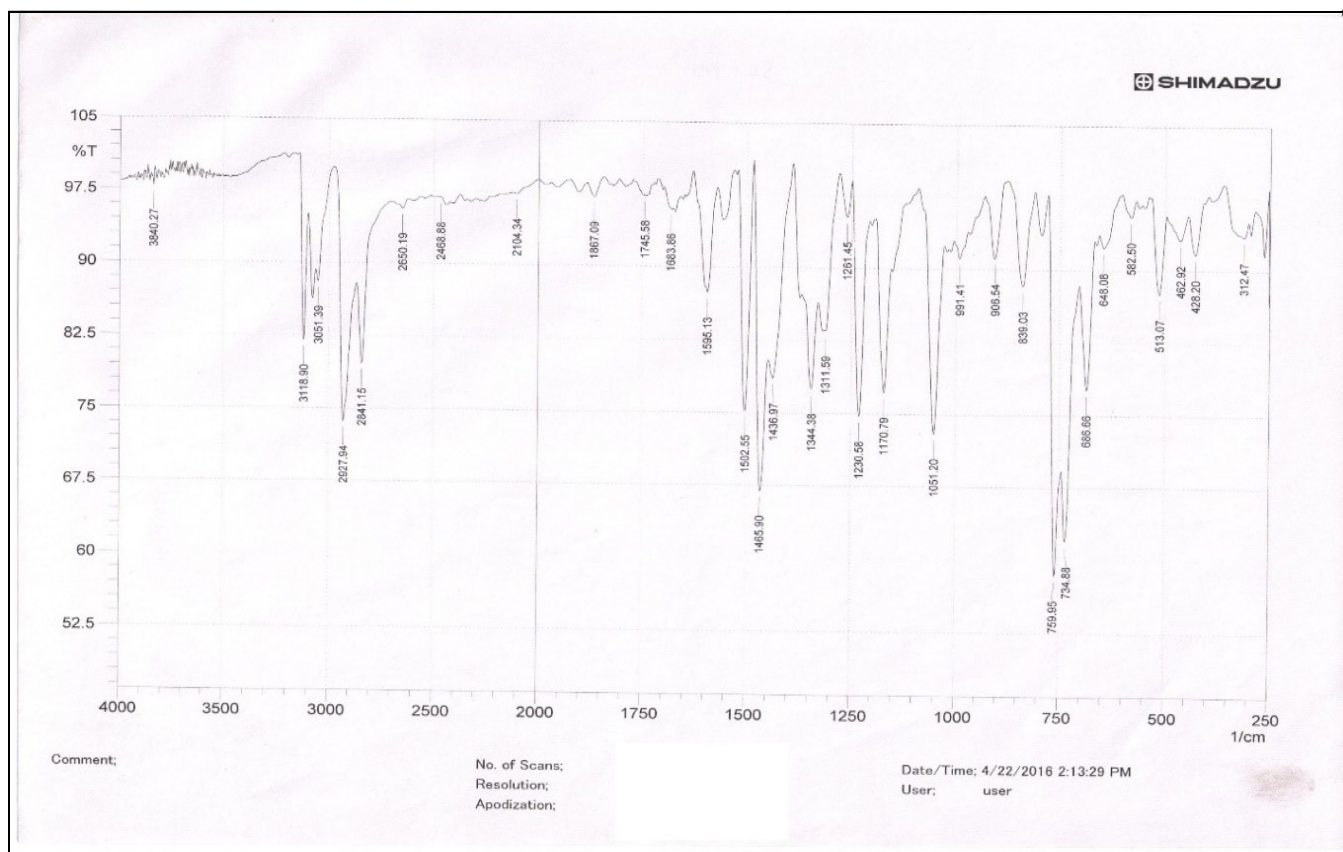


Figure S8: IR (KBr, cm^{-1}) spectrum of compound 9-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4a**)

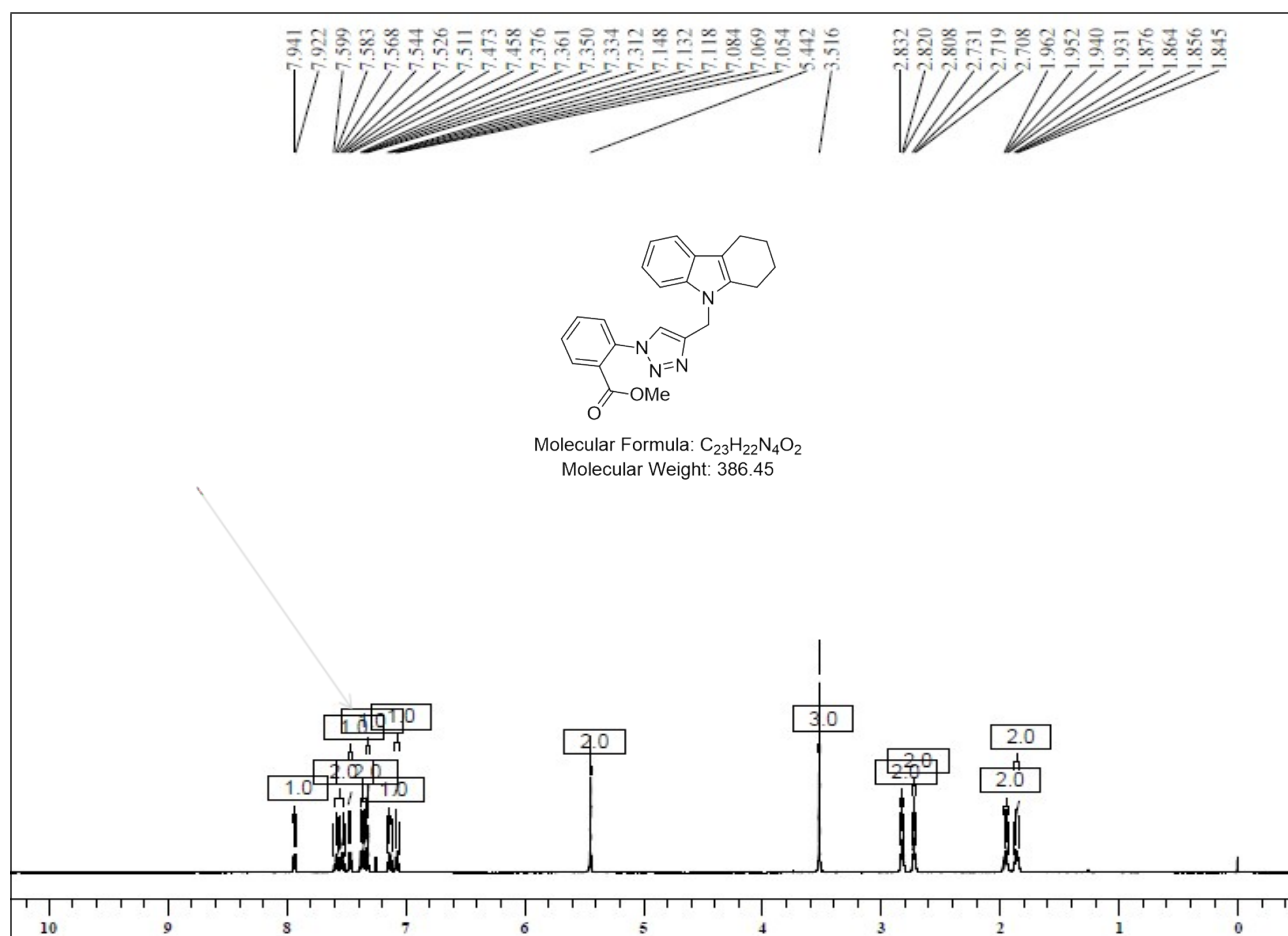


Figure S9: ¹H NMR (400 MHz, CDCl₃) of methyl 2-(4-((3,4-dihydro-1H-carbazol-9(2H)-yl)methyl)-1H-1,2,3-triazol-1-yl)benzoate (**4b**)

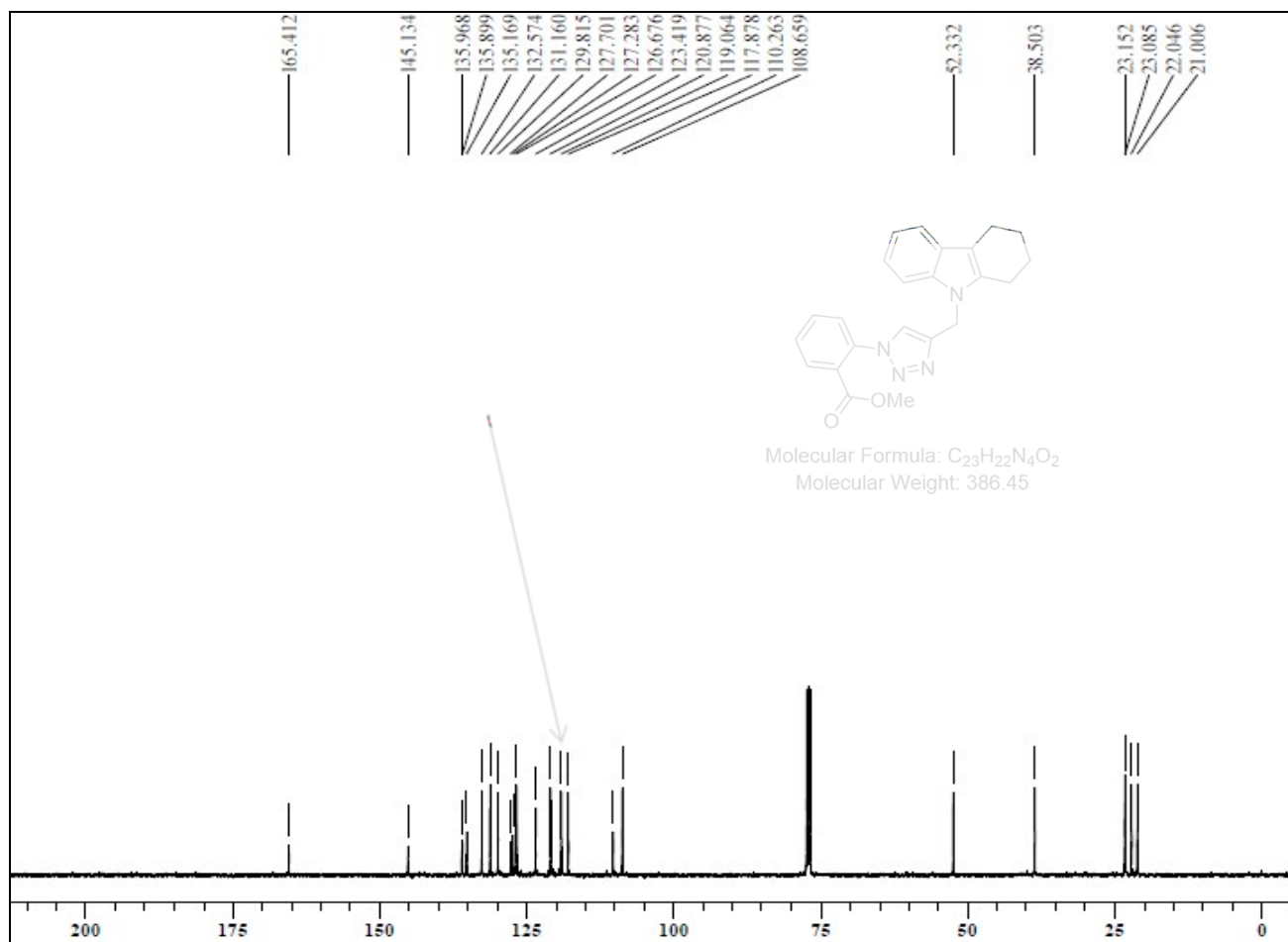


Figure S10: ¹³C NMR (100 MHz, CDCl₃) spectrum of compound methyl 2-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoate (**4b**)

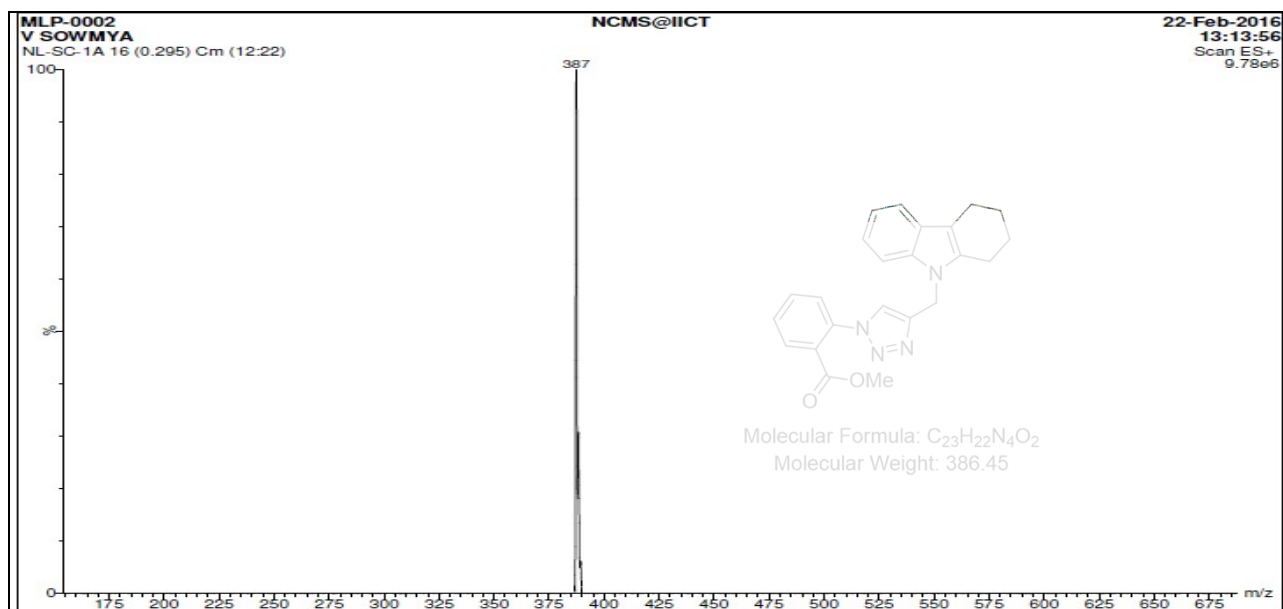


Figure S11: Mass (ES⁺) spectrum of methyl 2-(4-((3,4-dihydro-1H-carbazol-9(2H)-yl)methyl)-1H-1,2,3-triazol-1-yl)benzoate (**4b**)

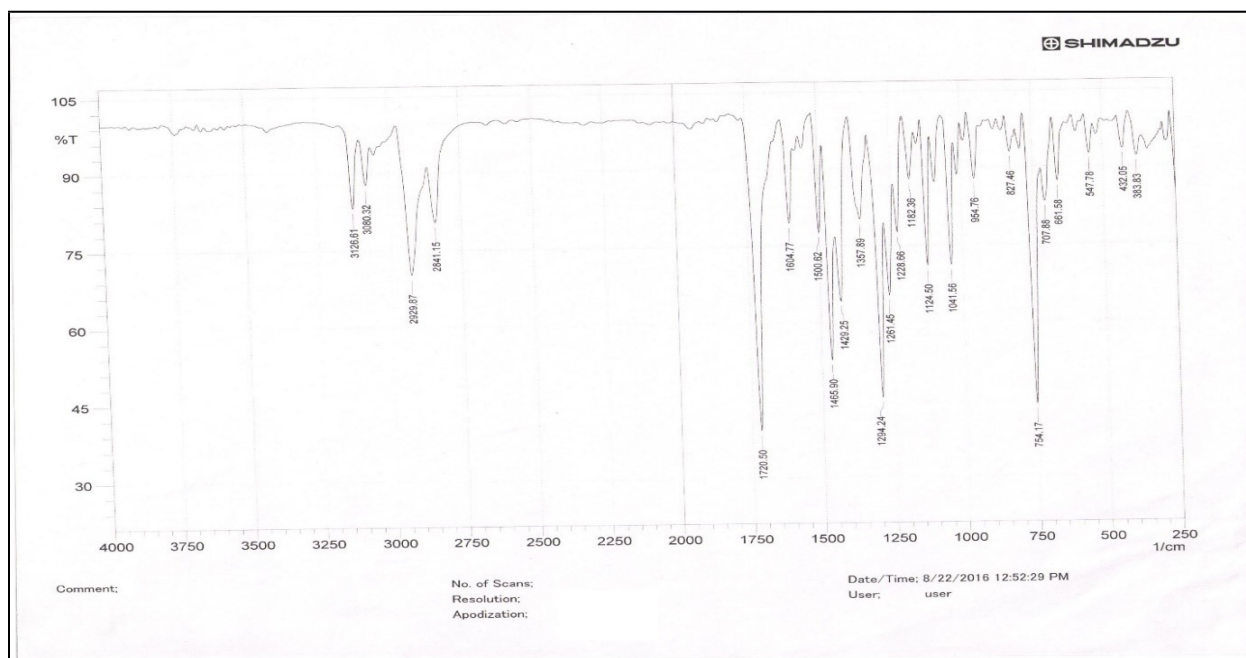


Figure S12: IR (KBr, cm⁻¹) spectrum of methyl 2-(4-((3,4-dihydro-1H-carbazol-9(2H)-yl)methyl)-1H-1,2,3-triazol-1-yl)benzoate (**4b**)

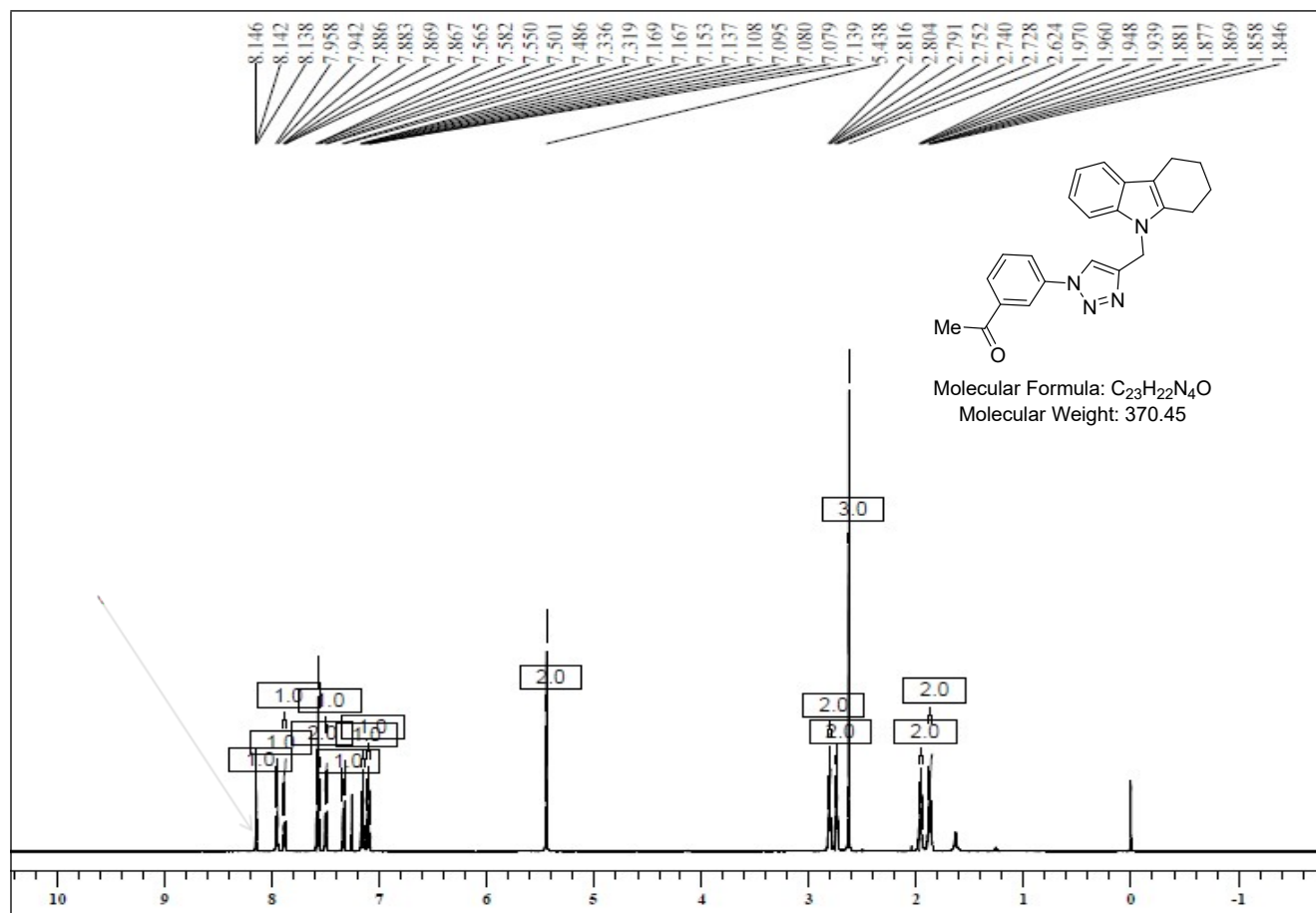


Figure S13: ¹H NMR (400 MHz, CDCl₃) of 1-(3-(4-((3,4-dihydro-1H-carbazol-9(2H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone (**4c**)

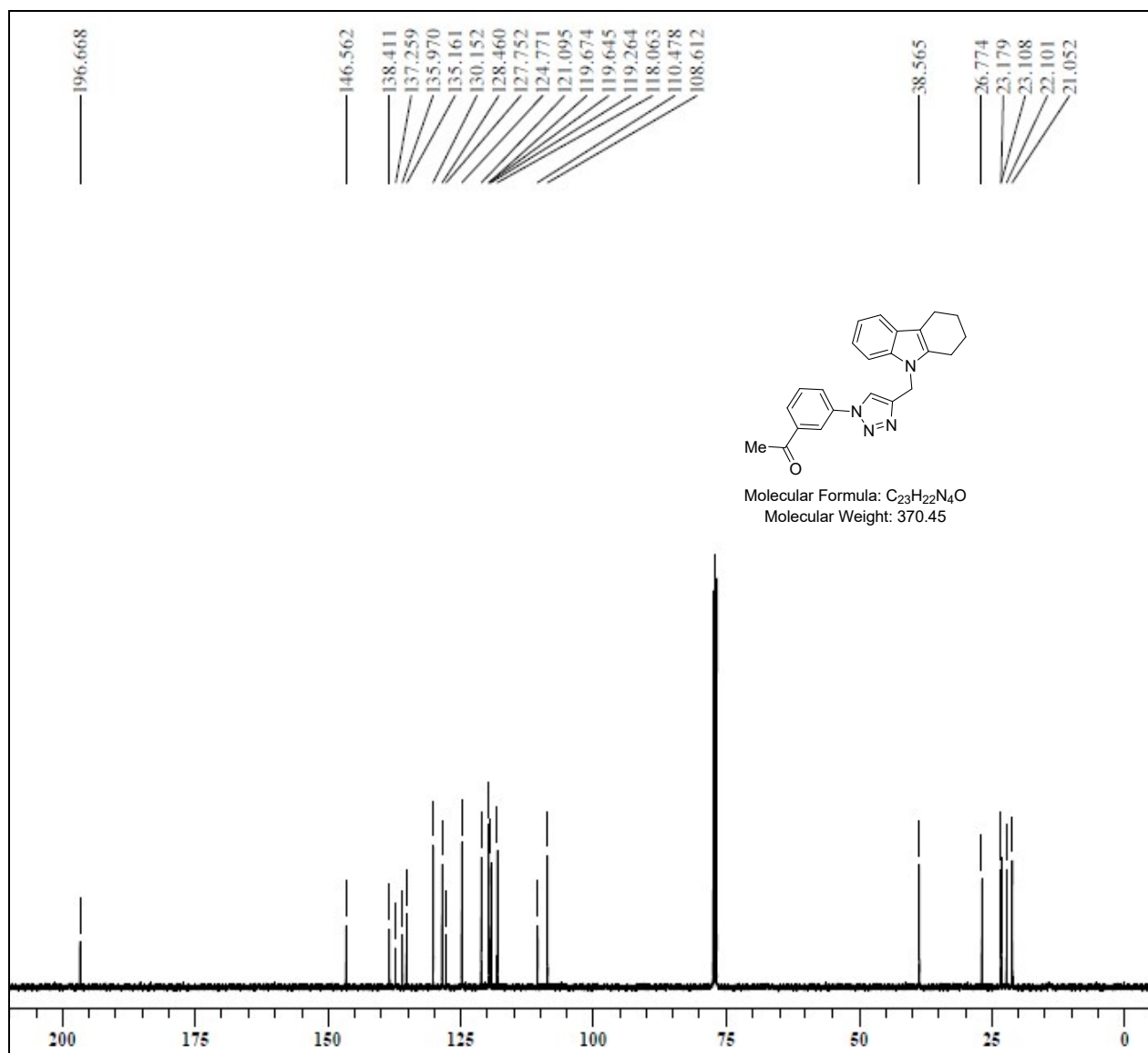


Figure S14: ¹³C NMR (100 MHz, CDCl₃) spectrum of 1-(3-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethanone (**4c**)

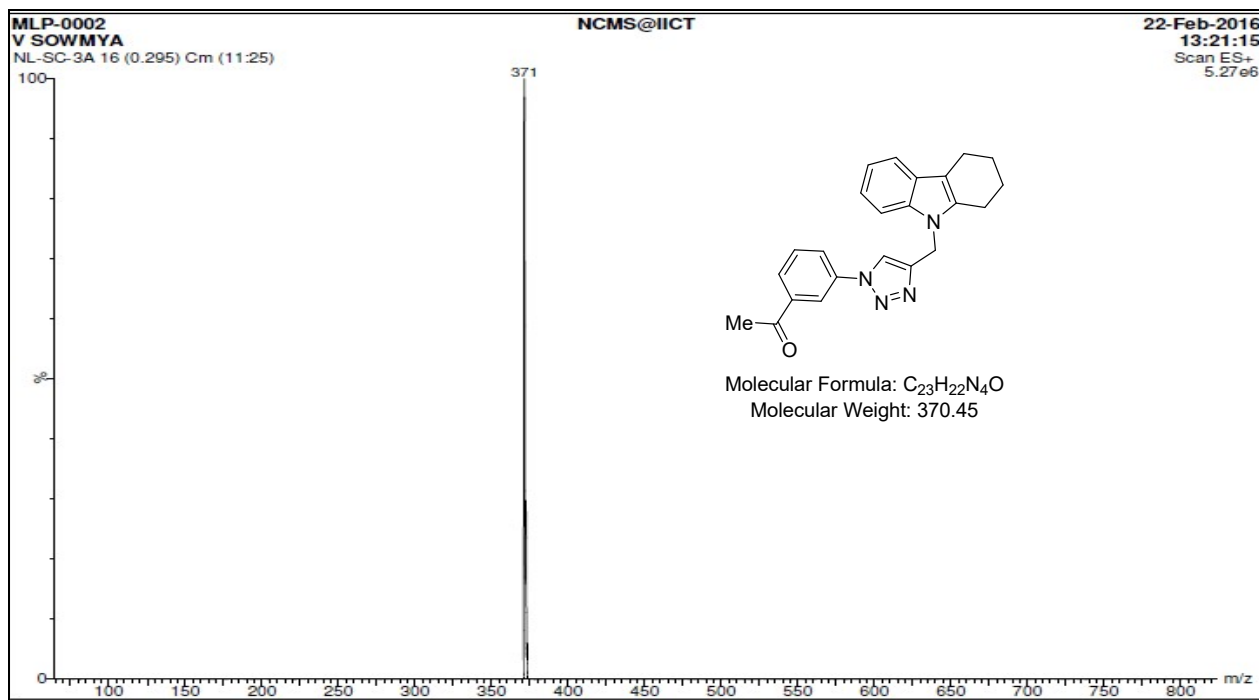


Figure S15: Mass (ES⁺) spectrum of 1-(3-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethanone (**4c**)

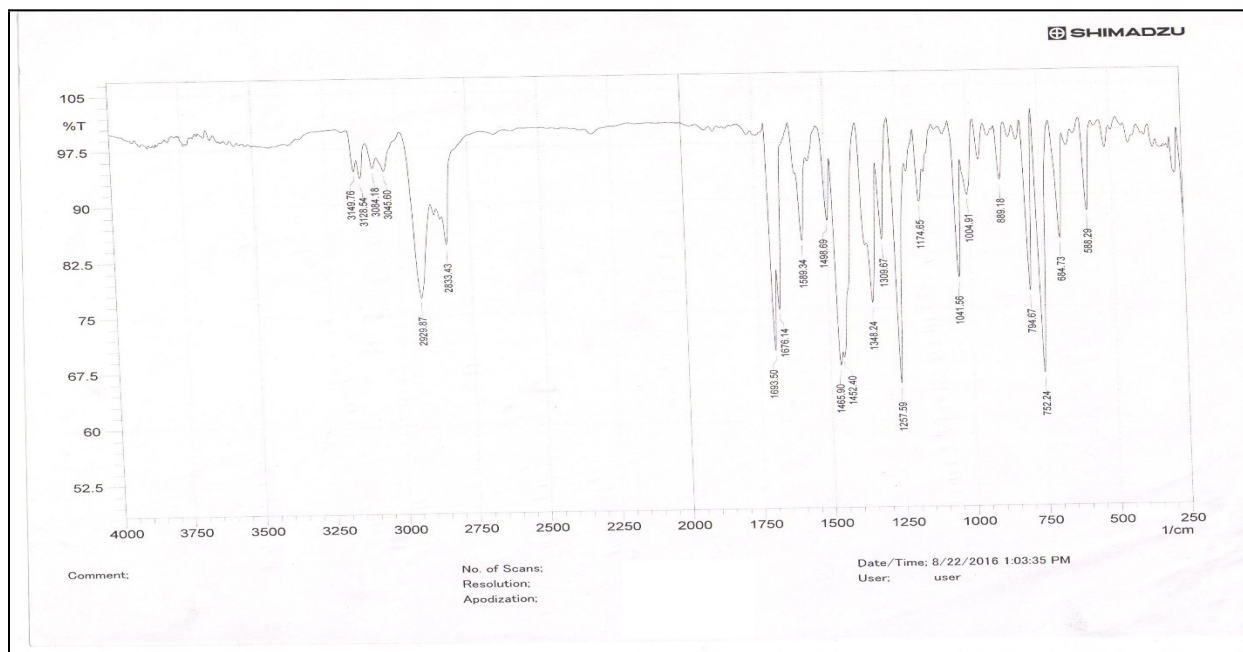


Figure S16: IR (KBr, cm⁻¹) spectrum of 1-(3-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethanone (**4c**)

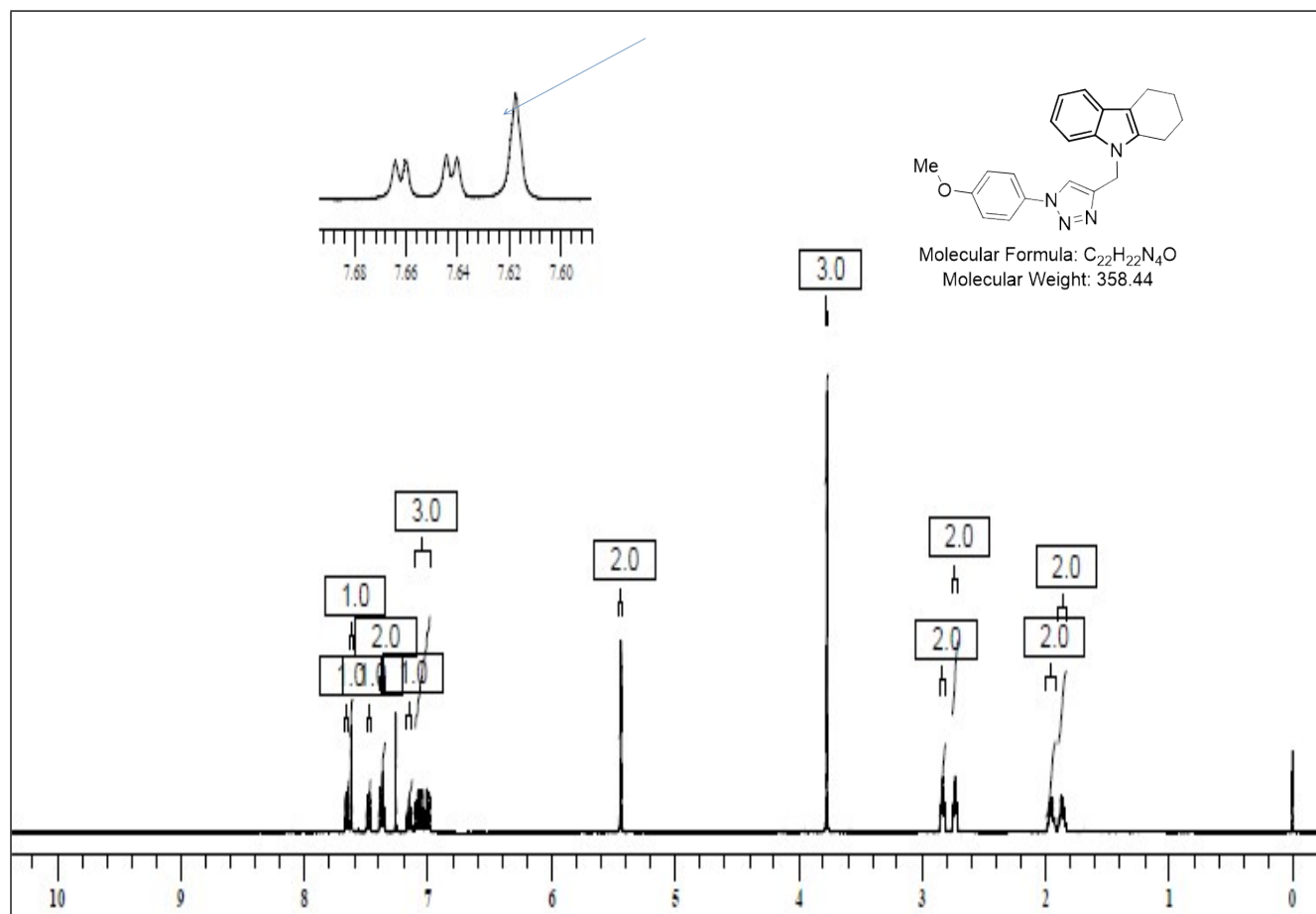


Figure S17: ^1H NMR (400 MHz, CDCl_3) of 9-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4d**)

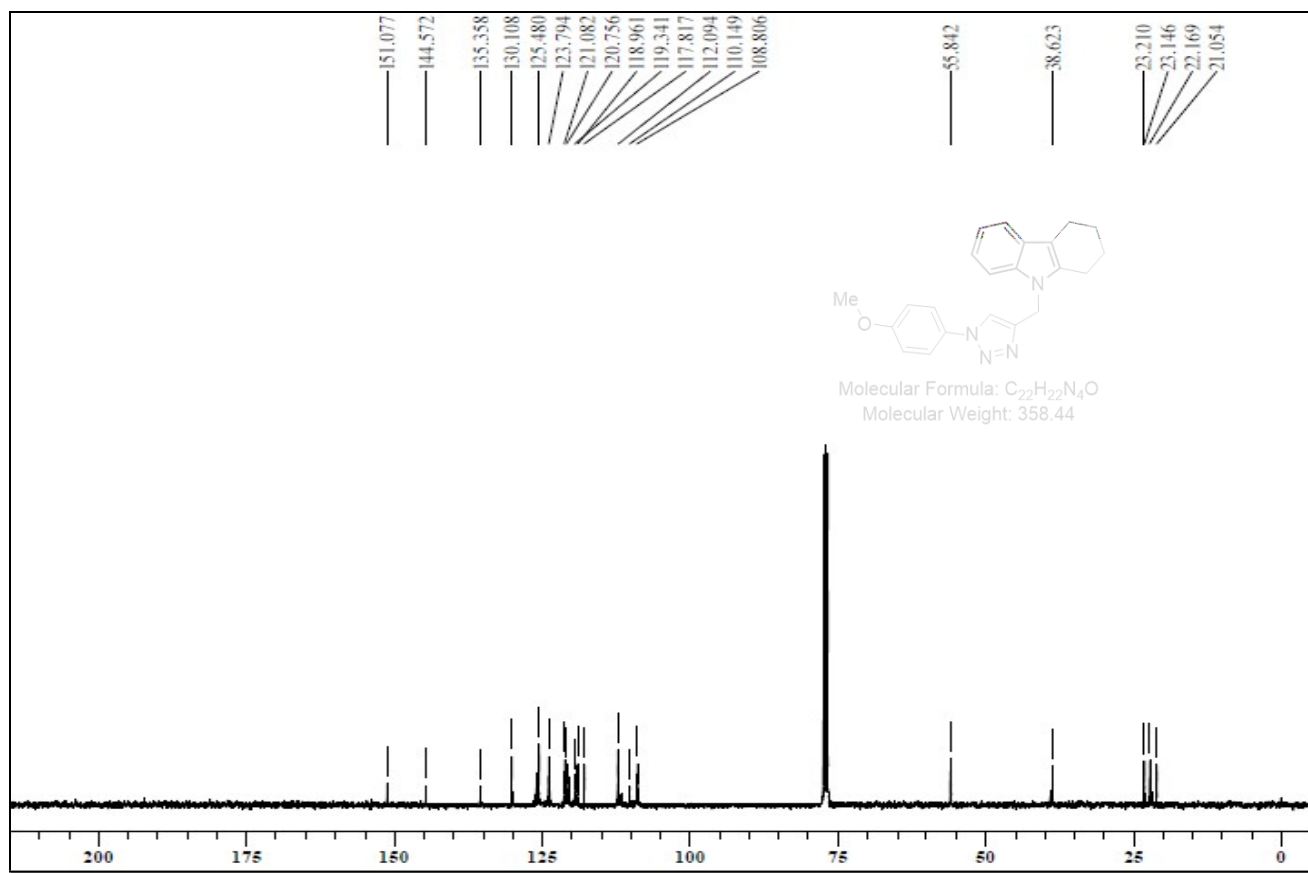


Figure S18: ¹³C NMR (100 MHz, CDCl₃) spectrum of 9-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4d**)

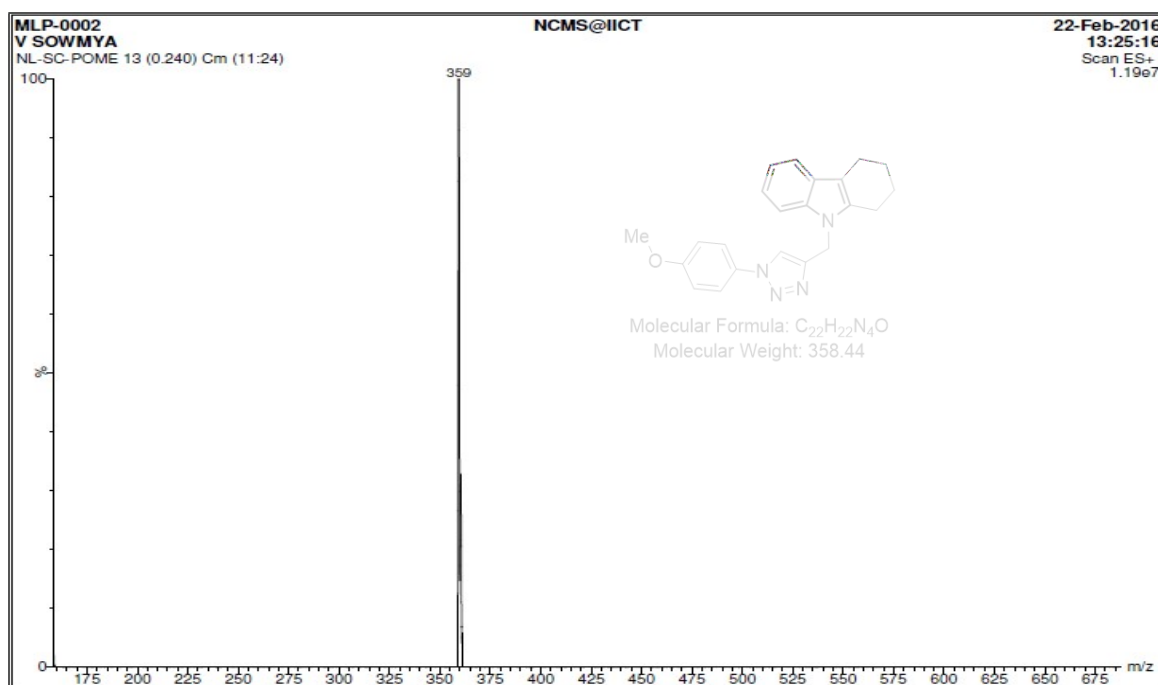


Figure S19: Mass (ES⁺) spectrum of 9-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4d**)

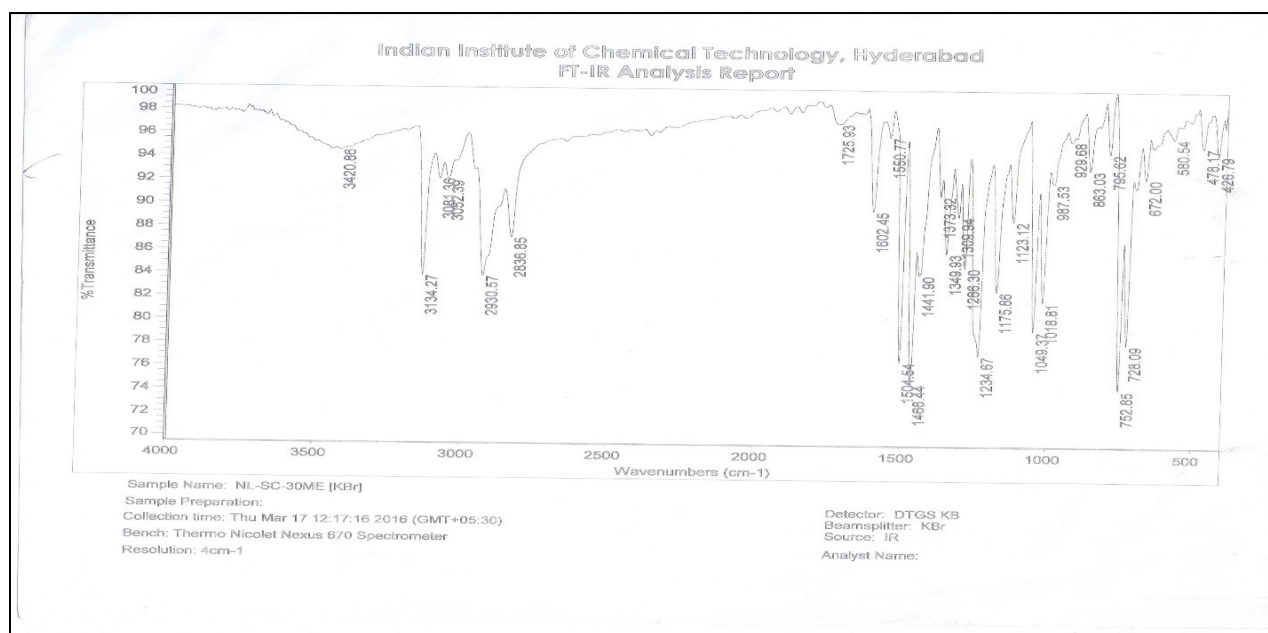


Figure S20: IR (KBr, cm⁻¹) spectrum of 9-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4d**)

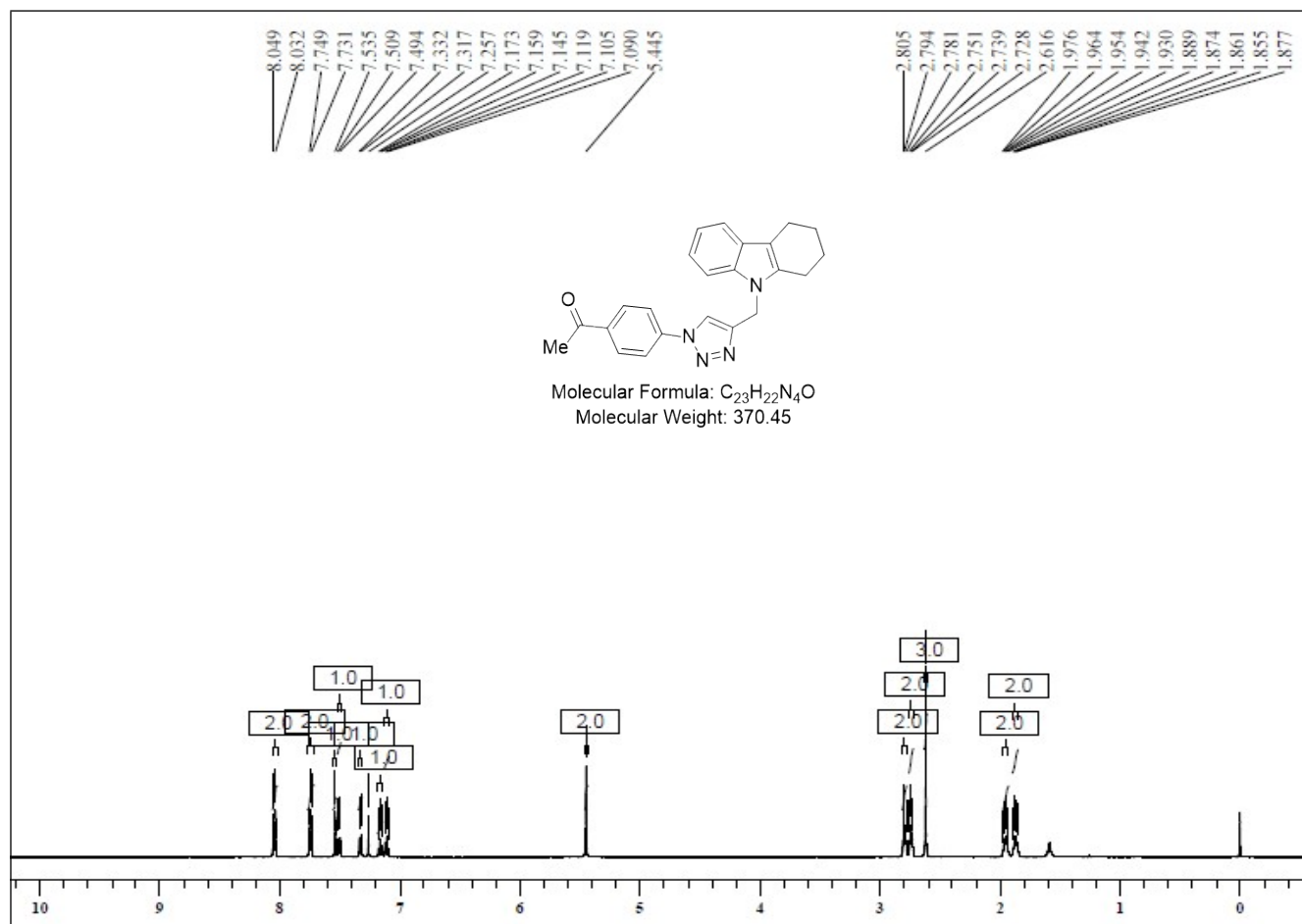


Figure S21: ¹H NMR (400 MHz, CDCl₃) of 1-(4-(4-((3,4-dihydro-1H-carbazol-9(2H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone (**4e**)

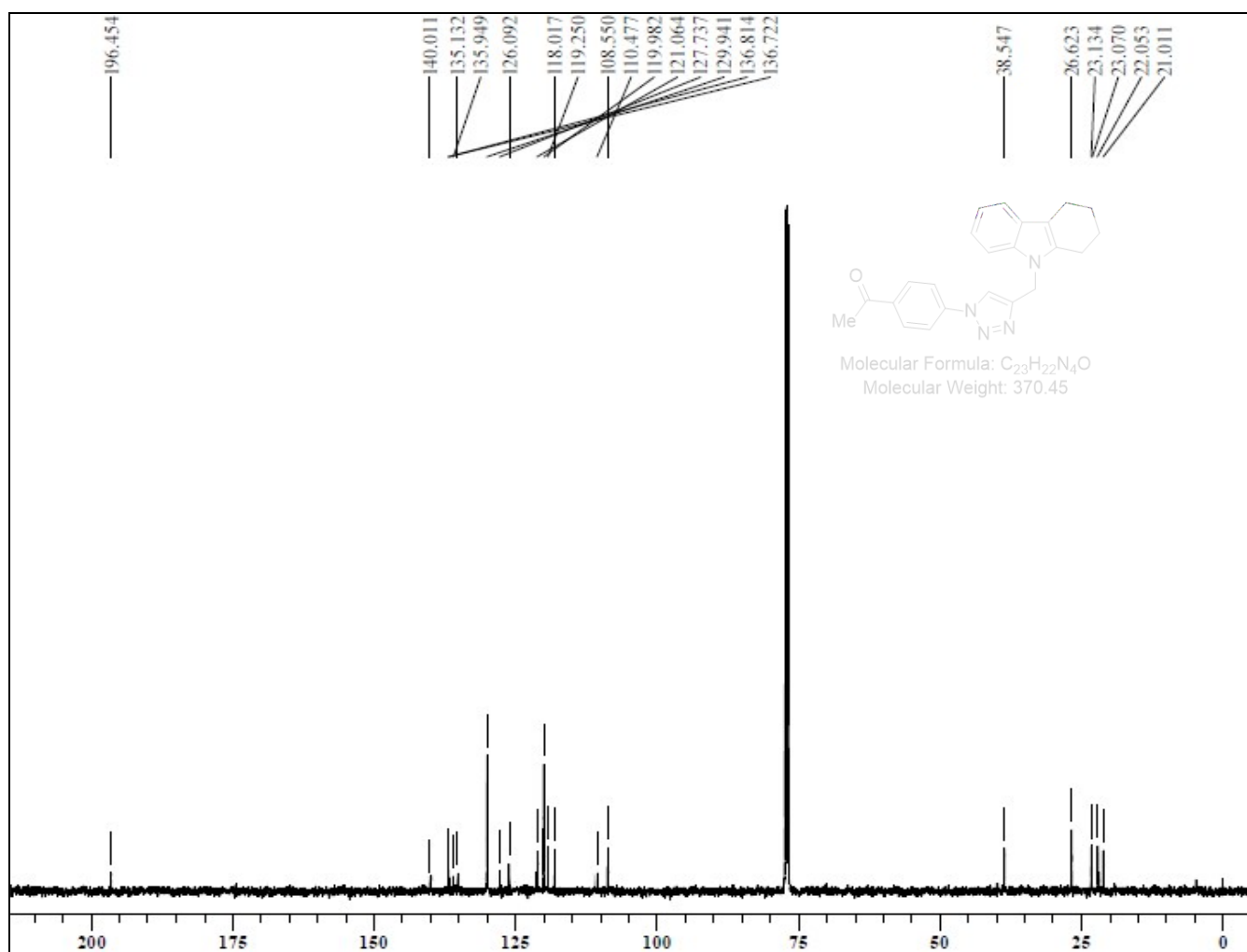


Figure S22: ¹³C NMR (100 MHz, CDCl₃) spectrum of 1-(4-(4-((3,4-dihydro-1H-carbazol-9(2H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone (**4e**)

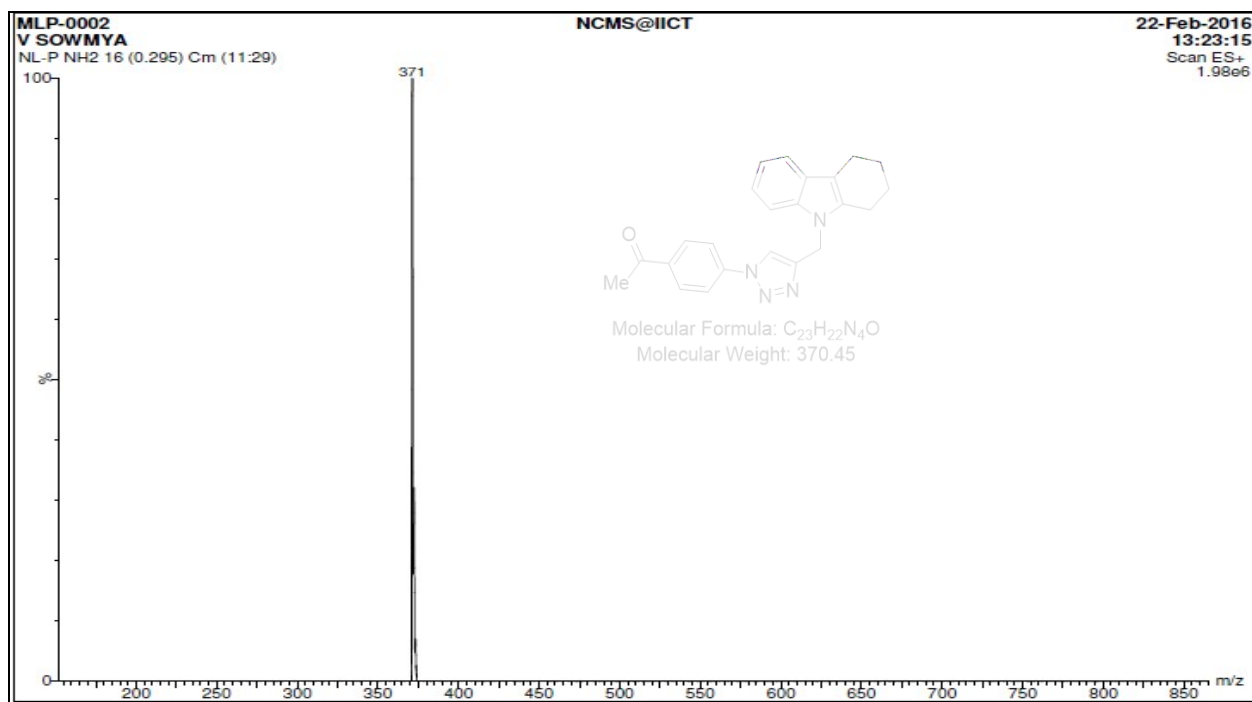


Figure S23: Mass (ES⁺) spectrum of 1-(4-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethanone (**4e**)

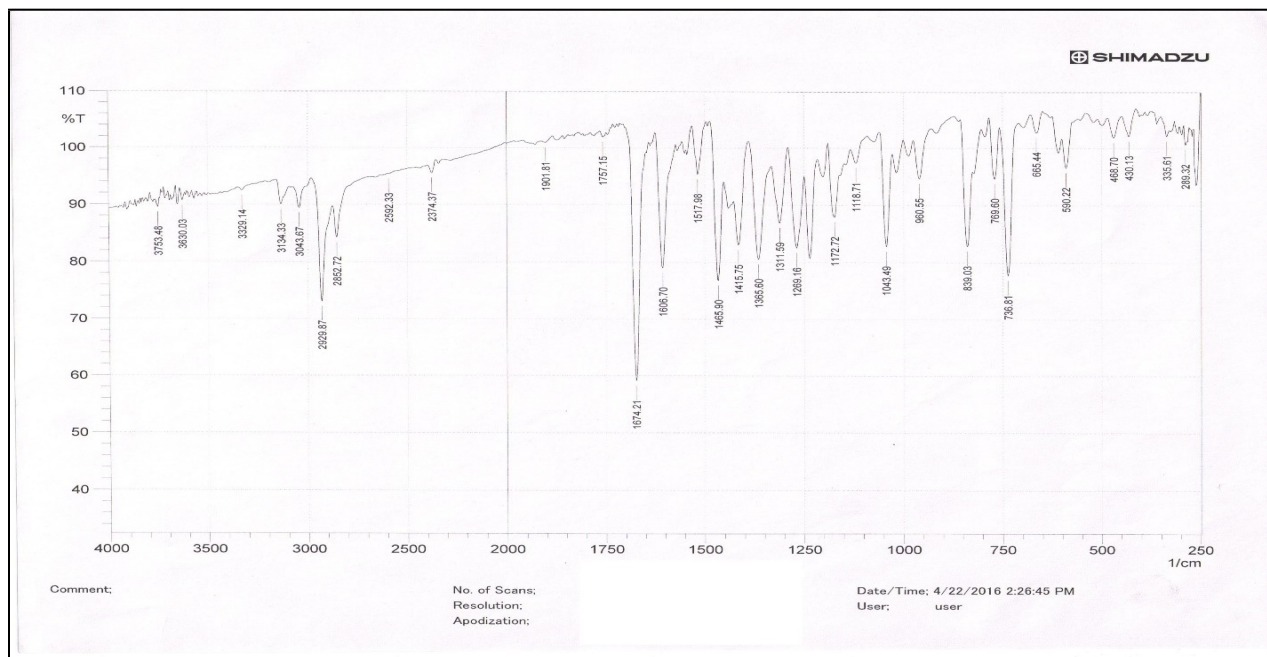


Figure S24: IR (KBr, cm⁻¹) spectrum of 1-(4-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethanone (**4e**)

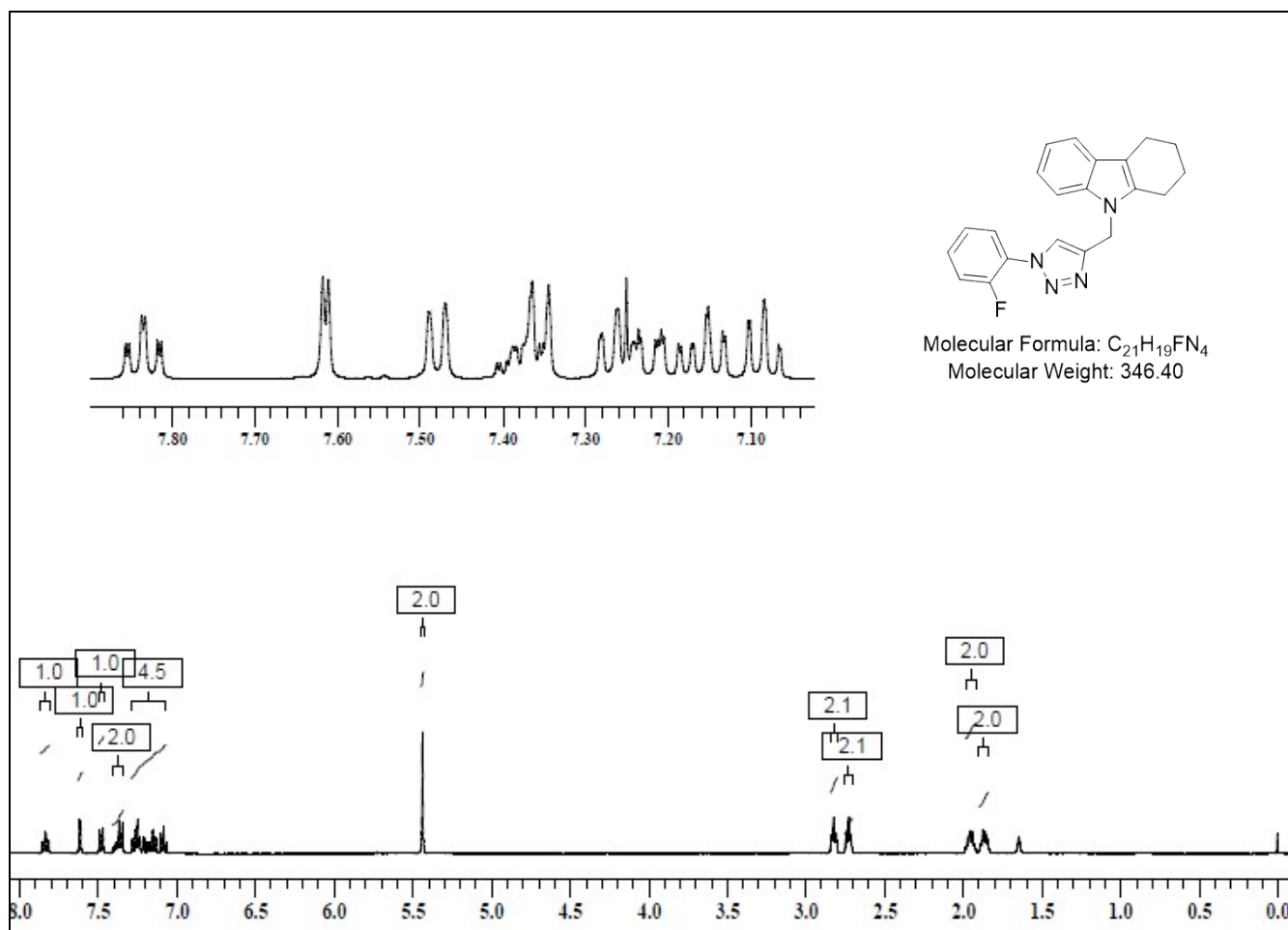


Figure S25: ¹H NMR (400 MHz, CDCl₃) of 9-((1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1H-carbazole (**4f**)

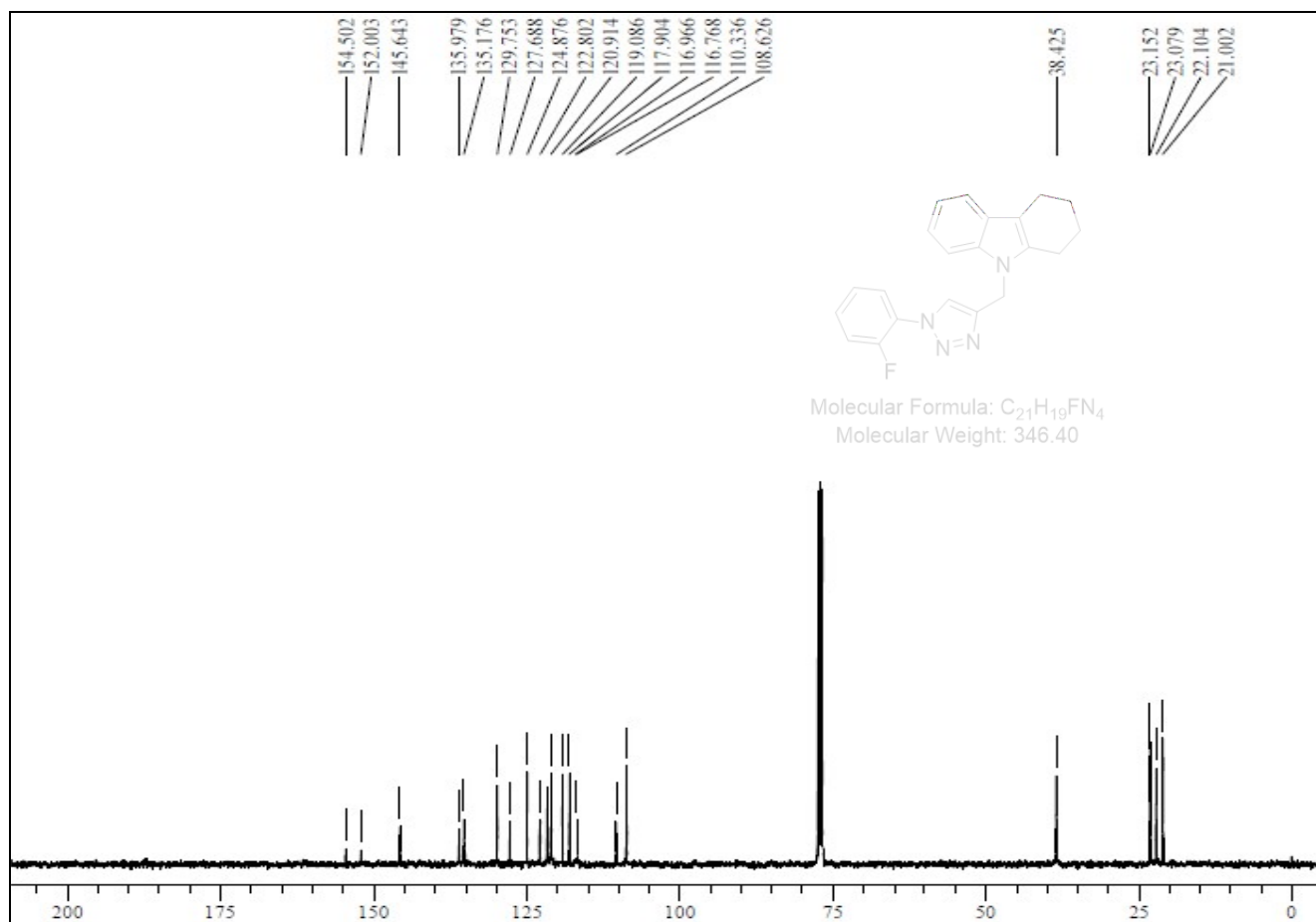


Figure S26: ¹³C NMR (100 MHz, CDCl₃) spectrum of 9-((1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1H-carbazole (**4f**)

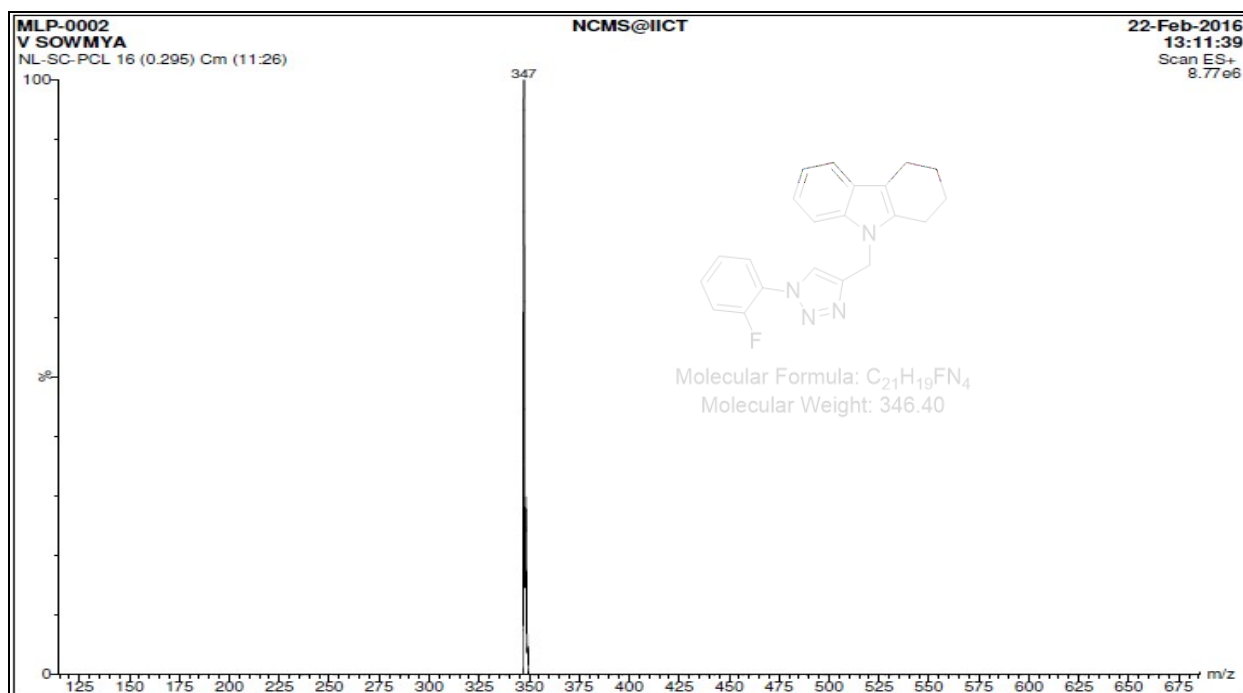


Figure S27: Mass (ES⁺) spectrum of 9-((1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1H-carbazole (**4f**)

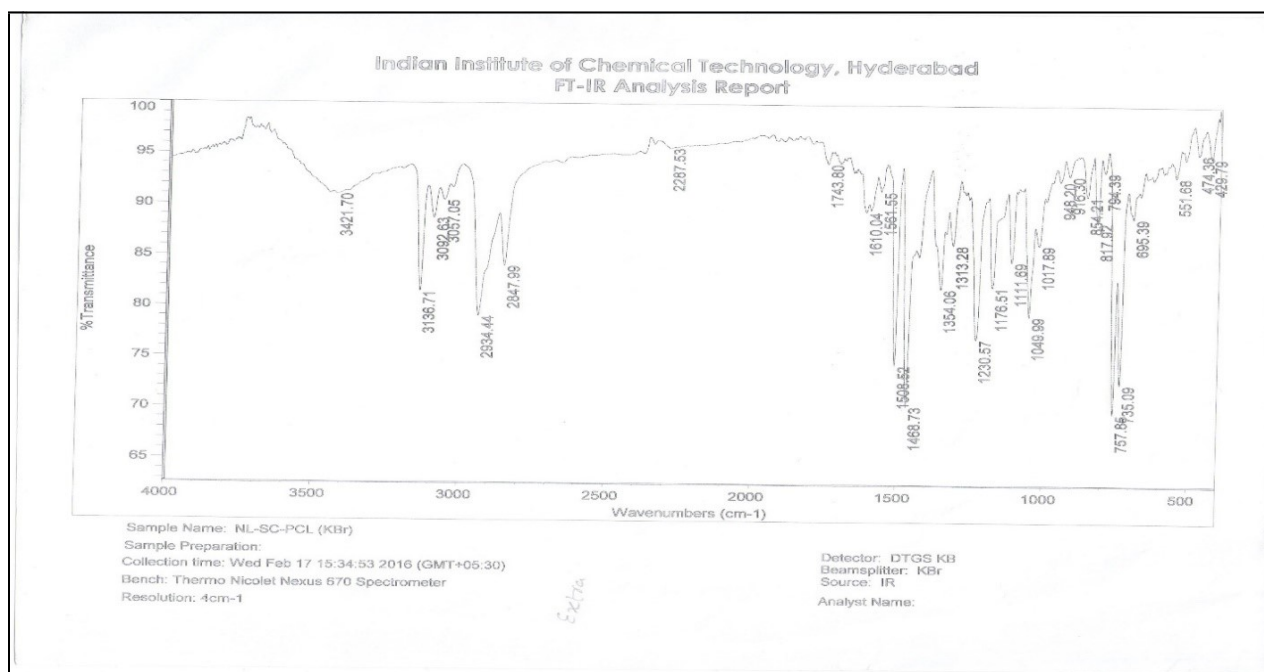
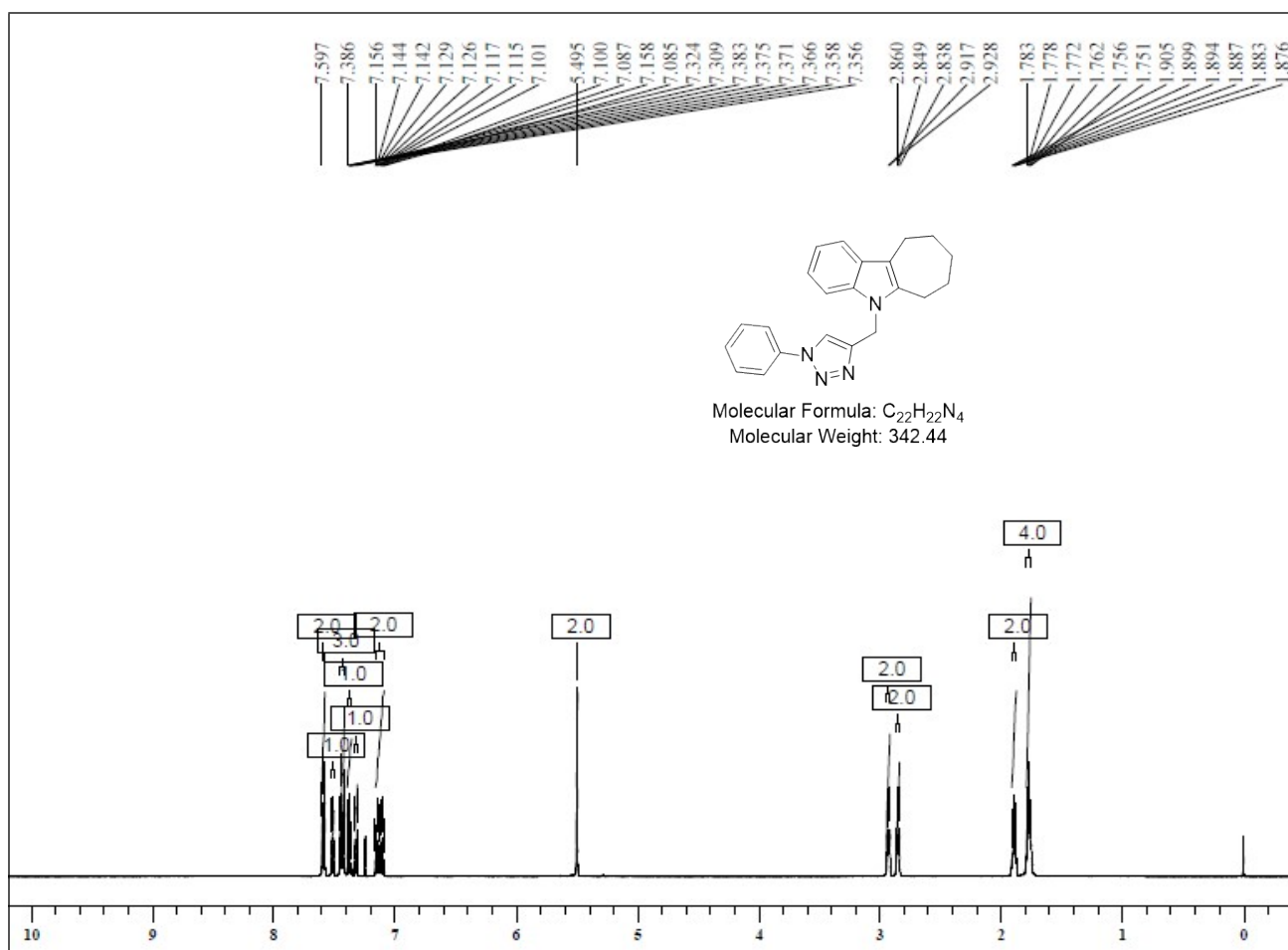


Figure S28: IR (KBr, cm⁻¹) spectrum of compound 9-((1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1H-carbazole (**4f**)



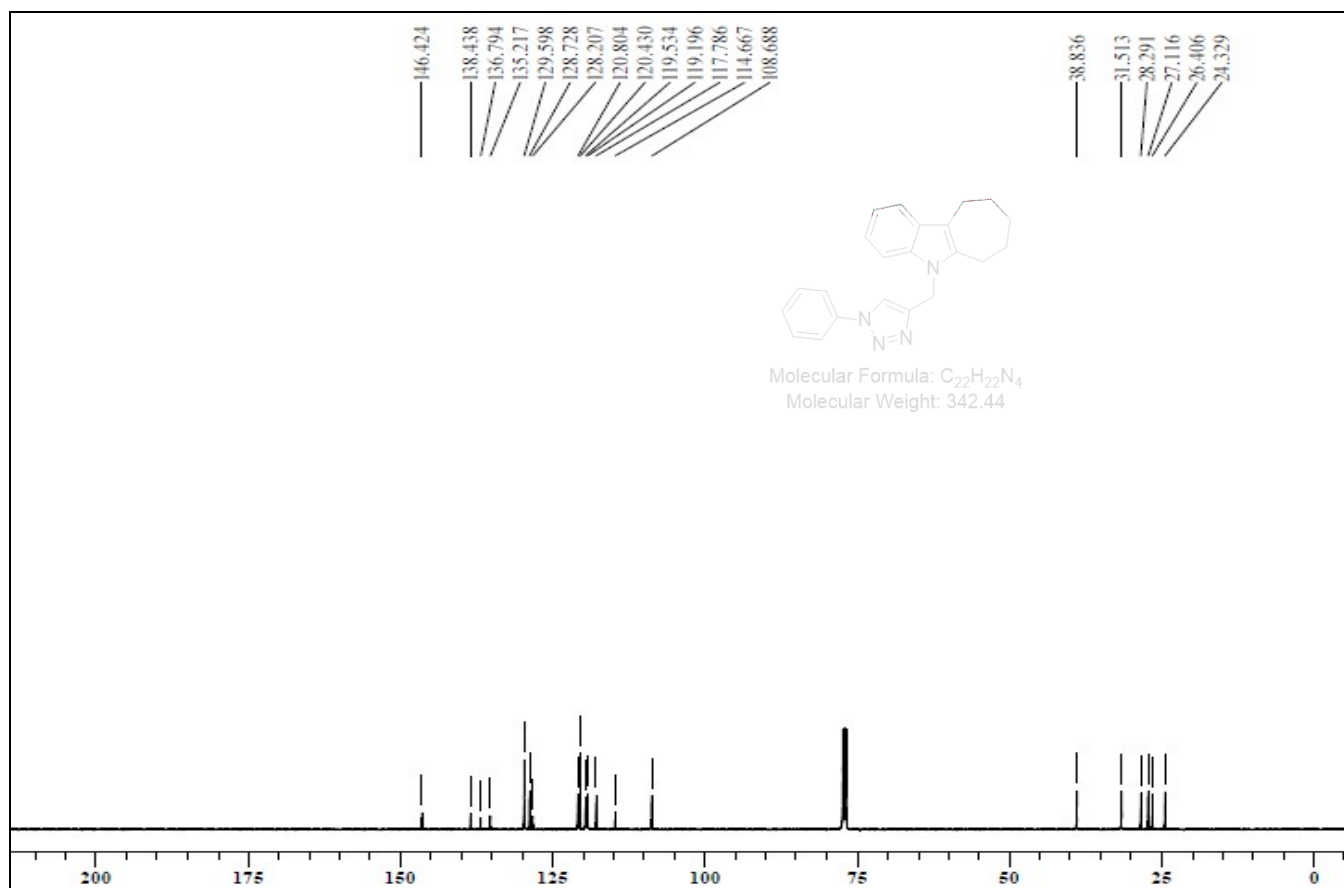


Figure S30: ¹³C NMR (100 MHz, CDCl₃) spectrum of 5-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl) 5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4g**)

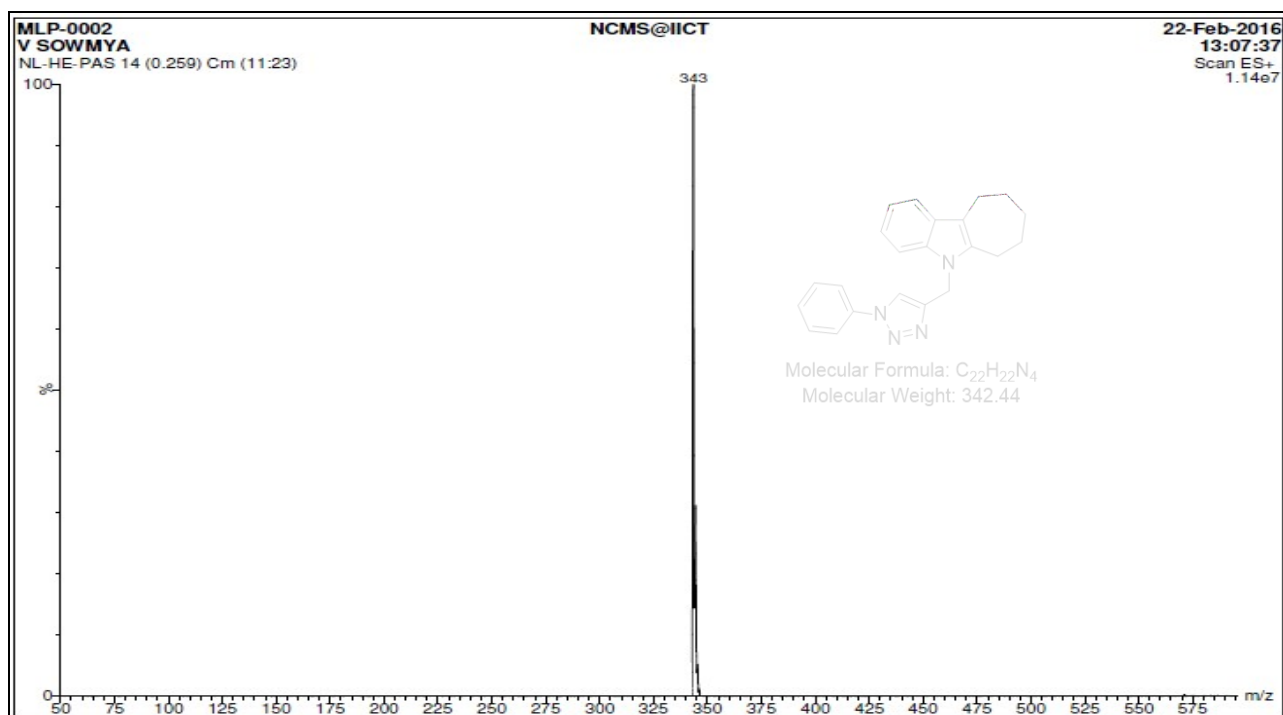


Figure S31: Mass (ES⁺) spectrum of 5-((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4g**)

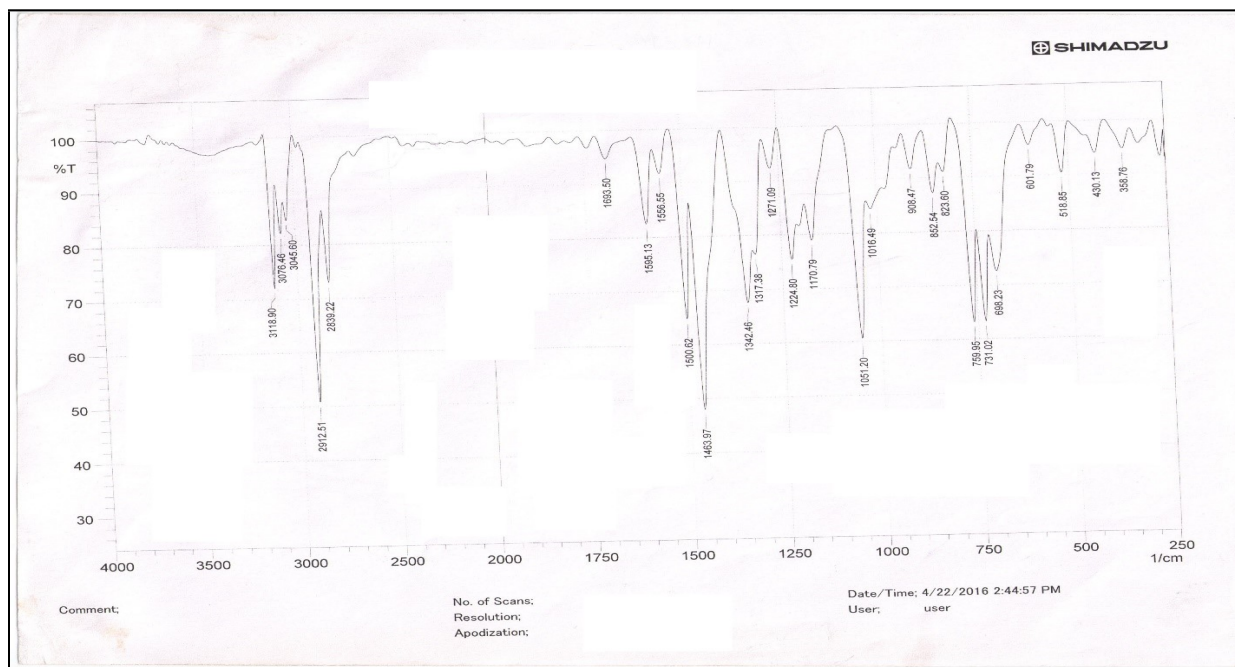


Figure S32: IR (KBr, cm⁻¹) spectrum of compound 5-((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4g**)

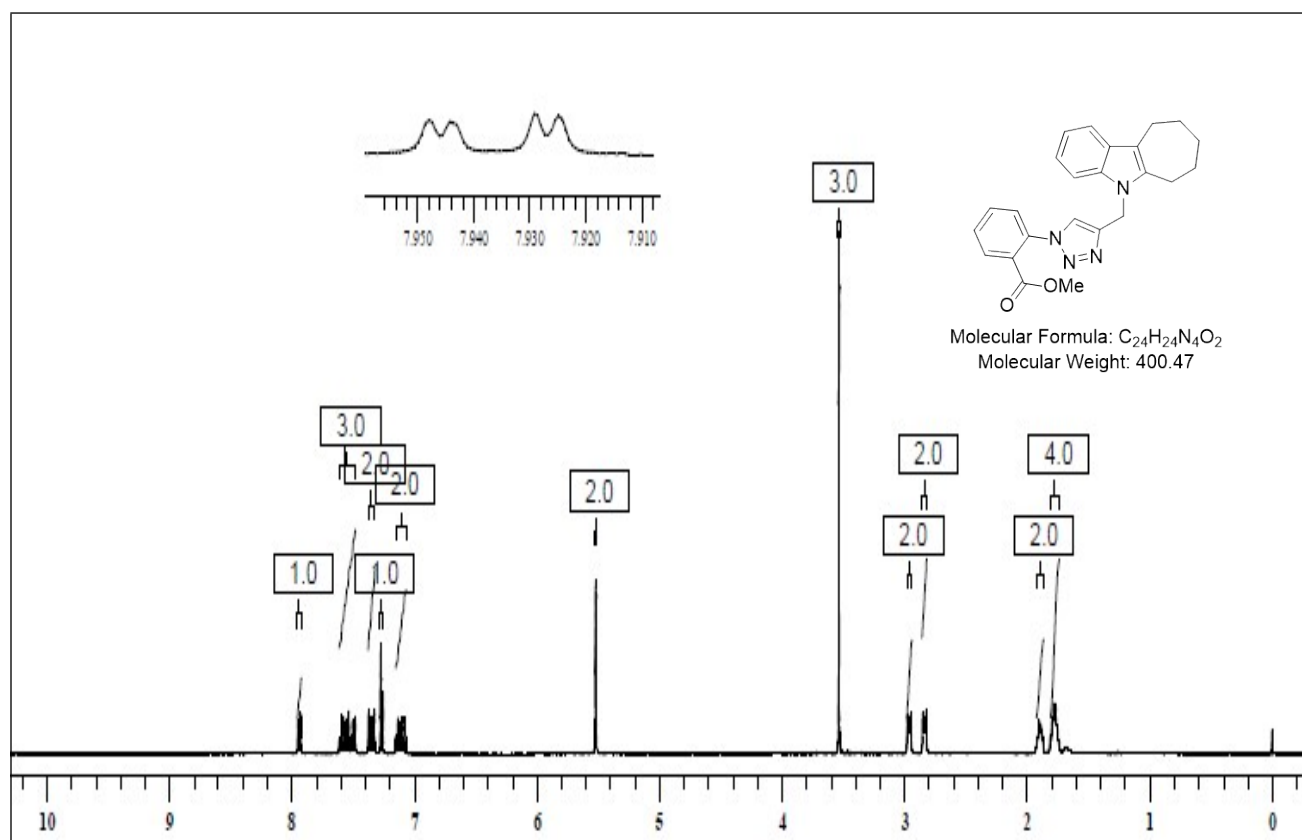


Figure S33: ¹H NMR (400 MHz, CDCl₃) of methyl 2-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)benzoate (**4h**)

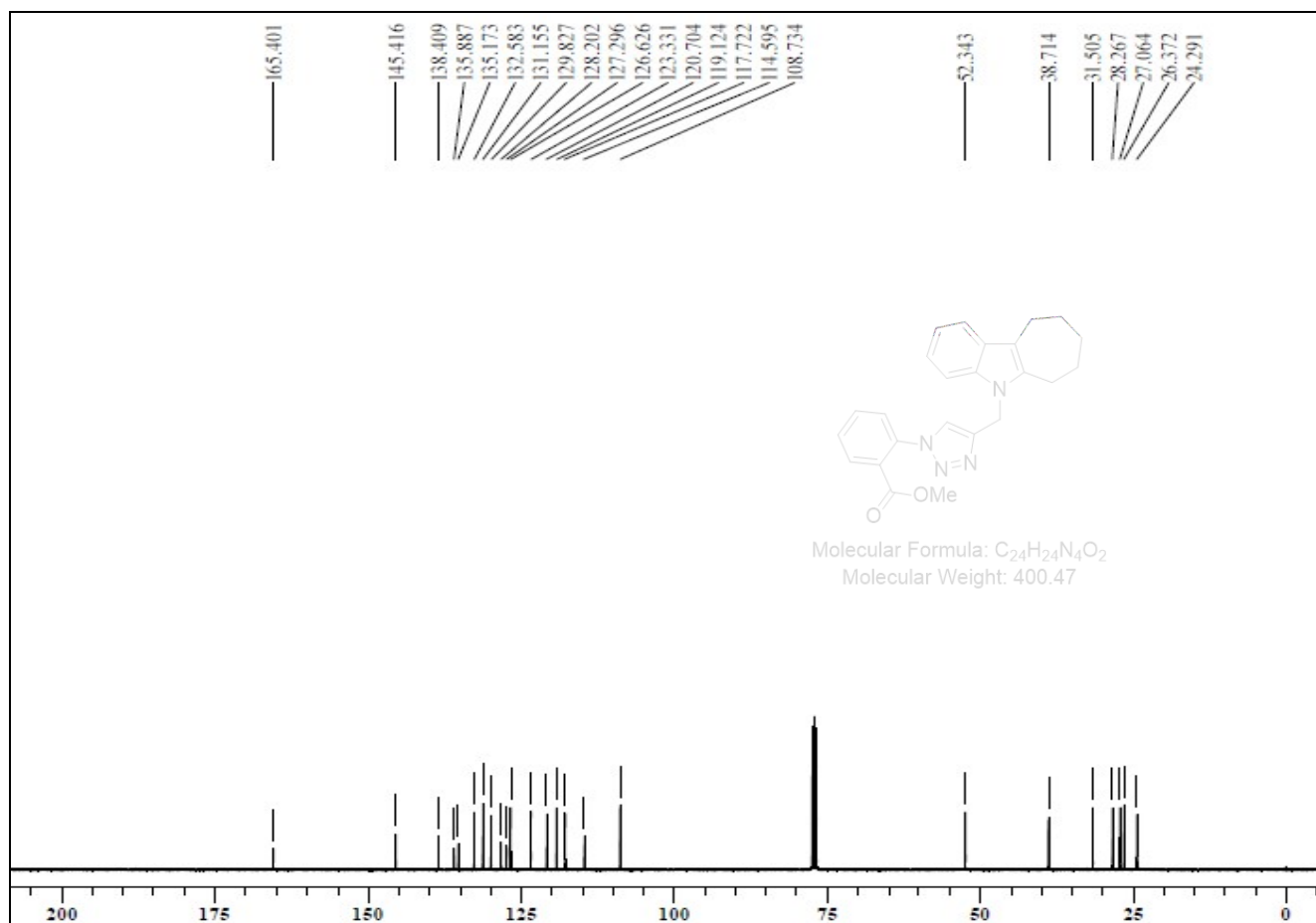


Figure S34: ¹³C NMR (100 MHz, CDCl₃) spectrum of methyl 2-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoate (**4h**)

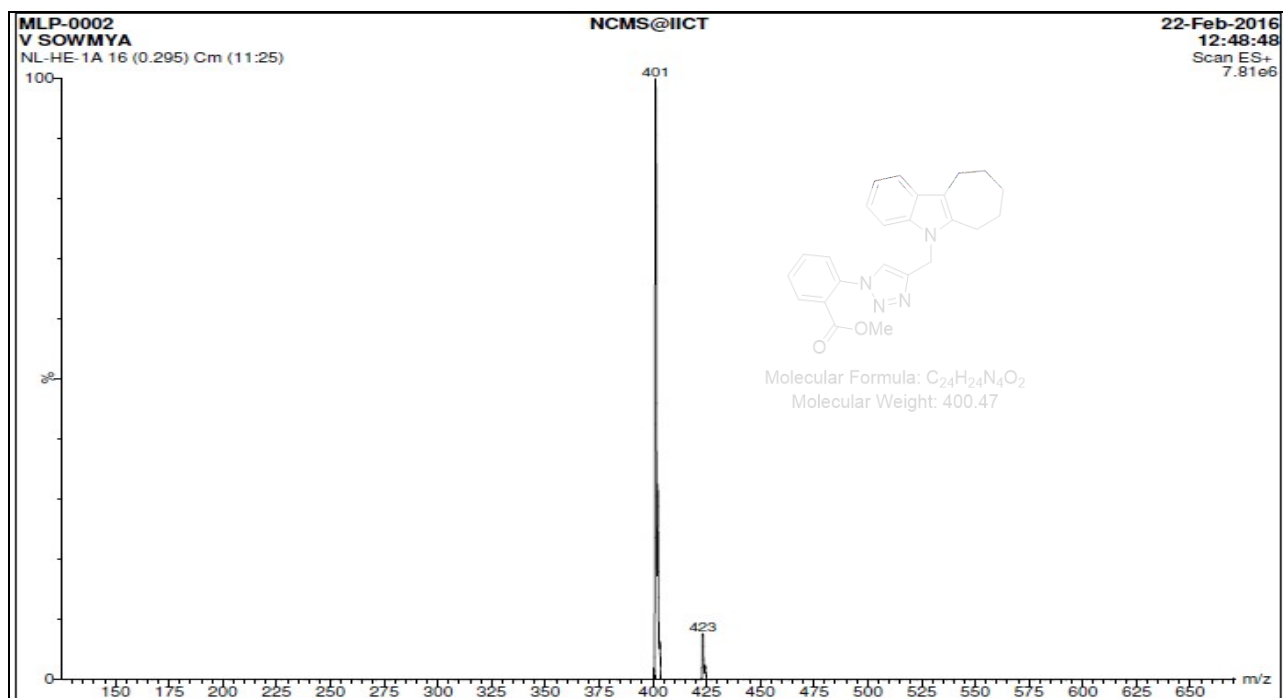


Figure S35: Mass (ES⁺) spectrum of compound methyl 2-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)benzoate (**4h**)

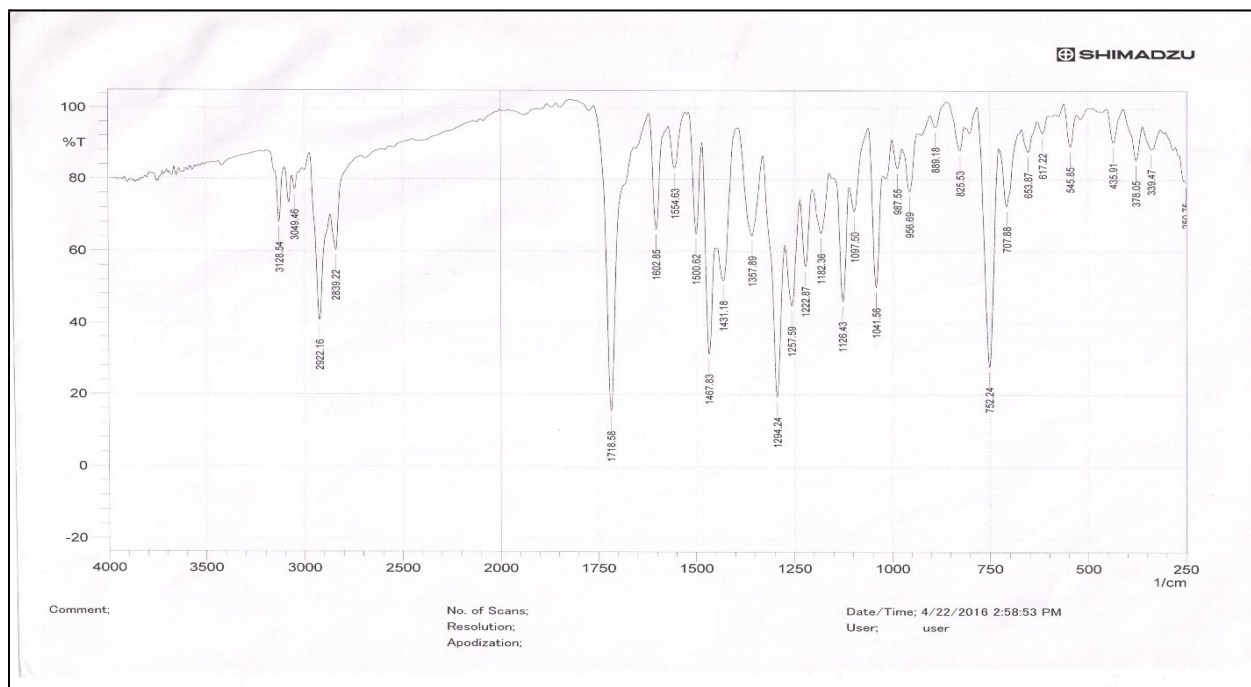


Figure S36: IR (KBr, cm⁻¹) spectrum of compound methyl 2-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)benzoate (**4h**)

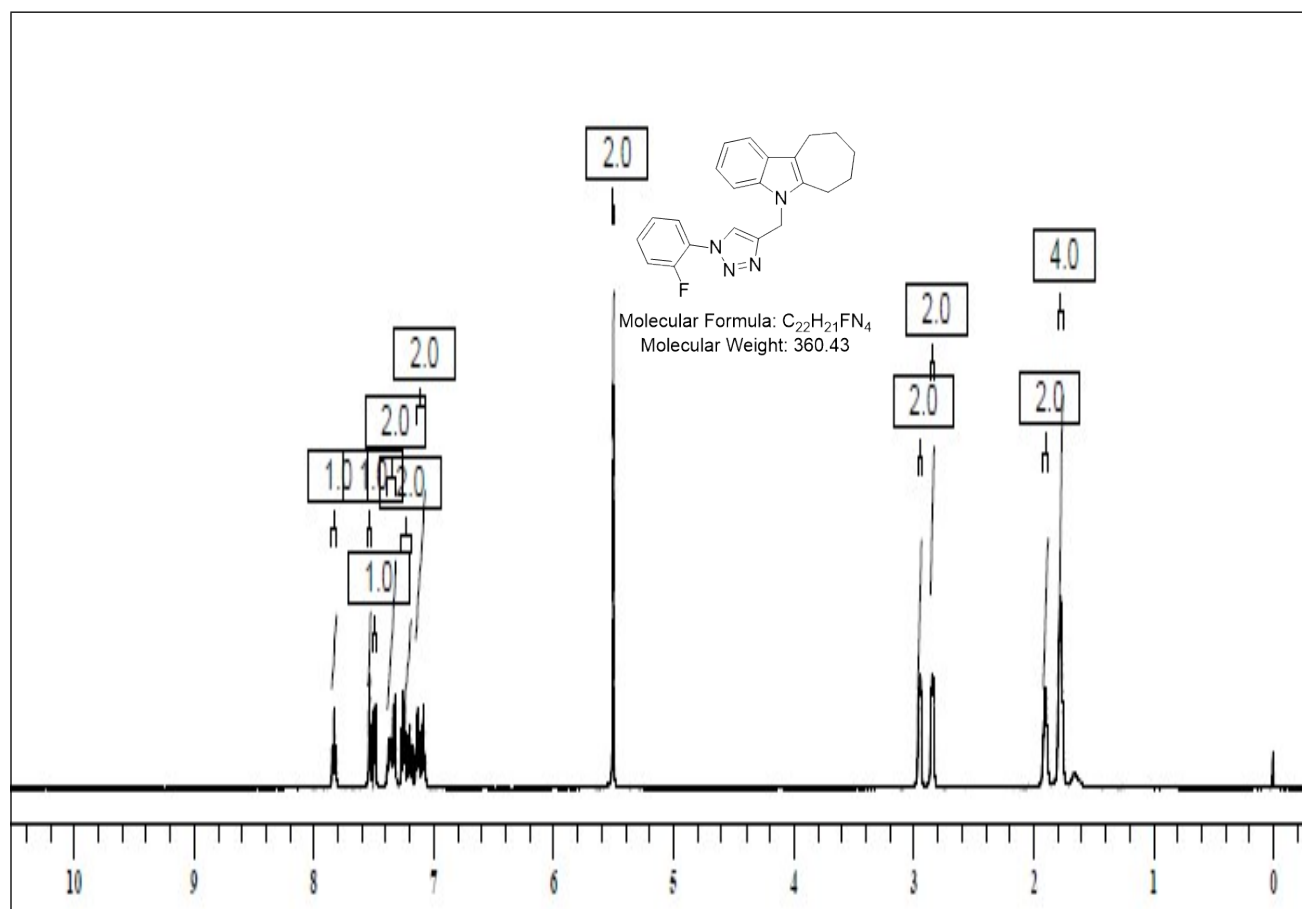


Figure S37: ¹H NMR (400 MHz, CDCl₃) of 5-((1-(2-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4i**)

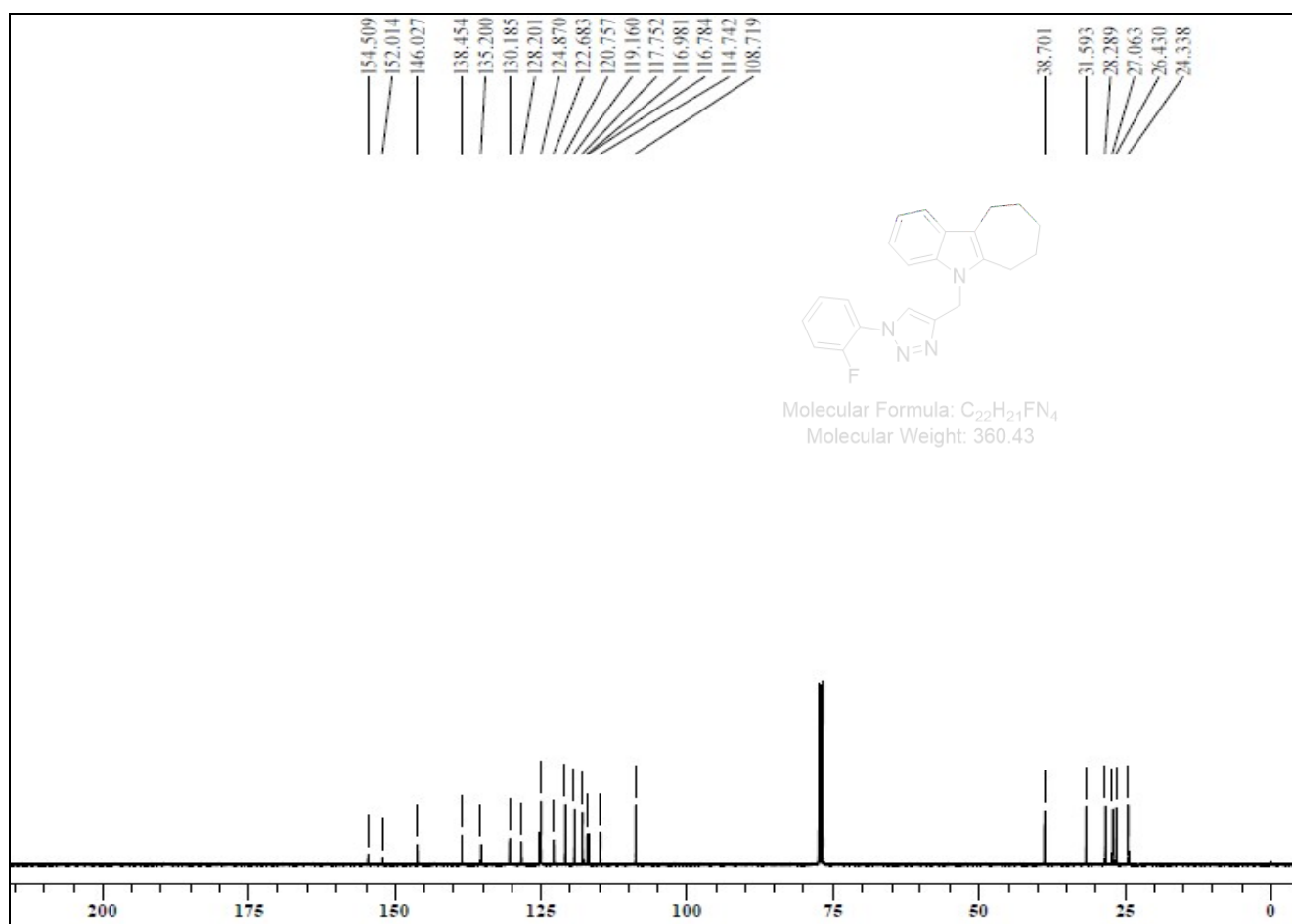


Figure S38: ¹³C NMR (100 MHz, CDCl₃) spectrum of 5-((1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4i**)

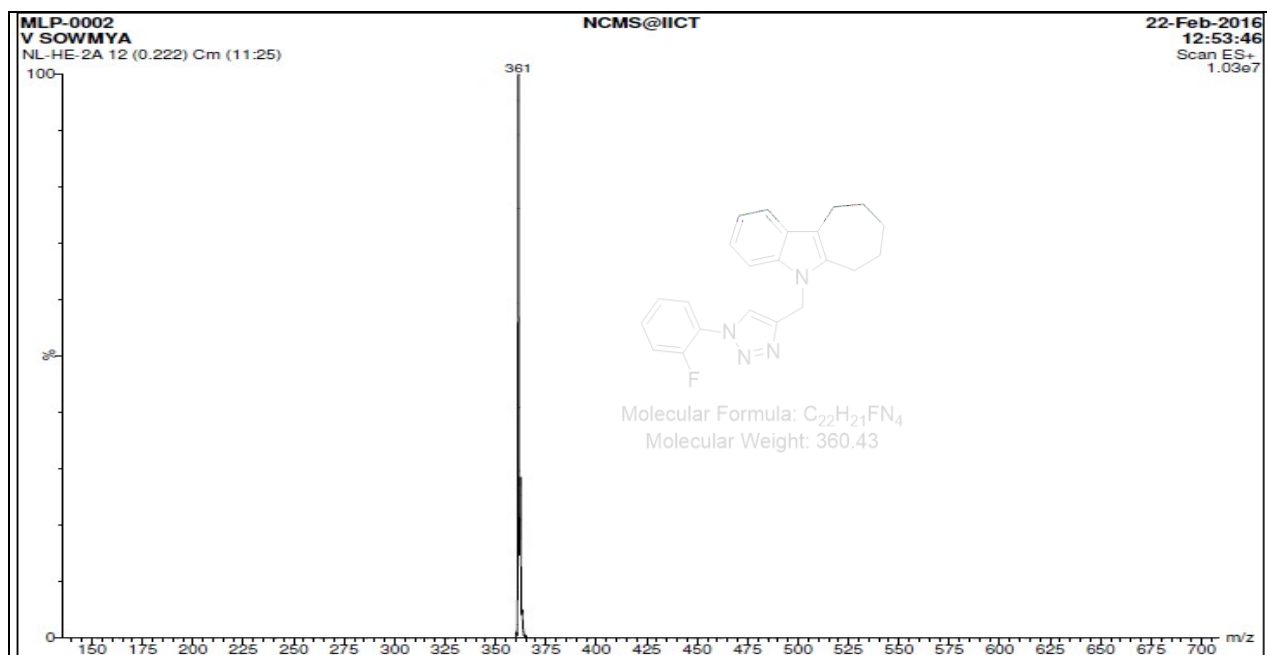


Figure S39: Mass (ES⁺) spectrum of 5-((1-(2-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4i**)

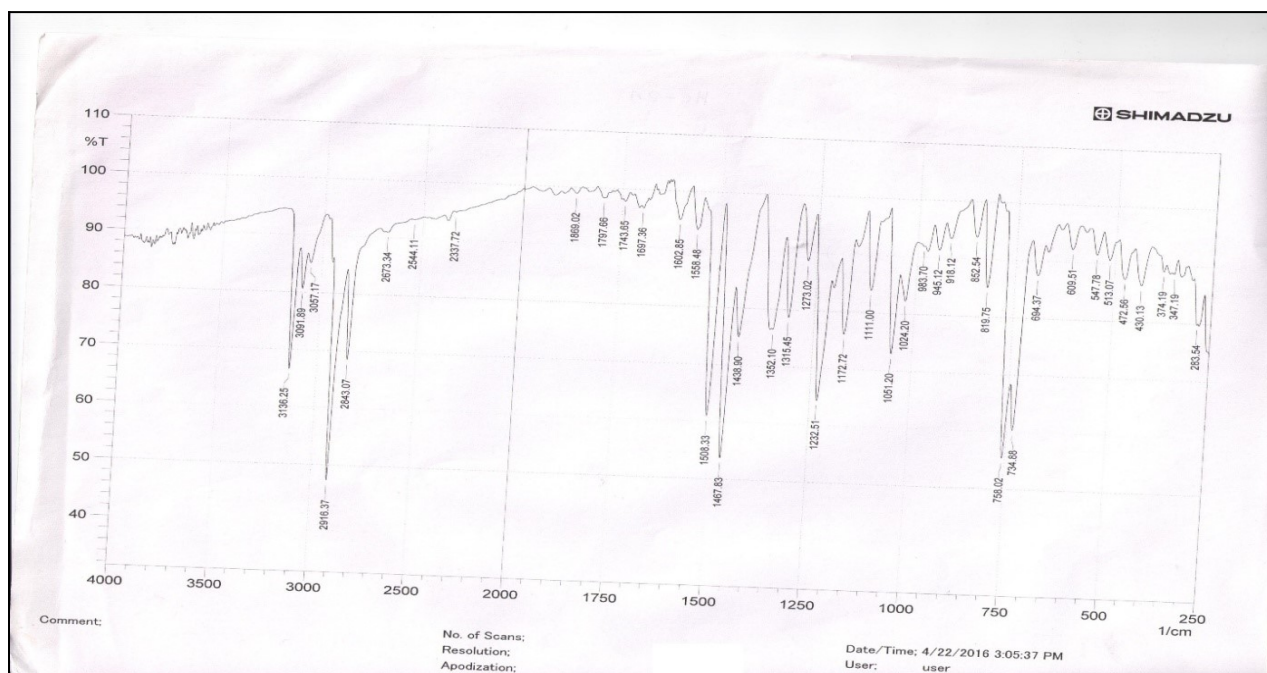


Figure S40: IR (KBr, cm⁻¹) spectrum of 5-((1-(2-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4i**)

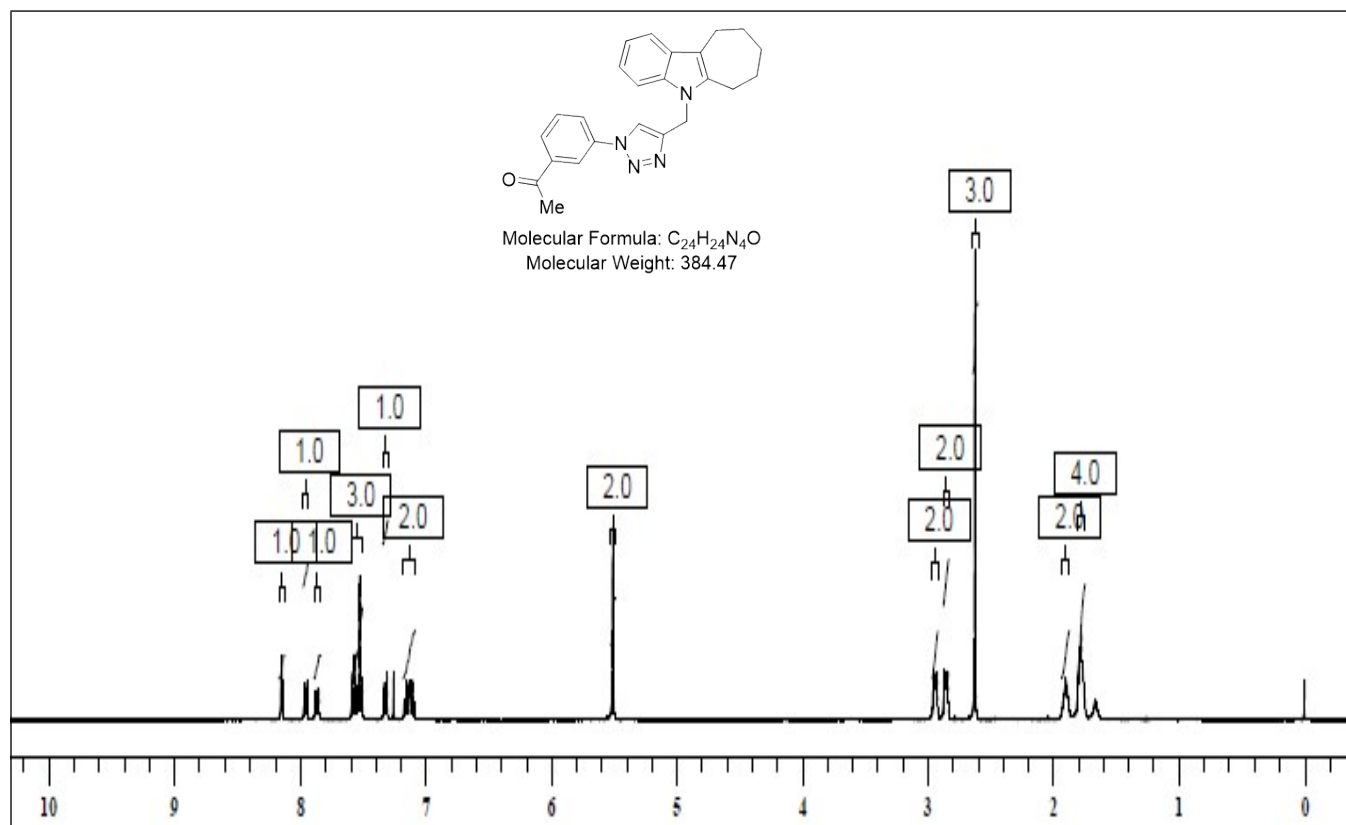


Figure S41: ¹H NMR (400 MHz, CDCl₃) of 1-(3-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethanone (**4j**)

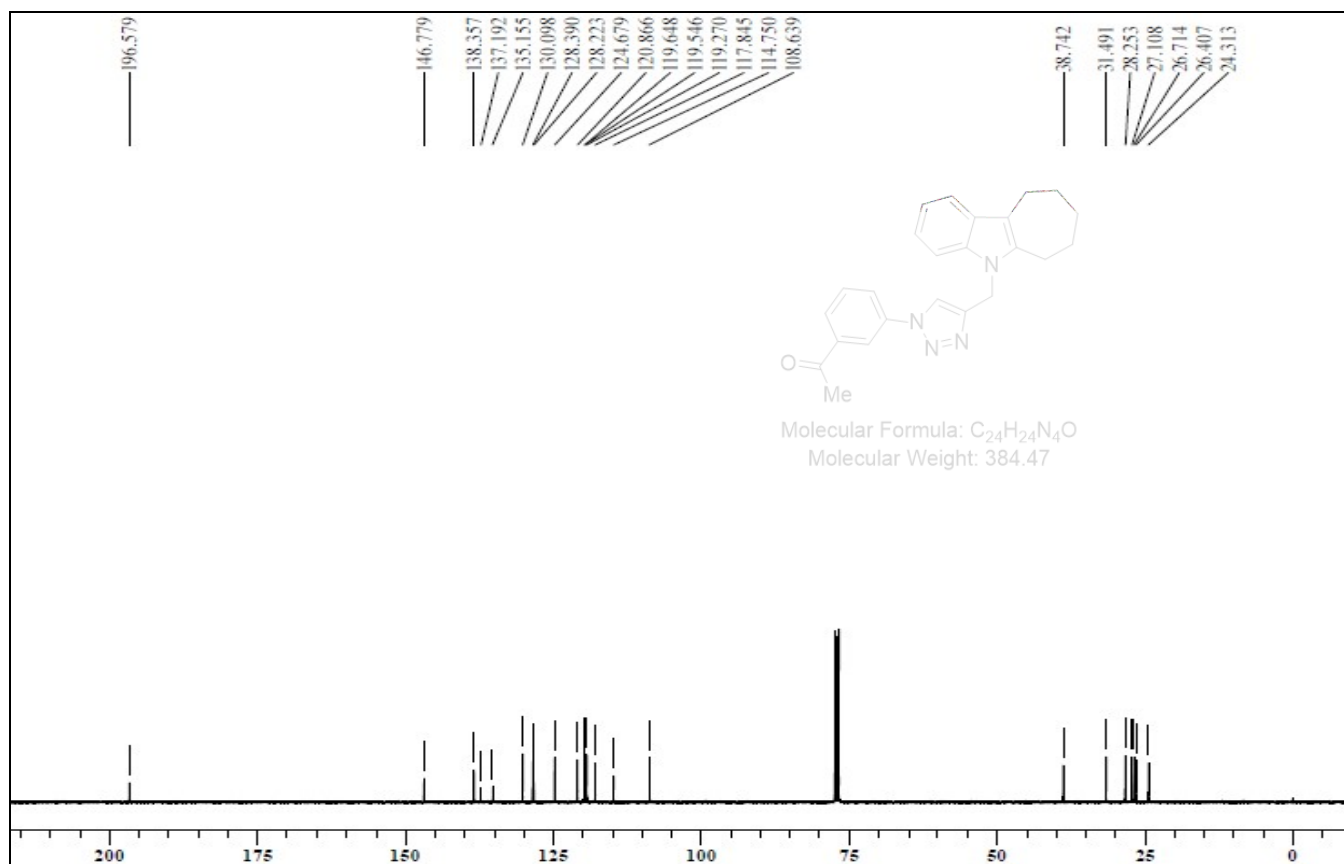


Figure S42: ¹³C NMR (100 MHz, CDCl₃) spectrum of 1-(3-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone (**4j**)

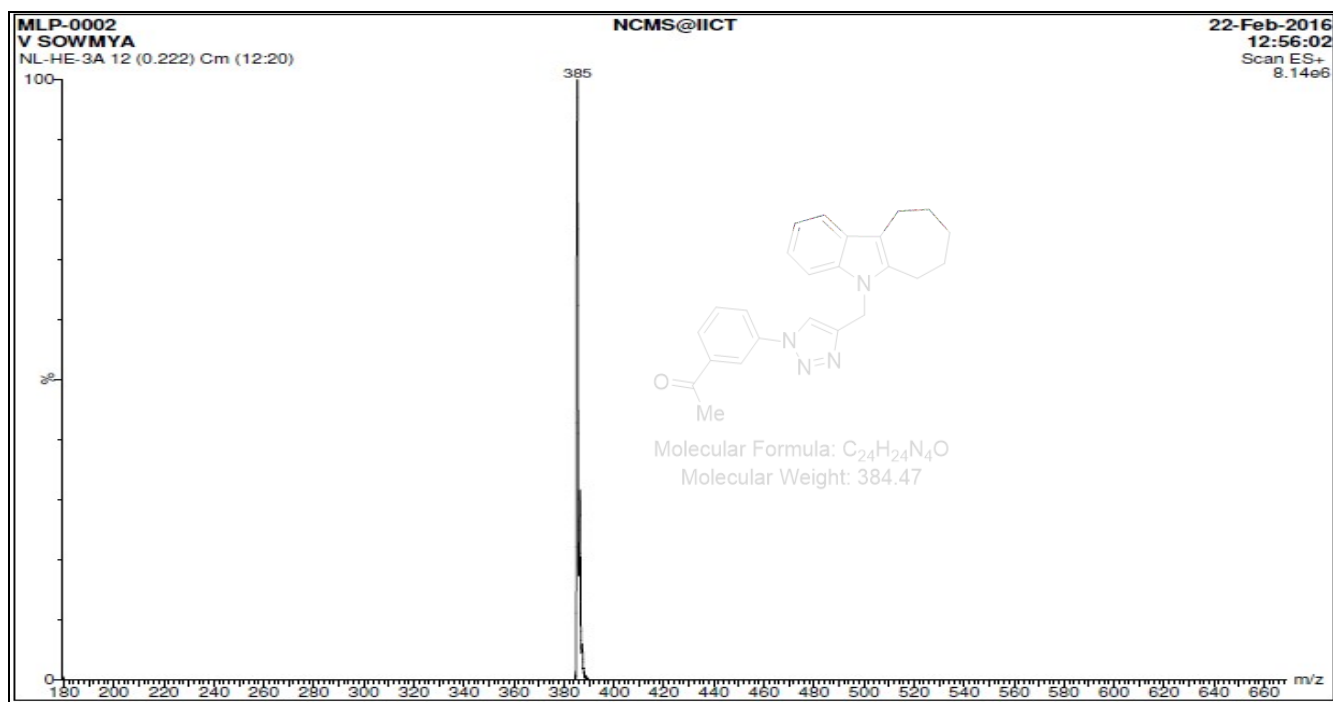


Figure S43: Mass (ES⁺) spectrum of 1-(3-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethanone (**4j**)

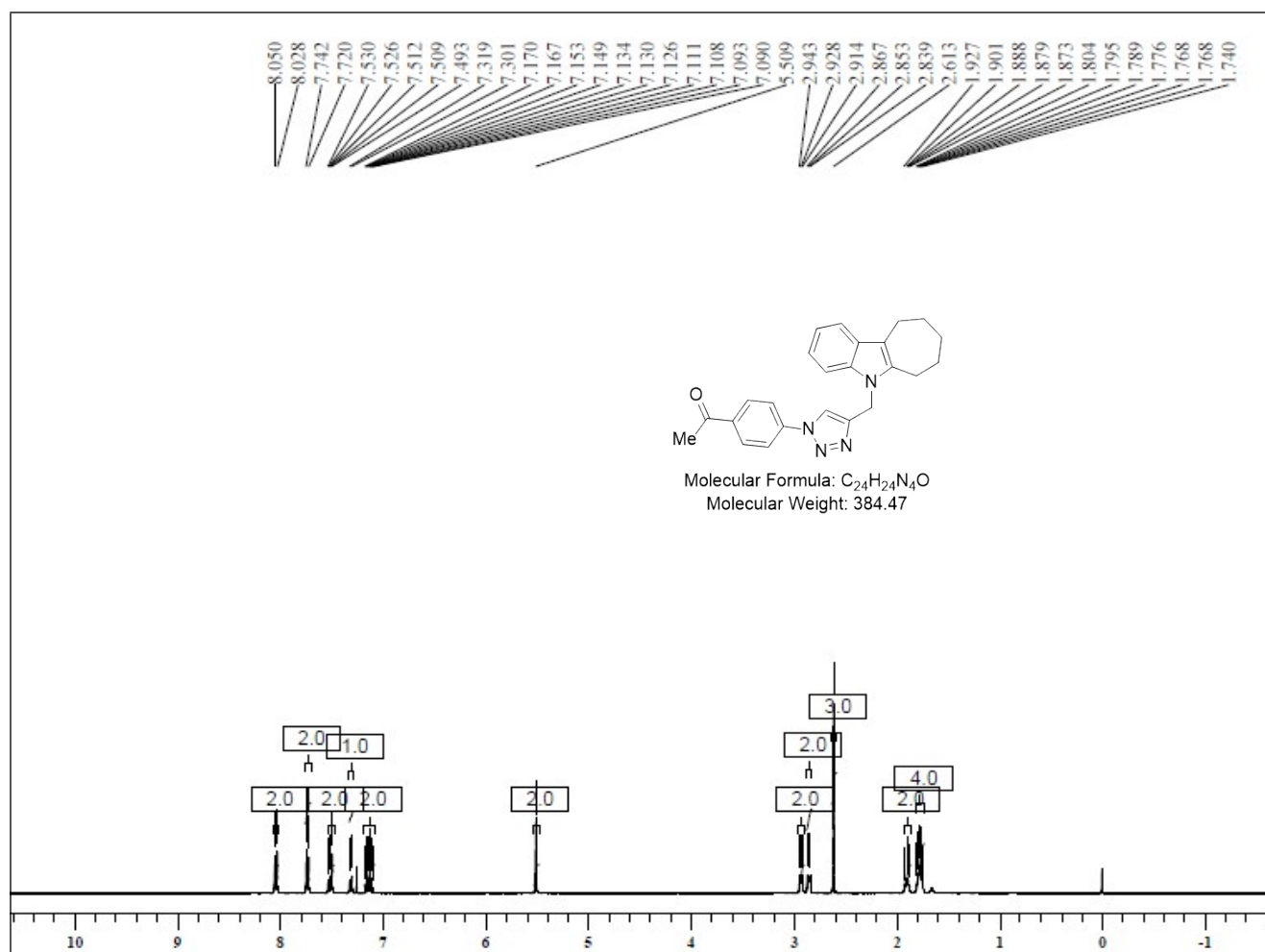


Figure S44: ¹H NMR (400 MHz, CDCl₃) of 1-(4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone (**4k**)

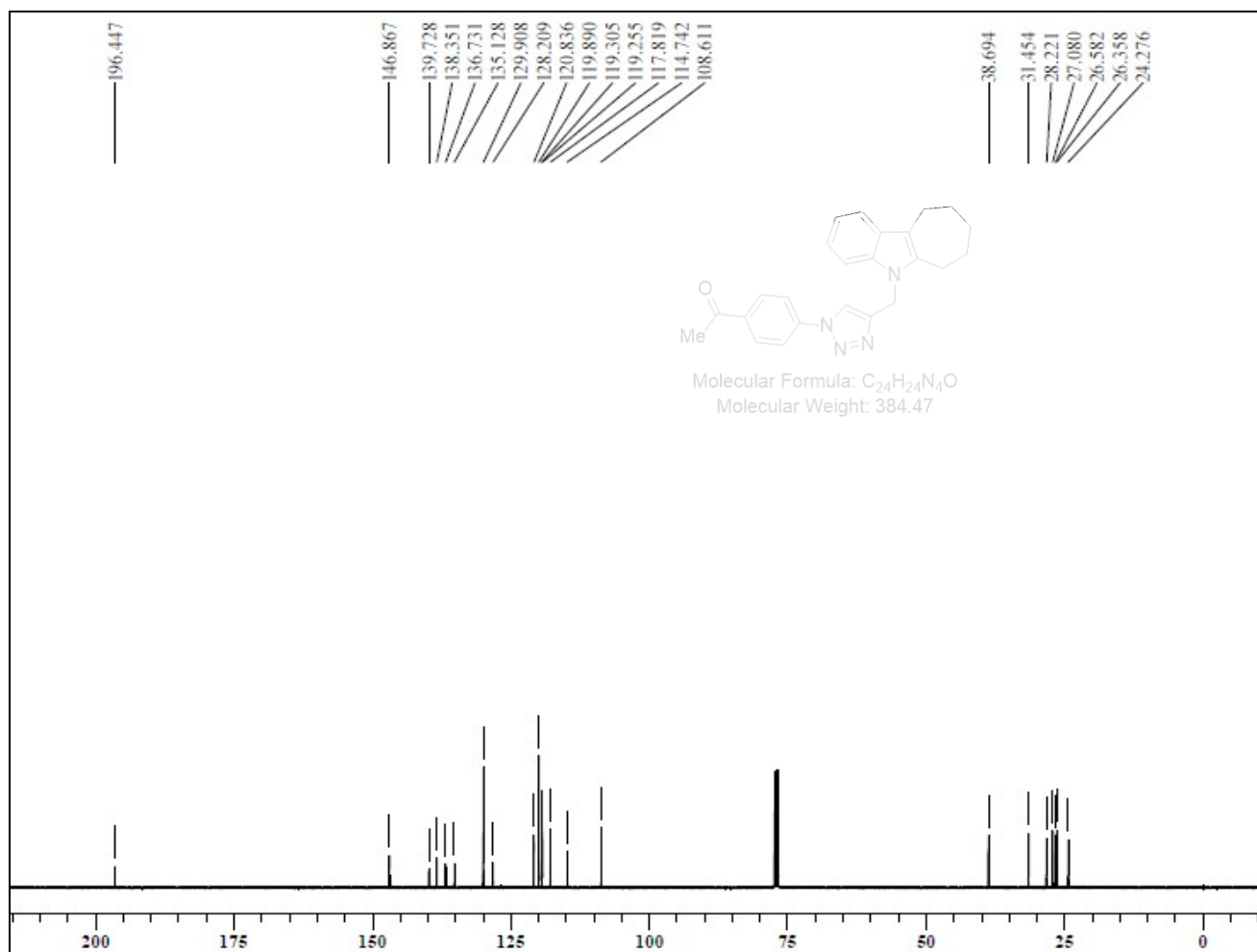


Figure S45: ¹³C NMR (100 MHz, CDCl₃) spectrum of 1-(4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone(**4k**)

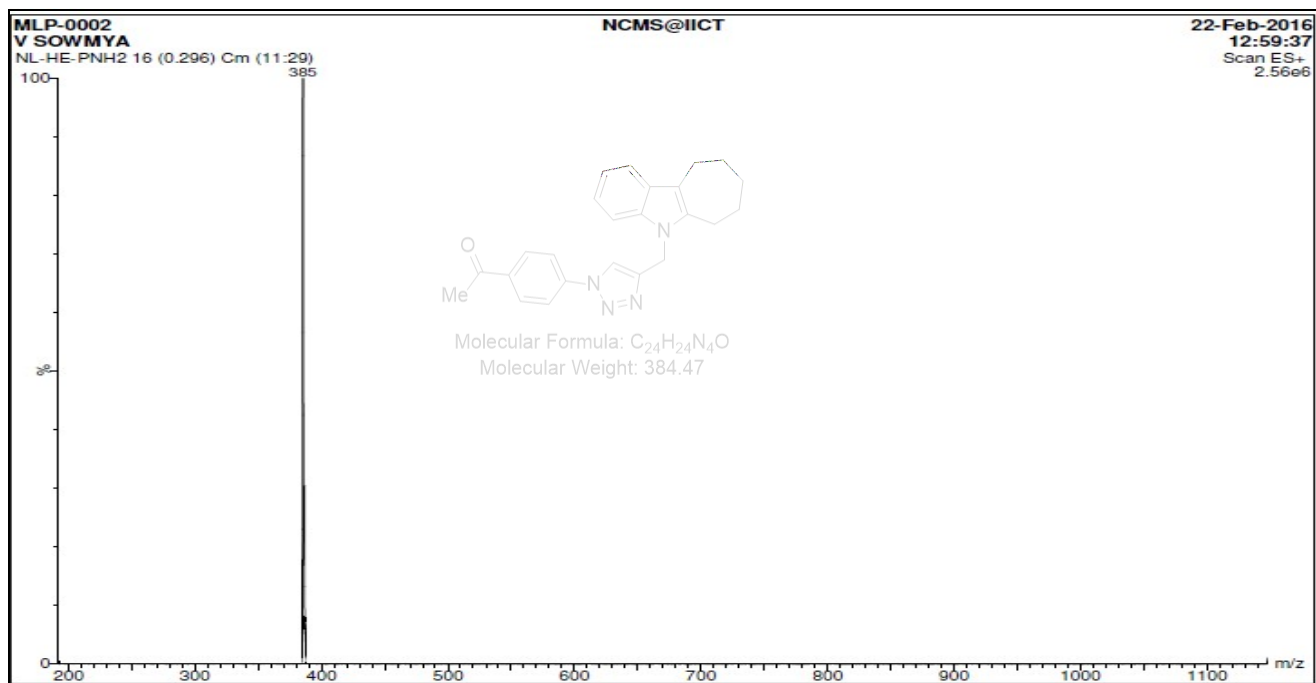


Figure S46: Mass (ES⁺) spectrum of 1-(4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone (**4k**)

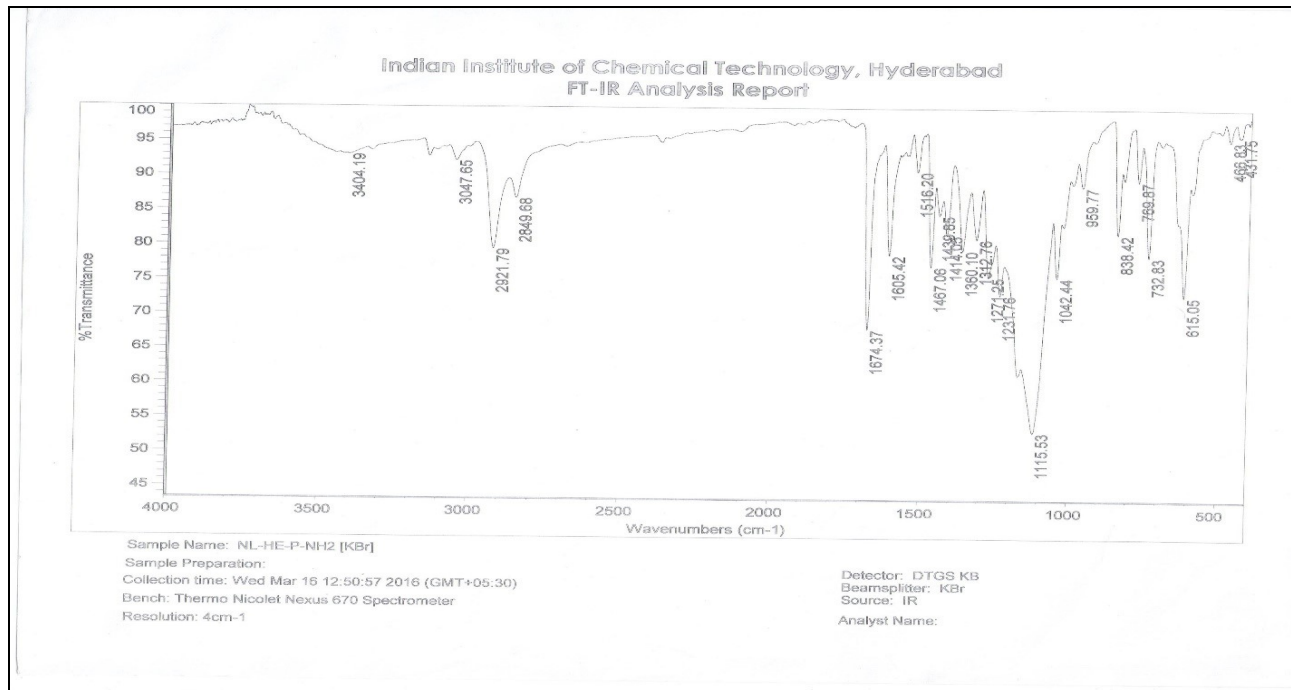


Figure S47: IR (KBr, cm⁻¹) spectrum of 1-(4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)ethanone (**4k**)

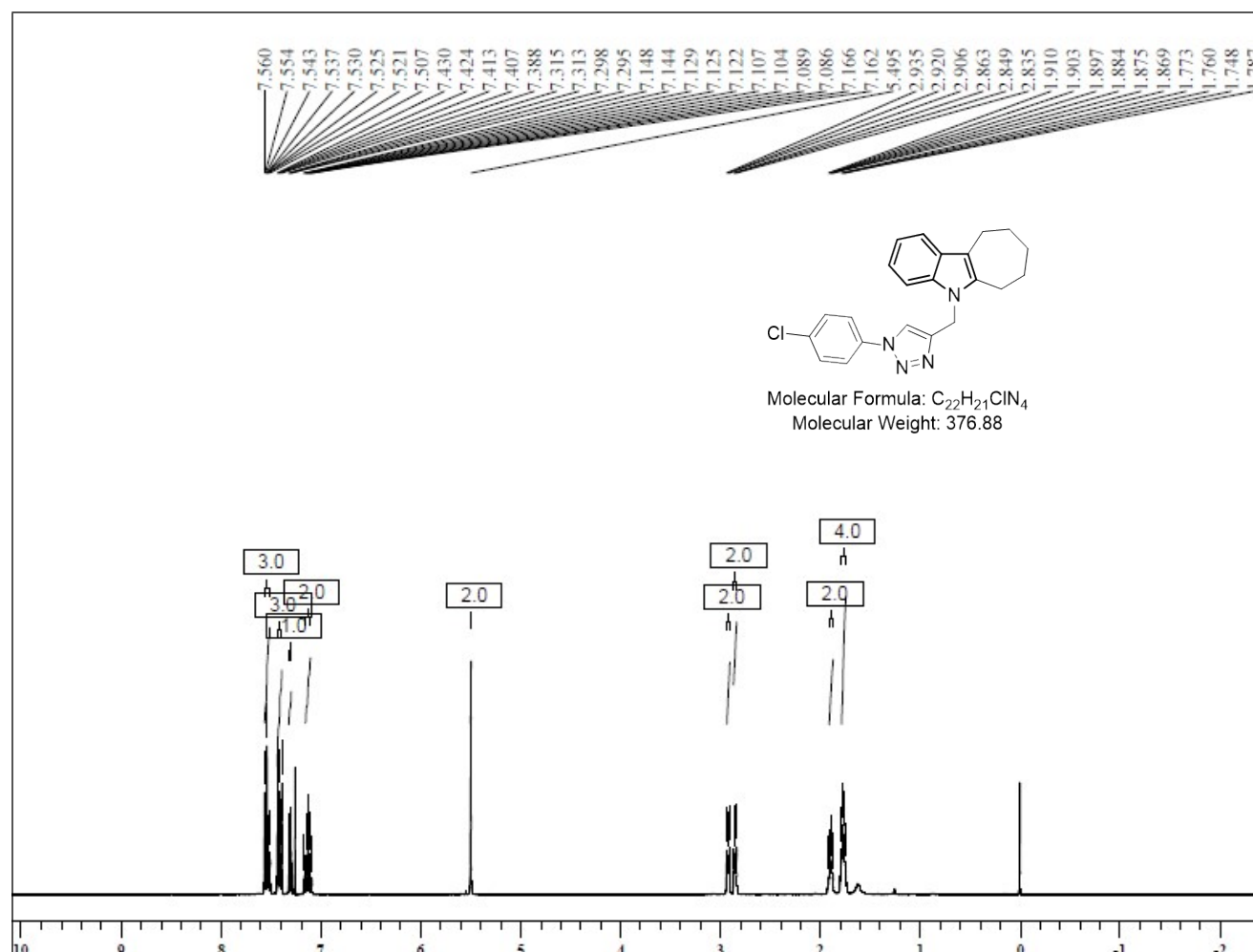


Figure S48: ¹H NMR (400 MHz, CDCl₃) of 5-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4l**)

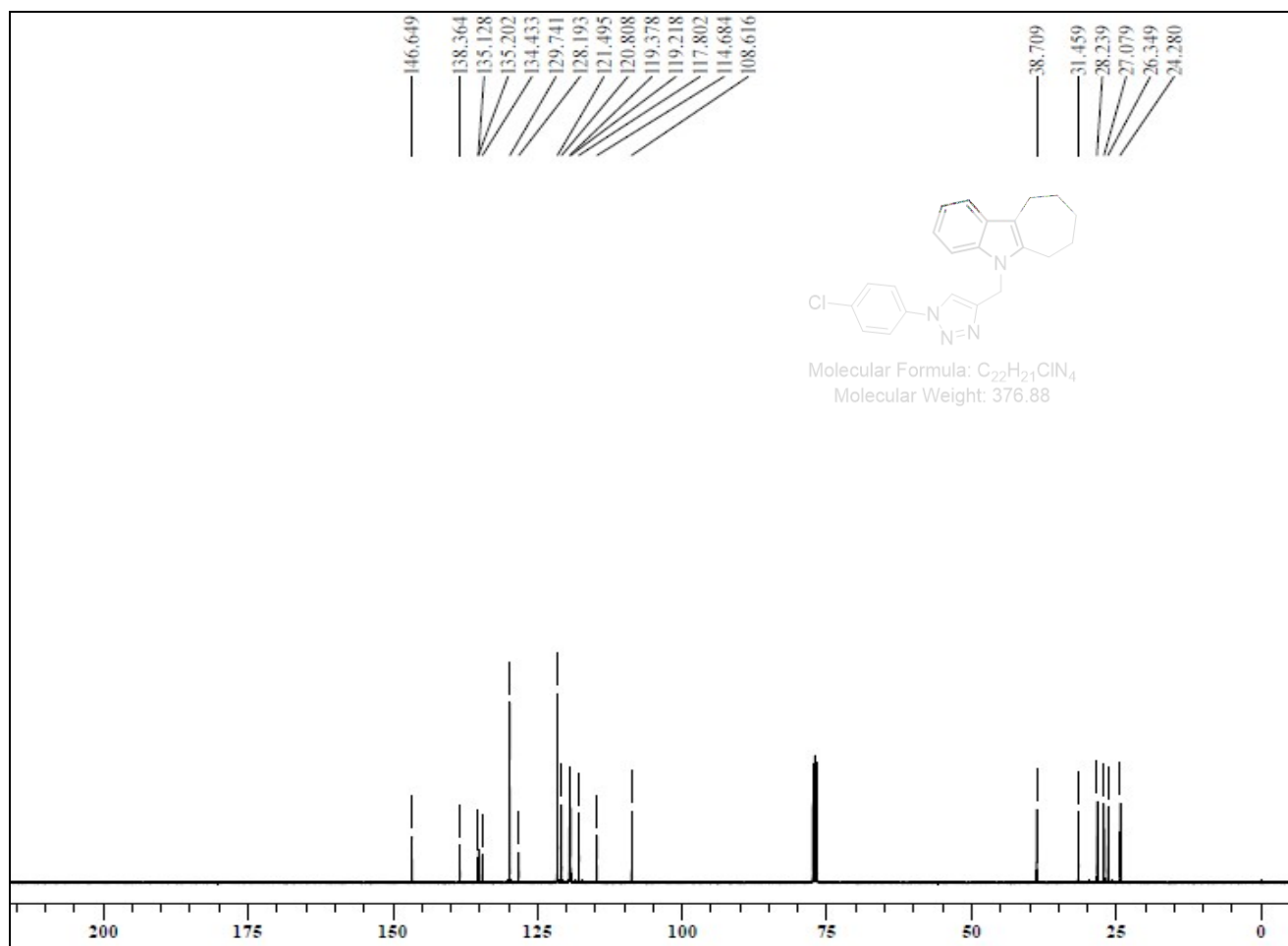


Figure S49: ¹³C NMR (100 MHz, CDCl₃) spectrum of 5-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4I**)

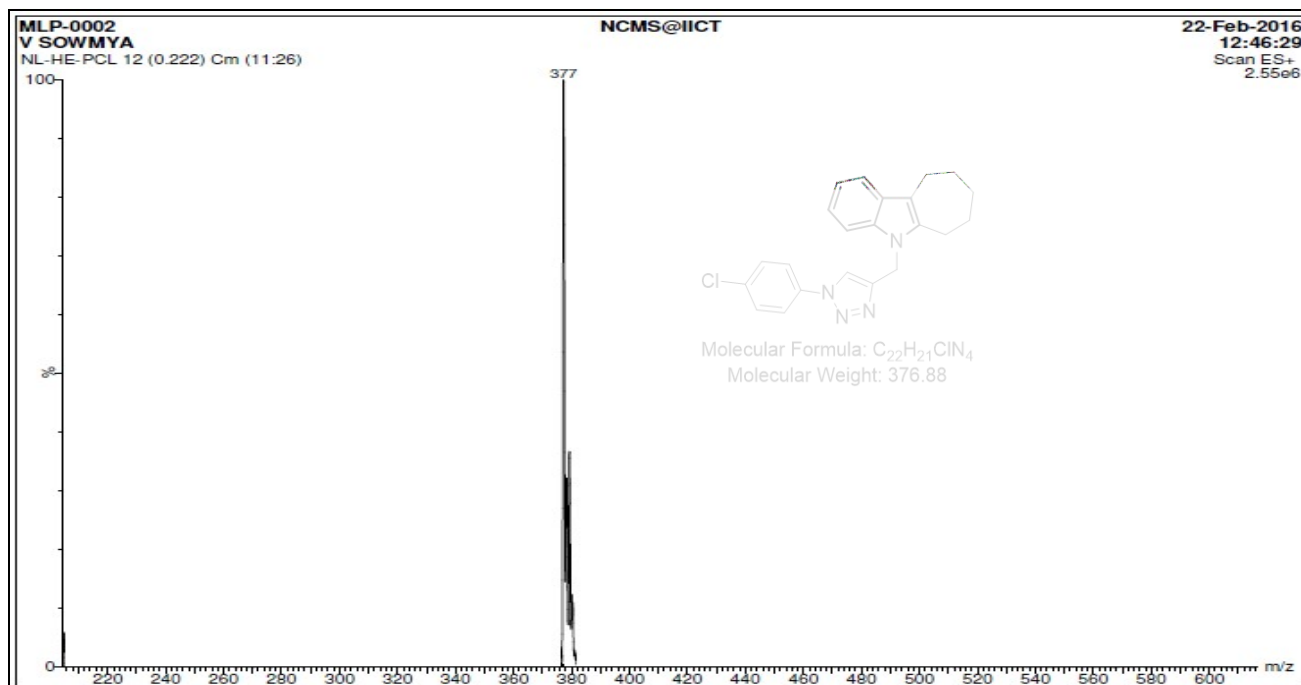


Figure S50: Mass (ES⁺) spectrum of 5-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4l**)

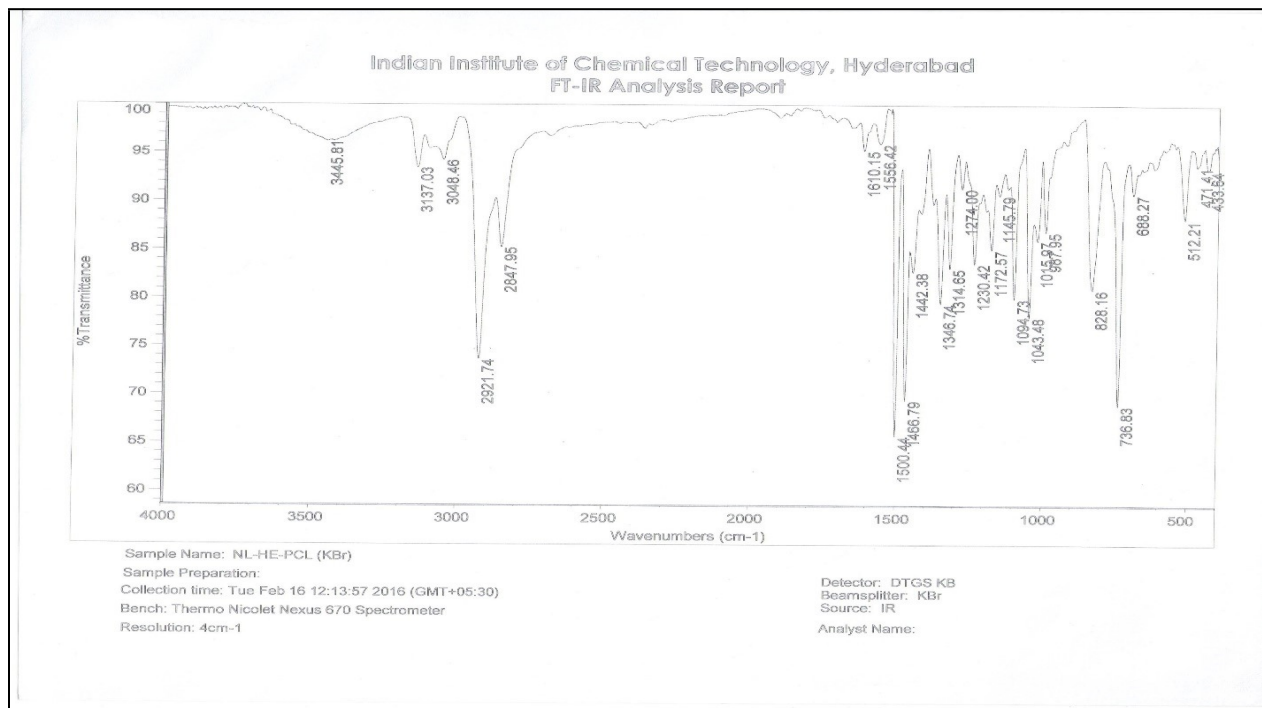


Figure S51: IR (KBr, cm⁻¹) spectrum of 5-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4l**)

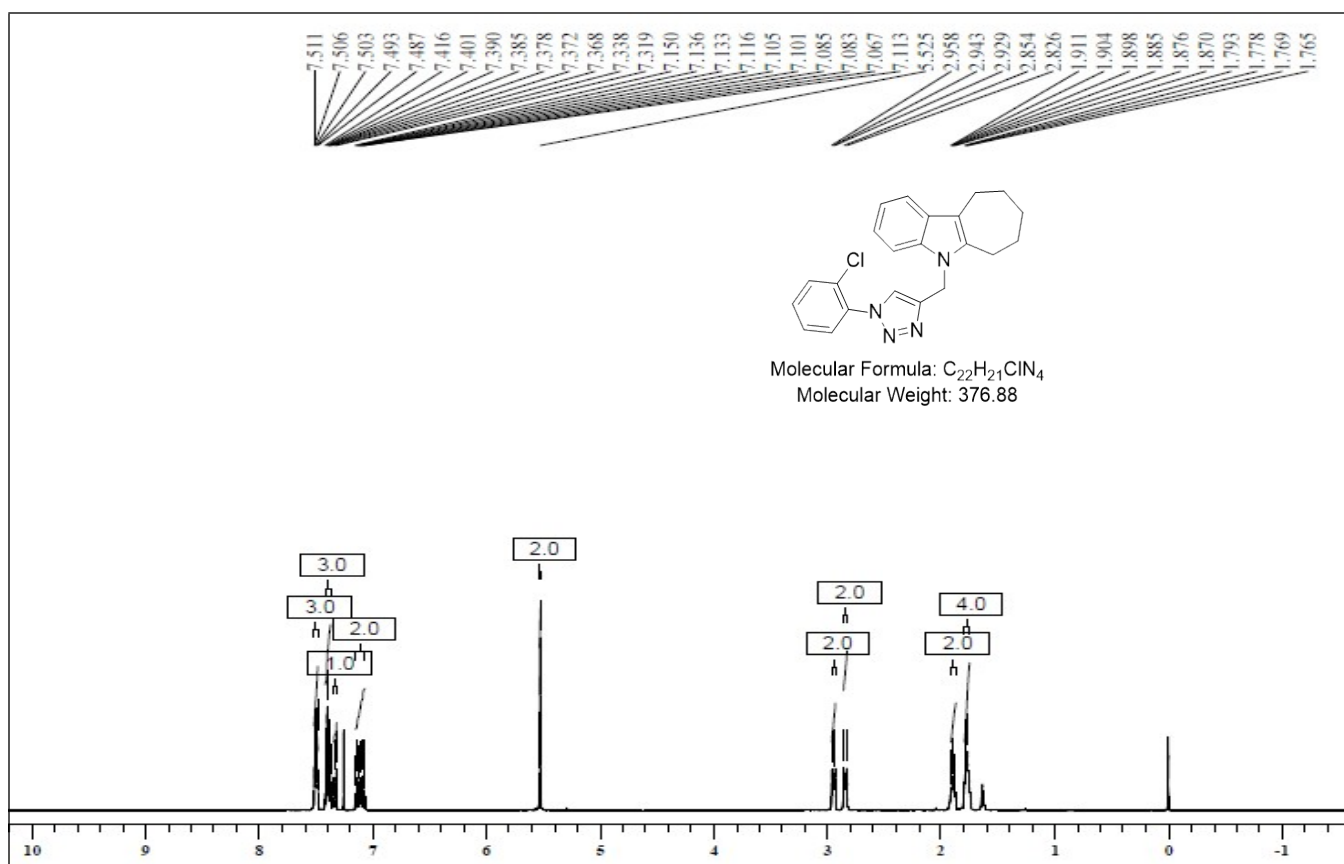


Figure S52: ¹H NMR (400 MHz, CDCl₃) of 4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl hypochlorite (**4m**)

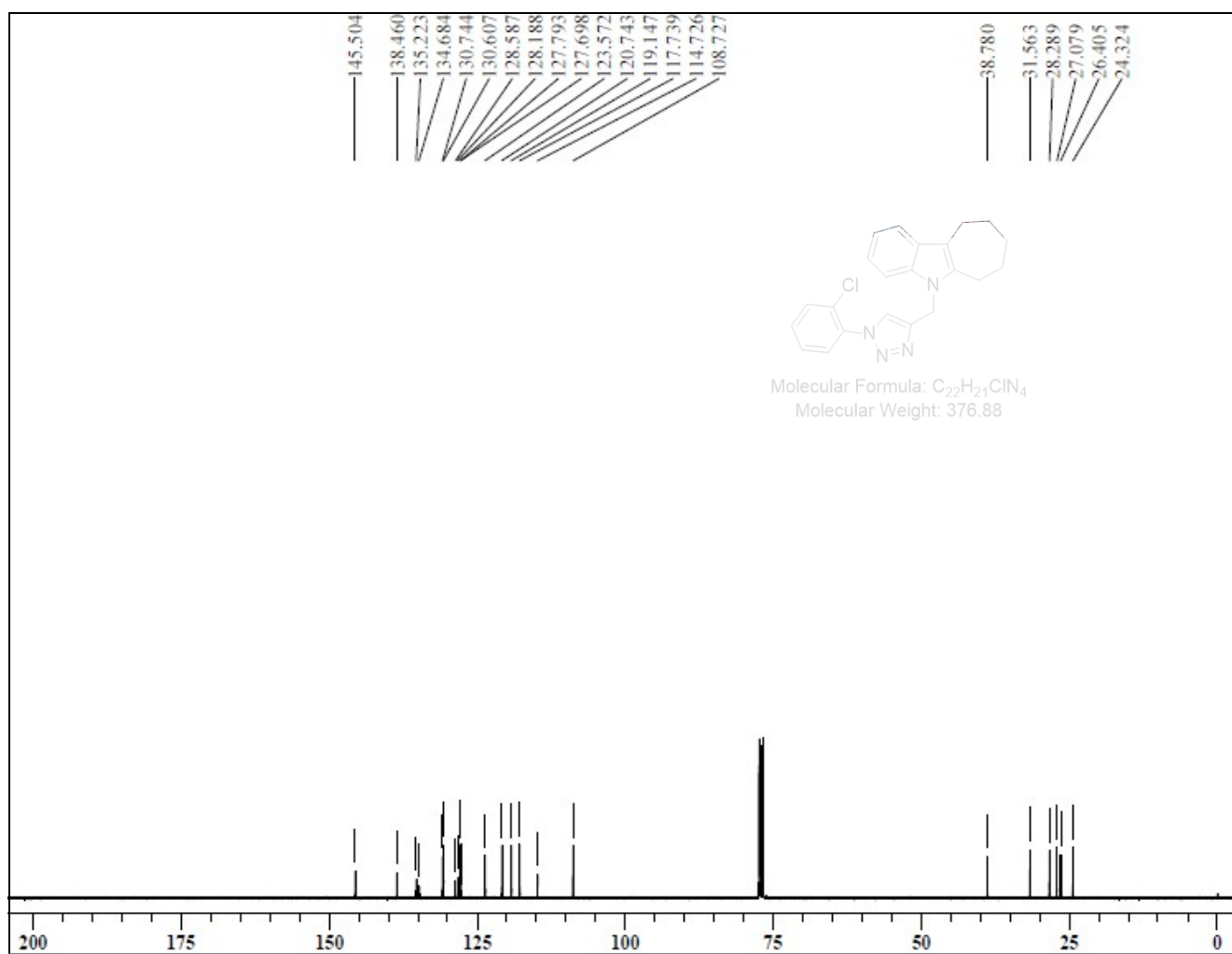


Figure S53: ¹³C NMR (100 MHz, CDCl₃) of 4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenyl hypochlorite (**4m**)

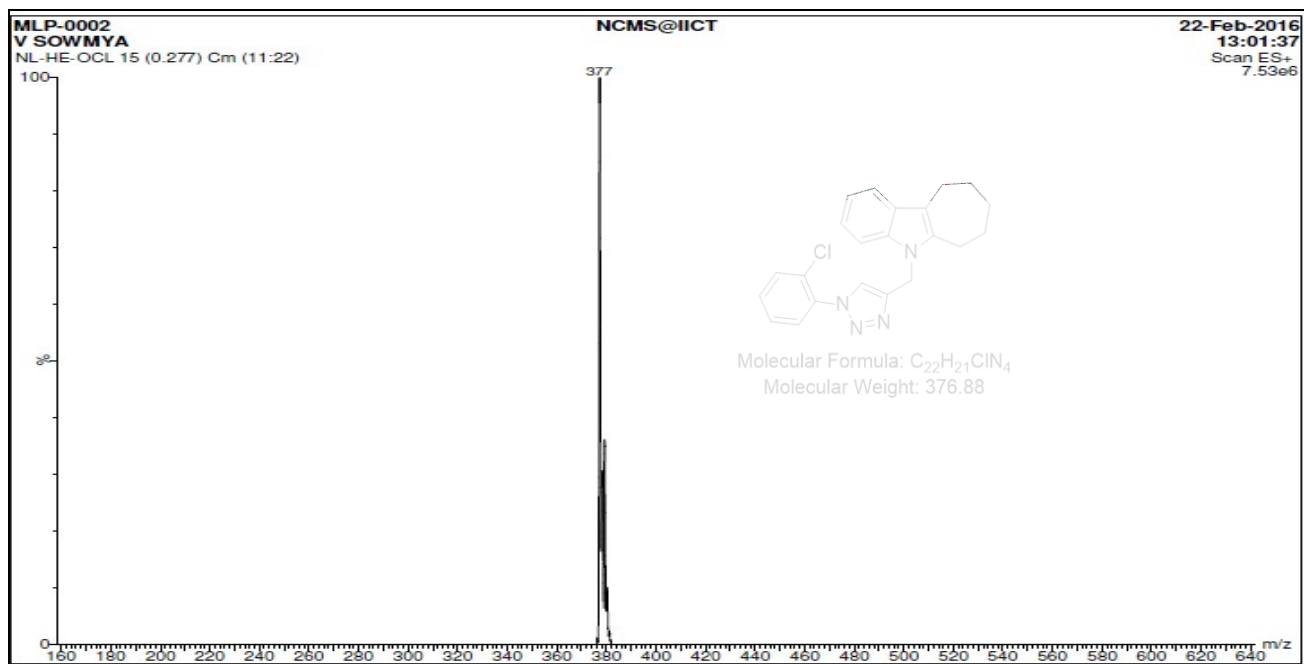


Figure S54: Mass (ES⁺) spectrum of 4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl hypochlorite (**4m**)

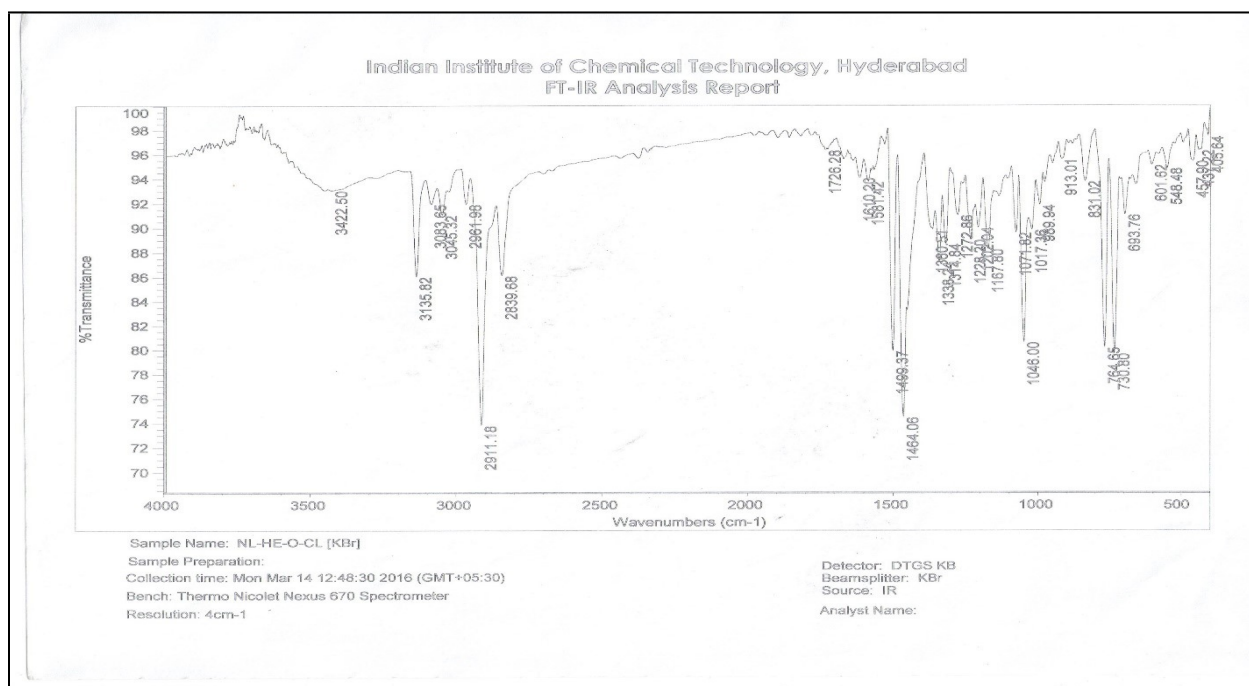


Figure S55: IR (KBr, cm⁻¹) spectrum of 4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenyl hypochlorite (**4m**)

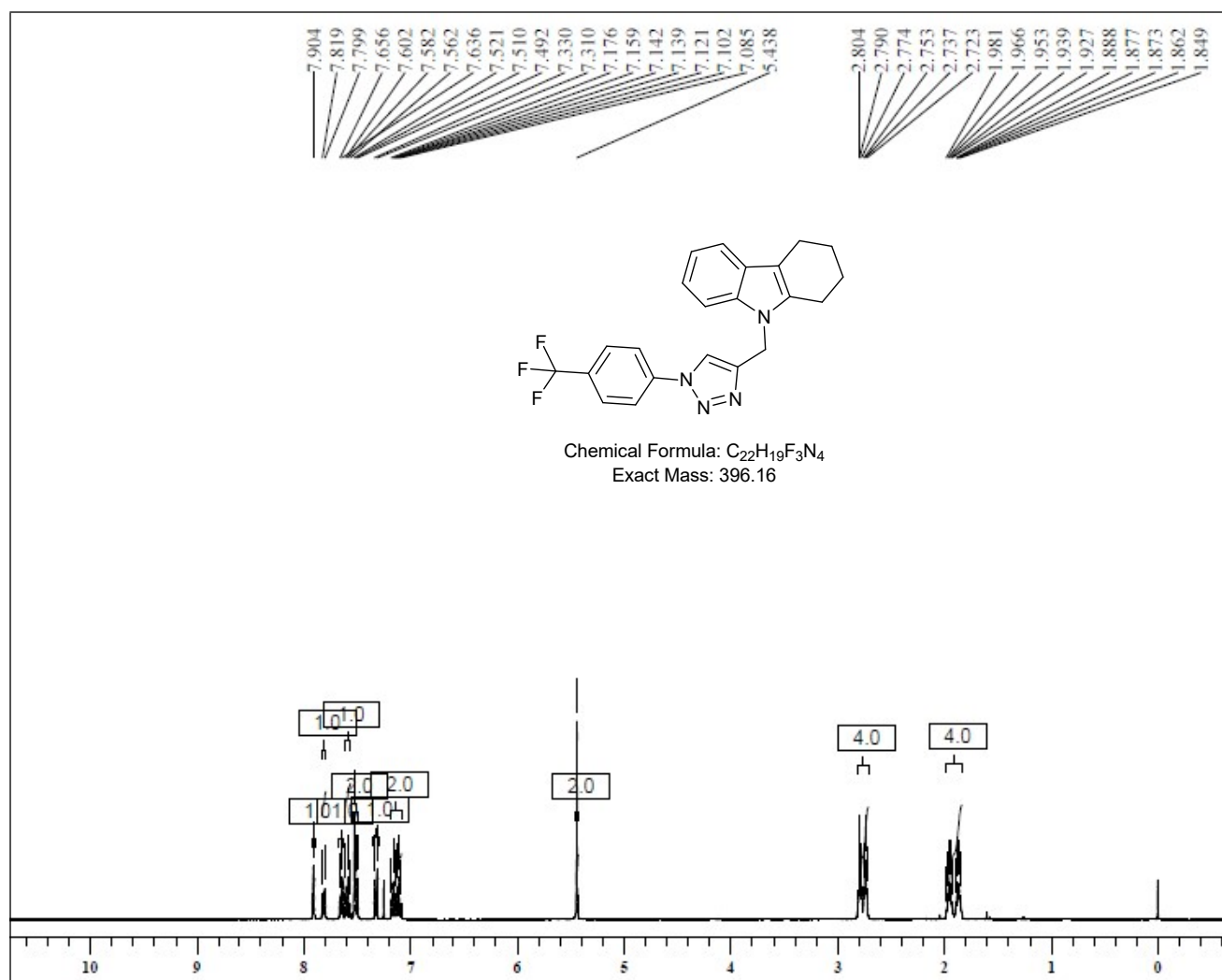


Figure S56: ¹H NMR (400 MHz, CDCl₃) of 9-((1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4n**)

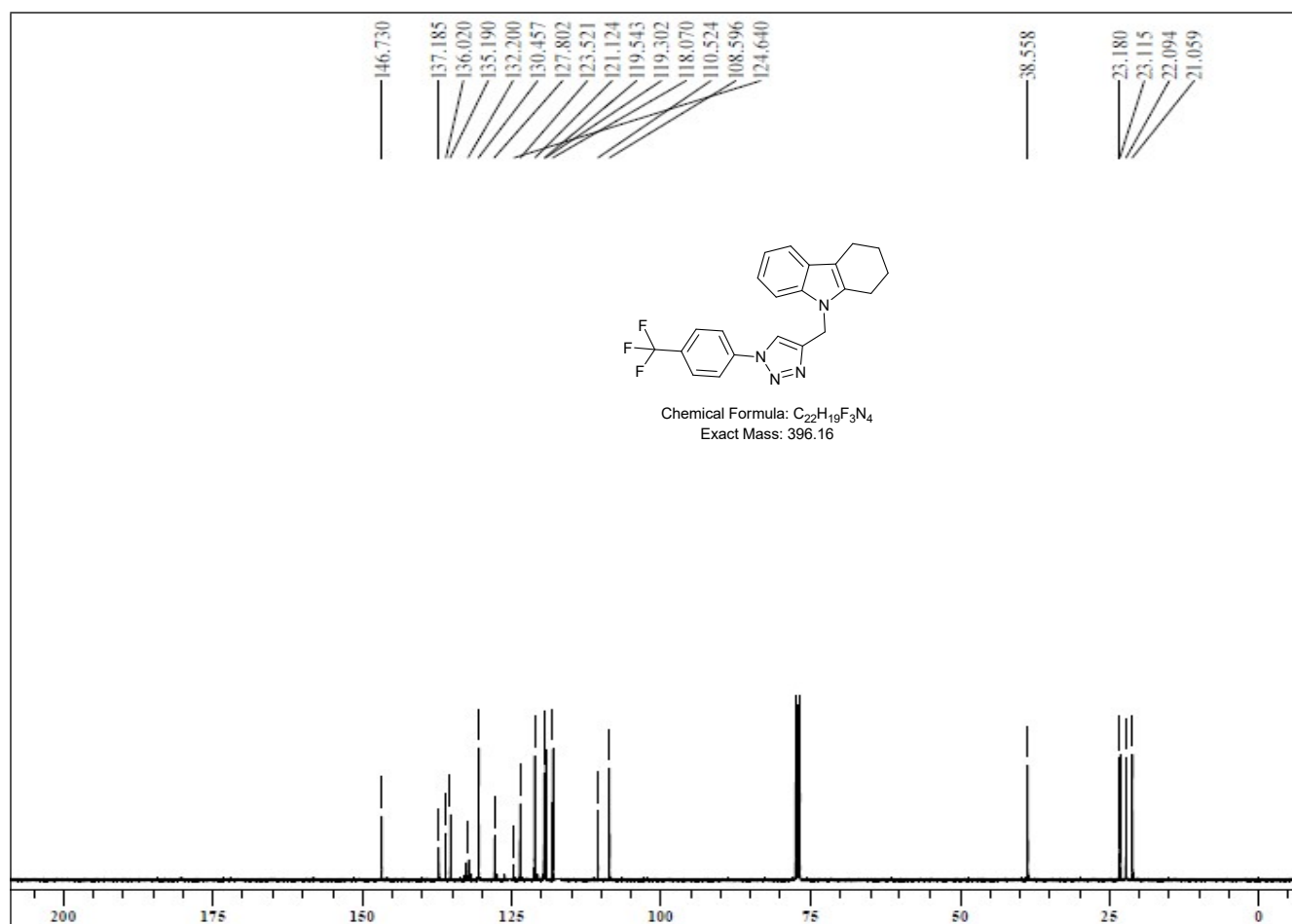


Figure S57: ¹³C NMR (100 MHz, CDCl₃) spectrum of 9-((1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4n**)

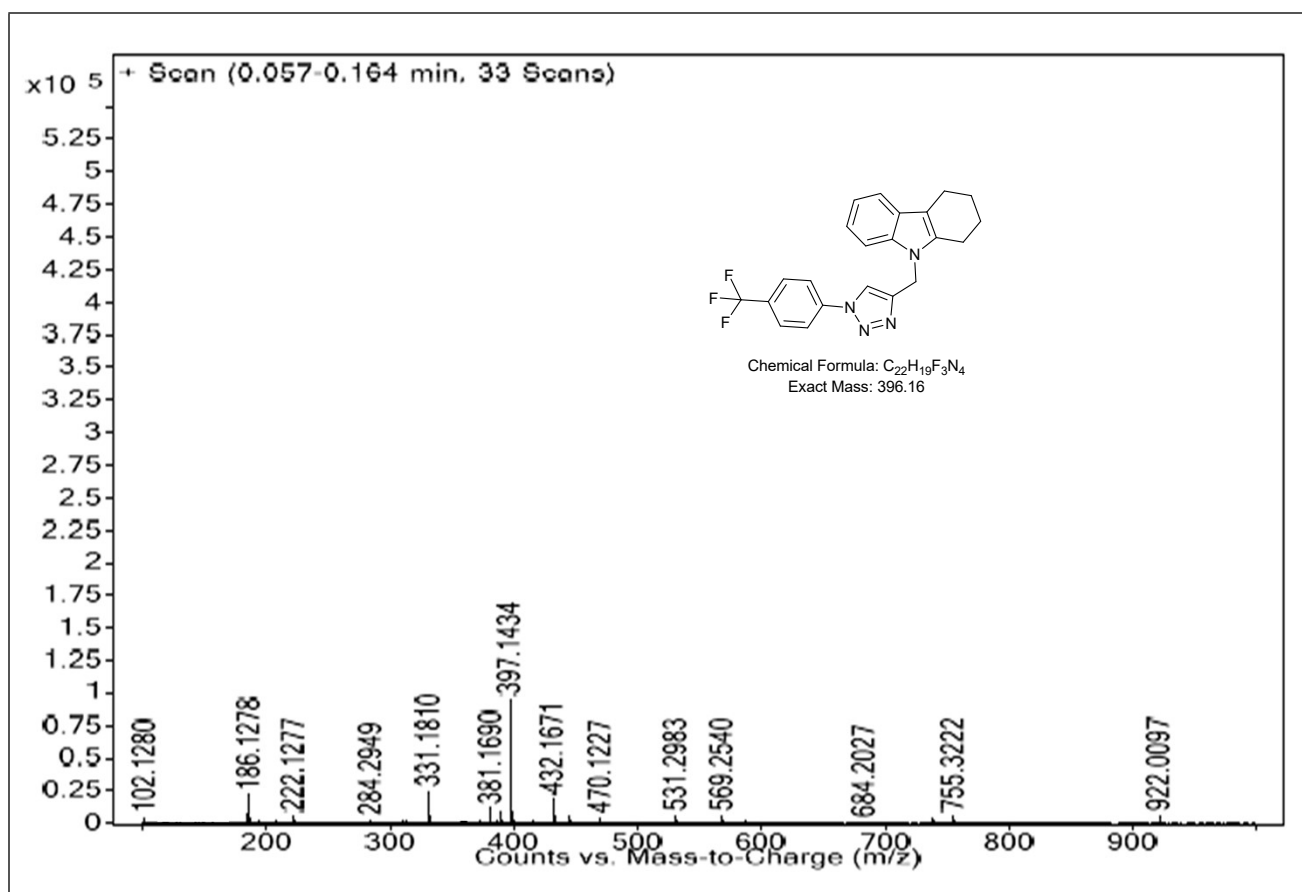


Figure S58: Mass (ES⁺) spectrum of 9-((1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4n**)

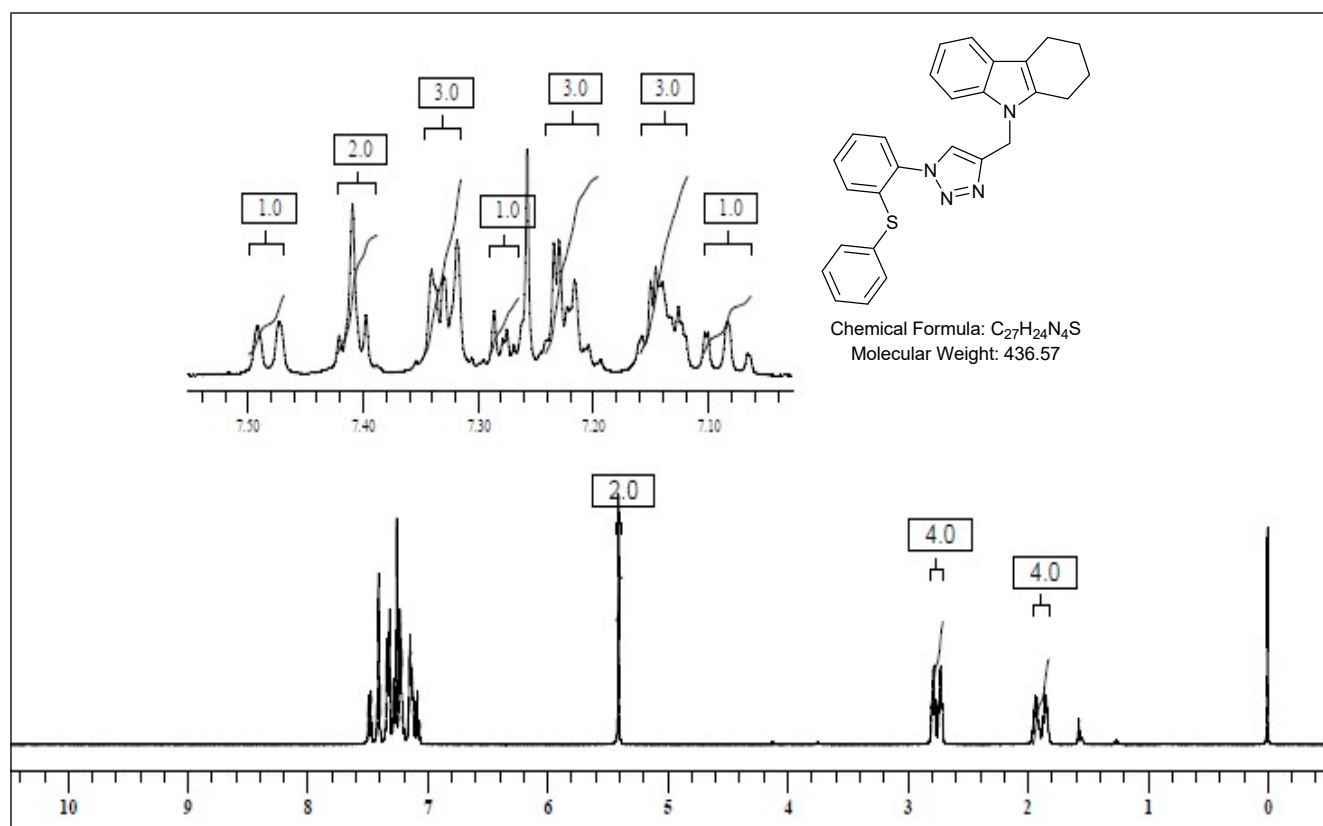


Figure S59: ¹H NMR (400 MHz, CDCl₃) of 9-((1-(2-(phenylthio)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**4o**)

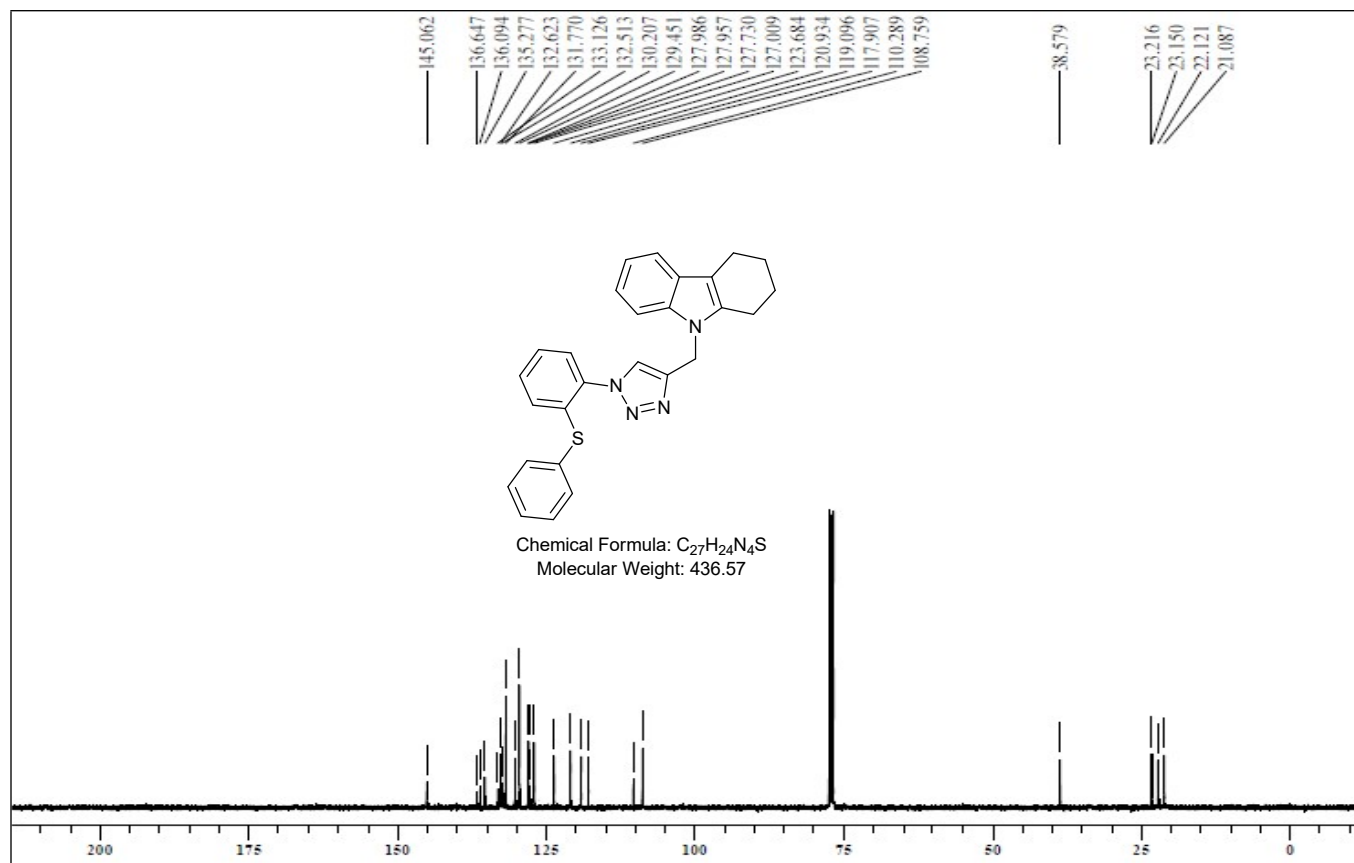


Figure S60: ¹³C NMR (100 MHz, CDCl₃) spectrum of 9-((1-(2-(phenylthio)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**40**)

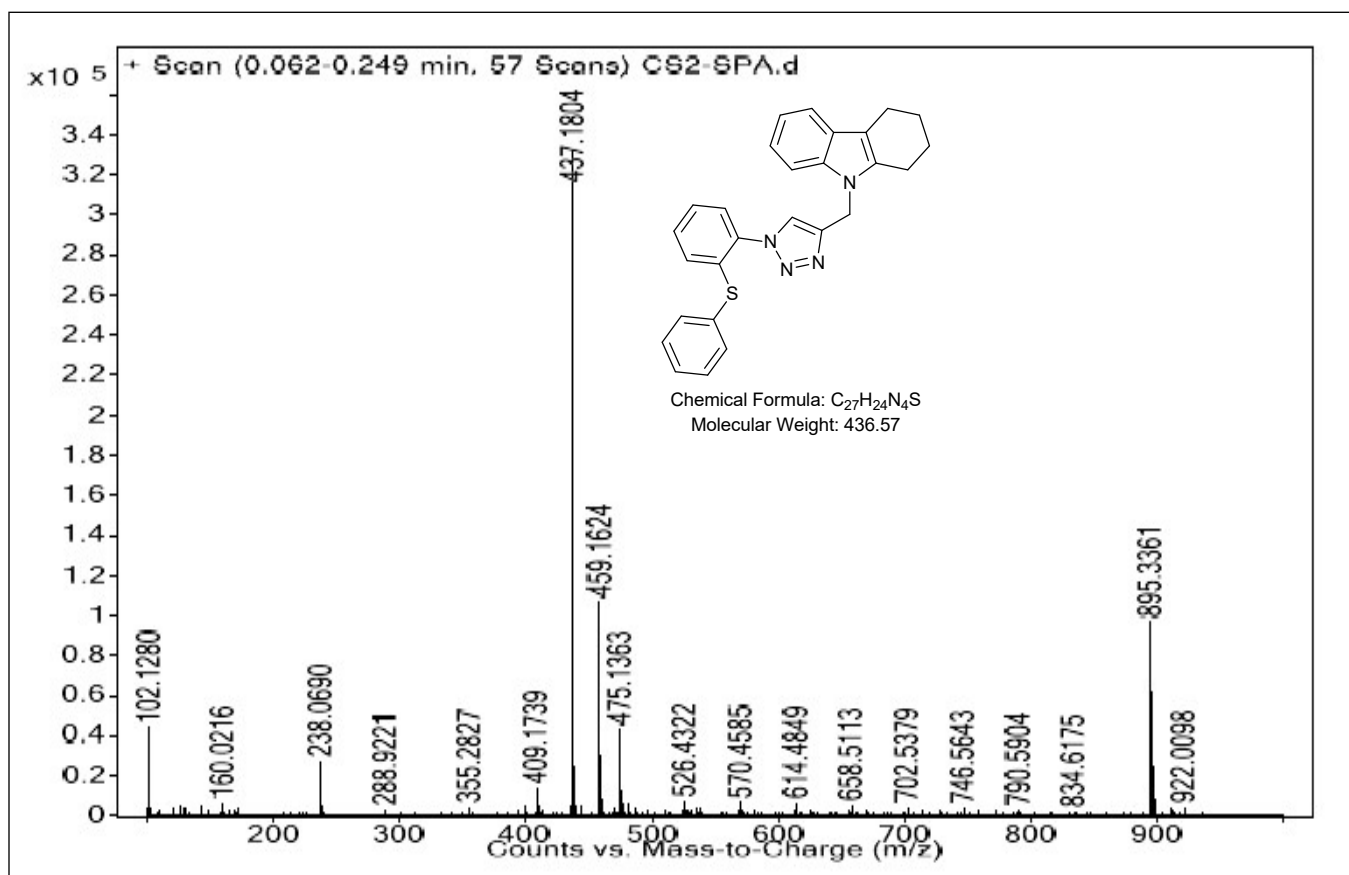


Figure S61: Mass (ES⁺) spectrum of 9-((1-(2-(phenylthio)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**40**)

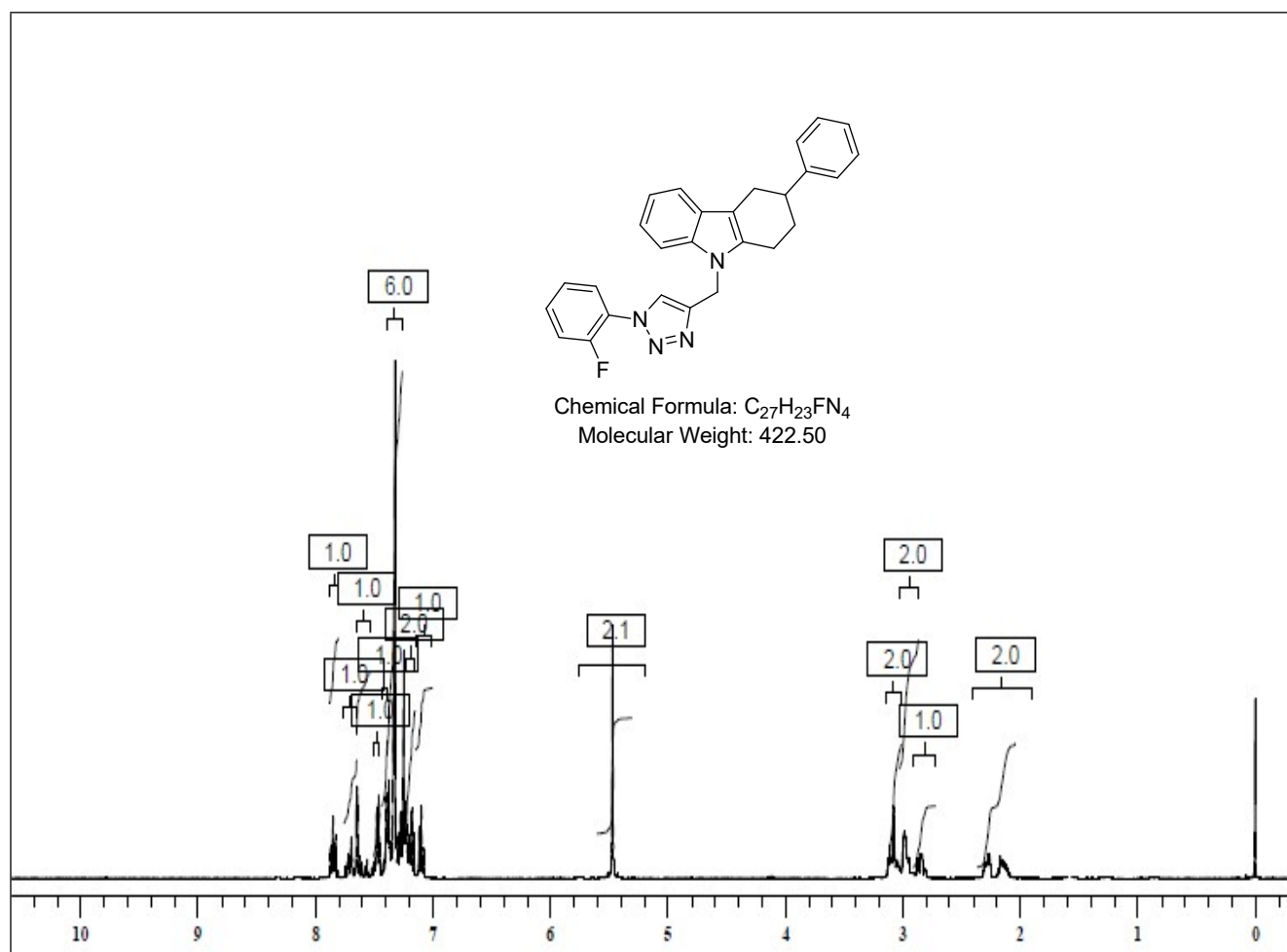


Figure S62: 1H NMR (400 MHz, $CDCl_3$) of 9-((1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-phenyl-2,3,4,9-tetrahydro-1H-carbazole (**4p**)

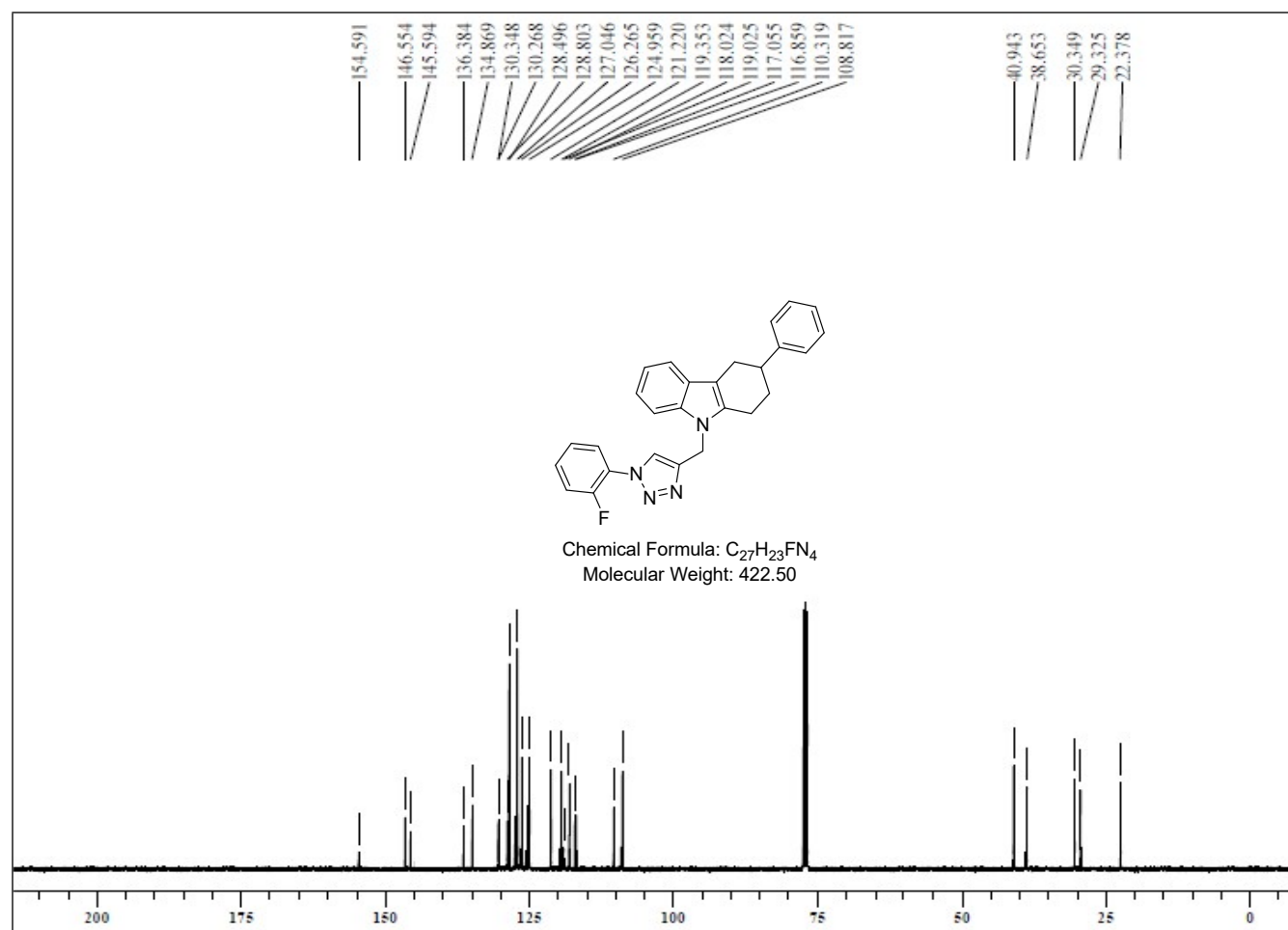


Figure S63: ¹³C NMR (100 MHz, CDCl₃) spectrum of 9-((1-(2-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-3-phenyl-2,3,4,9-tetrahydro-1*H*-carbazole (**4p**)

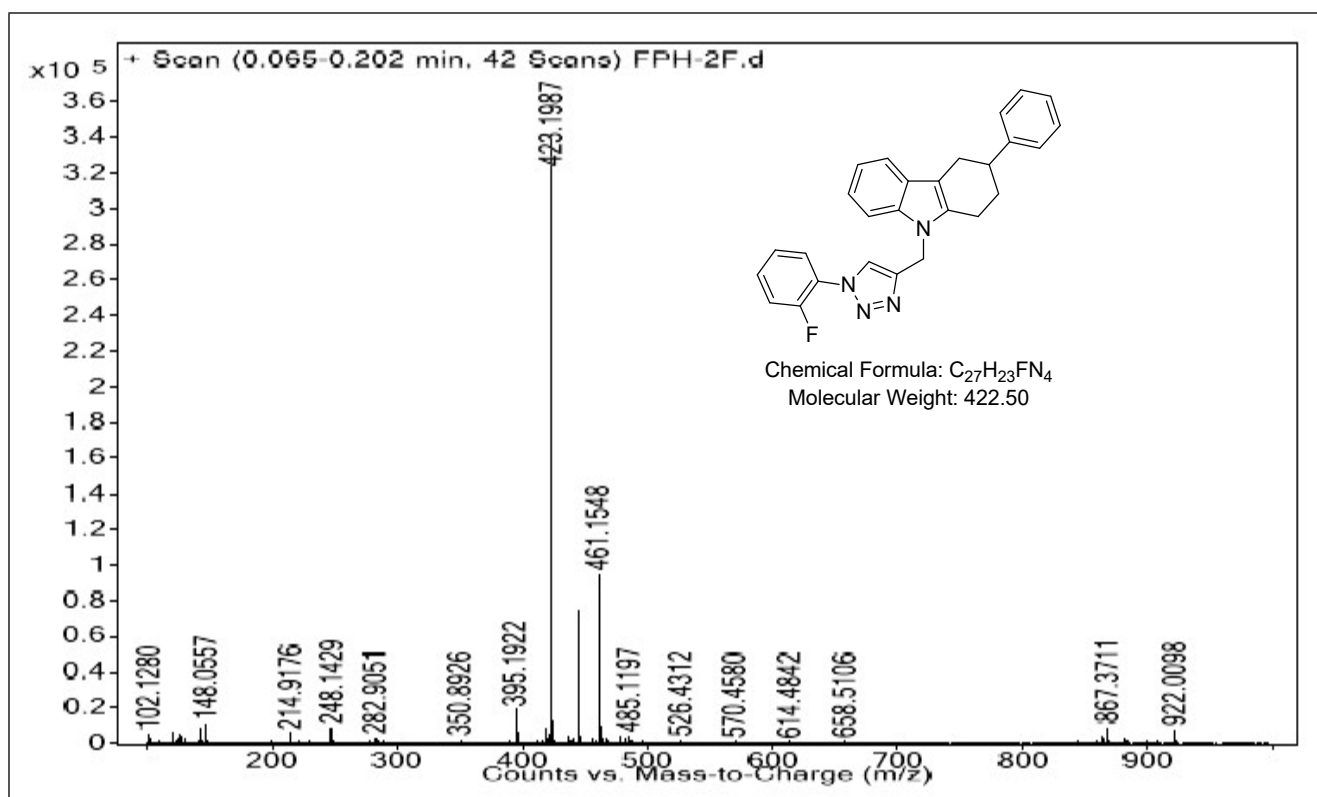


Figure S64: Mass (ES⁺) spectrum of 9-((1-(2-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-3-phenyl-2,3,4,9-tetrahydro-1*H*-carbazole (**4p**)

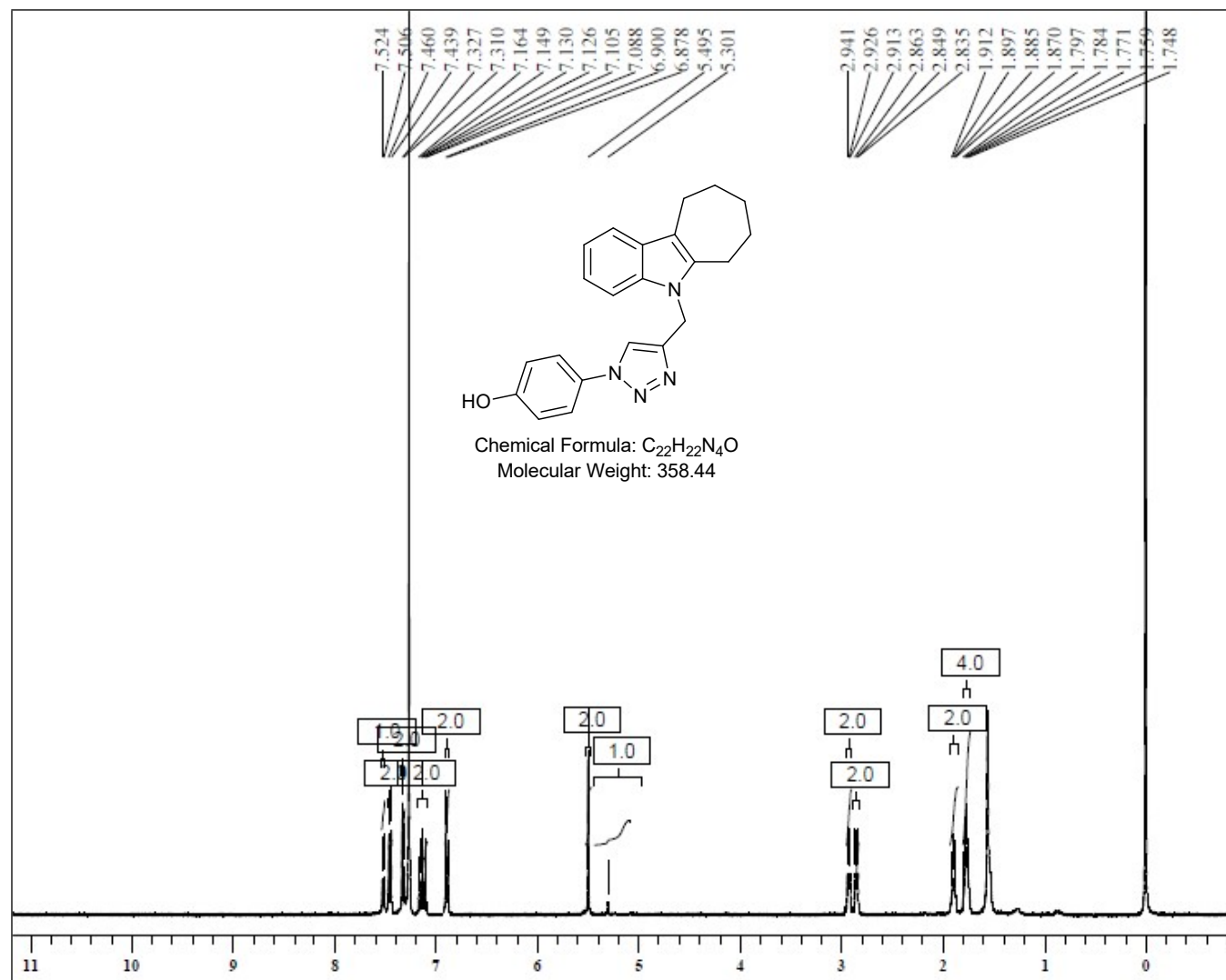


Figure S65: ¹H NMR (400 MHz, CDCl₃) of 4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenol (**4q**)

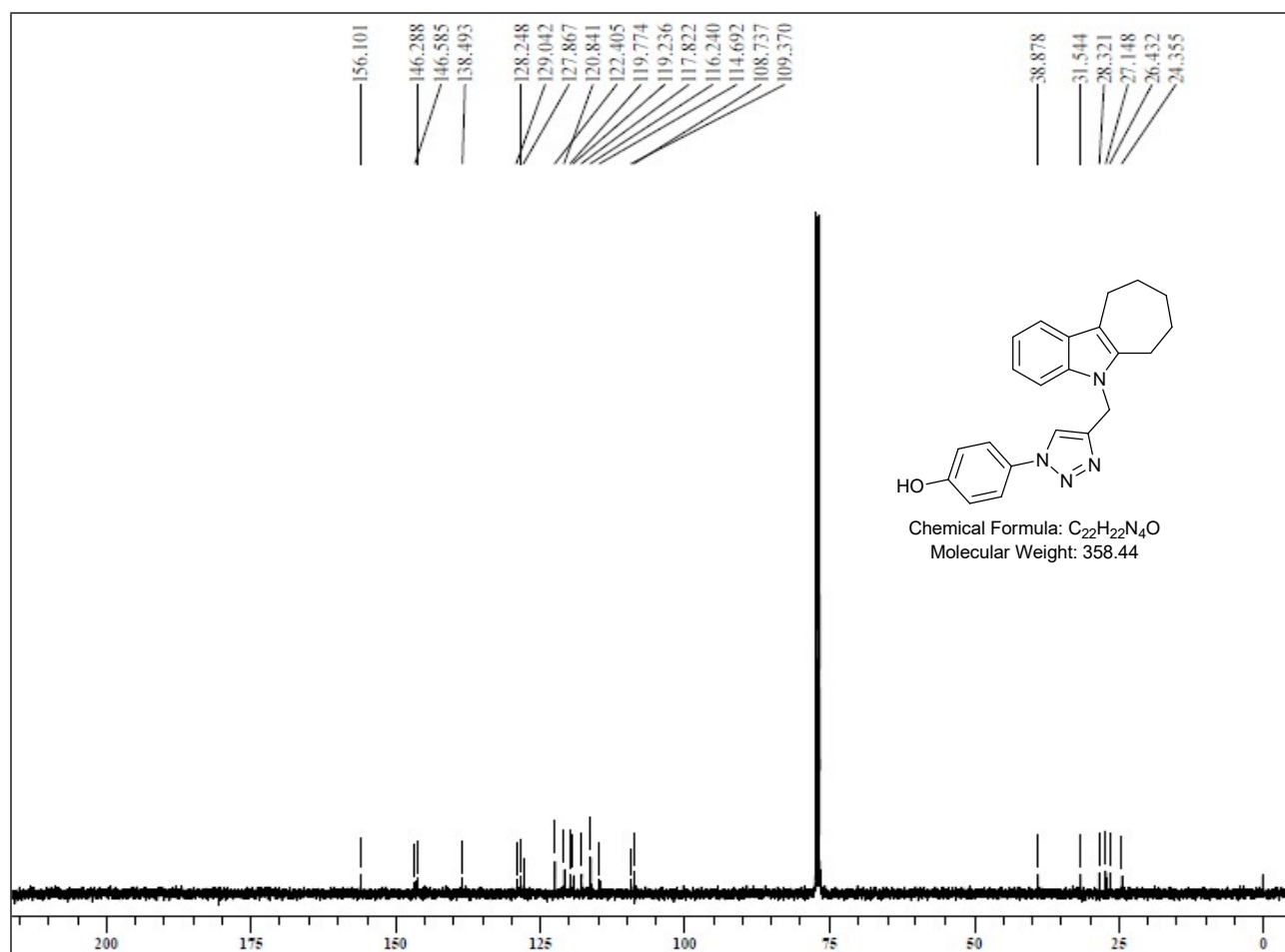


Figure S66: ^{13}C NMR (100 MHz, CDCl_3) spectrum of 4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)phenol (**4q**)

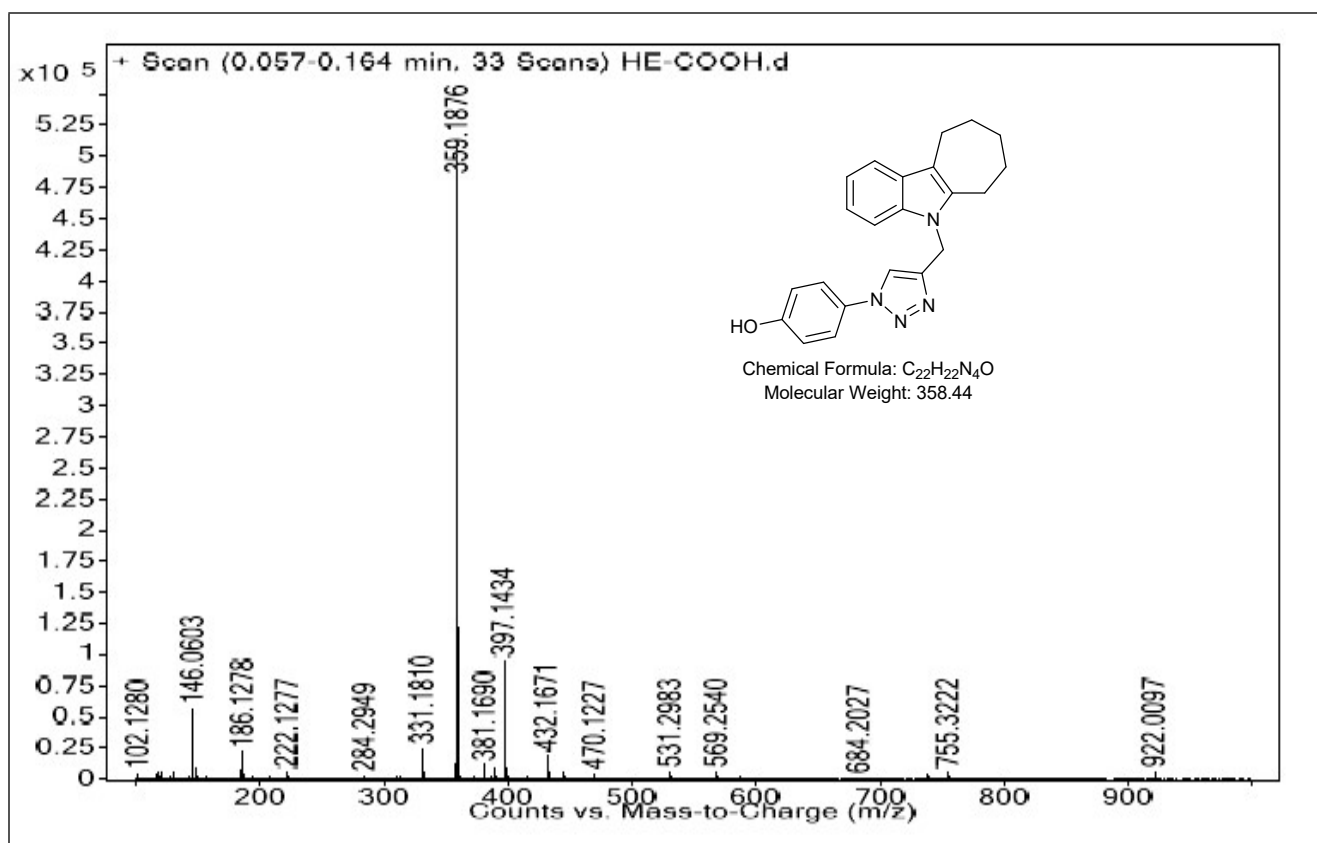


Figure S67: Mass (ES⁺) spectrum of 4-(4-((7,8,9,10-tetrahydrocyclohepta[b]indol-5(6H)-yl)methyl)-1H-1,2,3-triazol-1-yl)phenol (**4q**)

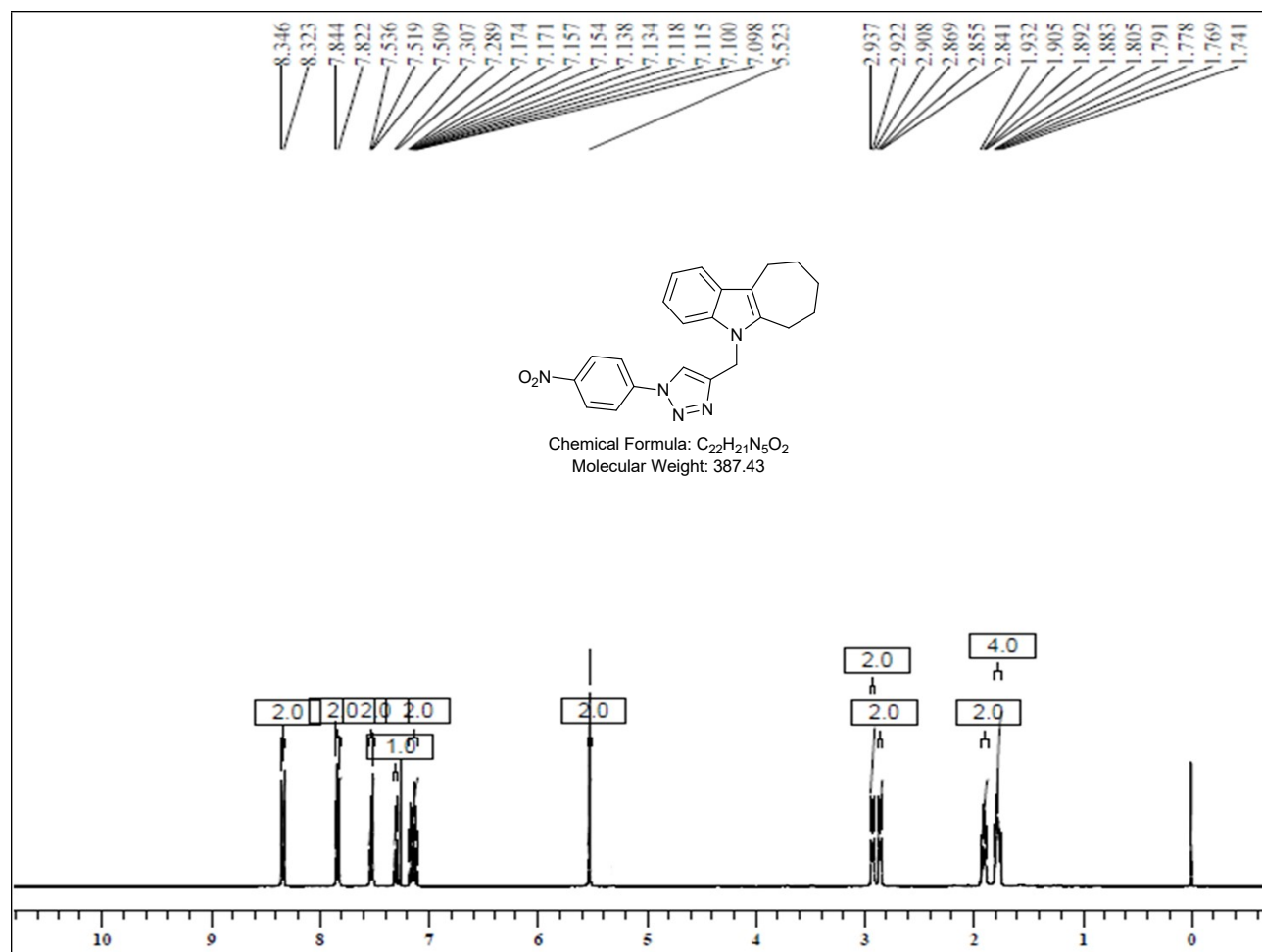


Figure S68: ^1H NMR (400 MHz, CDCl_3) of 5-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10 hexahydrocyclohepta[b]indole (**4r**)

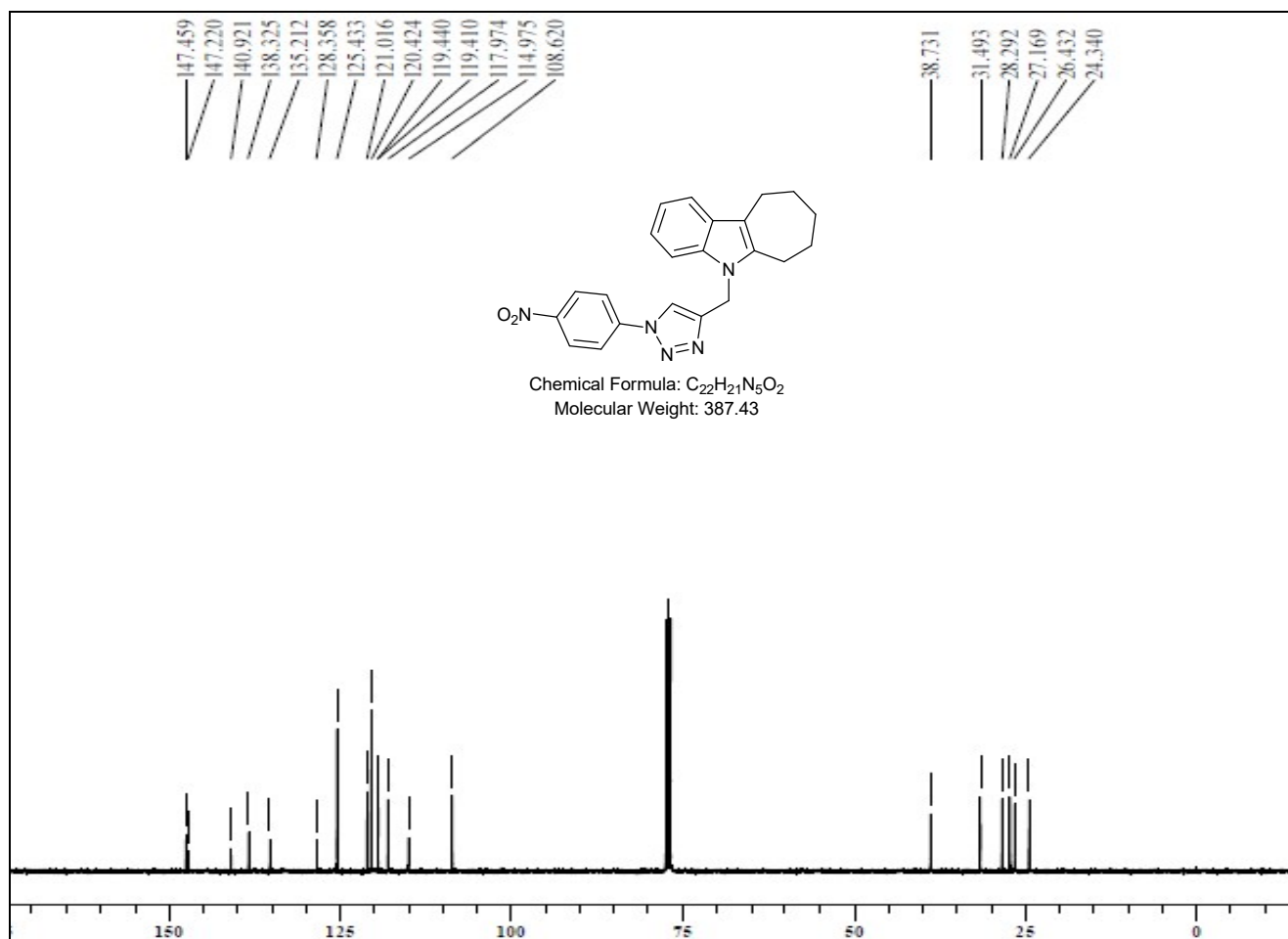


Figure S69: ¹³C NMR (100 MHz, CDCl₃) spectrum of 5-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4r**)

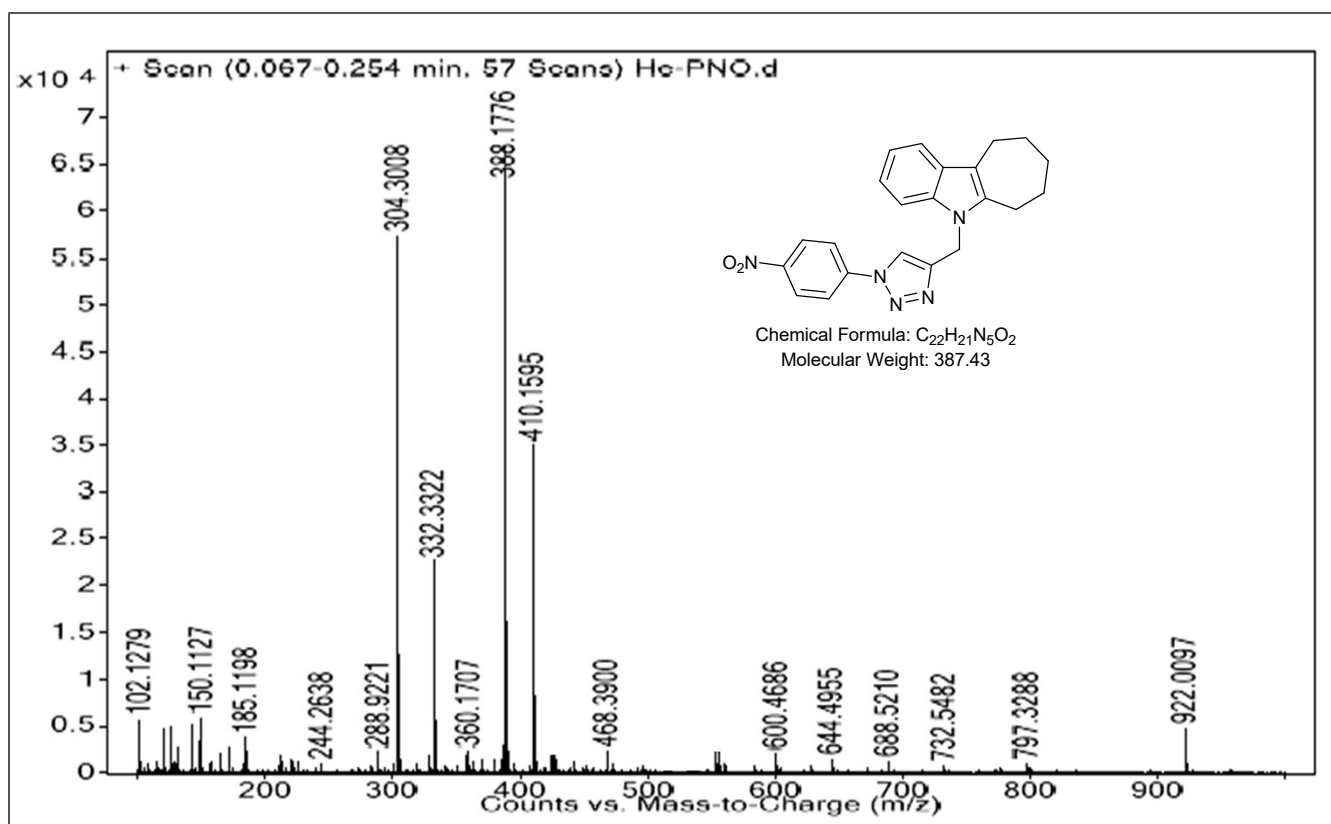


Figure S70: Mass (ES⁺) spectrum of 5-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4r**)

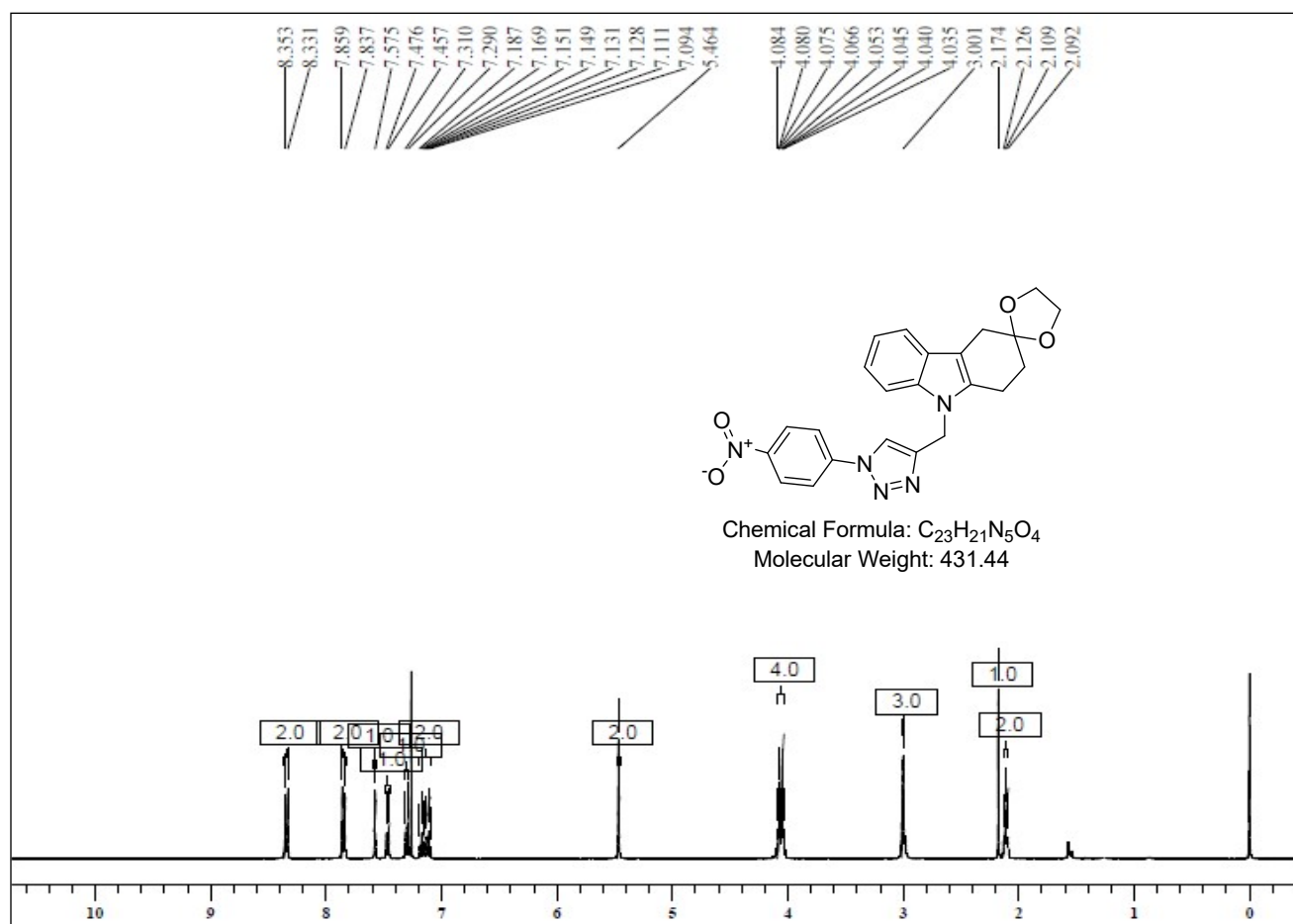


Figure S71: ^1H NMR (400 MHz, CDCl_3) of 9-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1,2,4,9-tetrahydrospiro[carbazole-3,2'-[1,3]dioxolane] (**4s**)

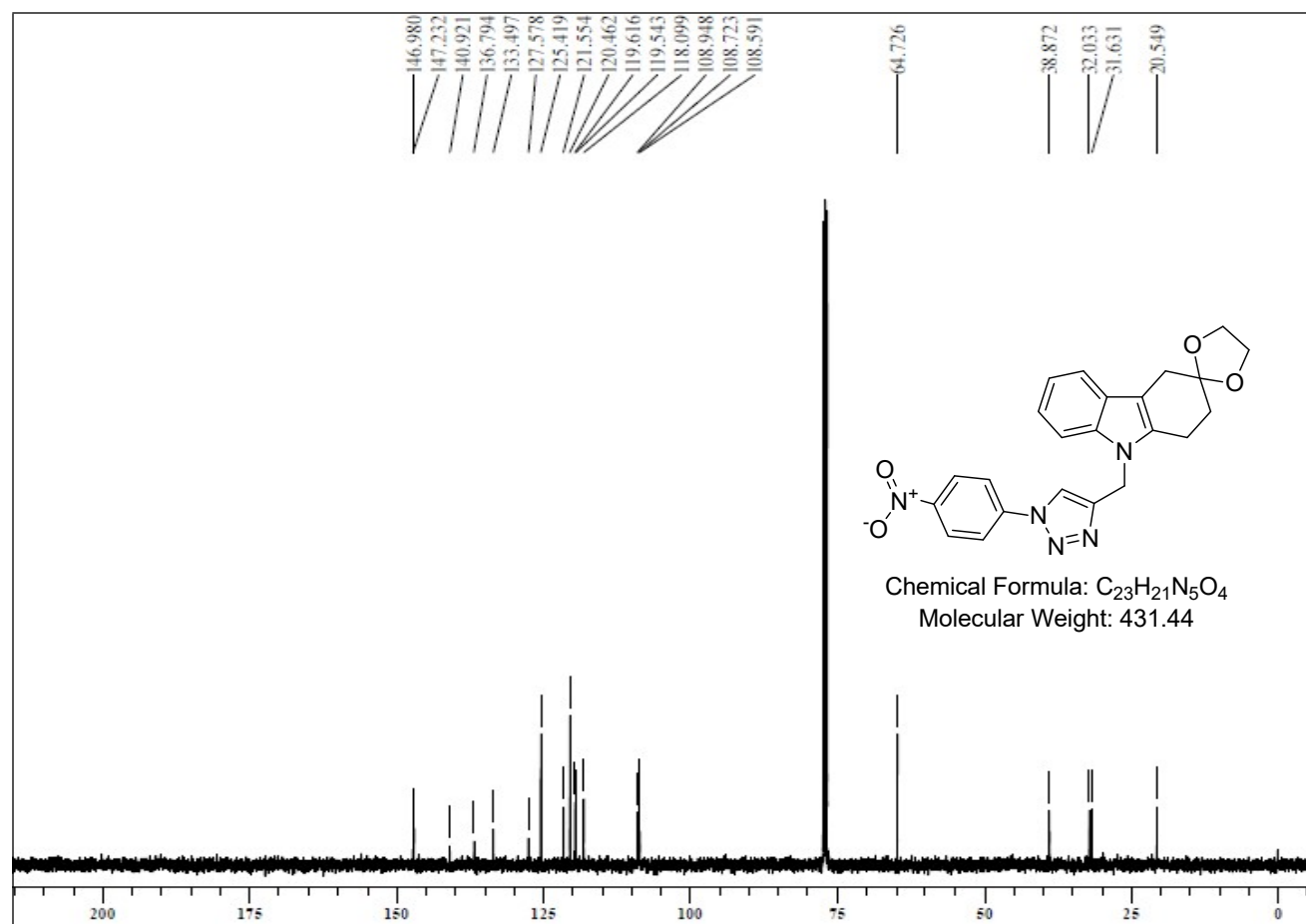


Figure S72: ¹³C NMR (100 MHz, CDCl₃) spectrum of 9-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1,2,4,9-tetrahydrospiro[carbazole-3,2'-[1,3]dioxolane] (**4s**)

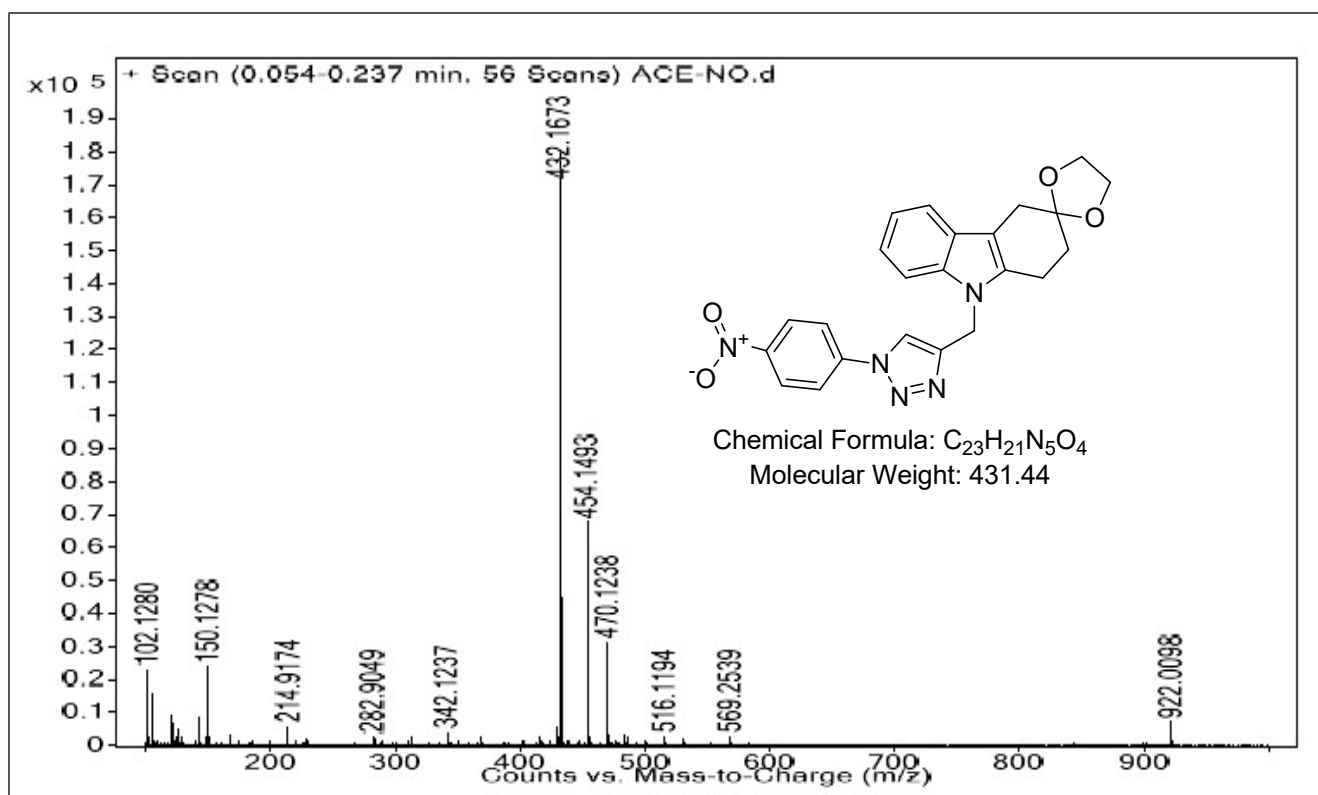


Figure S73: Mass (ES^+) spectrum of 9-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-1,2,4,9-tetrahydrospiro[carbazole-3,2'-[1,3]dioxolane] (**4s**)

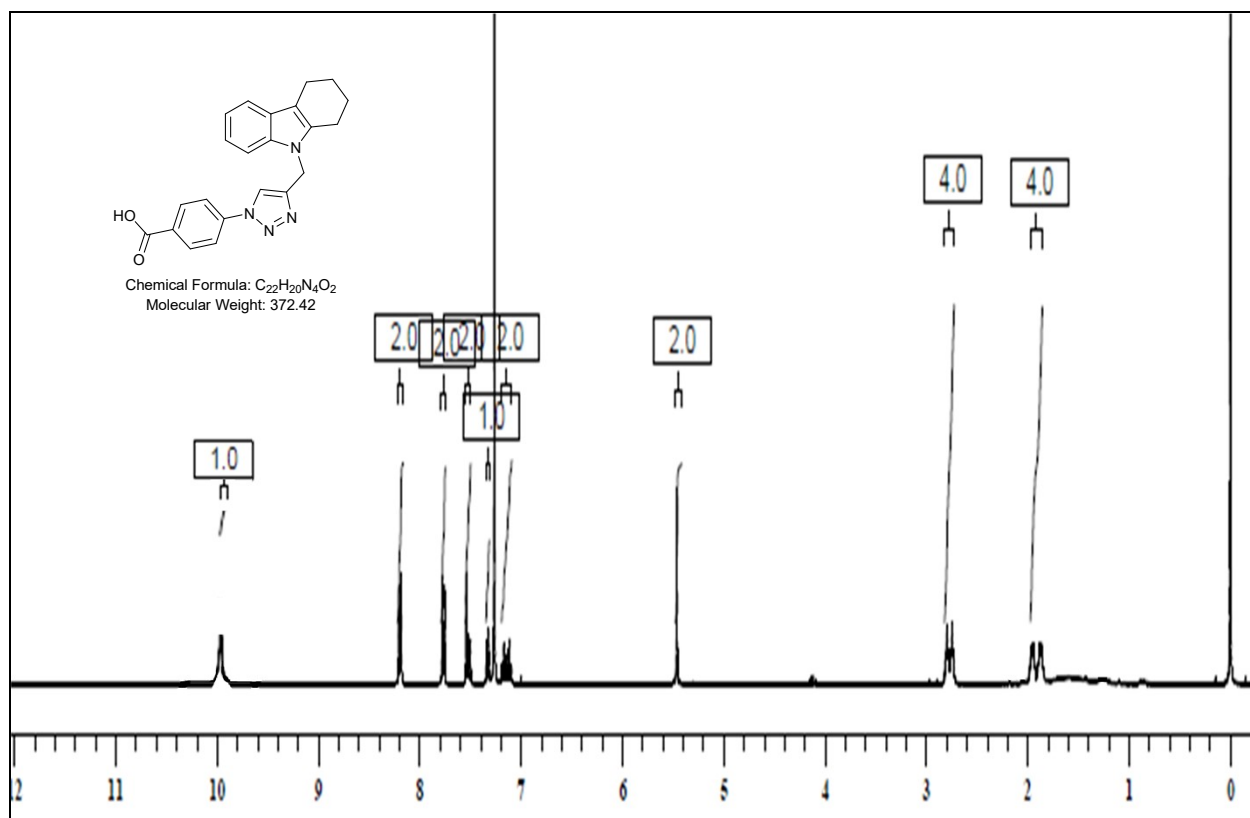


Figure S74: ¹H NMR (400 MHz, CDCl₃) of 4-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid (**4t**)

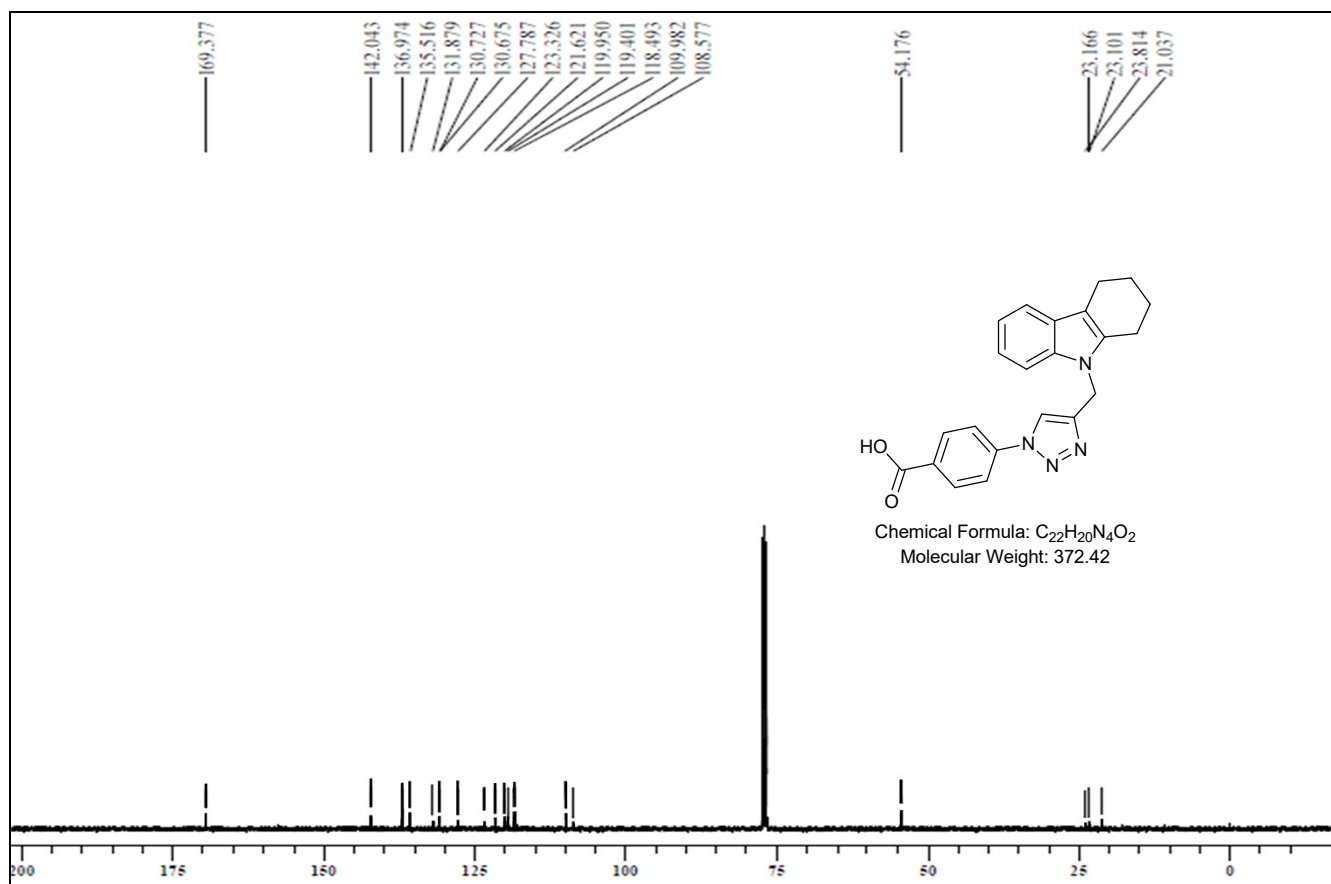


Figure S75: ¹³C NMR (100 MHz, CDCl₃) spectrum of 4-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid (**4t**)

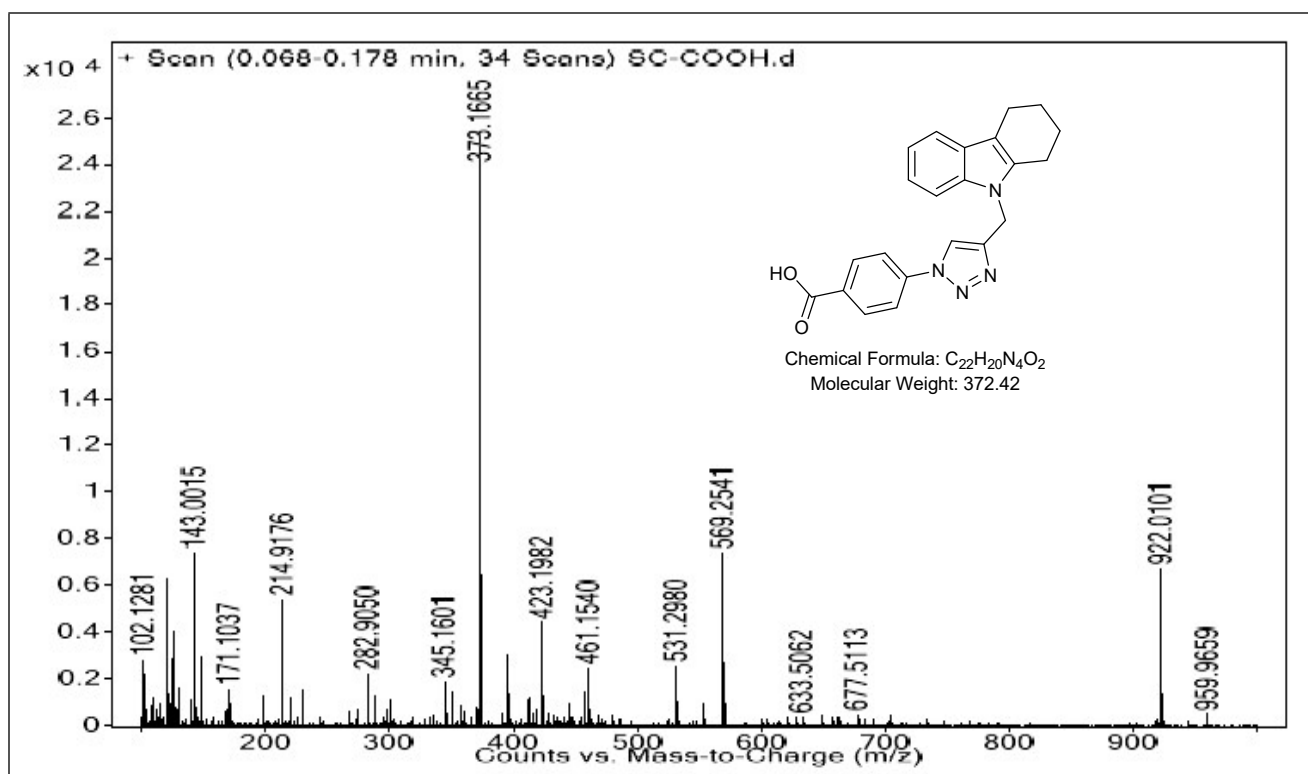


Figure S76: Mass (ES⁺) spectrum of 4-(4-((3,4-dihydro-1*H*-carbazol-9(2*H*)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid (**4t**)

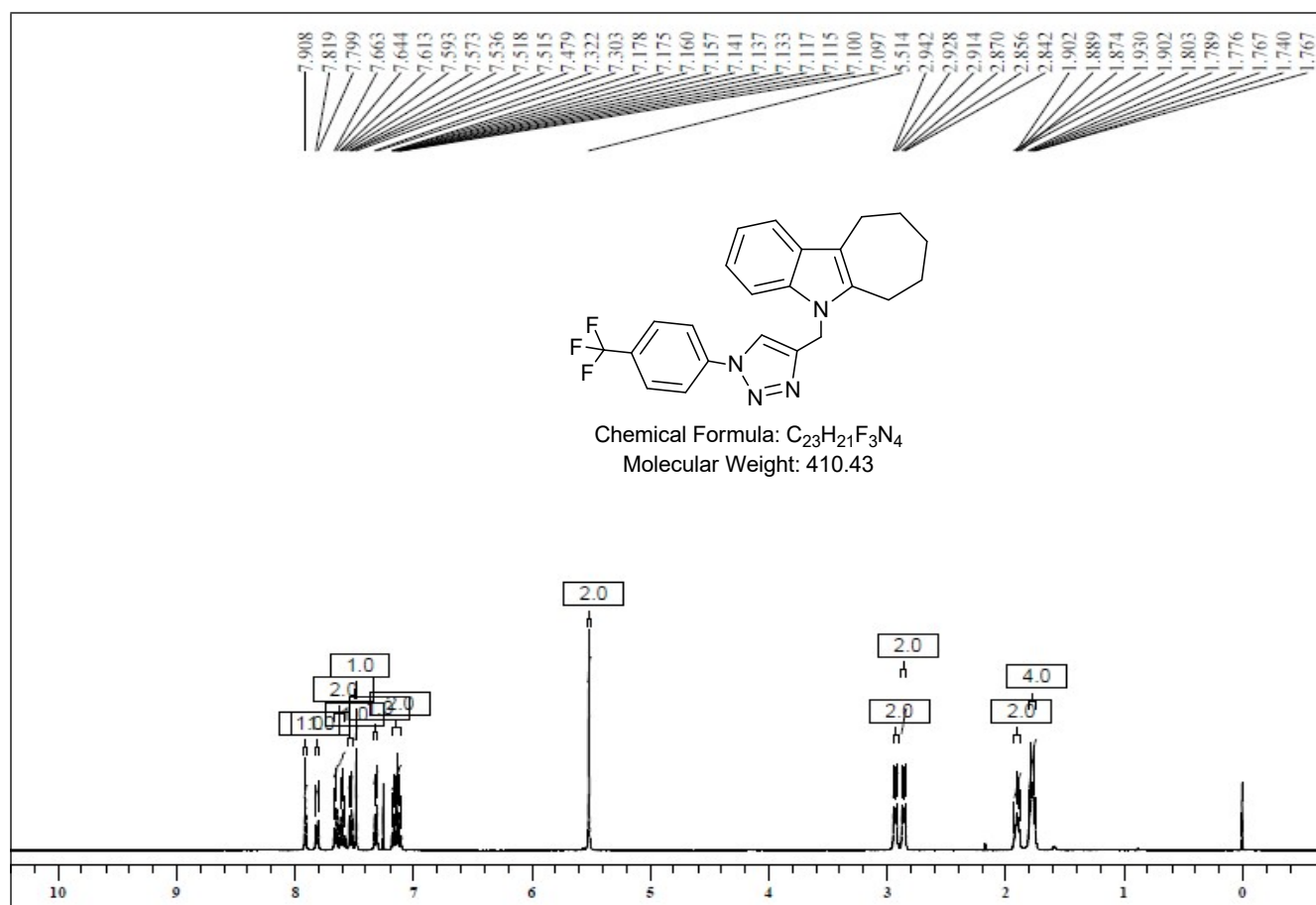


Figure S77: ^1H NMR (400 MHz, CDCl_3) of 5-((1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrohepta[b]indole (**4u**)

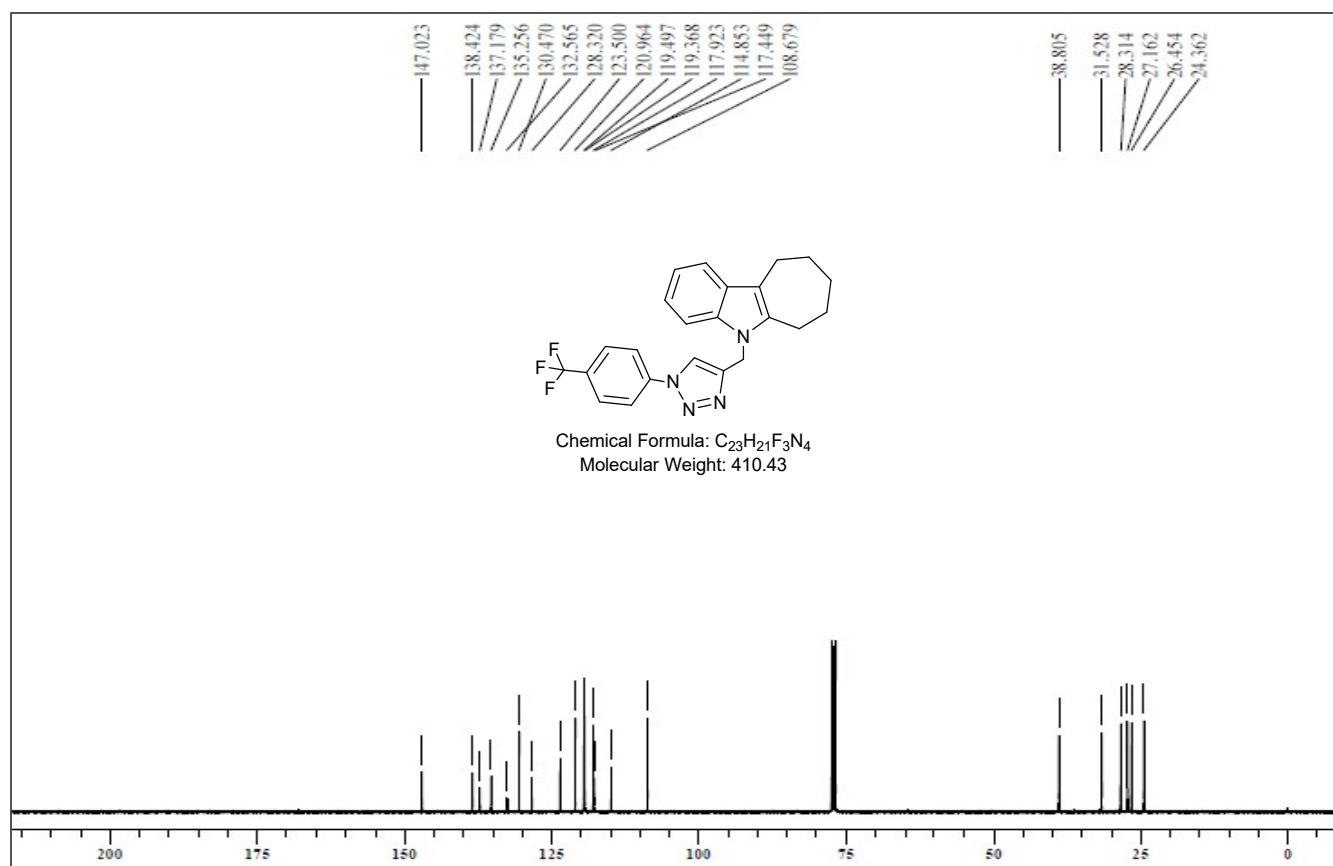


Figure S78: ¹³C NMR (100 MHz, CDCl₃) spectrum of 5-((1-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4u**)

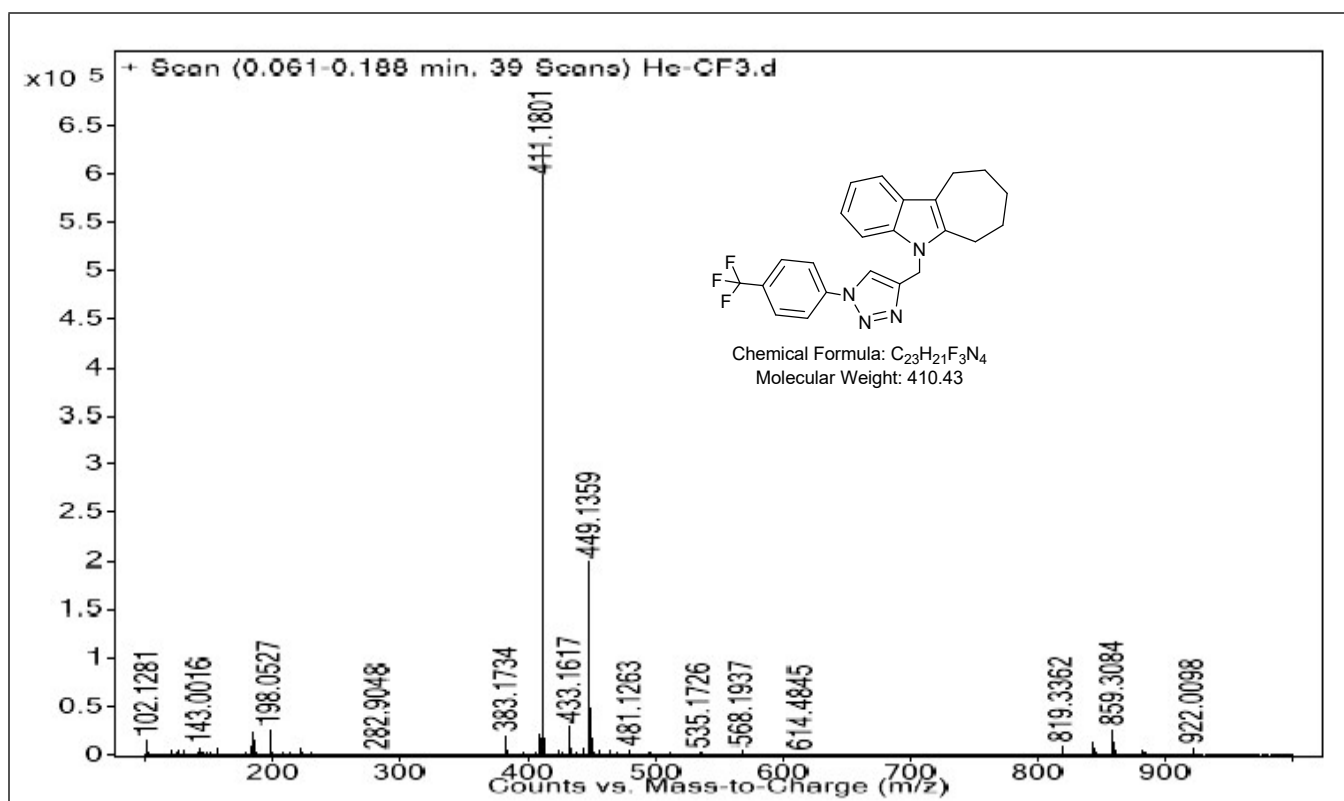


Figure S79: Mass (ES⁺) spectrum of 5-((1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5,6,7,8,9,10-hexahydrocyclohepta[b]indole (**4u**)