Supporting Information

Palladium-Catalyzed Tandem C-H Functionalization/Cyclization Strategy for the Synthesis of 5-Hydroxybenzofuran Derivatives

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Supporting Information Placeholder

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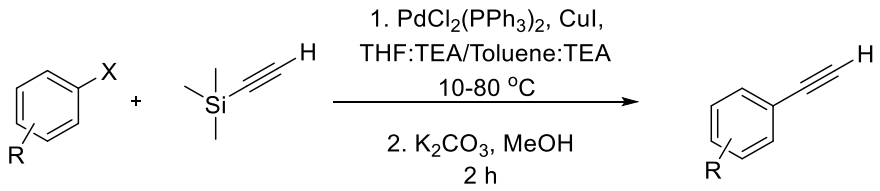
Table of contents

1. General Information

Unless otherwise stated, all reagents and solvents were purchased from commercial suppliers and were used directly without any further purification. Anhydrous solvents were distilled using CaH2 and stored under Argon. The 5ml sealed vials were cleaned dried in an oven for overnight and cooled to room temperature prior to use. All reactions that require anhydrous conditions were conducted under argon atmosphere. Flash column chromatography was performed on 63-200 mesh silica gel using distilled n-hexane(distilled) and ethyl acetate as eluents. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Ascend spectrometer 600, 400 and 150, 100 MHz, respectively. Chemical shifts are reported in parts per million (ppm) on the δ scale by using $CDCl_3$, DMSO-d_6 as an internal standard. multiplicities were indicated by using abbreviations s=singlet; d=doublet; t=triplet; q=quartet; m=multiplet. Coupling constants are expressed in Hertz (Hz). High Resolution Mass Spectra (HRMS) were recorded in ESI, EI^{+ve} and EI^{-ve} mode. The melting points (mp) were obtained on an ElectroThermal FARGO MP-2D capillary melting point apparatus.

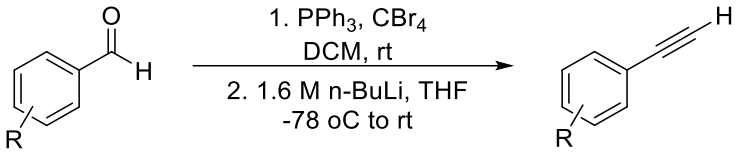
2. Preparation of Starting Materials.

a. Compounds 2b, 2c, 2f, 2g, 2h, 2j, 2k, 2l, 2m, 2n, 2r, 2s, 2t were synthesized using **general procedure A** from respective Iodo/bromo substituents.



General procedure A: To a stirred solution of 5.0 mmol of substituted Iodobenzene/bromobenzene, $PdCl_2(PPh_3)_2$ 0.014 mmol and CuI 0.05 mmol in 20 ml of THF: triethylamine /toluene: triethylamine (3:1) under argon atmosphere was added 6.0 mmol of TMS acetylene in a dropwise manner at 10 °C, then reaction mixture was stirred at rt (heated at 80 °C for bromo substituents) for 12 hrs. The progress of the reaction was monitored by TLC. After the completion of the reaction, the reaction mixture was added to brine and extracted with ethyl acetate. The residue was purified by column chromatography on silica gel using n-Hexane: Ethyl acetate as eluents. Resulted pure product was stirred in 10 ml of Methanol and 0.5 eq. of potassium carbonate for 2 hrs. after completion of the reaction the reaction mixture was extracted with Ethyl acetate. The acquired organic phase was then dried over anhydrous Na_2SO_4. After removing the volatile solvent, the resulting residue was purified by flash chromatography to afford the product in good to excellent isolated yields. ^1H NMR spectra of all the isolated products were matched with previously reported compounds.

b. Compounds 2d, 2e, 2i, 2o, 2p, 2q were synthesized using **general procedure B** from respective aldehyde substituents.



General procedure B: To a stirred solution of 4.0 mmol of PPh_3 and 8.0 mmol of CBr_4 in 50 ml of Dichloromethane was added benzaldehyde 2.0 mmol at 0 °c. stirred the reaction mixture at rt for 40 minutes. The progress of the reaction was monitored by TLC. After the completion of the reaction, the reaction mixture was added to brine and extracted with ethyl acetate. The residue was purified by column chromatography on silica gel using n-Hexane: Ethyl acetate as eluents. Resulted pure dibromo alkene product was added dropwise to a solution of 1.6 M n-butyl lithium (4.0 eq.) in dry THF (20 ml) at -78 °C under argon atmosphere. The reaction mixture was stirred at -78 °C for 1 h and then, room temperature for 2 h reaction mixture was quenched with sat. NH_4Cl solution and extracted with ethyl acetate. The acquired organic phase was then dried over anhydrous Na_2SO_4. After removing the volatile solvent, the resulting residue was purified by flash chromatography to afford the product. ^1H NMR spectra of all the isolated products were matched with previously reported compounds.

3. The Single Crystal X-Ray Diffraction Data of 3c, 5a & 5a'.

(1) 2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)benzofuran-5-ol **3c** (CCDC 1509374)

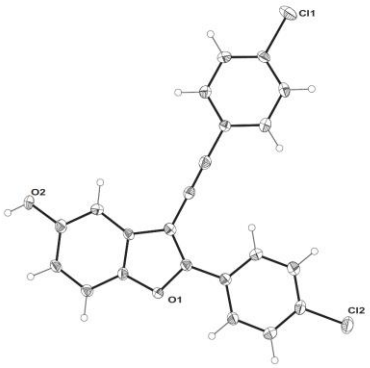


Table 1. Crystal data and structure refinement for a17766.

Identification code	a17766	
Empirical formula	C22 H12 Cl2 O2	
Formula weight	379.22	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 45.598(9) Å	= 90°.
	b = 3.8935(8) Å	= 110.747(10)°.
	c = 20.311(4) Å	= 90°.
Volume	3372.2(12) $Å^3$	
Z	8	
Density (calculated)	1.494 Mg/m^3	
Absorption coefficient	0.399 mm^{-1}	
F(000)	1552	
Crystal size	0.68 x 0.06 x 0.01 mm^3	

Theta range for data collection	2.64 to 25.26°.
Index ranges	-54<=h<=54, -4<=k<=4, -23<=l<=24
Reflections collected	11745
Independent reflections	3003 [R(int) = 0.1463]
Completeness to theta = 25.26°	97.6 %
Absorption correction	multi-scan
Max. and min. transmission	0.9960 and 0.7731
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3003 / 0 / 235
Goodness-of-fit on F^2	0.947
Final R indices [I>2sigma(I)]	R1 = 0.0600, wR2 = 0.0812
R indices (all data)	R1 = 0.1811, wR2 = 0.1095
Largest diff. peak and hole	0.317 and -0.303 e.$Å^{-3}$

(2) 6-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol **5a** (CCDC 1511959)

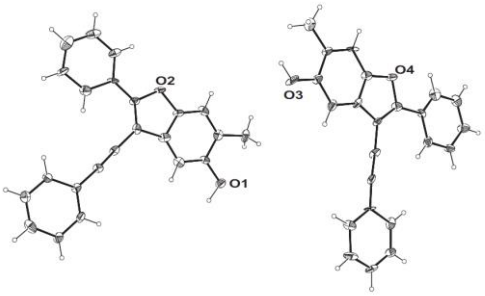


Table 1. Crystal data and structure refinement for a18122.

Identification code	a18122
Empirical formula	C23 H16 O2
Formula weight	324.36
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	P 21	
Unit cell dimensions	a = 15.545(14) Å	= 90°.
	b = 5.684(5) Å	= 96.35(3)°.
	c = 18.734(16) Å	= 90°.
Volume	1645(2) $Å^3$	
Z	4	
Density (calculated)	1.310 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	680	
Crystal size	0.34 x 0.06 x 0.01 mm^3	
Theta range for data collection	1.09 to 25.27°.	
Index ranges	-18<=h<=18, -6<=k<=6, -21<=l<=22	
Reflections collected	11039	
Independent reflections	5467 [R(int) = 0.1276]	
Completeness to theta = 25.27°	98.6 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9992 and 0.9725	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5467 / 1 / 439	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.1241, wR2 = 0.2379	
R indices (all data)	R1 = 0.2854, wR2 = 0.3070	
Absolute structure parameter	-4(4)	
Largest diff. peak and hole	0.298 and -0.308 $e.Å^{-3}$	

(3) 7-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol **5a'** (CCDC 1509527)

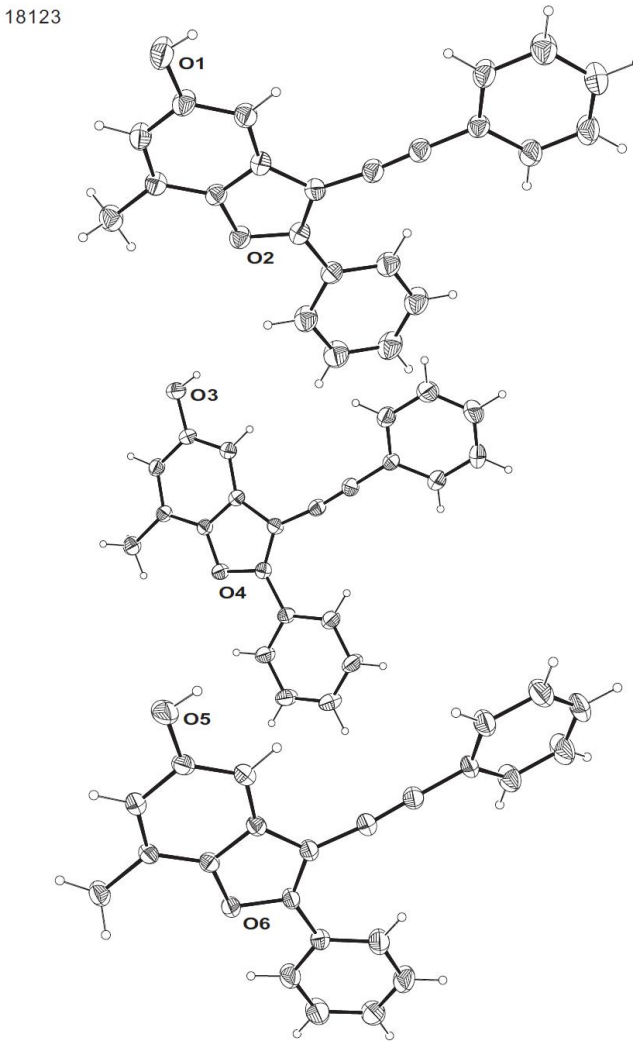


Table 1. Crystal data and structure refinement for ch18123.

Identification code	ch18123
Empirical formula	C23 H16 O2
Formula weight	324.36
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic

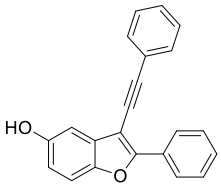
Space group	P -1
Unit cell dimensions	a = 10.186(3) Å = 72.886(5)°.
	b = 14.690(4) Å = 86.219(5)°.
	c = 19.103(5) Å = 71.026(5)°.
Volume	2582.0(11) $Å^3$
Z	6
Density (calculated)	1.252 Mg/m^3
Absorption coefficient	0.079 mm^{-1}
F(000)	1020
Crystal size	0.16 x 0.14 x 0.04 mm^3
Theta range for data collection	2.18 to 25.07°.
Index ranges	-12<=h<=12, -17<=k<=17, -22<=l<=22
Reflections collected	21011
Independent reflections	8772 [R(int) = 0.0511]
Completeness to theta = 25.07°	95.8 %
Absorption correction	multi-scan
Max. and min. transmission	0.9969 and 0.9875
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8772 / 0 / 670
Goodness-of-fit on F^2	0.930
Final R indices [I>2sigma(I)]	R1 = 0.0696, wR2 = 0.1586
R indices (all data)	R1 = 0.1826, wR2 = 0.2175
Largest diff. peak and hole	0.258 and -0.288 $e.Å^{-3}$

4. General Experimental Procedure and analysis data of 3a-3p, 5a, 5a', 5b, 5b', 5c and 5c'.

General procedure for the synthesis of compound 3a-3p, 5a, 5a', 5b, 5b', 5c and 5c'.

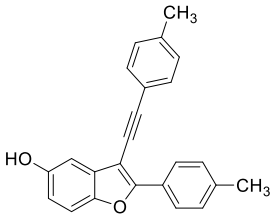
5 ml sealed vial was charged with 0.5 mmol of terminal alkyne and 1.5 mmol of quinone in 2 ml of DMSO under argon atmosphere was added 10 mol% of $Pd(OAc)_2$, stirred the resulted reaction mixture at rt for 10 min and heated to 100 ^oC for 12 hrs. The progress of reaction was monitored by TLC. After the completion of reaction, the reaction mixture was added to brine and extracted with ethyl acetate (2 x 10 ml). The residue was purified by column chromatography on silica gel using n-Hexane: Ethyl acetate as eluents to obtain pure products 3a-3p, 5a, 5a', 5b, 5b', 5c and 5c'.

2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**3a**)



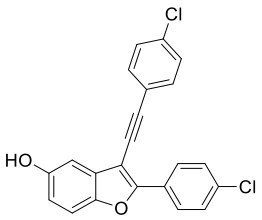
Eluent: n-hexane/ ethyl acetate (90/10); Off white Solid; Yield: 57 mg (74%); Mp: 138-140 °C. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.32 (d, *J* = 7.8 Hz, 2H), 7.62 (dd, *J* = 7.5, 1.8 Hz, 2H), 7.50 (t, *J*= 7.7 Hz, 2H), 7.43-7.36(m, 5H), 7.16 (d, *J* = 2.5 Hz, 1H),6.87 (dd, *J*=8.7, 2.6 Hz, 1H), 5.03 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.4, 152.3, 148.7, 131.6, 131.1, 130.3, 129.3, 128.8, 128.6, 128.6, 126.2, 123.5, 114.1, 111.9, 105.5, 99.2, 96.9, 81.2. HRMS (ES-): Calcd for $C_{22}H_{13}O_2$ [M-H] 309.0916, found: 309.0919.

2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**3b**)



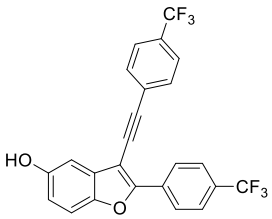
Eluent: n-hexane/ ethyl acetate (90/10); White Solid; Yield: 64 mg (76%); Mp: 188-190 °C. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.21 (d, *J* = 8.2 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J*= 8.7 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 2.4 Hz, 1H), 6.84 (dd, *J*=8.7, 2.5 Hz, 1H), 4.87 (s, 1H), 2.42 (s, 3H), 2.40 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.6, 152.2, 148.6, 139.5, 138.7, 131.5, 131.2, 129.5, 129.4, 127.7, 126.1, 120.5, 113.8, 111.8, 105.5, 98.7, 96.9, 80.7, 21.7, 21.7. HRMS (EI): Calcd for $C_{24}H_{18}O_2$ [M+] 338.1307, found: 338.1307.

2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)benzofuran-5-ol (**3c**)



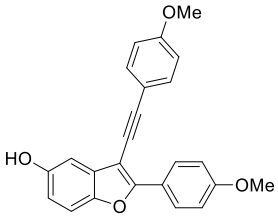
Eluent: n-hexane/ ethyl acetate (85/15); White Solid; Yield: 65 mg (69%); Mp: 262-264 °C. ^{1}H NMR (DMSO, 400 MHz): δ 9.52(s, 1H), 8.21 (d, *J* = 8.7 Hz, 2H), 7.71 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J*= 8.6 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.06 (d, *J* = 2.4 Hz, 1H), 6.88 (dd, *J*=8.8, 2.5 Hz, 1H). ^{13}C NMR (DMSO, 100 MHz): δ 155.2, 154.5, 147.2, 134.2, 133.9, 133.1, 129.7, 129.4, 129.1, 128.1, 127.1, 121.0, 115.2, 112.1, 104.3, 98.7, 96.1, 81.6. HRMS (ES-): Calcd for $C_{22}H_{11}Cl_2O_2$ [M-H] 377.0136, found: 377.0140.

2-(4-(trifluoromethyl)phenyl)-3-((4-(trifluoromethyl)phenyl)ethynyl)benzofuran-5-ol (**3d**)



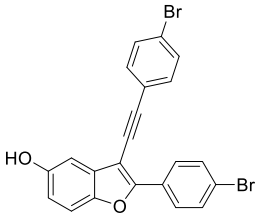
Eluent: n-hexane/ ethyl acetate (88/12); White Solid; Yield: 69 mg (62%); Mp: 226-228 °C. ^{1}H NMR (DMSO, 600 MHz): δ 9.61 (s, 1H), 8.40 (d, *J* = 8.2 Hz, 2H), 7.96 (d, *J* = 8.3 Hz, 2H), 7.93 (d, *J*= 8.0 Hz, 2H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.11 (d, *J* = 2.3 Hz, 1H), 6.93 (dd, *J*=8.8, 2.4 Hz, 1H). ^{13}C NMR (DMSO, 150 MHz): δ 154.8, 154.6, 147.5, 132.7, 132.2, 129.4, 129.3 (d, *J*= 32.0 Hz), 129.1 (d, *J*= 31.7 Hz), 126.2 (d, *J*= 4.0 Hz), 126.0, 125.7 (d, *J*= 3.9 Hz), 124.9(d, *J*= 270.4 Hz), 124.9 (d, *J*= 270.8 Hz), 115.8, 112.3, 104.4, 99.8, 96.2, 82.8. HRMS (ES-): Calcd for $C_{24}H_{11}F_6O_2$ [M-H] 445.0663, found: 445.0663.

2-(4-methoxyphenyl)-3-((4-methoxyphenyl)ethynyl)benzofuran-5-ol (**3e**)



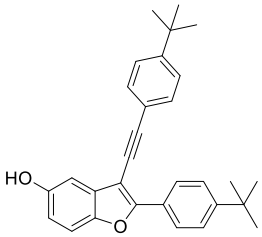
Eluent: n-hexane/ ethyl acetate (85/15); Off white Solid; Yield: 54 mg (58%); Mp: 125-127 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.25 (d, *J* = 8.9 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.33 (d, *J*= 8.7 Hz, 1H), 7.12 (d, *J* = 2.3 Hz, 1H), 7.01 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 6.82 (dd, *J*=8.7, 2.3 Hz, 1H), 4.87 (s, 1H), 3.88 (s, 3H), 3.86 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.5, 159.9, 157.3, 152.2, 148.5, 133.1, 131.4, 127.7, 123.3, 115.8, 114.3, 114.3, 113.4, 111.6, 105.4, 97.8, 96.4, 80.1, 55.5. HRMS (EI): Calcd for $C_{24}H_{18}O_4$ [M+] 370.1205, found: 370.1205.

2-(4-bromophenyl)-3-((4-bromophenyl)ethynyl)benzofuran-5-ol (**3f**)



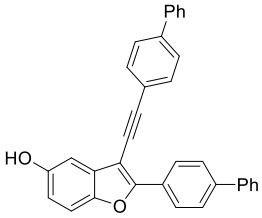
Eluent: n-hexane/ ethyl acetate (85/15); White Solid; Yield: 48 mg (41%); Mp: 268-270 °C. ^{1}H NMR (DMSO, 400 MHz): δ 9.52(s, 1H), 8.14 (d, *J* = 8.6 Hz, 2H), 7.81 (d, *J* = 8.7 Hz, 2H), 7.68 (d, *J*= 8.5 Hz, 2H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.06 (d, *J* = 2.4 Hz, 1H), 6.89 (dd, *J*=8.8, 2.5 Hz, 1H). ^{13}C NMR (DMSO, 100 MHz): δ 155.2, 154.5, 147.1, 133.2,132.2, 131.9, 129.6, 128.4, 127.3, 122.9, 122.6, 121.3, 115.2, 112.1, 104.2, 98.7, 96.2, 81.7. HRMS (EI): Calcd for $C_{22}H_{11}O_2Br_2$ [M-H] 464.9126, found: 464.9130.

2-(4-(tert-butyl)phenyl)-3-((4-(tert-butyl)phenyl)ethynyl)benzofuran-5-ol (**3g**)



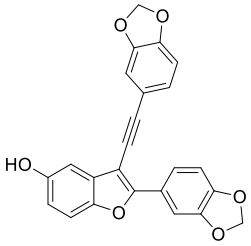
Eluent: n-hexane/ ethyl acetate (90/10); Brown Solid; Yield: 73 mg (70%); Mp: 214-216 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.25 (d, *J* = 8.6 Hz, 2H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J*= 8.6 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.7 Hz, 1H), 7.14 (d, *J* = 2.5 Hz, 1H), 6.84 (dd, *J*=8.7, 2.6 Hz, 1H), 4.76 (s, 1H), 1.37 (s, 9H), 1.36 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.6, 152.6, 152.2, 151.9, 148.7, 131.4, 131.3, 127.6, 125.9, 125.8(2xC), 125.6, 120.6, 113.7, 118.8, 105.5, 98.8, 96.6, 80.1, 35.0, 35.0, 31.4. HRMS (EI): Calcd for $C_{30}H_{30}O_2$ [M+] 422.2246, found: 422.2247.

2-([1,1'-biphenyl]-4-yl)-3-([1,1'-biphenyl]-4-ylethynyl)benzofuran-5-ol (**3h**)



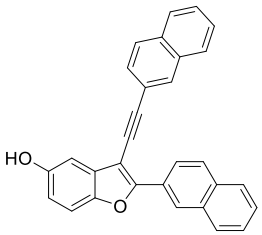
Eluent: n-hexane/ ethyl acetate (85/15); Brown Solid; Yield: 90 mg (78%); Mp: 246-248 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.41 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 2H), 7.72-7.63(m, 8H), 7.48 (t, *J*= 7.6 Hz, 4H), 7.41-7.37 (m, 3H), 7.19 (d, *J* = 2.5 Hz, 1H), 6.88 (dd, *J*=8.8, 2.6 Hz, 1H), 4.84 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.3, 152.3, 148.8, 141.9, 141.4, 140.6, 140.5, 132.1, 131.1, 129.3, 129.1, 127.9, 127.5, 127.3, 127.2, 126.6, 122.4, 114.2, 111.9, 105.5, 99.4, 97.1, 82.0. HRMS (EI): Calcd for $C_{34}H_{22}O_2$ [M+] 462.1620, found: 462.1620.

2-(benzo[d][1,3]dioxol-5-yl)-3-(benzo[d][1,3]dioxol-5-ylethynyl)benzofuran-5-ol (**3i**)



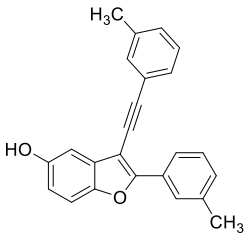
Eluent: n-hexane/ ethyl acetate (80/20); Light brown Solid; Yield: 60 mg (60%); Mp: 216-218 °C. ^{1}H NMR (DMSO, 400 MHz): δ 9.44(s, 1H), 7.78 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.69 (d, *J* = 1.7 Hz, 1H), 7.44 (d, *J*= 8.8 Hz, 1H), 7.19-7.14 (m, 3H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.00 (d, *J* = 2.4 Hz, 1H), 6.82 (dd, *J*=8.8, 2.5 Hz, 1H), 6.13(s, 2H), 6.11(s, 2H). ^{13}C NMR (DMSO, 100 MHz): δ 155.8, 154.2, 148.4, 148.1, 147.8, 147.6, 146.7, 129.9, 126.1, 123.4, 120.2, 115.4, 114.3, 111.7, 110.9, 109.1, 109.0, 105.1, 104.1, 101.7, 101.6, 97.1, 96.7, 79.2. HRMS (ES-): Calcd for $C_{24}H_{13}O_6$ [M-H] 397.0712, found: 397.0709.

2-(naphthalen-2-yl)-3-(naphthalen-2-ylethynyl)benzofuran-5-ol (**3j**)



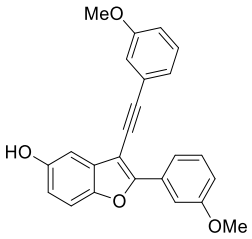
Eluent: n-hexane/ ethyl acetate (90/10); Brown Solid; Yield: 69 mg (67%); Mp: 204-206 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.84(s, 1H), 8.49 (d, *J* = 8.7 Hz, 1H), 8.16(s, 1H), 7.96 (d, *J* = 8.6 Hz, 2H), 7.90-7.87(m, 4H), 7.70 (d, *J*= 8.4 Hz, 1H), 7.57-7.51 (m, 4H), 7.42 (d, *J* = 8.8 Hz, 1H), 7.23 (d, *J* = 2.5 Hz, 1H), 6.89 (dd, *J*=8.7, 2.6 Hz, 1H), 4.82 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.6, 152.3, 148.9, 133.7, 133.4, 133.3, 133.1, 131.4, 131.2, 128.8, 128.5, 128.4, 128.3, 128.0(2xC), 127.9, 127.8, 127.1, 127.0, 126.9, 126.8, 125.9, 123.4, 120.8, 114.2, 111.9, 105.6, 99.7, 97.6, 81.9. HRMS (ES-): Calcd for $C_{30}H_{17}O_2$ [M-H] 409.1229, found: 409.1227.

2-(m-tolyl)-3-(m-tolylethynyl)benzofuran-5-ol (**3k**)



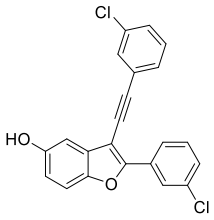
Eluent: n-hexane/ ethyl acetate (88/12); White Solid; Yield: 59 mg (70%); Mp: 125-127 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.16 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.43-7.35 (m, 4H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J*= 7.7 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 2.4 Hz, 1H), 6.85 (dd, *J*=8.7, 2.5 Hz, 1H), 4.88 (s, 1H), 2.46(s, 3H), 2.40(s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.6, 152.3, 148.7, 138.4, 138.3, 132.1, 131.1, 130.3, 130.1, 129.4, 128.7, 128.6, 128.5, 126.7, 123.4, 123.3, 114.0, 111.8, 105.5, 99.2, 97.1, 81.1, 21.8, 21.4. HRMS (EI): Calcd for $C_{24}H_{18}O_2$ [M+] 338.1307, found: 338.1307.

2-(3-methoxyphenyl)-3-((3-methoxyphenyl)ethynyl)benzofuran-5-ol (**3l**)



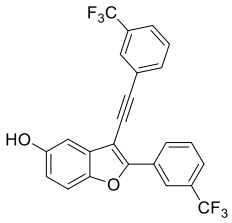
Eluent: n-hexane/ ethyl acetate (80/20); Brown Solid; Yield: 50 mg (54%); Mp: 114-116 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.89 (m, 2H), 7.42-7.37(m, 2H), 7.31 (t, *J* = 7.9 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.15 (d, *J*= 2.5 Hz, 1H), 7.13 (s, 1H), 6.97-6.93 (m, 2H), 6.86 (dd, *J*=8.8, 2.5 Hz, 1H), 4.80 (s, 1H), 3.89 (s, 3H), 3.86 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.9, 159.6, 157.3, 152.3, 148.7, 131.5, 131.0, 129.9, 129.7, 124.4, 124.2, 118.7, 116.5, 115.8, 115.2, 114.2, 111.9, 110.9, 105.5, 99.4, 97.1, 81.1, 55.5(2xC). HRMS (ES-): Calcd for $C_{24}H_{17}O_4$ [M-H] 369.1127, found: 369.1125.

2-(3-chlorophenyl)-3-((3-chlorophenyl)ethynyl)benzofuran-5-ol (**3m**)



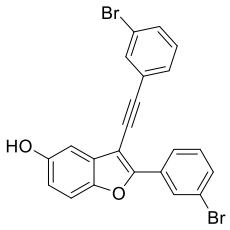
Eluent: n-hexane/ ethyl acetate (85/15); White Solid; Yield: 59 mg (63%); Mp: 182-184 °C. ^{1}H NMR (DMSO, 400 MHz): δ 9.54 (s, 1H), 8.23 (s, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 7.75 (s, 1H), 7.65-7.61 (m, 2H), 7.56-7.50(m, 4H) 7.10 (d, *J* = 2.2 Hz, 1H), 6.90 (dd, *J*=8.8, 2.3 Hz, 1H). ^{13}C NMR (DMSO, 100 MHz): δ 154.6, 154.5, 147.2, 133.8, 133.5, 131.2, 131.0, 130.8, 130.6, 129.8, 129.4, 129.3, 129.2, 124.8, 123.9, 115.4, 112.1, 104.4, 99.0, 95.6, 81.8. HRMS (ES-): Calcd for $C_{22}H_{11}O_2Cl_2$ [M-H] 377.0136, found: 377.0140.

2-(3-(trifluoromethyl)phenyl)-3-((3-(trifluoromethyl)phenyl)ethynyl)benzofuran-5-ol (**3n**)



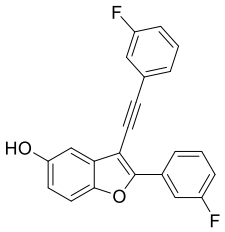
Eluent: n-hexane/ ethyl acetate (90/10); White Solid; Yield: 81 mg (73%); Mp: 165-167 °C. ^{1}H NMR (DMSO, 600 MHz): δ 9.54 (s, 1H), 8.55 (s, 1H), 8.36-8-34 (m, 1H), 7.93 (s, 1H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.81-7.77 (m, 3H), 7.71 (t, *J* = 7.8 Hz, 1H), 7.49 (d, *J*= 8.8 Hz, 1H), 7.10 (d, *J*= 2.4 Hz, 1H), 6.89 (dd, *J*=8.8, 2.5 Hz, 1H). ^{13}C NMR (DMSO, 150 MHz): δ 154.7, 154.6, 147.3, 134.8, 130.5, 130.1, 130.0, 130.0 (d, J = 32.1 Hz), 129.9 (d, J = 31.8 Hz), 129.3, 128.9, 127.5 (d, J = 3.8 Hz), 125.9 (d, J = 3.3 Hz), 125.6 (d, J = 3.6 Hz), 124.8 (d, J = 270.8 Hz), 124.6 (d, J = 270.8 Hz), 123.1, 121.5 (d, J = 3.9 Hz), 115.6, 112.1, 104.5, 99.3, 95.8, 82.0 HRMS (ES-): Calcd for $C_{24}H_{11}O_2F_6$ [M-H] 445.0663, found: 445.0663.

2-(3-bromophenyl)-3-((3-bromophenyl)ethynyl)benzofuran-5-ol (**3o**)



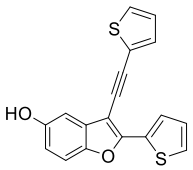
Eluent: n-hexane/ ethyl acetate (80/20); Brown Solid; Yield: 42 mg (36%); Mp: 200-202 °C. ^{1}H NMR (DMSO, 400 MHz): δ 9.54 (s, 1H), 8.42 (s, 1H), 8.18 (d, *J* = 7.9 Hz, 1H), 7.91 (s, 1H), 7.70-7.68 (m, 3H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.46 (d, *J* = 7.9 Hz, 1H), 7.10 (d, *J* = 2.4 Hz, 1H), 6.90 (dd, *J*=8.8, 2.5 Hz, 1H). ^{13}C NMR (DMSO, 100 MHz): δ 154.6, 154.5, 147.2, 133.4, 132.2, 132.1, 131.5, 131.3, 131.0, 130.2, 129.4, 127.7, 124.3, 124.2, 122.2, 121.9, 115.4, 112.1, 104.4, 99.0, 95.8, 81.9. HRMS (EI): Calcd for $C_{22}H_{12}Br_2O_2$ [M+] 465.9204, found: 465.9207.

2-(3-fluorophenyl)-3-((3-fluorophenyl)ethynyl)benzofuran-5-ol (**3p**)



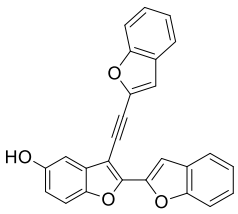
Eluent: n-hexane/ ethyl acetate (85/15); White Solid; Yield: 52 mg (61%); Mp: 127-129 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.07 (d, *J* = 7.9 Hz, 1H), 8.00 (d, J=10.1Hz, 1H), 7.39-7.35 (m, 4H), 7.29 (t, *J* = 9.4 Hz, 1H), 7.14-7.11 (m, 3H), 6.89 (d, *J*=8.0, 1H), 4.83 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.3 (d, *J*=245 Hz), 163.9 (d, *J*=246 Hz), 156.3, 152.5, 148.8, 132.2 (d, *J*=8 Hz), 130.7, 130.5 (d, *J*=9 Hz), 130.4 (d, *J*=9 Hz), 127.5 (d, *J*=3 Hz), 125.1 (d, *J*=10 Hz), 121.8 (d, *J*=2 Hz), 118.5 (d, J=23 Hz), 116.4, 116.2, 116.0, 114.7, 113.1 (d, *J*=24 Hz), 112.1, 105.5, 99.8, 96.3, 81.8. HRMS (ES-): Calcd for $C_{22}H_{11}O_2F_2$ [M-H] 345.0727, found: 345.0724.

2-(thiophen-2-yl)-3-(thiophen-2-ylethynyl)benzofuran-5-ol (**3s**)



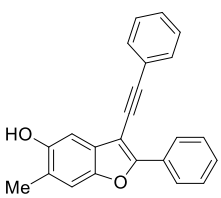
Eluent: n-hexane/ ethyl acetate (90/10); Gray Solid; Yield: 20 mg (25%); Mp: 149-151 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86 (d, *J* = 3.9 Hz, 1H), 7.44 (dd, J=4.9, 0.7Hz, 1H), 7.38-7.33 (m, 3H), 7.16 (t, *J* = 4.4 Hz, 1H), 7.10-7.07 (m, 2H), 6.83 (dd, *J*=8.7, 2.6 Hz, 1H), 4.87 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 154.4, 152.5, 148.6, 132.4, 132.2, 130.3, 127.9, 127.8, 127.5, 127.4, 126.7, 123.4, 114.0, 111.9, 105.5, 97.9, 91.3, 84.5. HRMS (EI): Calcd for $C_{18}H_{10}O_2S_2$ [M+] 322.0122, found: 322.0121.

3-(benzofuran-2-ylethynyl)-[2,2'-bibenzofuran]-5-ol (**3t**)



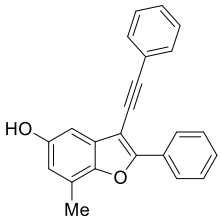
Eluent: n-hexane/ ethyl acetate (80/20); Brown Solid; Yield: 35 mg (36%); Mp: 250-252 °C. ^{1}H NMR (DMSO, 400 MHz): δ 9.68 (s, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.70-7.68 (m, 2H), 7.61-7.58 (m, 2H), 7.49-7.44 (m, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.07 (d, *J* = 2.3 Hz, 1H), 6.94 (dd, *J* = 8.8, 2.4 Hz, 1H). ^{13}C NMR (DMSO, 100 MHz): δ 154.9, 154.6, 154.4, 149.2, 147.6, 145.4, 137.5, 128.4, 127.7, 127.3, 126.4, 124.0, 123.8, 122.2, 121.8, 115.8, 113.1, 112.5, 111.5, 111.3, 106.7, 104.1, 98.5, 87.7, 85.8. HRMS (ES-): Calcd for $C_{26}H_{13}O_4$ [M-H] 389.0814, found: 389.0815.

6-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**5a**)



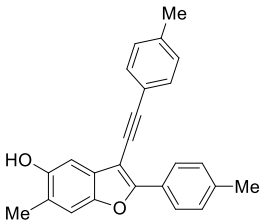
Eluent: n-hexane/ ethyl acetate (90/10); Off white solid; Yield: 32 mg (40%); Mp: 155-157 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.30 (d, *J* = 7.4 Hz, 2H), 7.60 (dd, *J* = 7.7, 1.7 Hz 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.43-7.37 (m, 4H), 7.28 (s, 1H), 7.09 (s, 1H), 4.79 (s, 1H), 2.39 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.5, 150.8, 148.8, 131.6(2xC), 130.5, 129.1, 128.8(3xC), 128.6(2xC), 128.5, 125.1(2xC), 123.6, 123.2, 112.8, 104.9, 99.0, 96.7, 81.6, 16.9. HRMS (ES-): Calcd for $C_{23}H_{15}O_2$ [M-H] 323.1072, found: 323.1075.

7-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**5a'**)



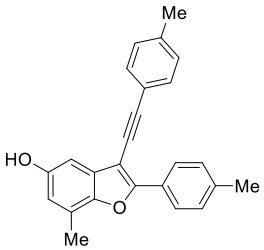
Eluent: n-hexane/ ethyl acetate (88/12); Brown solid; Yield: 26 mg (32%); Mp: 150-152 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.33 (d, *J* = 7.7 Hz, 2H), 7.61 (d, *J* = 7.7, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.42-7.36 (m, 4H), 6.98 (d, *J* = 2.2, 1H), 6.69 (s, 1H), 4.73 (s, 1H), 2.54 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.7, 152.2, 147.9, 131.6(2xC), 130.5, 130.4, 129.2, 128.8(2xC), 128.6(2xC), 128.5, 126.1(2xC), 123.6, 122.6, 115.1, 102.8, 99.4, 96.7, 81.5, 15.1. HRMS (ES+): Calcd for $C_{23}H_{16}O_2$ [M+] 325.1229, found: 325.1226.

6-methyl-2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**5b**)



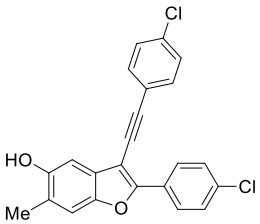
Eluent: n-hexane/ ethyl acetate (88/12); Brown solid; Yield: 37 mg (42%); Mp: 148-150 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 7.9, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.26 (s, 1H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.08 (s, 1H), 4.74 (s, 1H), 2.41 (s, 3H), 2.40 (s, 3H), 2.38 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.7, 150.7, 148.7, 139.3, 138.6, 131.5(2xC), 129.5(2xC), 129.4(2xC), 128.9, 127.9, 125.9(2xC), 122.8, 120.7, 112.7, 104.8, 98.4, 96.7, 81.0, 21.7, 21.6, 16.6. HRMS (EI): Calcd for $C_{25}H_{20}O_2$ [M+] 352.1463, found: 352.1463.

7-methyl-2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**5b'**)



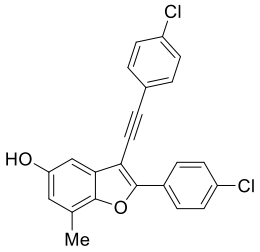
Eluent: n-hexane/ ethyl acetate (86/14); Off white solid; Yield: 32 mg (36%);Mp: 167-169 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.21 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 8.0, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 6.96 (d, *J* = 2.4 Hz, 1H), 6.66 (d, *J* = 2.0 Hz, 1H), 4.74 (s, 1H), 2.53 (s, 3H), 2.42 (s, 3H), 2.40 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.2, 152.1, 147.7, 139.3, 138.6, 131.5(2xC), 130.6, 129.5(2xC), 129.4(2xC), 127.9, 126.0(2xC), 122.4, 120.6, 114.8, 102.7, 98.9, 96.7, 81.0, 21.7, 21.7, 15.1. HRMS (ES-): Calcd for $C_{25}H_{20}O_2$ [M+] 352.1463, found: 352.1463.

2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)-6-methylbenzofuran-5-ol (**5c**)



Eluent: n-hexane/ ethyl acetate (88/12); Brown solid; Yield: 36 mg (38%); Mp: 217-219 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.3, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.27 (s, 1H), 7.06 (s, 1H), 4.74 (s, 1H), 2.38 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.6, 151.0, 148.8, 135.0, 134.8, 132.8(2xC), 129.1(2xC), 129.0(2xC), 128.9, 128.5, 127.1(2xC), 123.7, 121.8, 112.9, 104.8, 99.2, 96.0, 82.3, 16.9. HRMS (ES-): Calcd for $C_{23}H_{13}O_2Cl_2$ [M-H] 391.0293, found: 391.0291.

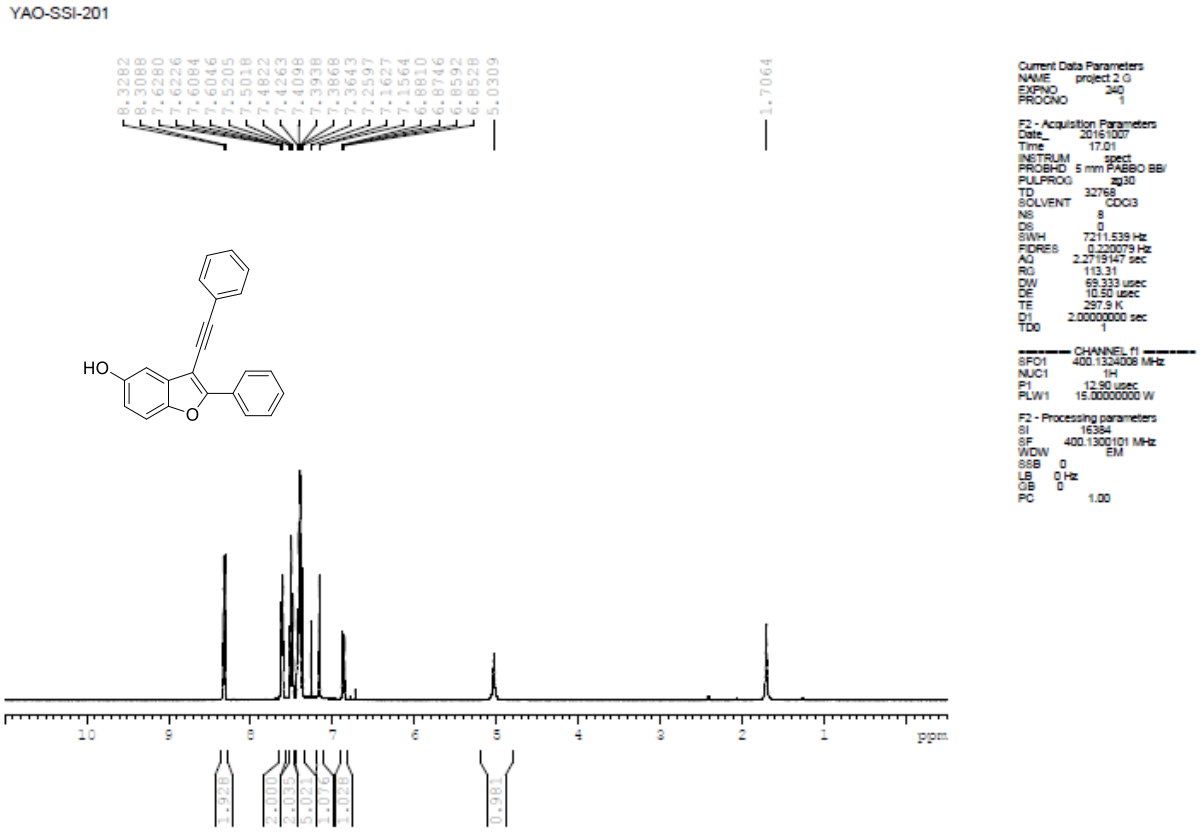
2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)-7-methylbenzofuran-5-ol (**5c'**)



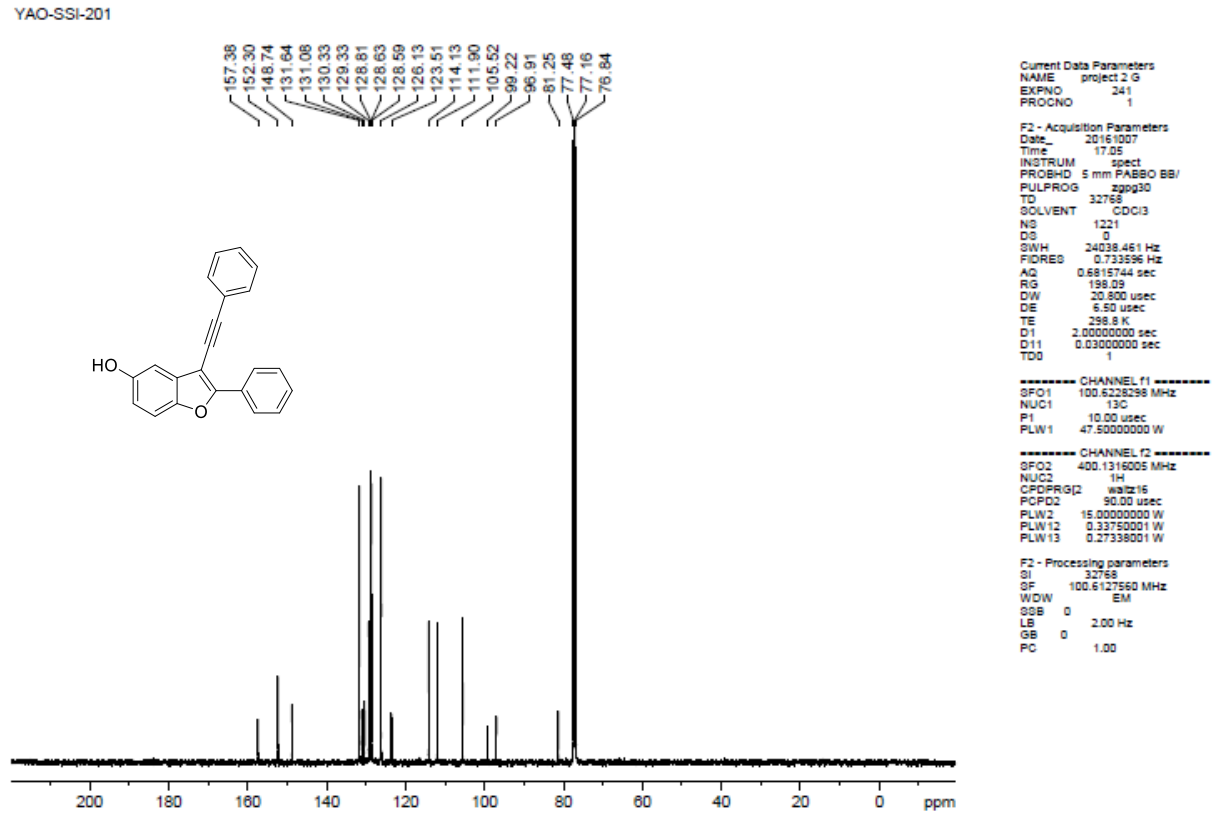
Eluent: n-hexane/ ethyl acetate (87/13); Off white solid; Yield: 25 mg (25%);Mp: 206-208 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.22 (d, *J* = 8.6 Hz, 2H), 7.51 (d, *J* = 8.5, 2H), 7.46 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 8.5 Hz, 2H), 6.94 (s, 1H), 6.70 (s, 1H), 4.70 (s, 1H), 2.52 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.0, 152.3, 147.9, 135.1, 134.8, 132.8(2xC), 130.2, 129.1(2xC), 129.0(2xC), 128.9, 127.3(2xC), 122.7, 121.8, 115.5, 102.8, 99.6, 96.0, 82.2, 15.1. HRMS (ES-): Calcd for $C_{23}H_{13}O_2\ Cl_2$ [M-H] 391.0293, found: 391.0289.

^{1}H and ^{13}C NMR Spectra copies of all compounds

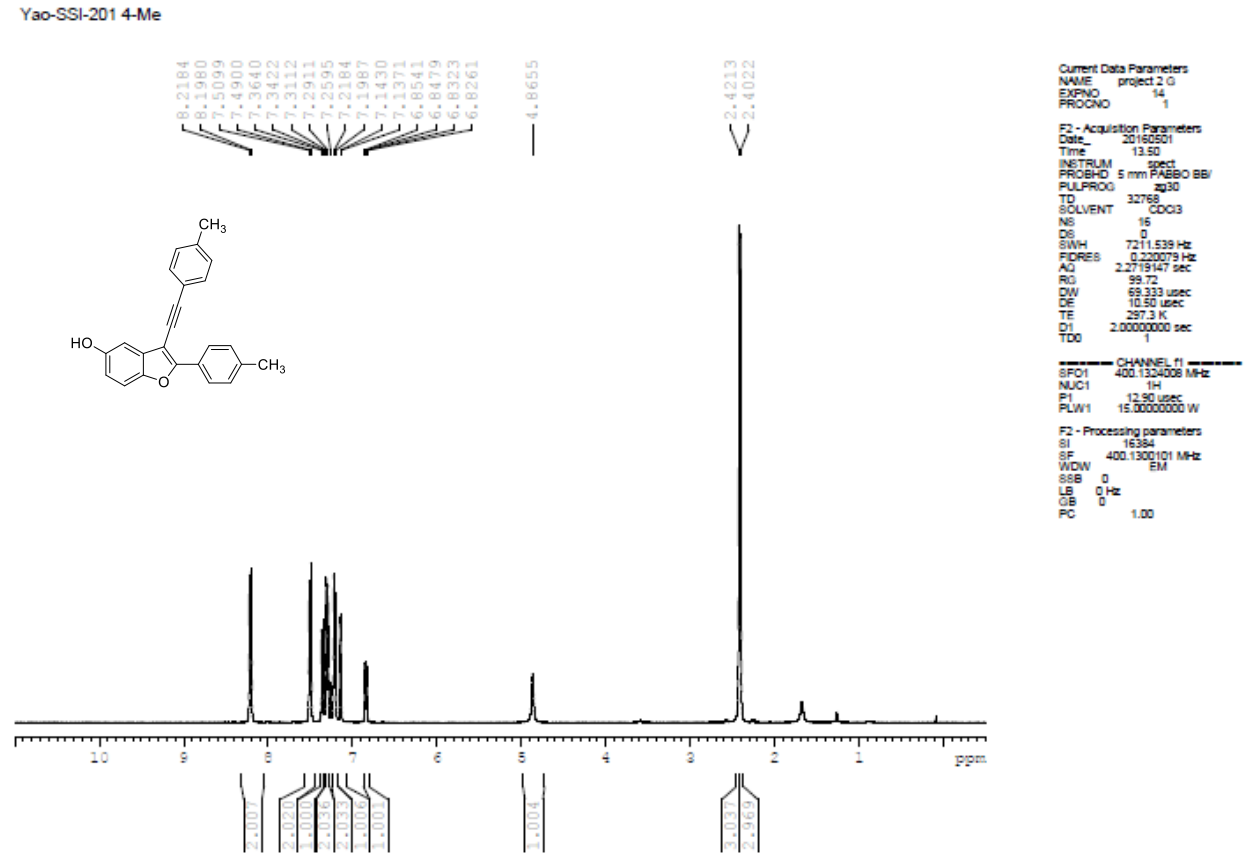
2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**3a**): ^{1}H NMR (400 MHz, $CDCl_3$)



2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**3a**): ^{13}C NMR (100 MHz, $CDCl_3$)



2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**3b**): ^{1}H NMR (400 MHz, $CDCl_3$)



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PROCNO 1

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DE 10.50 usec
TE 297.3 K
D1 2.00000000 sec
TD0 1

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NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

F2 - Processing parameters
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SF 400.1300101 MHz
WDW EM
SSB 0
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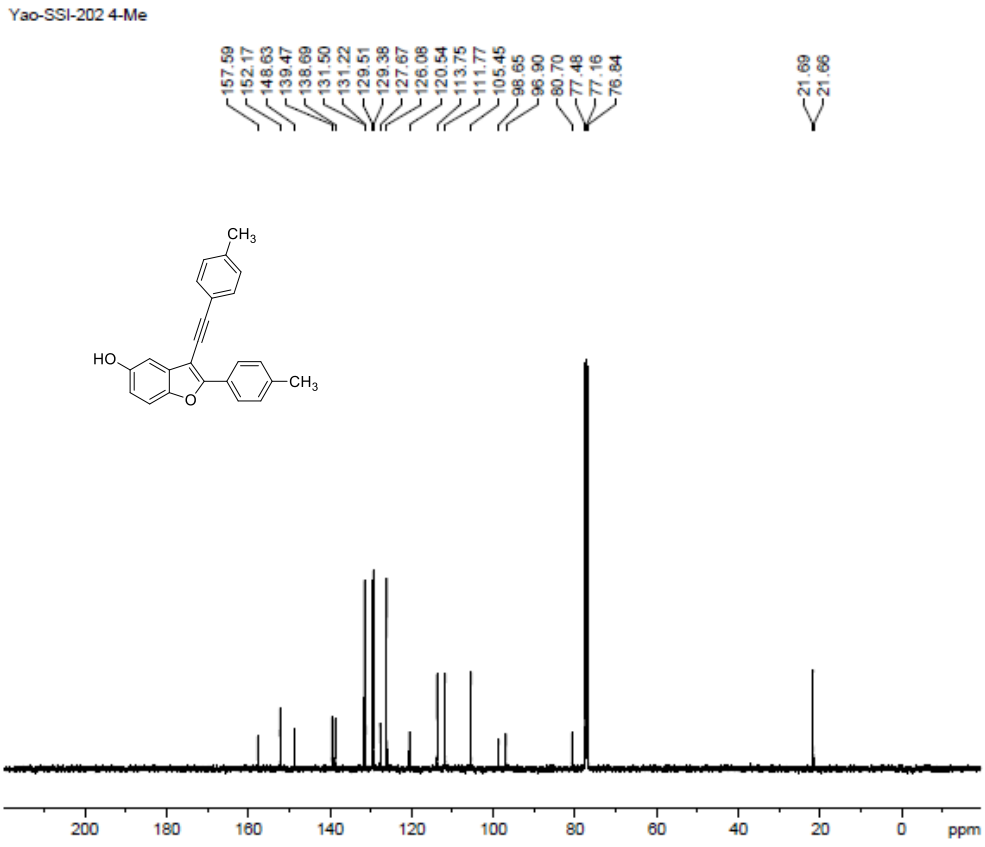
2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**3b**): ^{13}C NMR (100 MHz, $CDCl_3$)



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D11 0.03000000 sec
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PLW13 0.27338001 W

F2 - Processing parameters
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WDW EM
SSB 0
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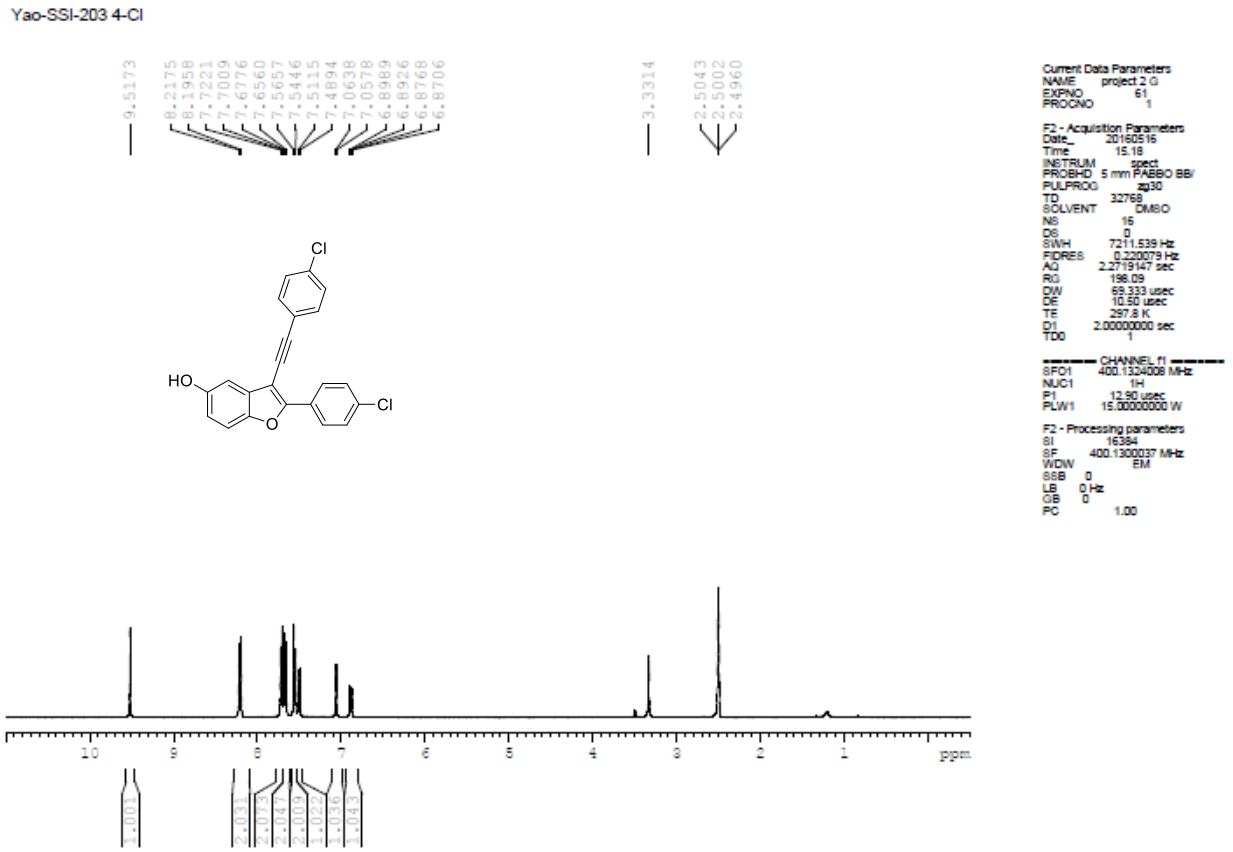
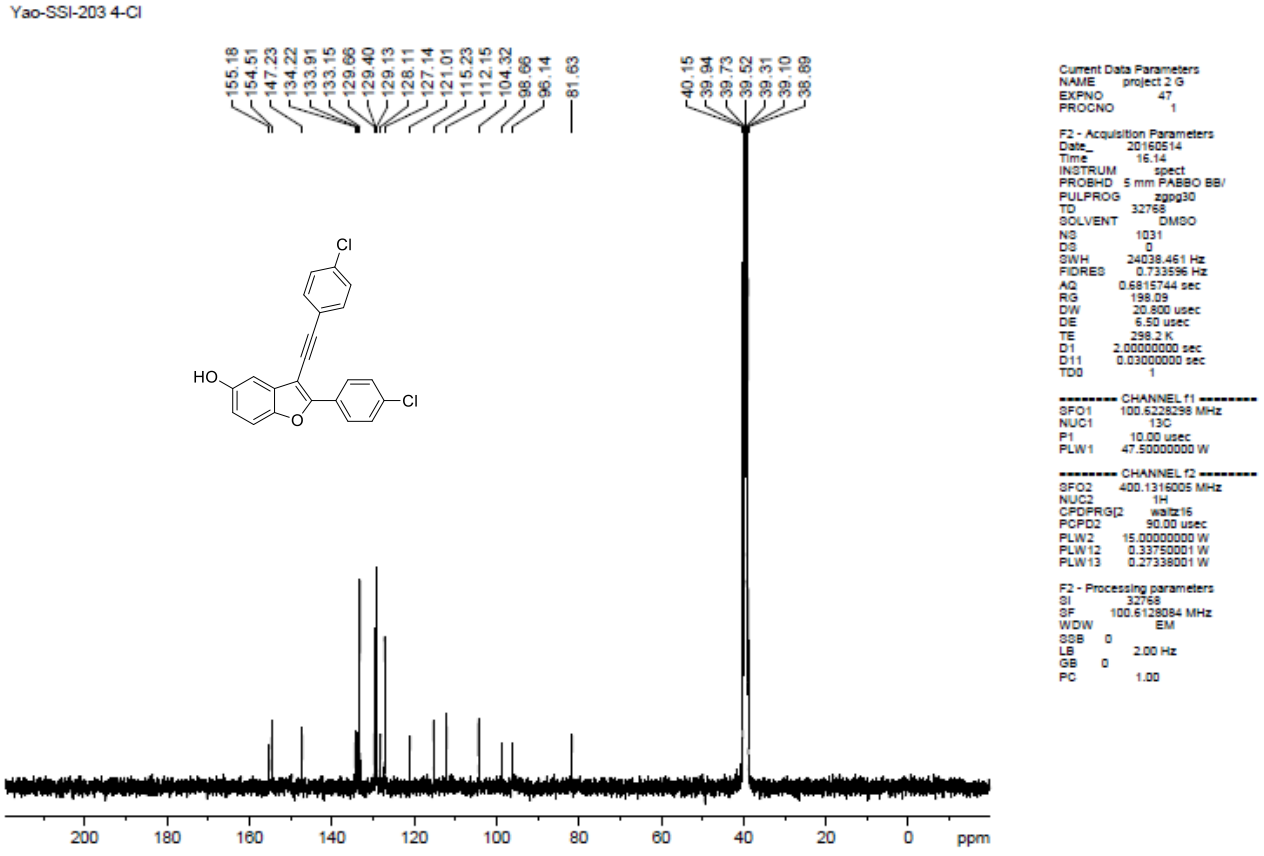
GB 0
PC 1.00

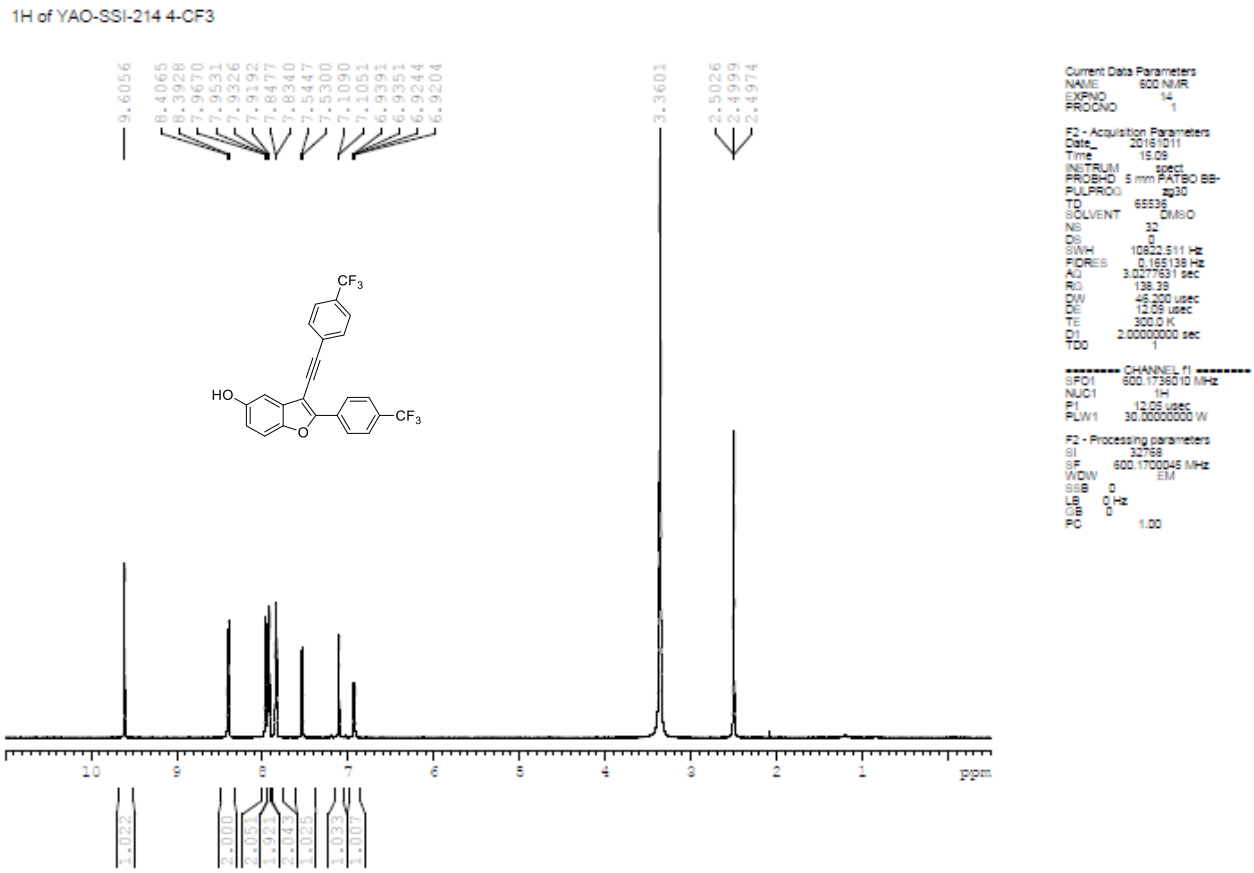
2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)benzofuran-5-ol (**3c**): ^{1}H NMR (400 MHz, DMSO)



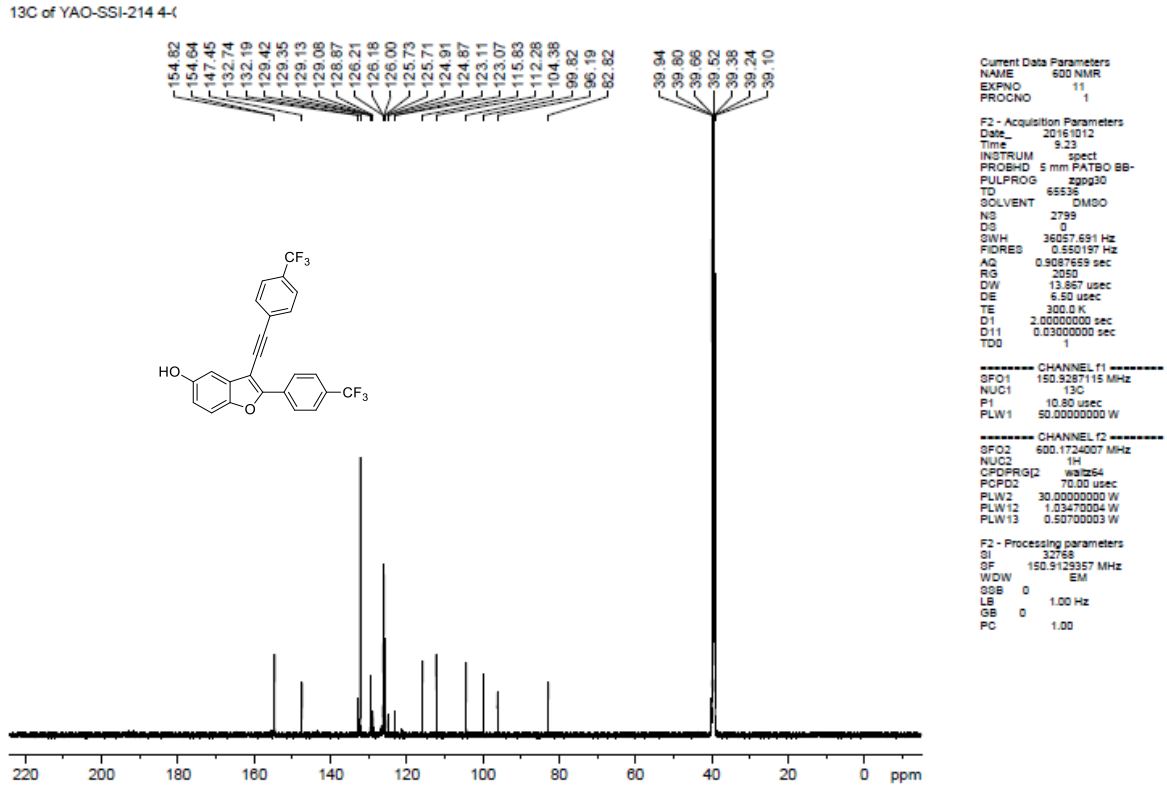
2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)benzofuran-5-ol (**3c**): ^{13}C NMR (100 MHz, DMSO)



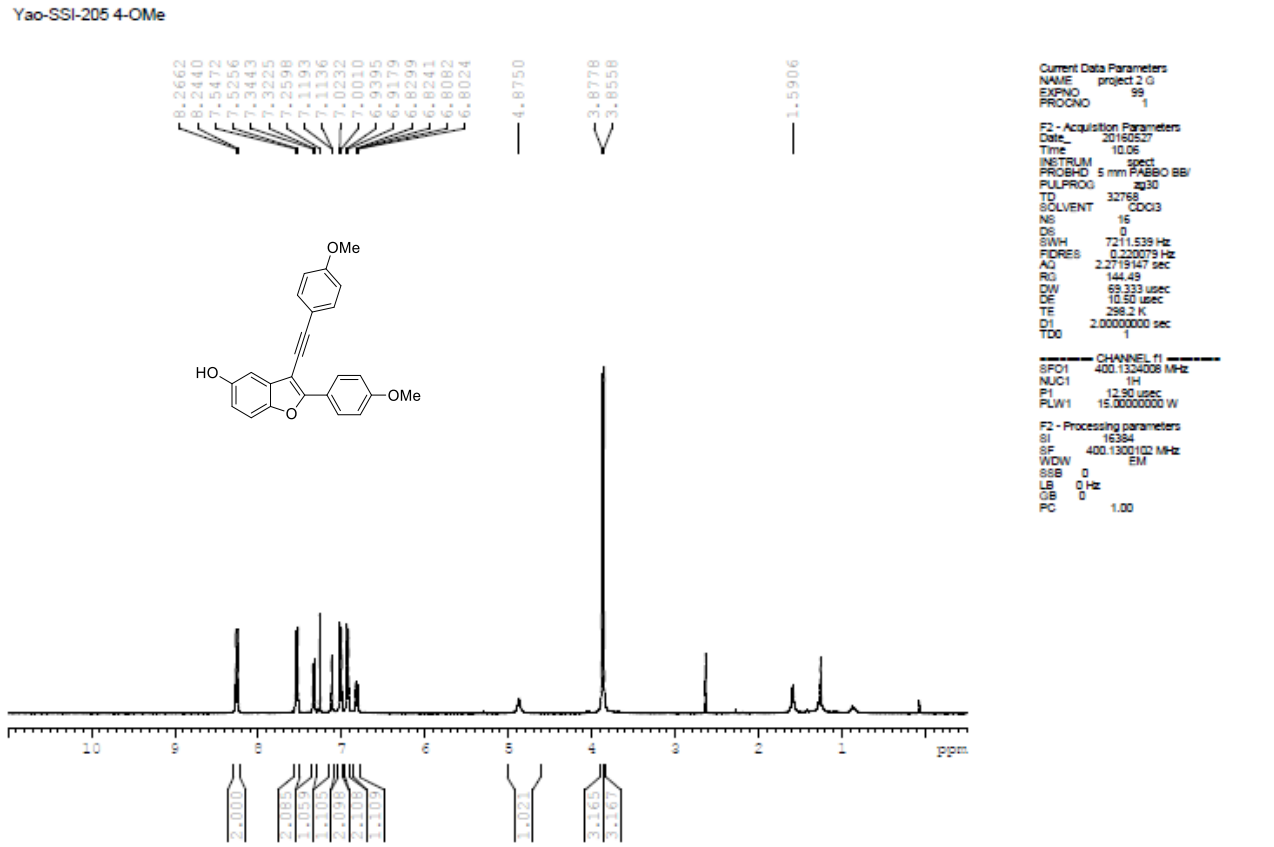
2-(4-(trifluoromethyl)phenyl)-3-((4-(trifluoromethyl)phenyl)ethynyl)benzofuran-5-ol (**3d**): ^{1}H NMR (600 MHz, $CDCl_3$)



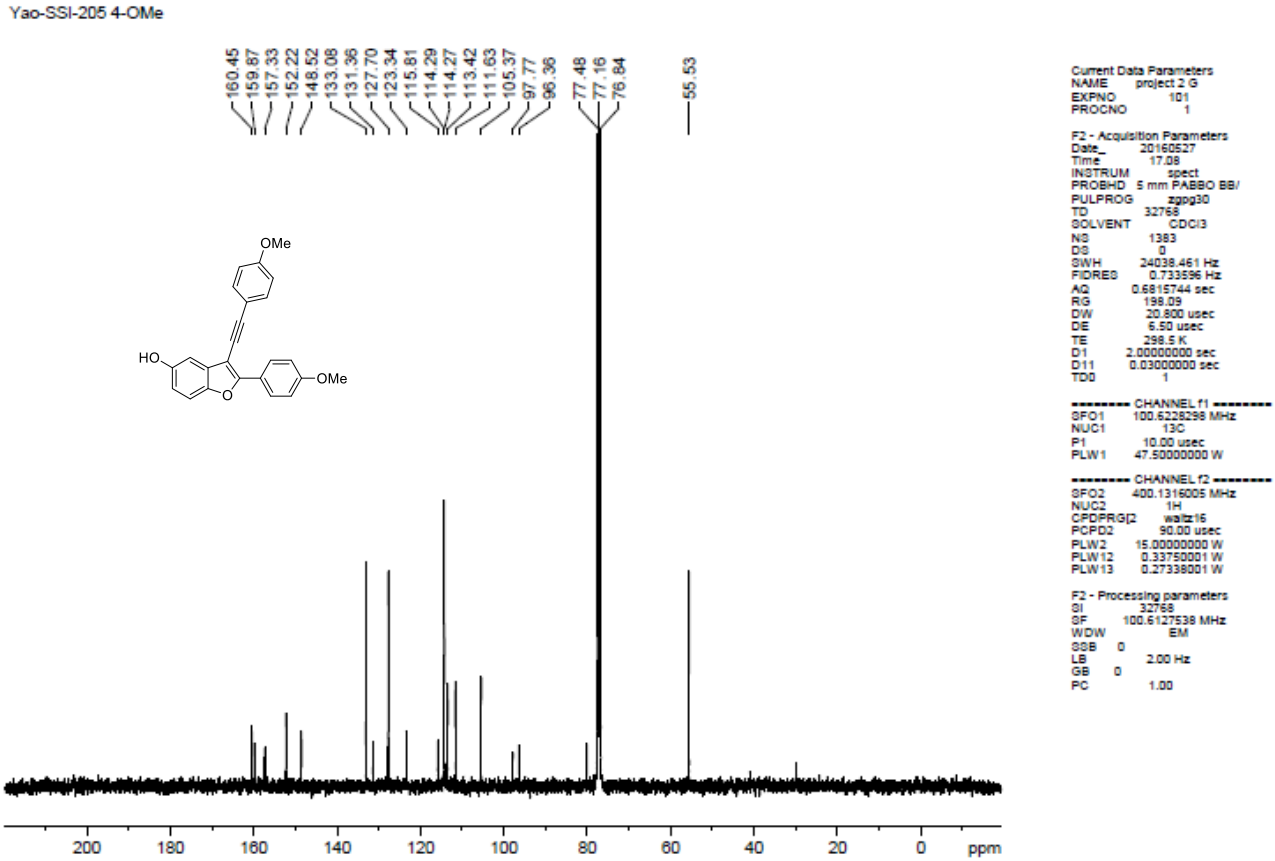
2-(4-(trifluoromethyl)phenyl)-3-((4-(trifluoromethyl)phenyl)ethynyl)benzofuran-5-ol (**3d**):): ^{13}C NMR (150 MHz, $CDCl_3$)



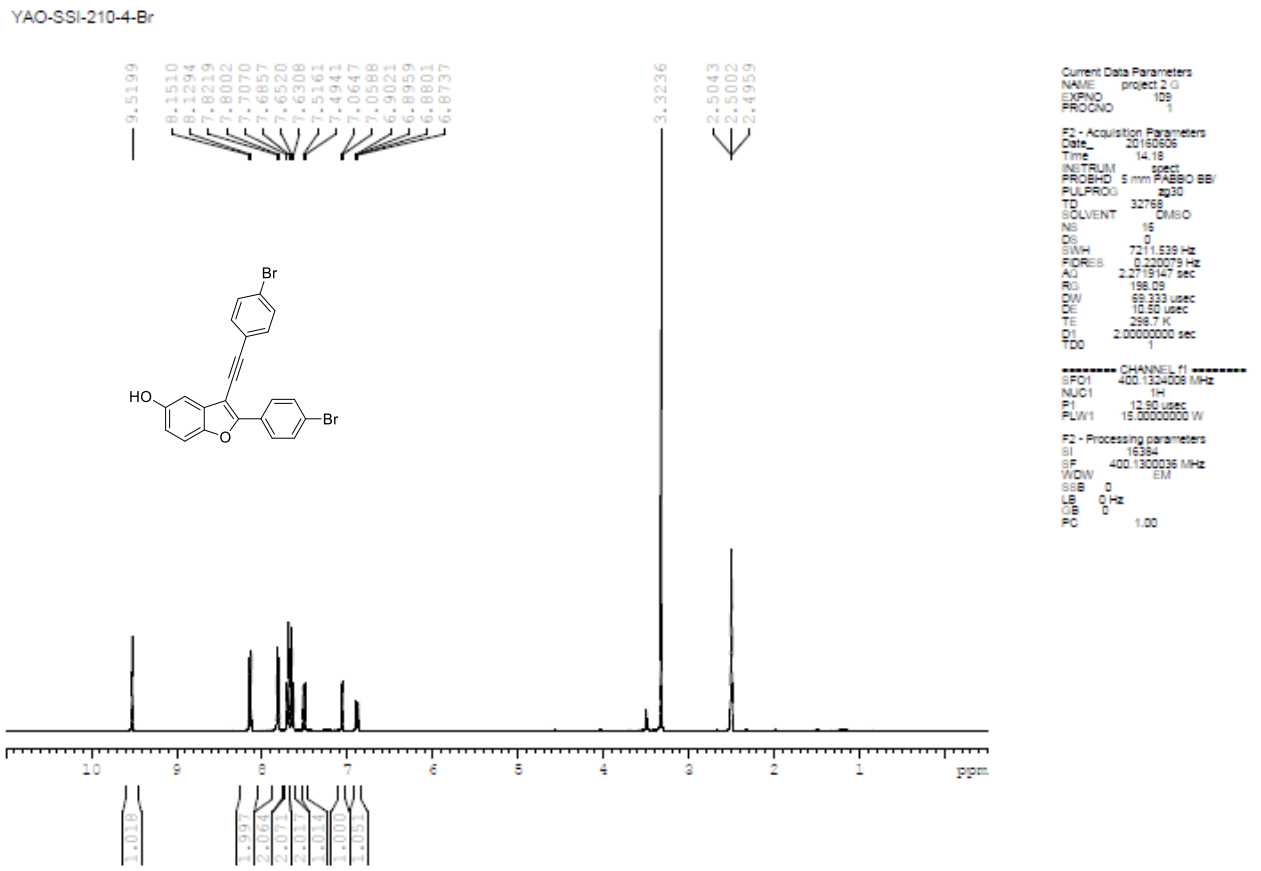
2-(4-methoxyphenyl)-3-((4-methoxyphenyl)ethynyl)benzofuran-5-ol (**3e**): ^{1}H NMR (400 MHz, $CDCl_3$)



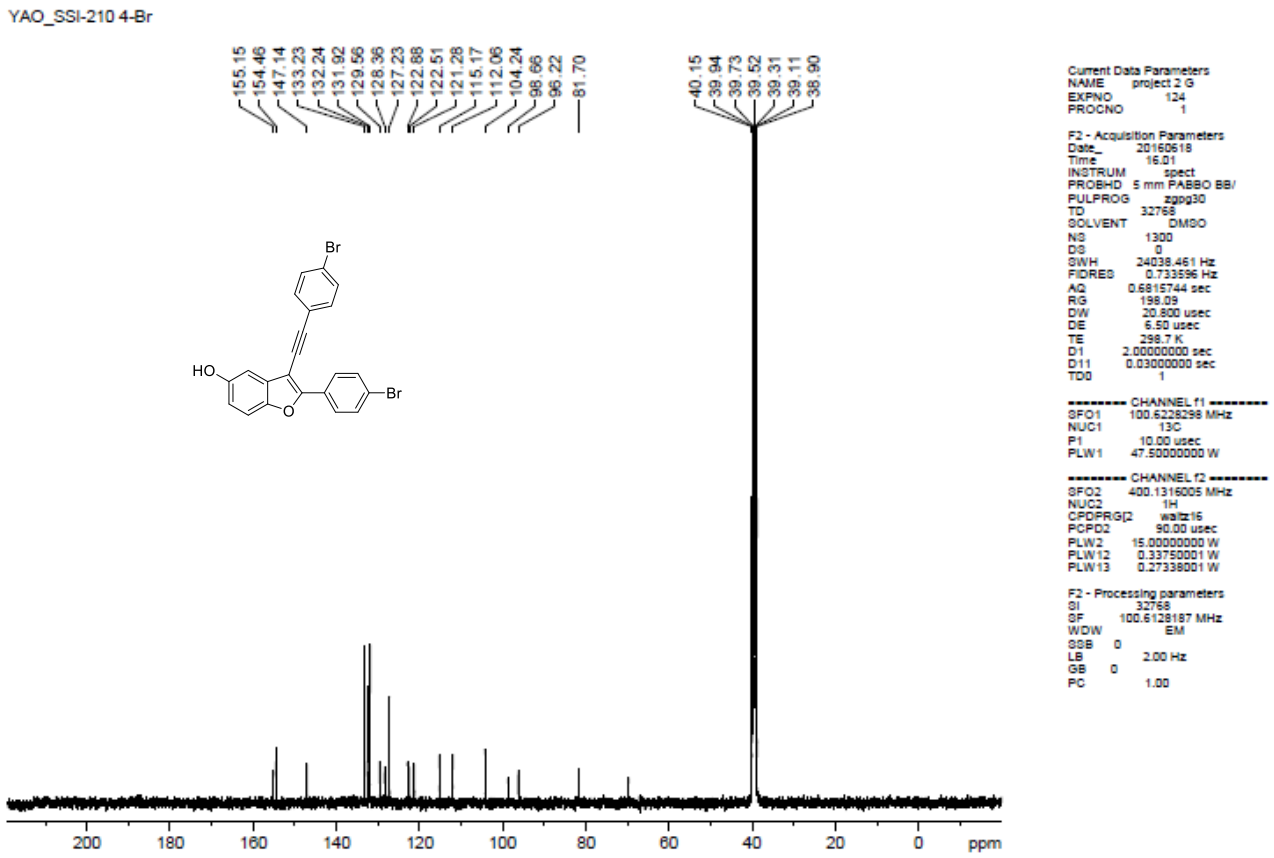
2-(4-methoxyphenyl)-3-((4-methoxyphenyl)ethynyl)benzofuran-5-ol (**3e**): ^{13}C NMR (100 MHz, $CDCl_3$)



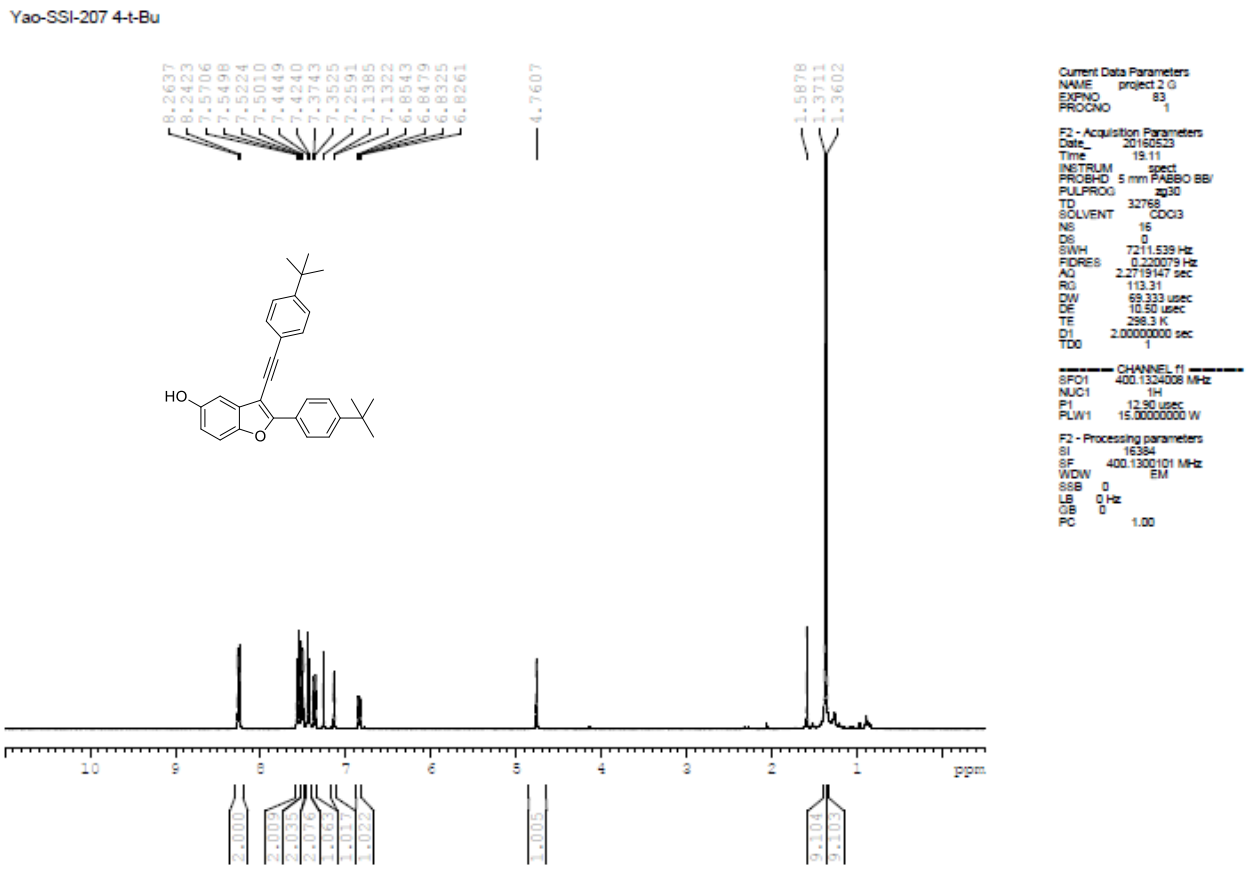
2-(4-bromophenyl)-3-((4-bromophenyl)ethynyl)benzofuran-5-ol (**3f**): ^{1}H NMR (400 MHz, DMSO)



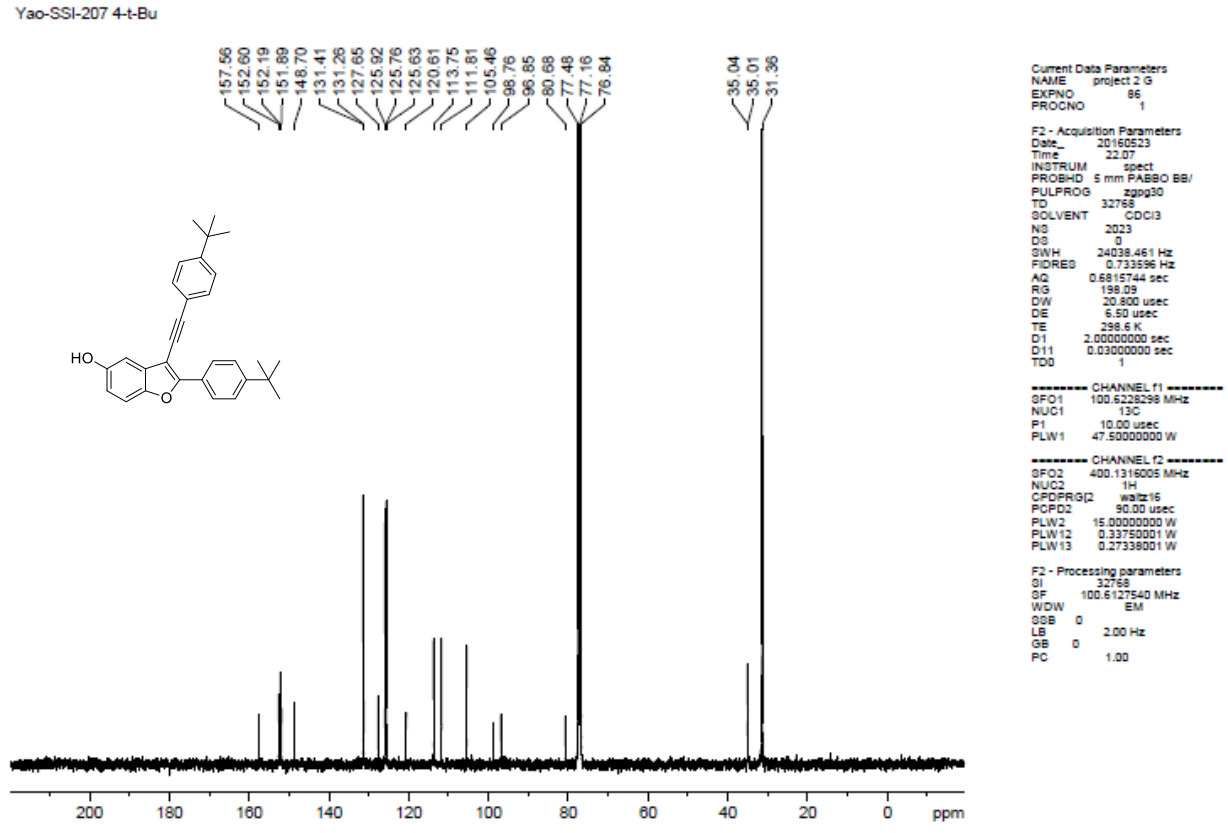
2-(4-bromophenyl)-3-((4-bromophenyl)ethynyl)benzofuran-5-ol (**3f**): ^{13}C NMR (100 MHz, DMSO)



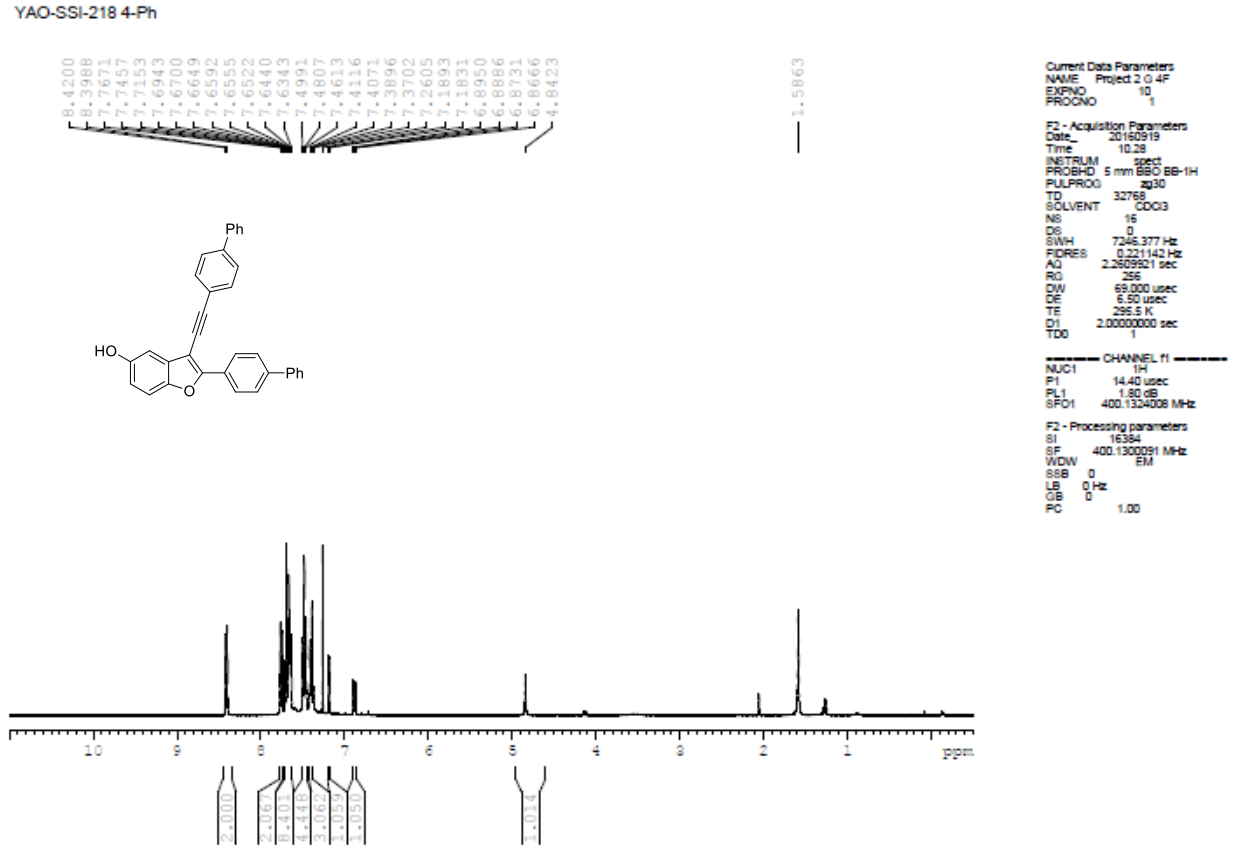
2-(4-(tert-butyl)phenyl)-3-((4-(tert-butyl)phenyl)ethynyl)benzofuran-5-ol (**3g**): ^{1}H NMR (400 MHz, $CDCl_3$)



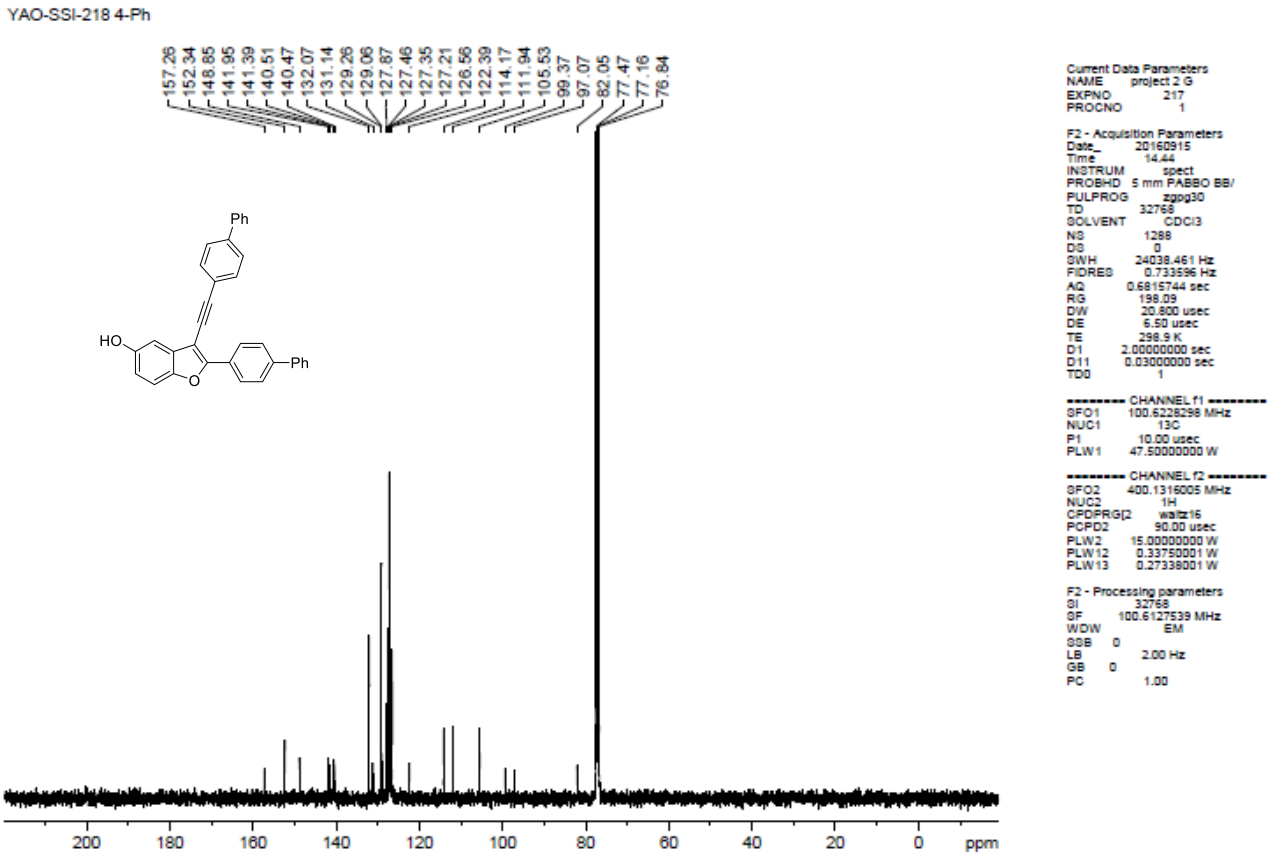
2-(4-(tert-butyl)phenyl)-3-((4-(tert-butyl)phenyl)ethynyl)benzofuran-5-ol (**3g**): ^{13}C NMR (100 MHz, $CDCl_3$)



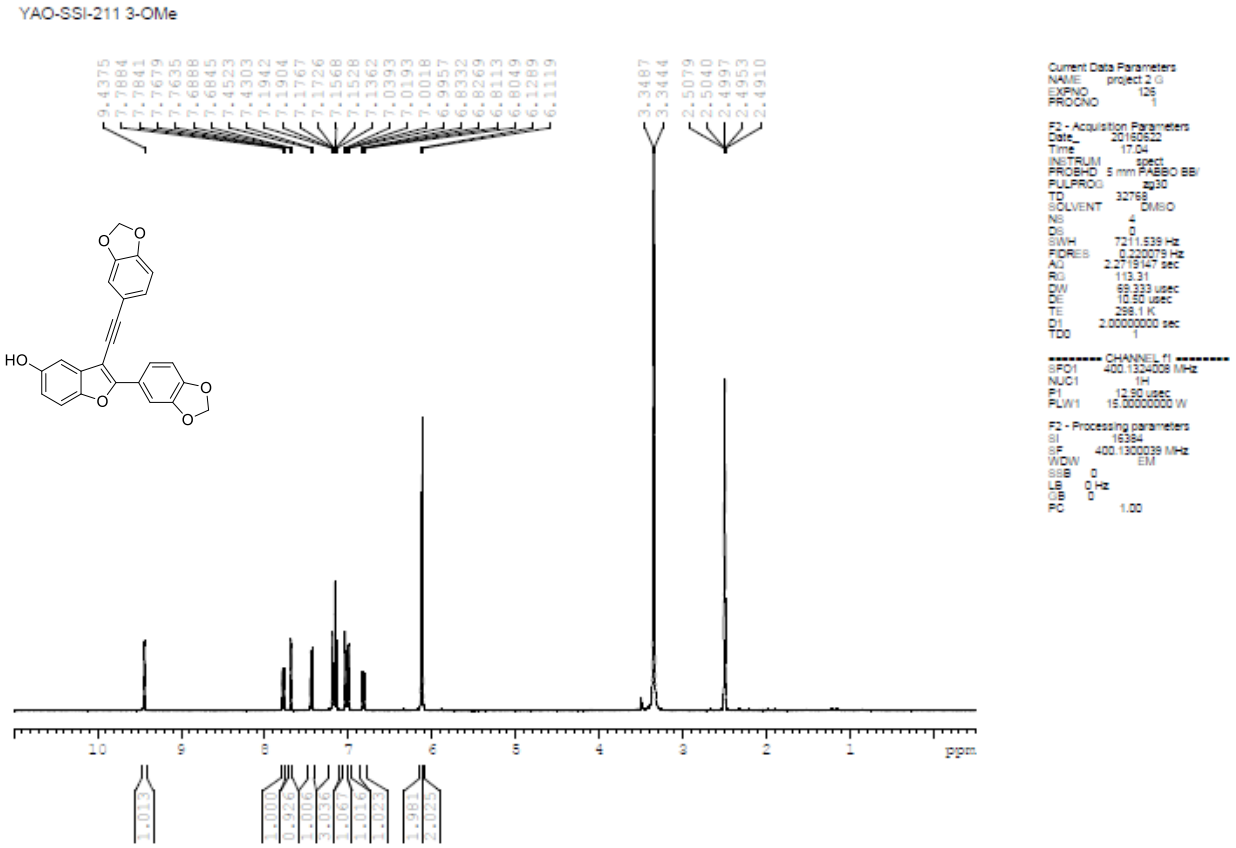
2-([1,1'-biphenyl]-4-yl)-3-([1,1'-biphenyl]-4-ylethynyl)benzofuran-5-ol (**3h**): ^{1}H NMR (400 MHz, $CDCl_3$)



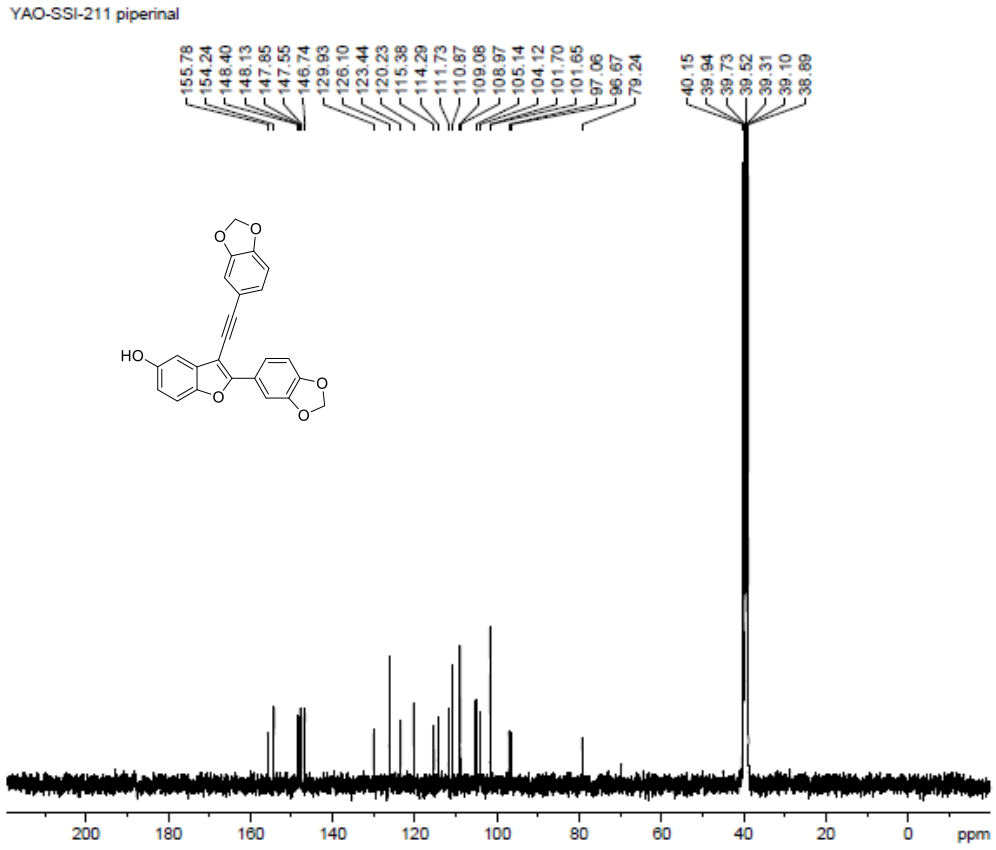
2-([1,1'-biphenyl]-4-yl)-3-([1,1'-biphenyl]-4-ylethynyl)benzofuran-5-ol (**3h**): ^{13}C NMR (100 MHz, $CDCl_3$)



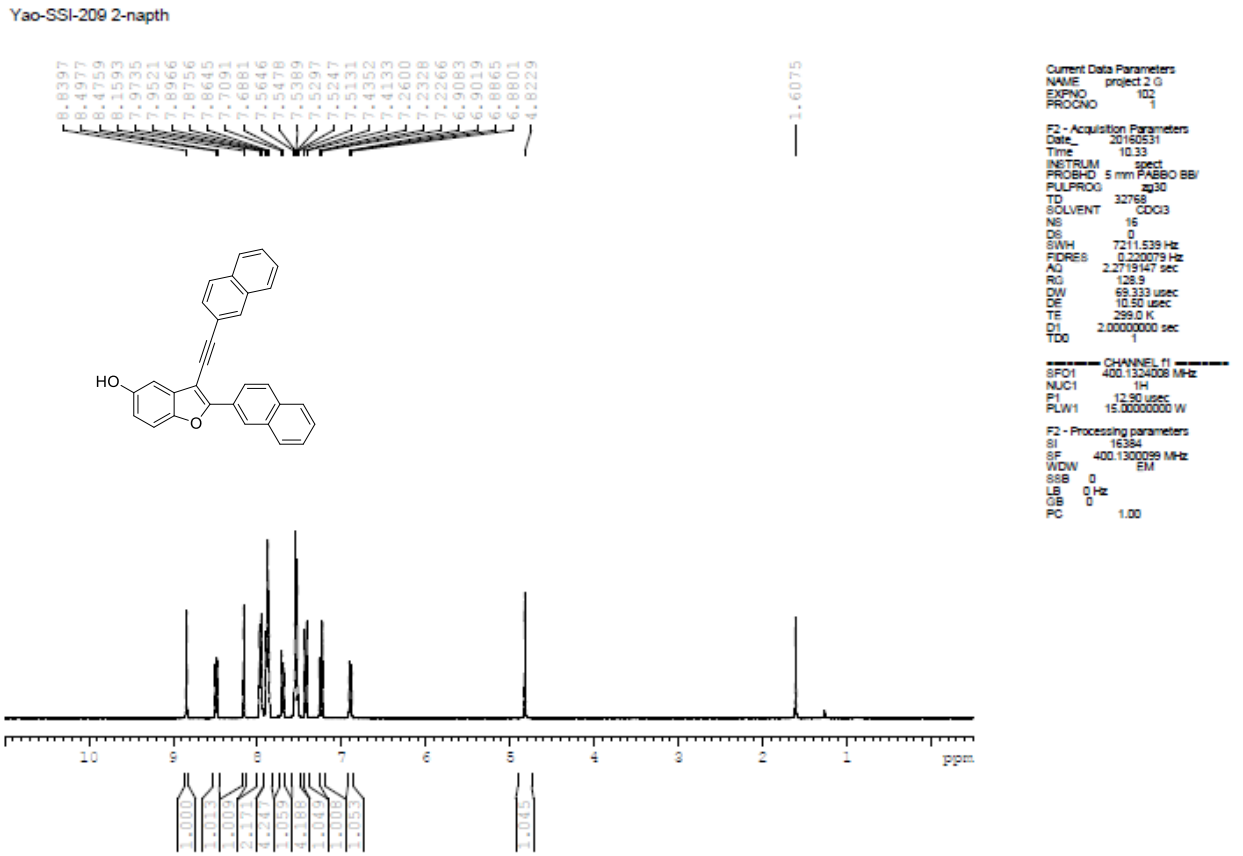
2-(benzo[d][1,3]dioxol-5-yl)-3-(benzo[d][1,3]dioxol-5-ylethynyl)benzofuran-5-ol (**3i**): ^{1}H NMR (400 MHz, DMSO)



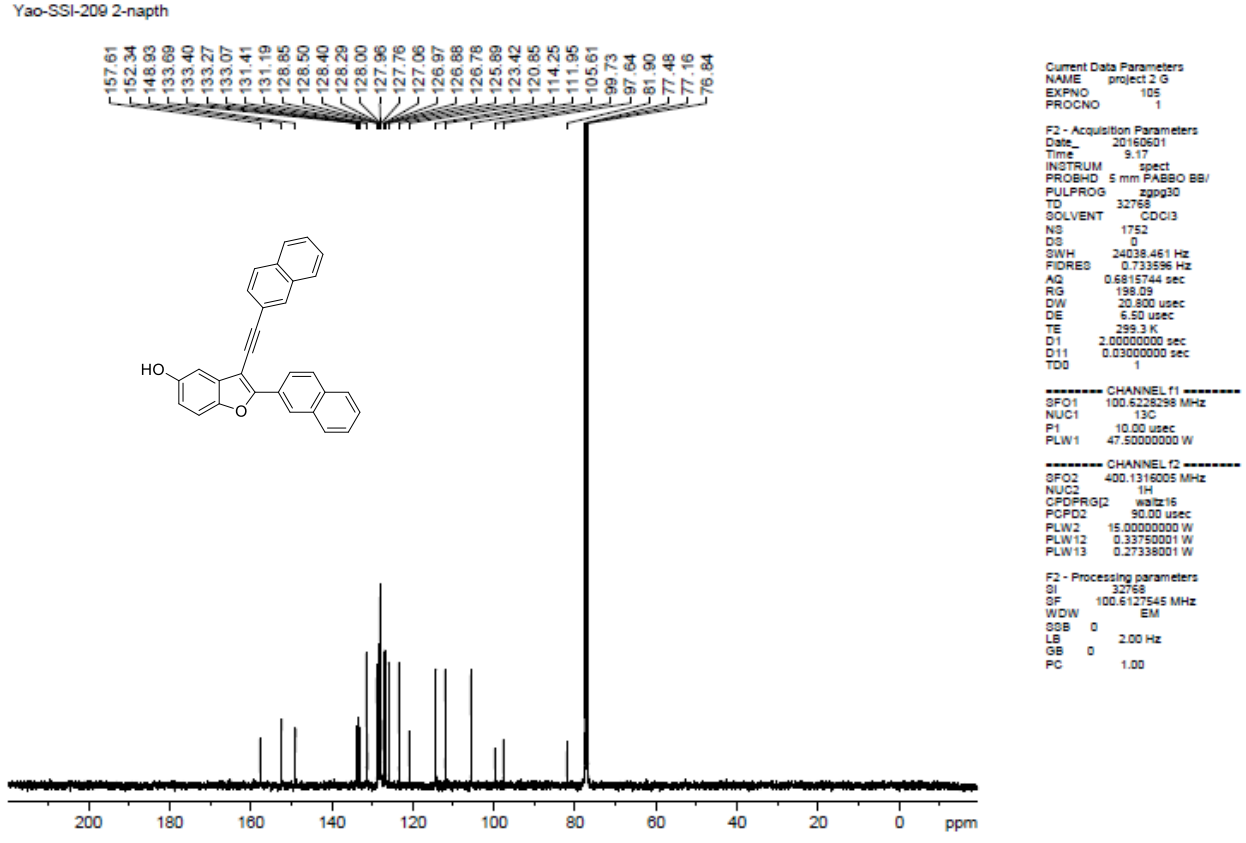
2-(benzo[d][1,3]dioxol-5-yl)-3-(benzo[d][1,3]dioxol-5-ylethynyl)benzofuran-5-ol (**3i**): ^{13}C NMR (100 MHz, DMSO)



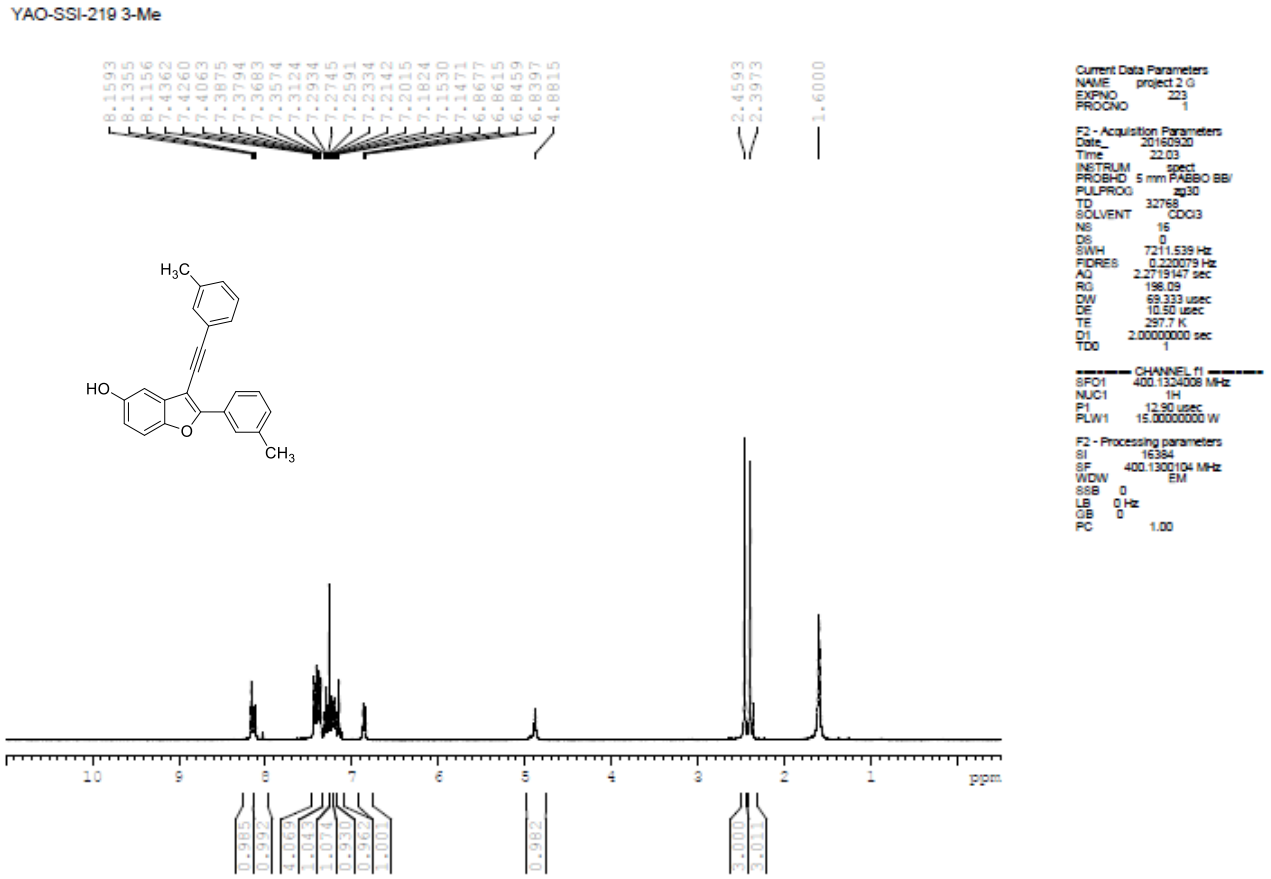
2-(naphthalen-2-yl)-3-(naphthalen-2-ylethynyl)benzofuran-5-ol (**3j**): ^{1}H NMR (400 MHz, $CDCl_3$)



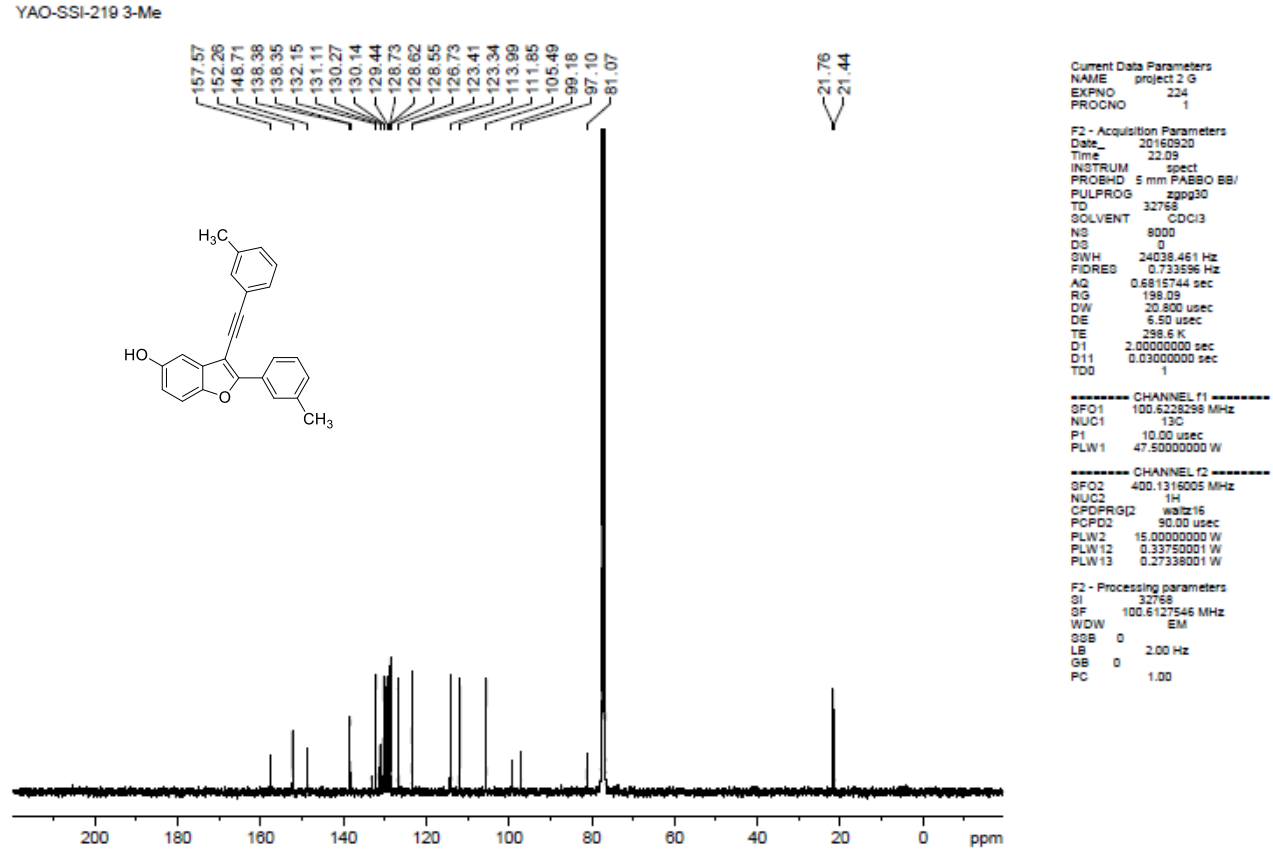
2-(naphthalen-2-yl)-3-(naphthalen-2-ylethynyl)benzofuran-5-ol (**3j**): ^{13}C NMR (100 MHz, $CDCl_3$)



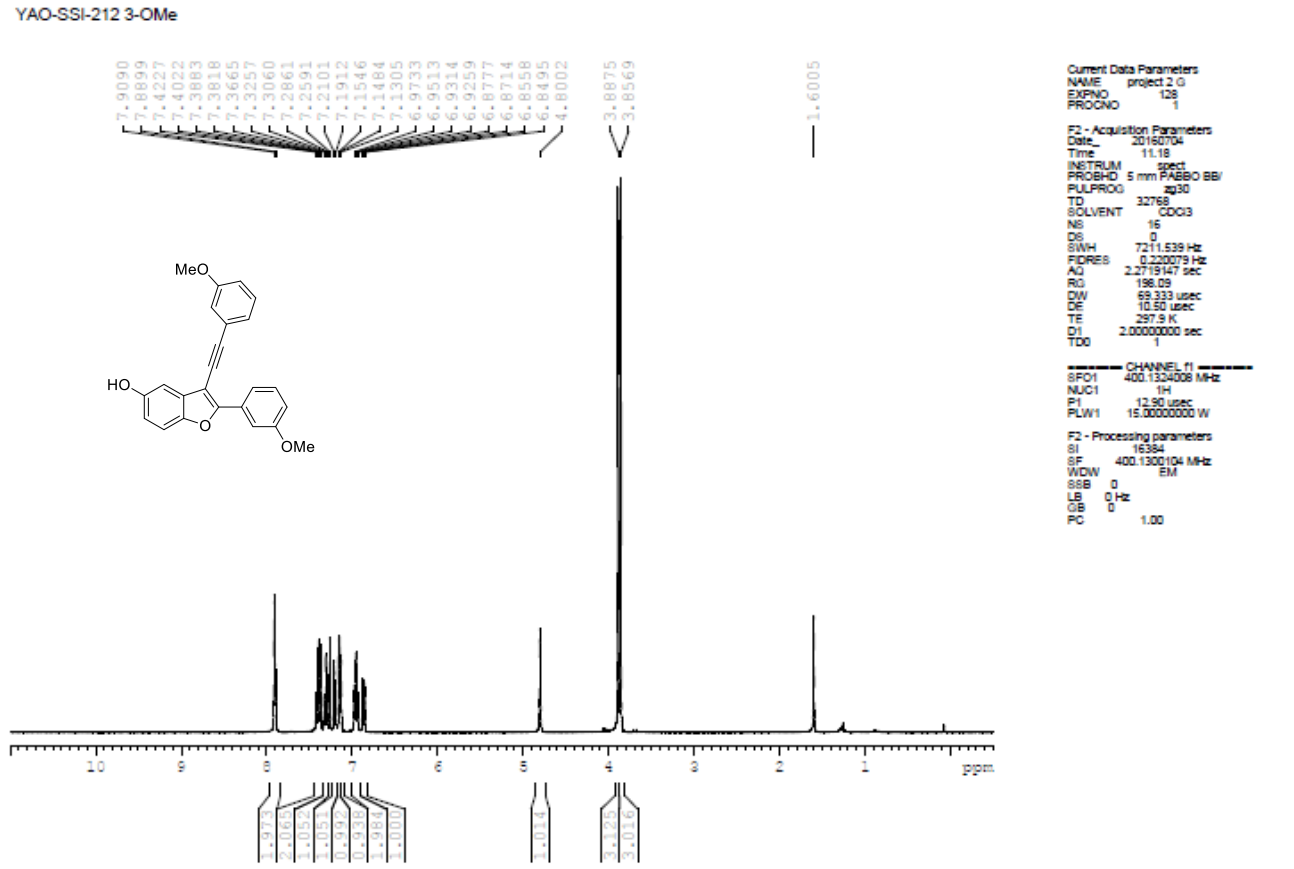
2-(m-tolyl)-3-(m-tolylethynyl)benzofuran-5-ol (**3k**): ^{1}H NMR (400 MHz, $CDCl_3$)



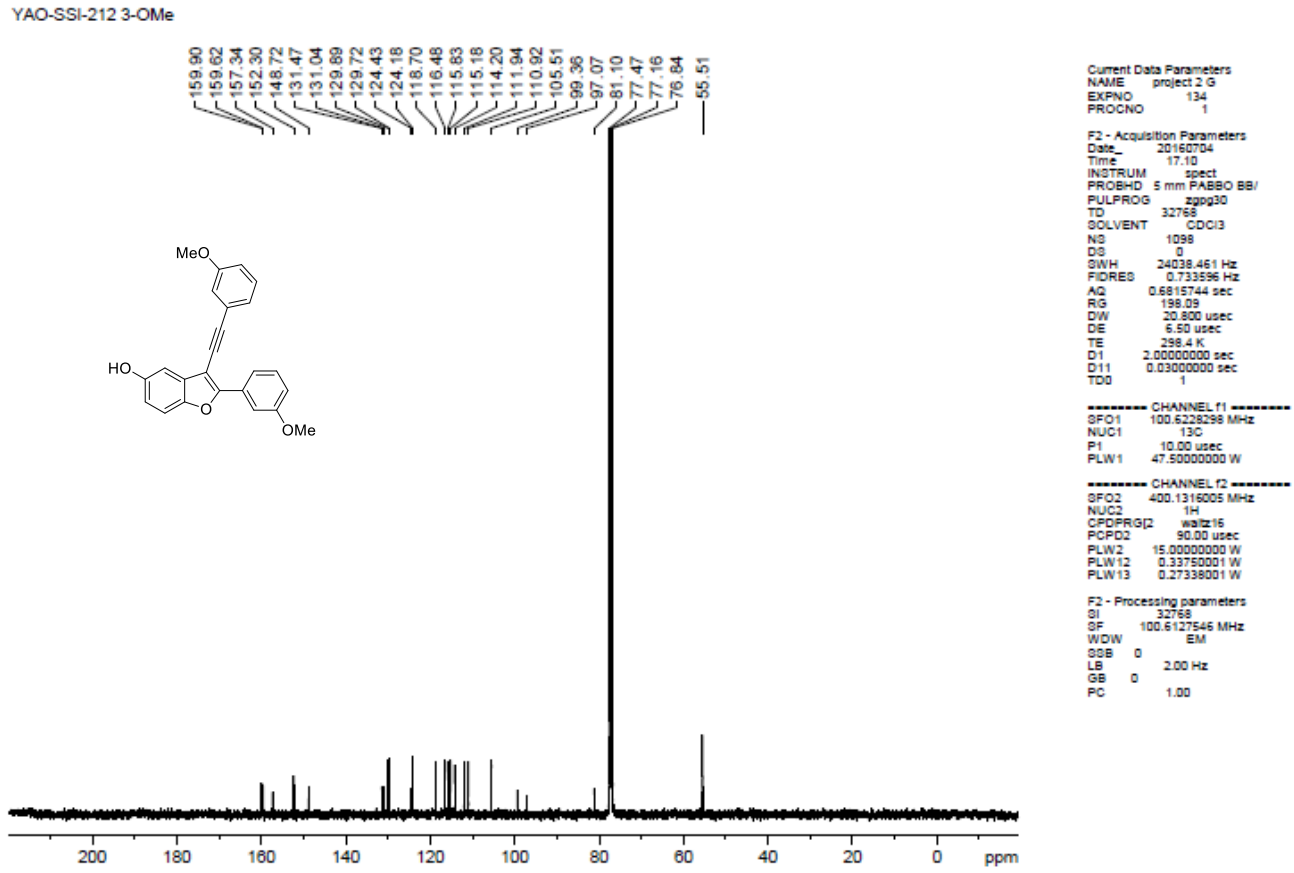
2-(m-tolyl)-3-(m-tolylethynyl)benzofuran-5-ol (**3k**): ^{13}C NMR (100 MHz, $CDCl_3$)



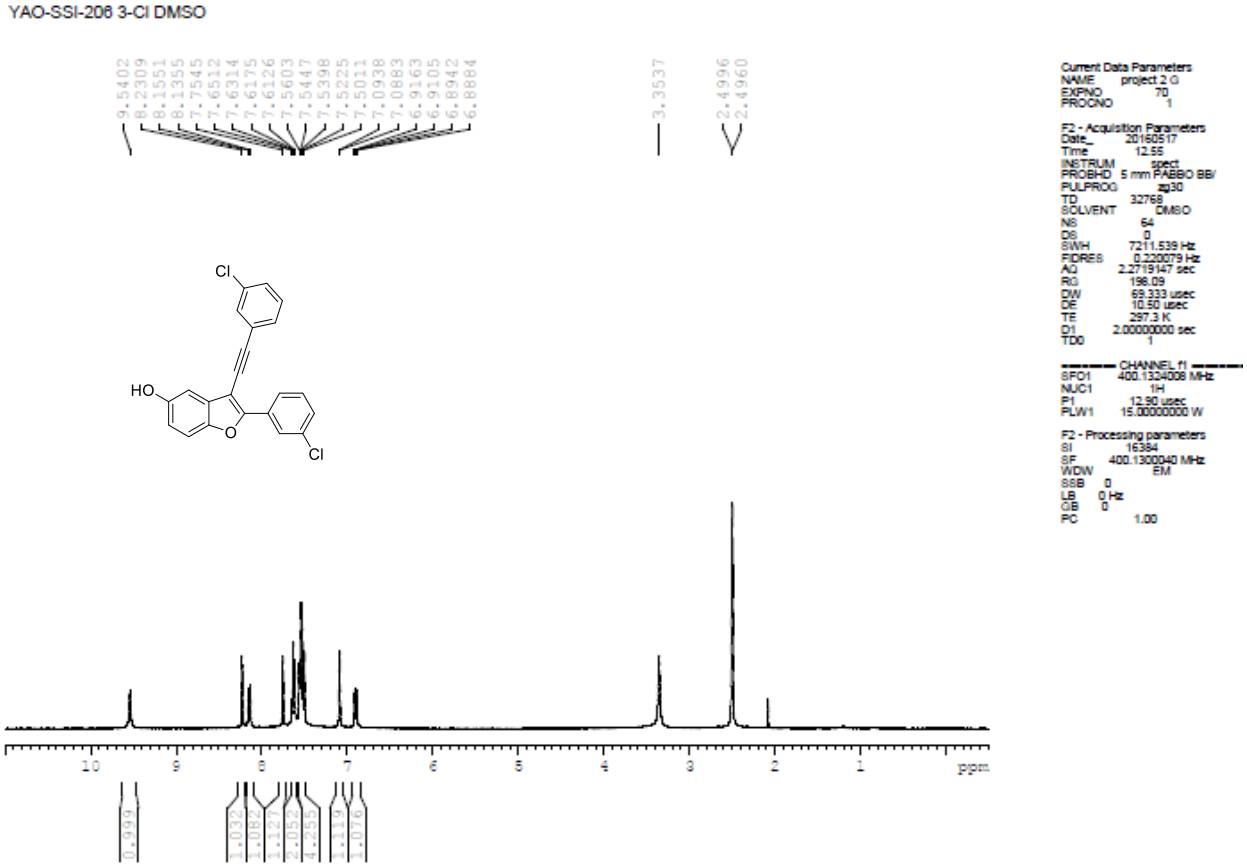
2-(3-methoxyphenyl)-3-((3-methoxyphenyl)ethynyl)benzofuran-5-ol (**3l**): ^{1}H NMR (400 MHz, DMSO)



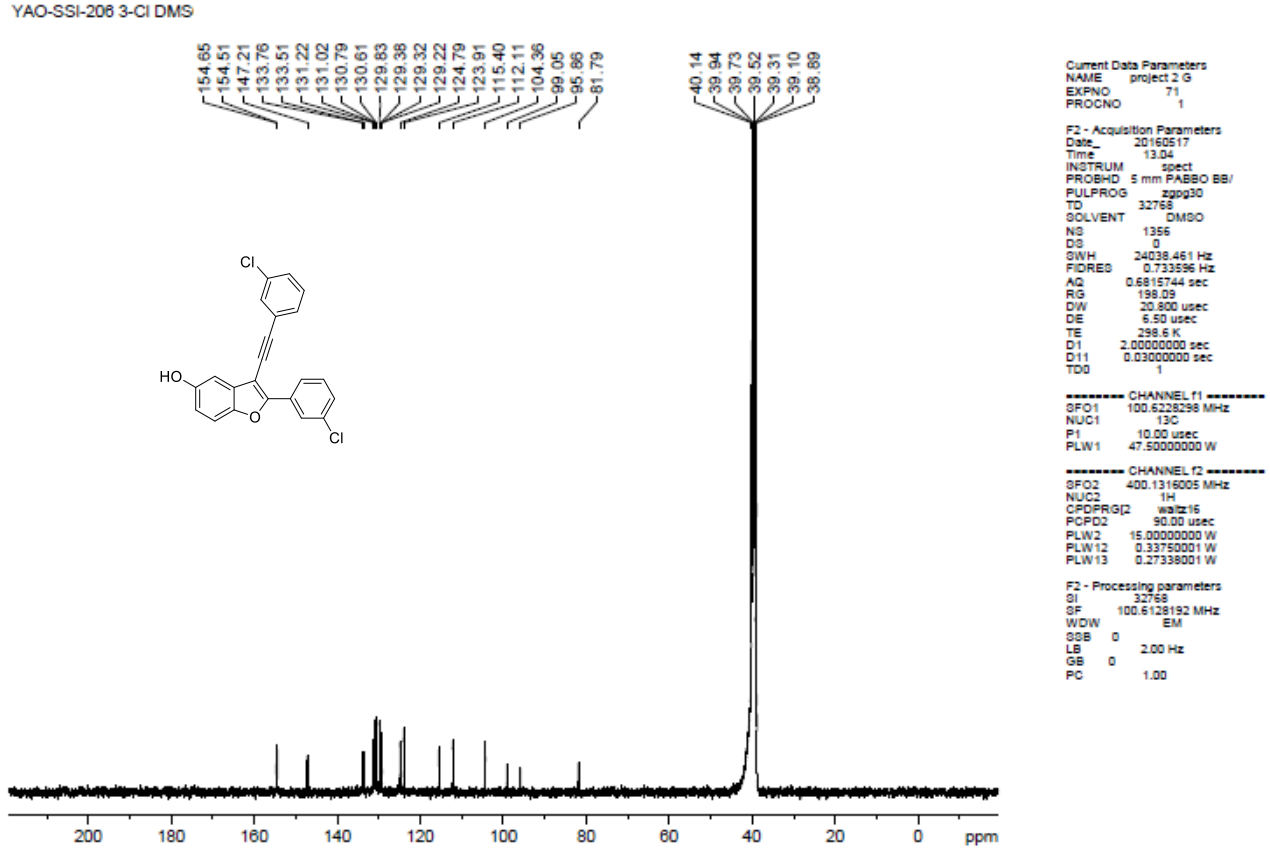
2-(3-methoxyphenyl)-3-((3-methoxyphenyl)ethynyl)benzofuran-5-ol (**3l**): ^{13}C NMR (100 MHz, DMSO)



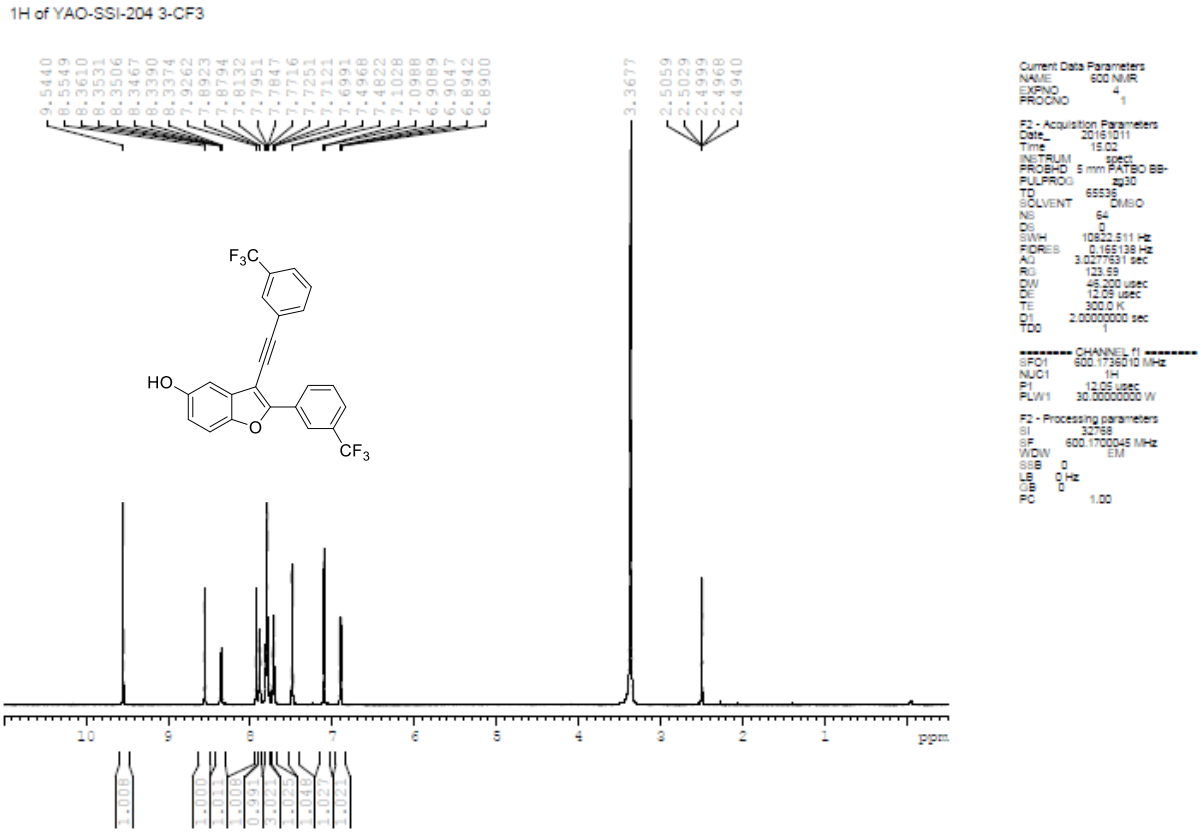
2-(3-chlorophenyl)-3-((3-chlorophenyl)ethynyl)benzofuran-5-ol (**3m**): ^{1}H NMR (400 MHz, DMSO)



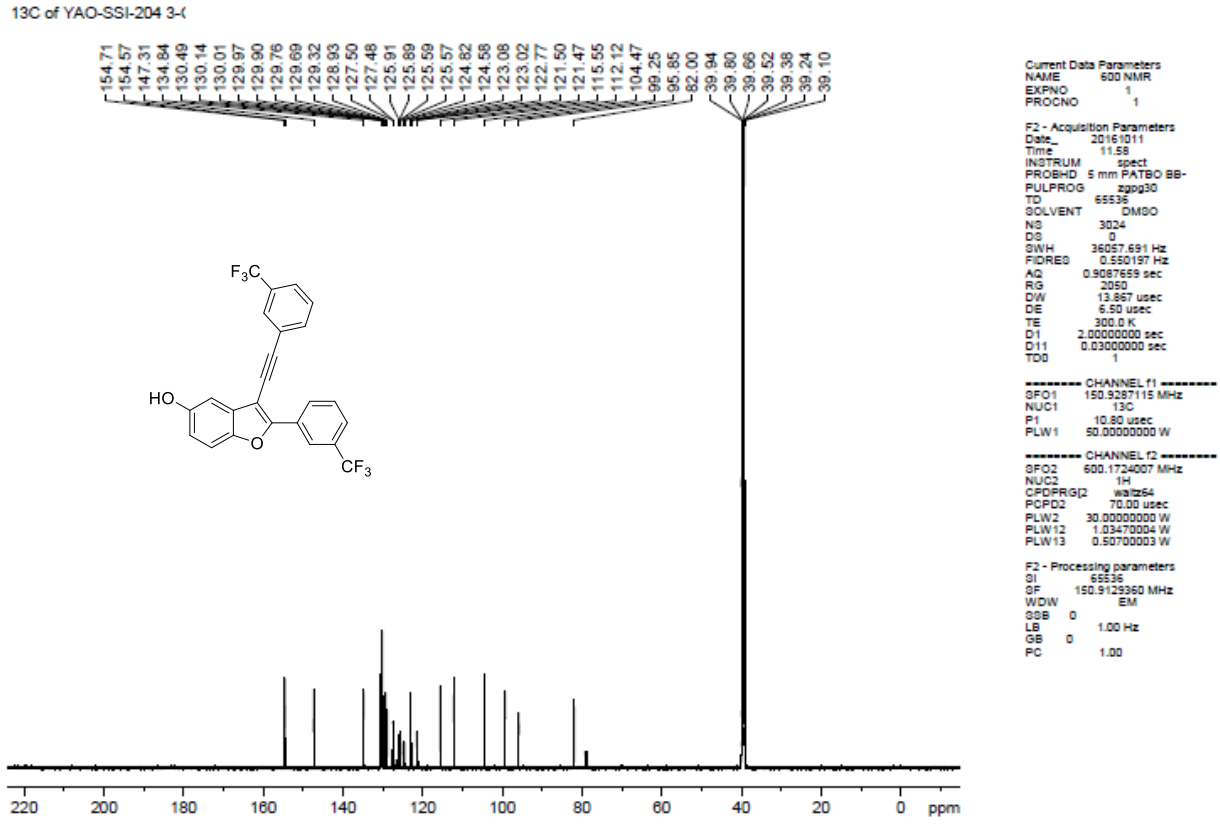
2-(3-chlorophenyl)-3-((3-chlorophenyl)ethynyl)benzofuran-5-ol (**3m**): ^{13}C NMR (100 MHz, DMSO)



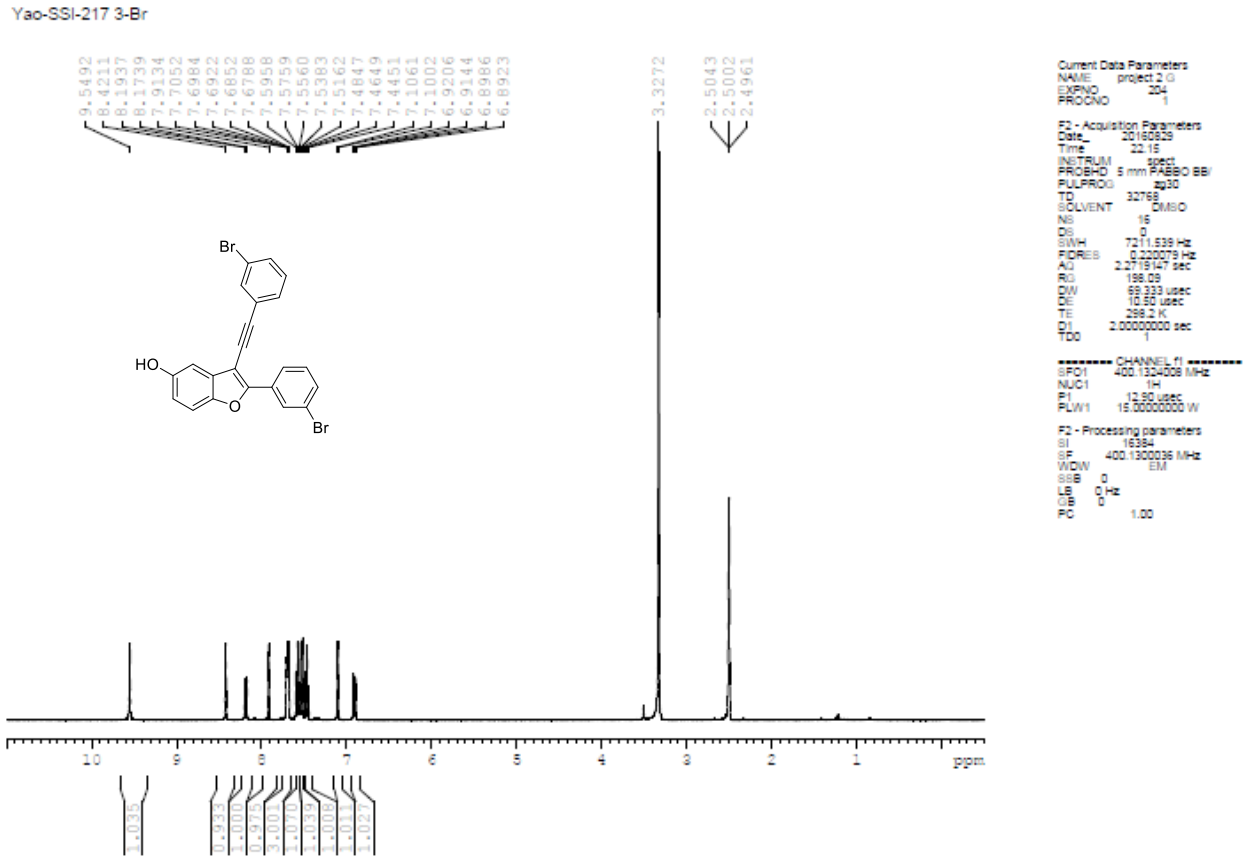
2-(3-(trifluoromethyl)phenyl)-3-((3-(trifluoromethyl)phenyl)ethynyl)benzofuran-5-ol (**3n**): ^{1}H NMR (400 MHz, $CDCl_3$)



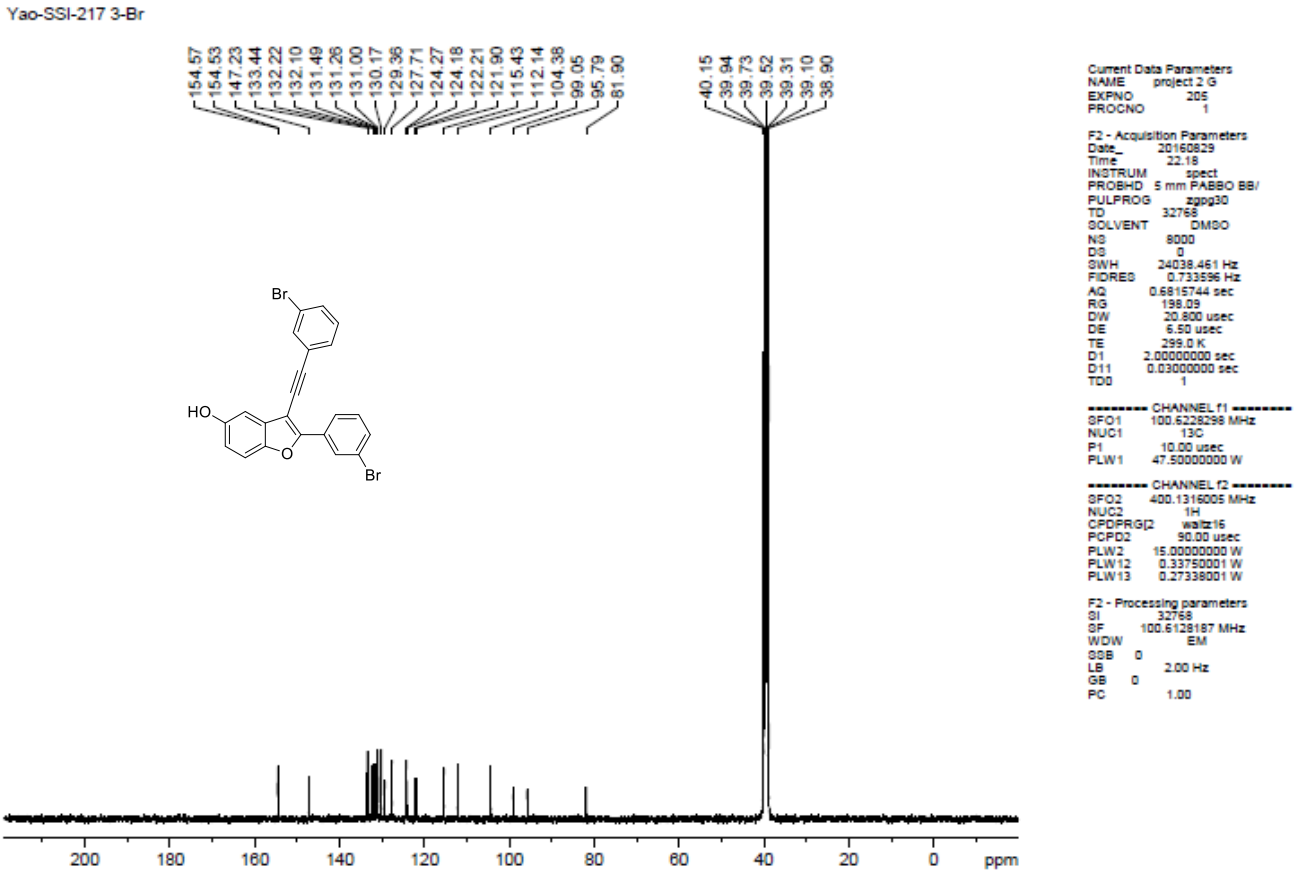
2-(3-(trifluoromethyl)phenyl)-3-((3-(trifluoromethyl)phenyl)ethynyl)benzofuran-5-ol (**3n**): ^{13}C NMR (100 MHz, $CDCl_3$)



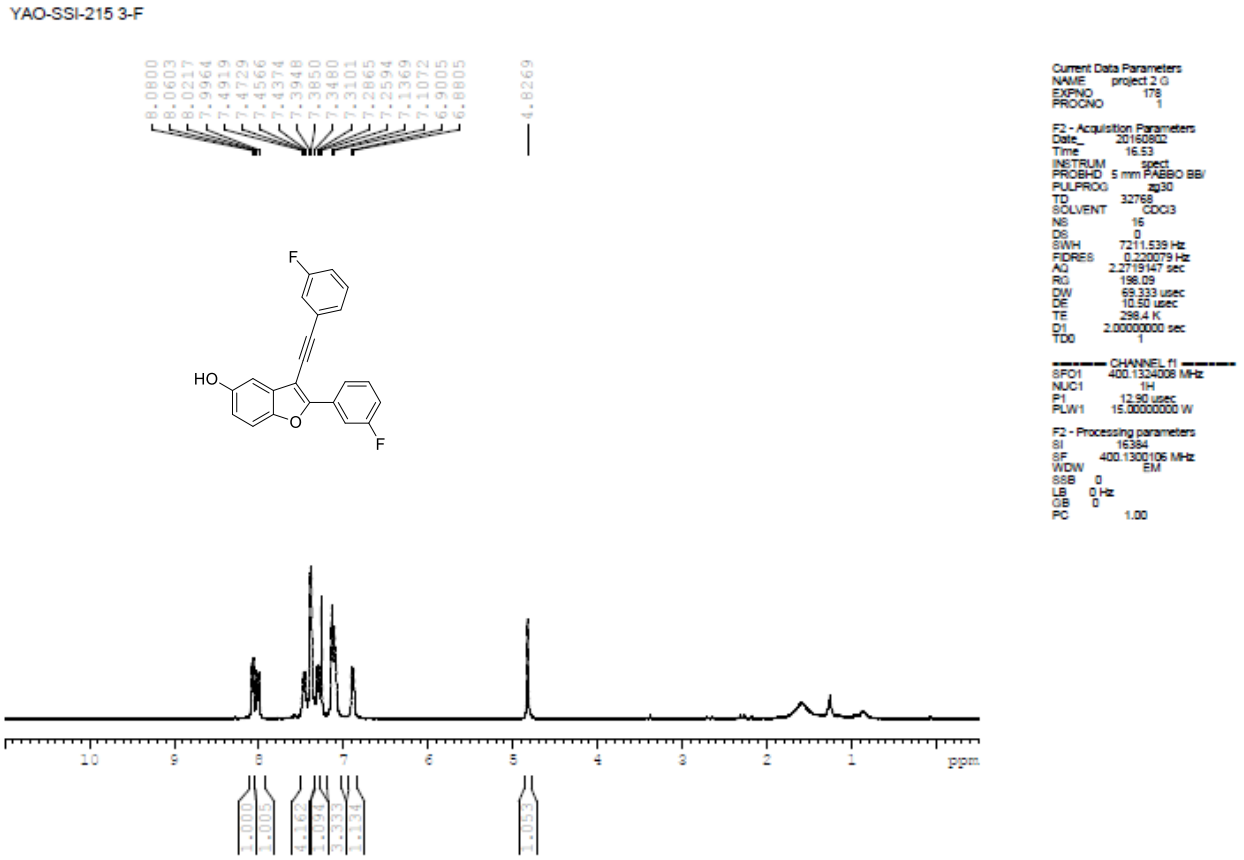
2-(3-bromophenyl)-3-((3-bromophenyl)ethynyl)benzofuran-5-ol (**3o**): ^{1}H NMR (400 MHz, DMSO)



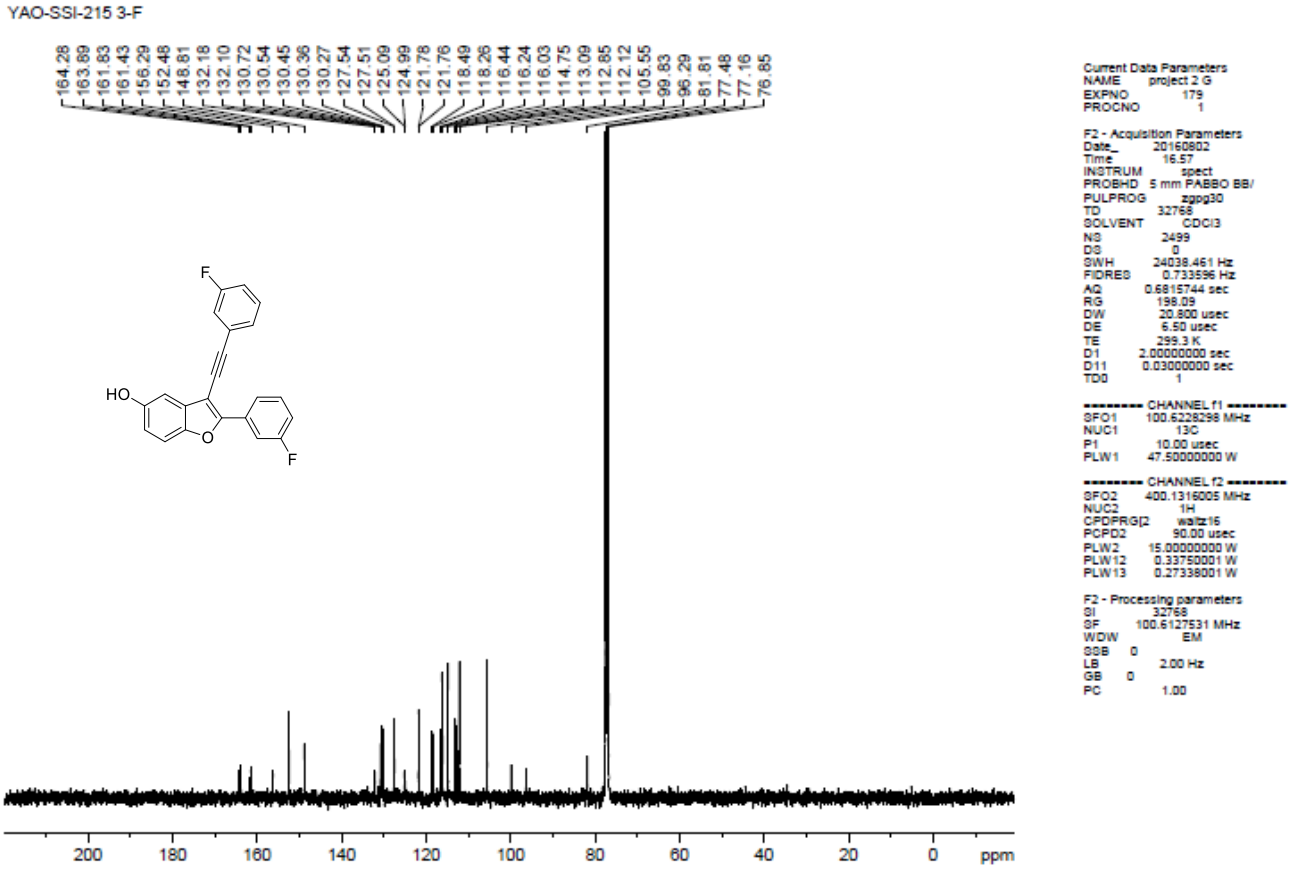
2-(3-bromophenyl)-3-((3-bromophenyl)ethynyl)benzofuran-5-ol (**3o**): ^{13}C NMR (100 MHz, DMSO)



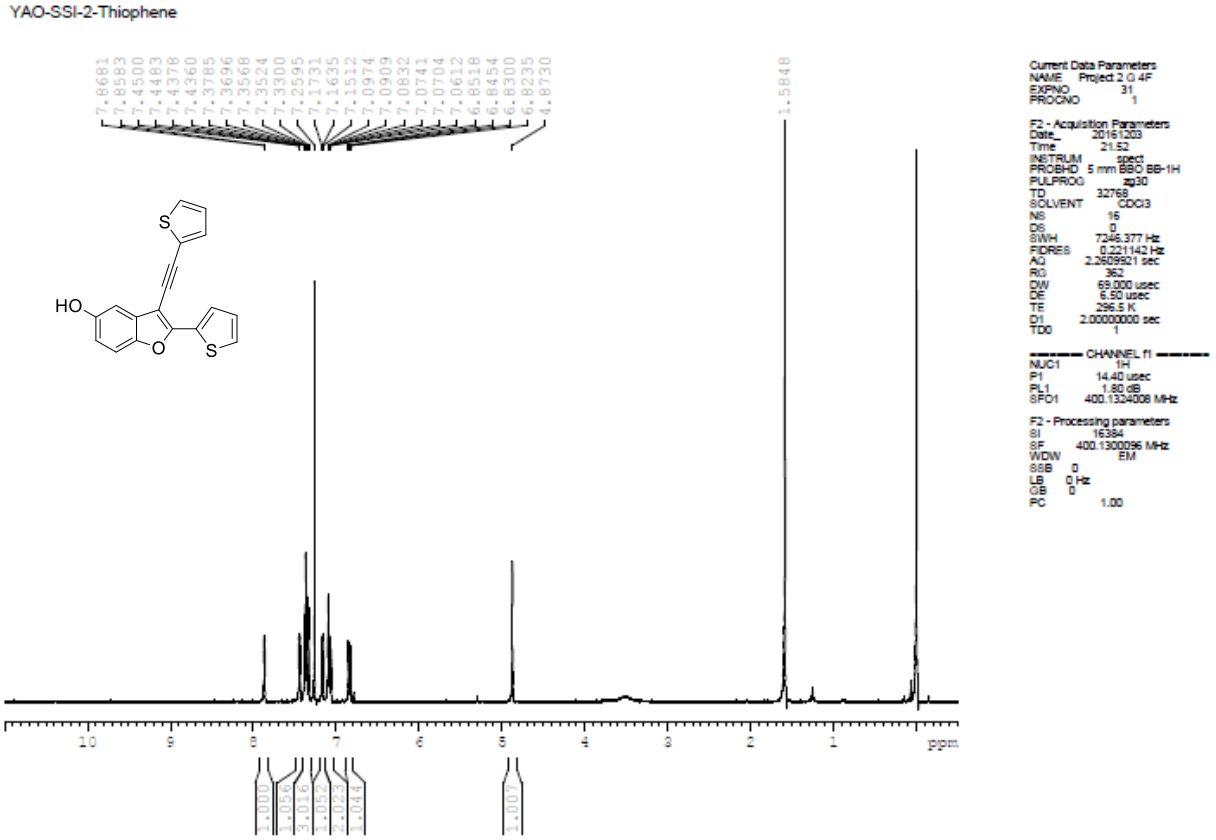
2-(3-fluorophenyl)-3-((3-fluorophenyl)ethynyl)benzofuran-5-ol (**3p**): ^{1}H NMR (400 MHz, $CDCl_3$)



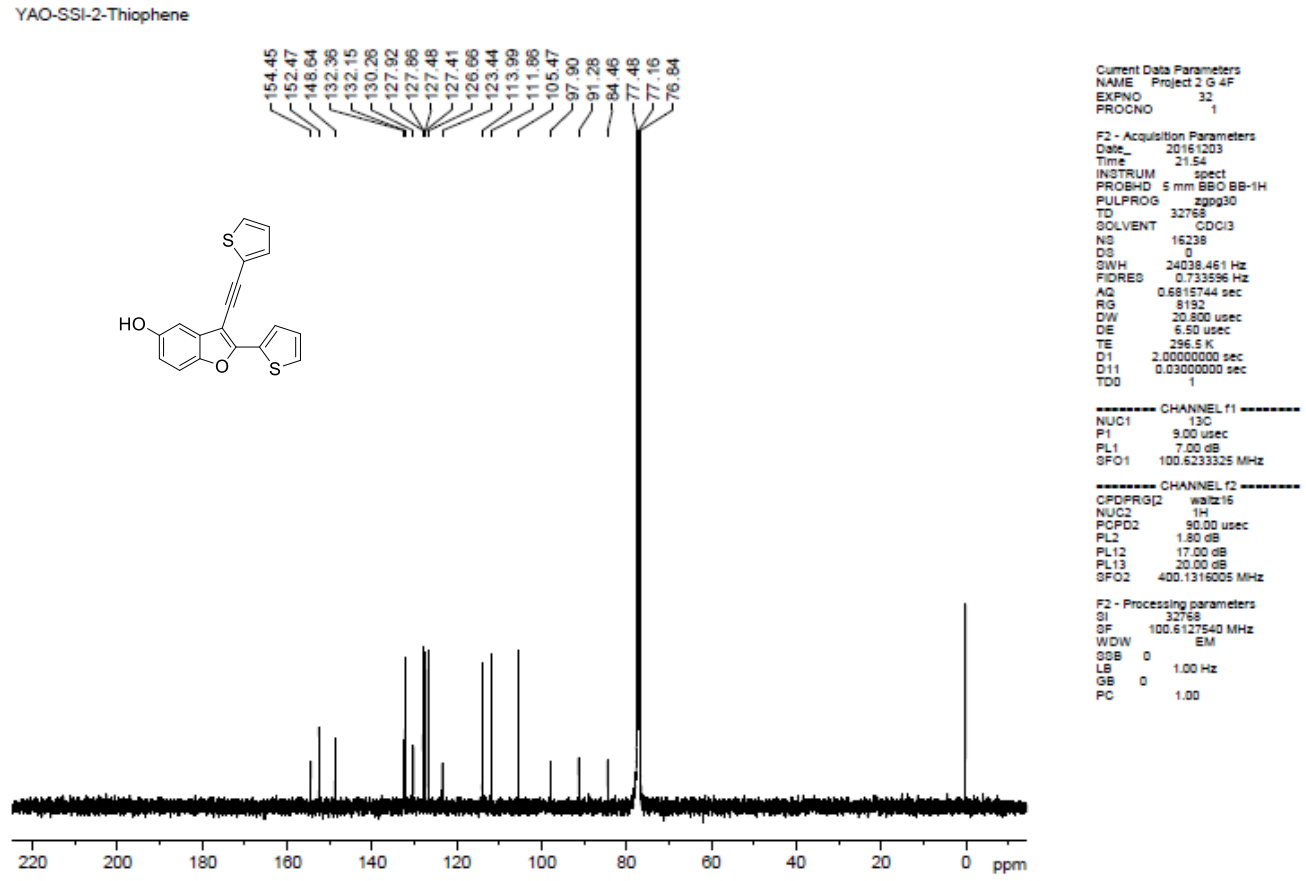
2-(3-fluorophenyl)-3-((3-fluorophenyl)ethynyl)benzofuran-5-ol (**3p**): ^{13}C NMR (100 MHz, $CDCl_3$)



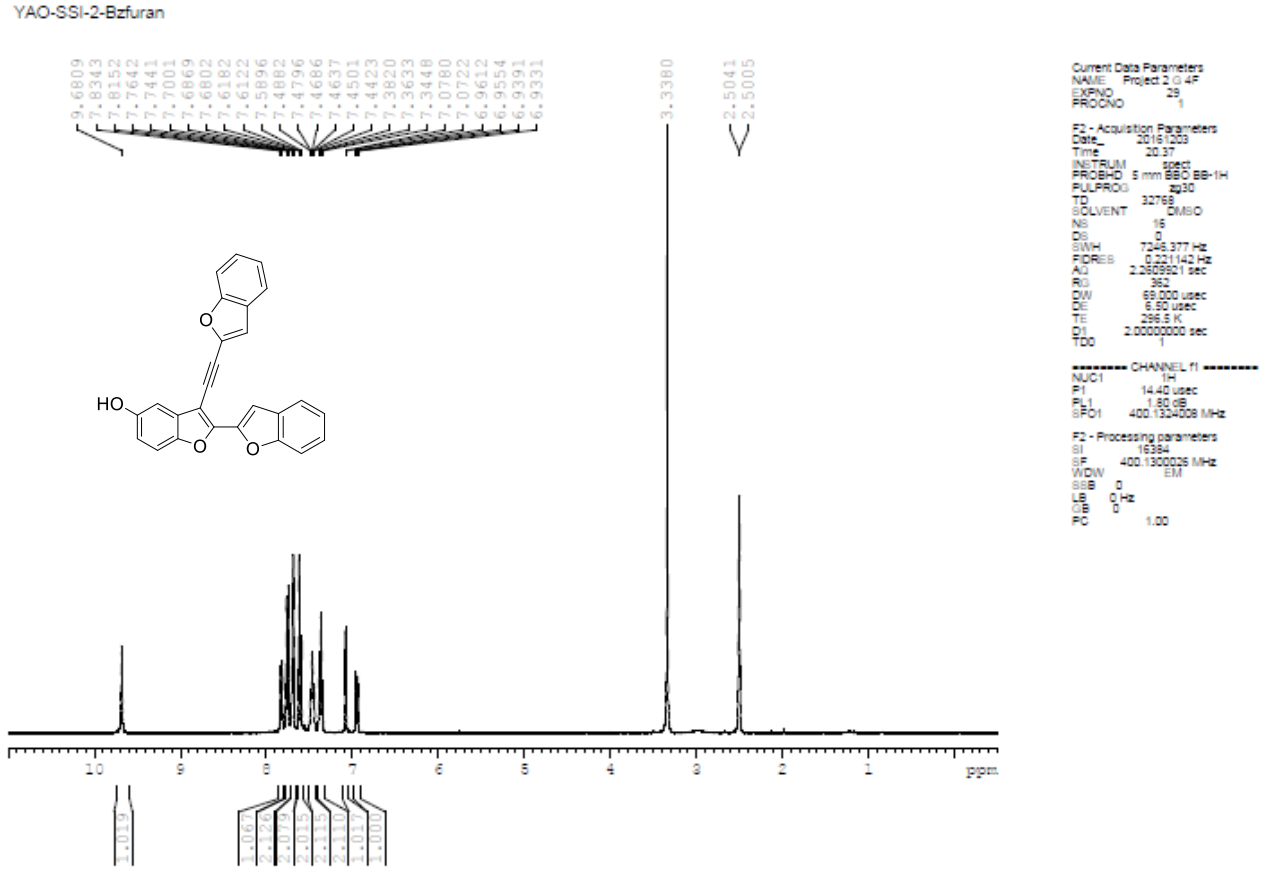
2-(thiophen-2-yl)-3-(thiophen-2-ylethynyl)benzofuran-5-ol (**3s**): ^{1}H NMR (400 MHz, $CDCl_3$)



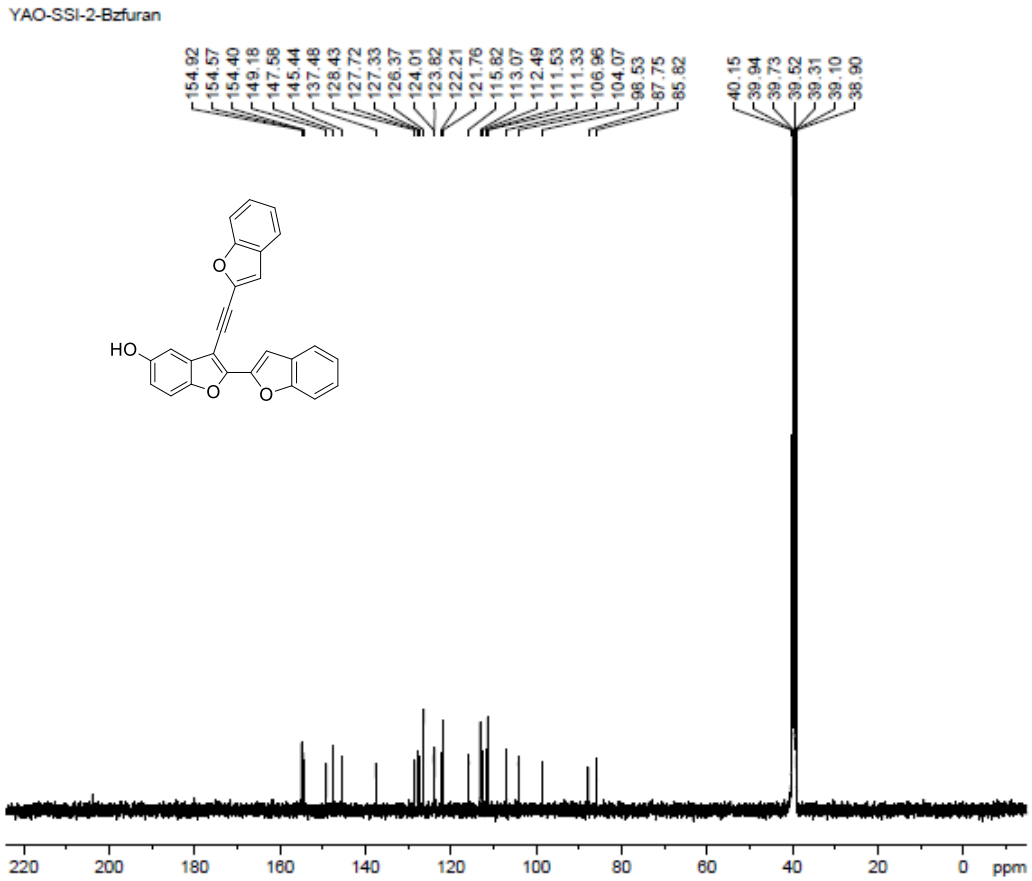
2-(thiophen-2-yl)-3-(thiophen-2-ylethynyl)benzofuran-5-ol (**3s**): ^{13}C NMR (100 MHz, $CDCl_3$)



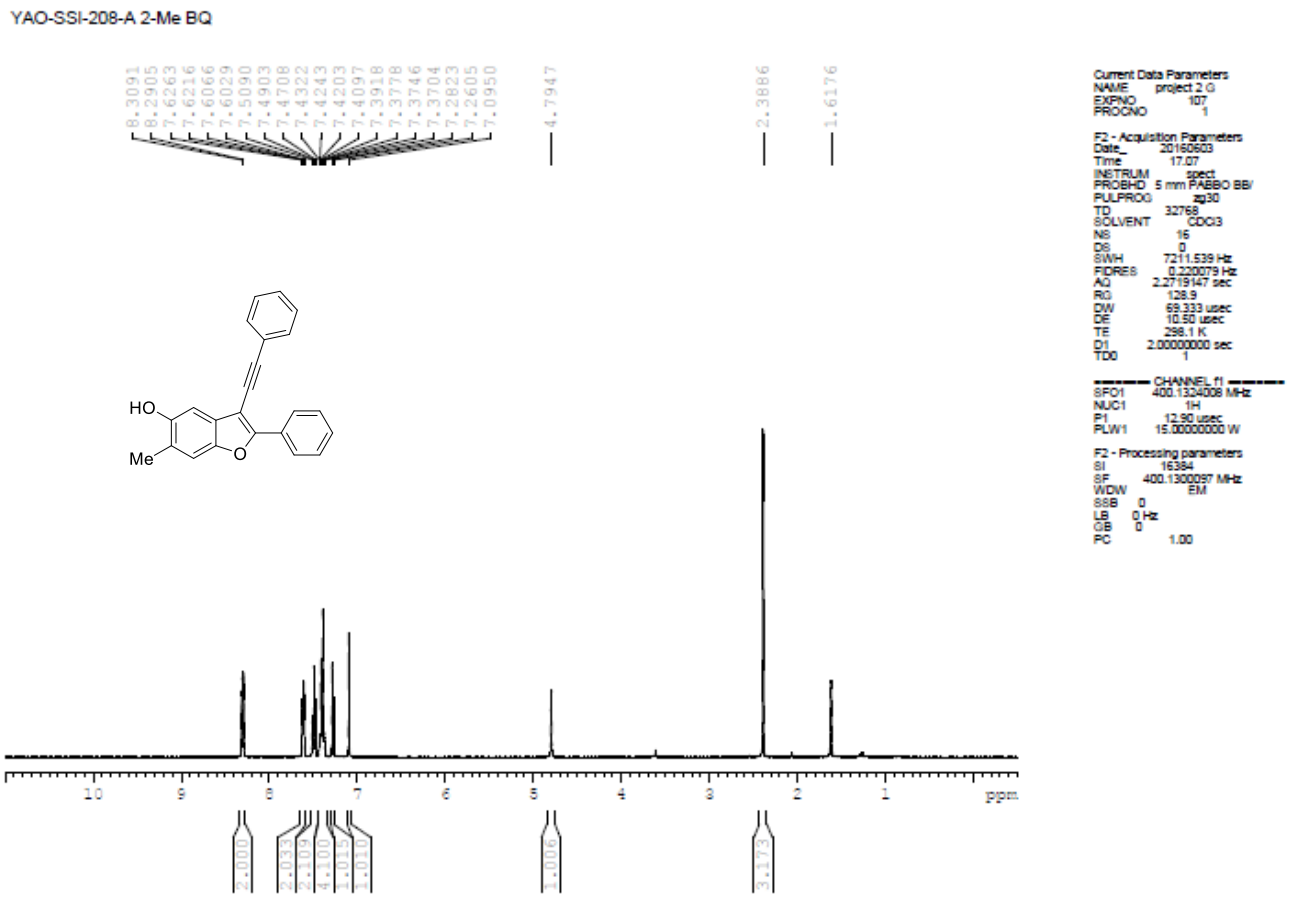
3-(benzofuran-2-ylethynyl)-[2,2'-bibenzofuran]-5-ol (**3t**): ^{1}H NMR (400 MHz, DMSO)



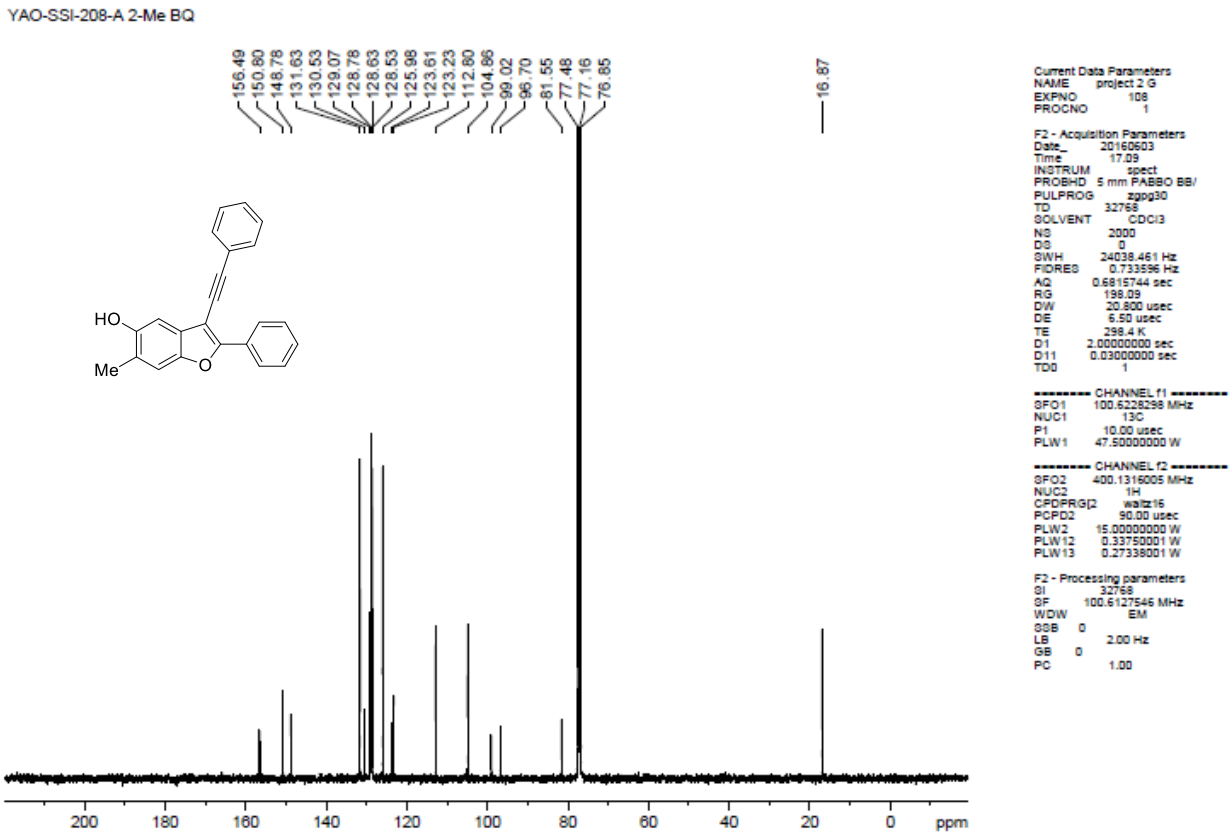
3-(benzofuran-2-ylethynyl)-[2,2'-bibenzofuran]-5-ol (**3t**): ^{13}C NMR (100 MHz, DMSO)



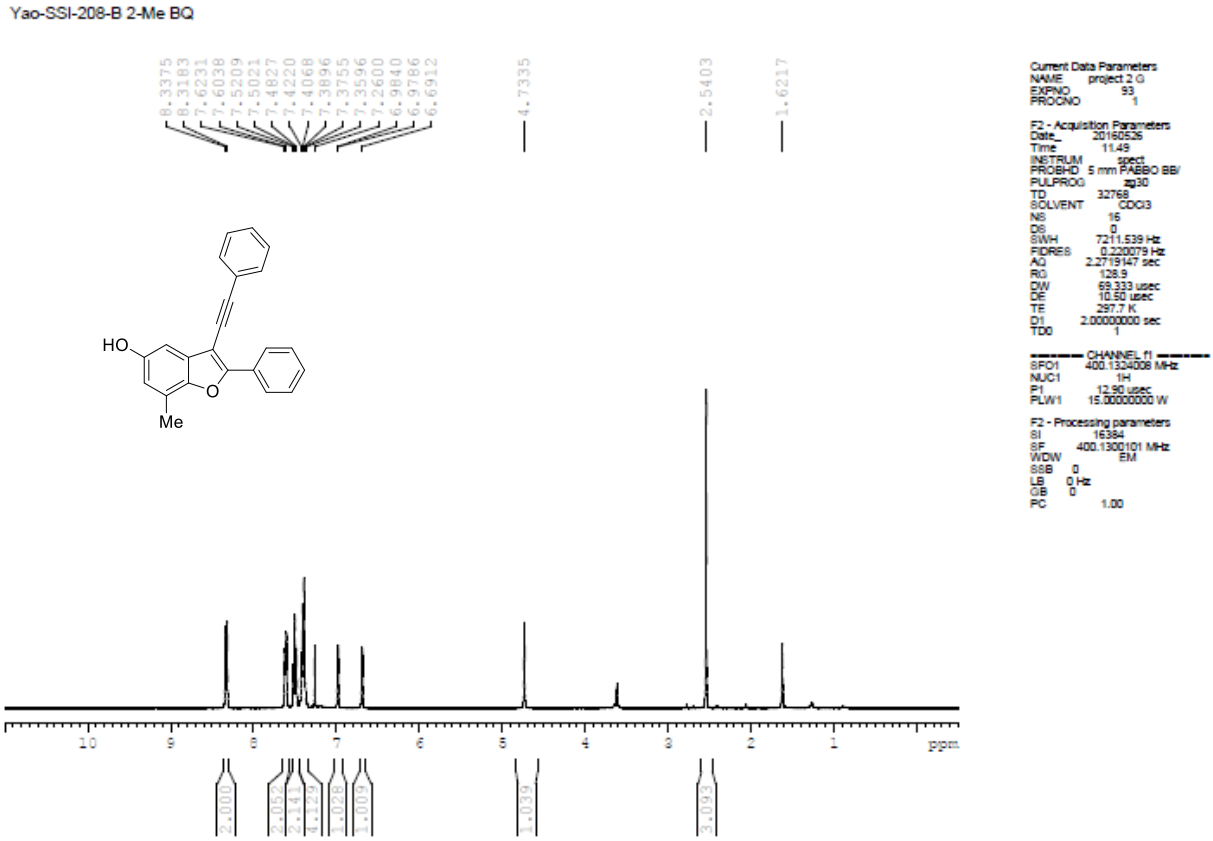
6-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**5a**): ^{1}H NMR (400 MHz, $CDCl_3$)



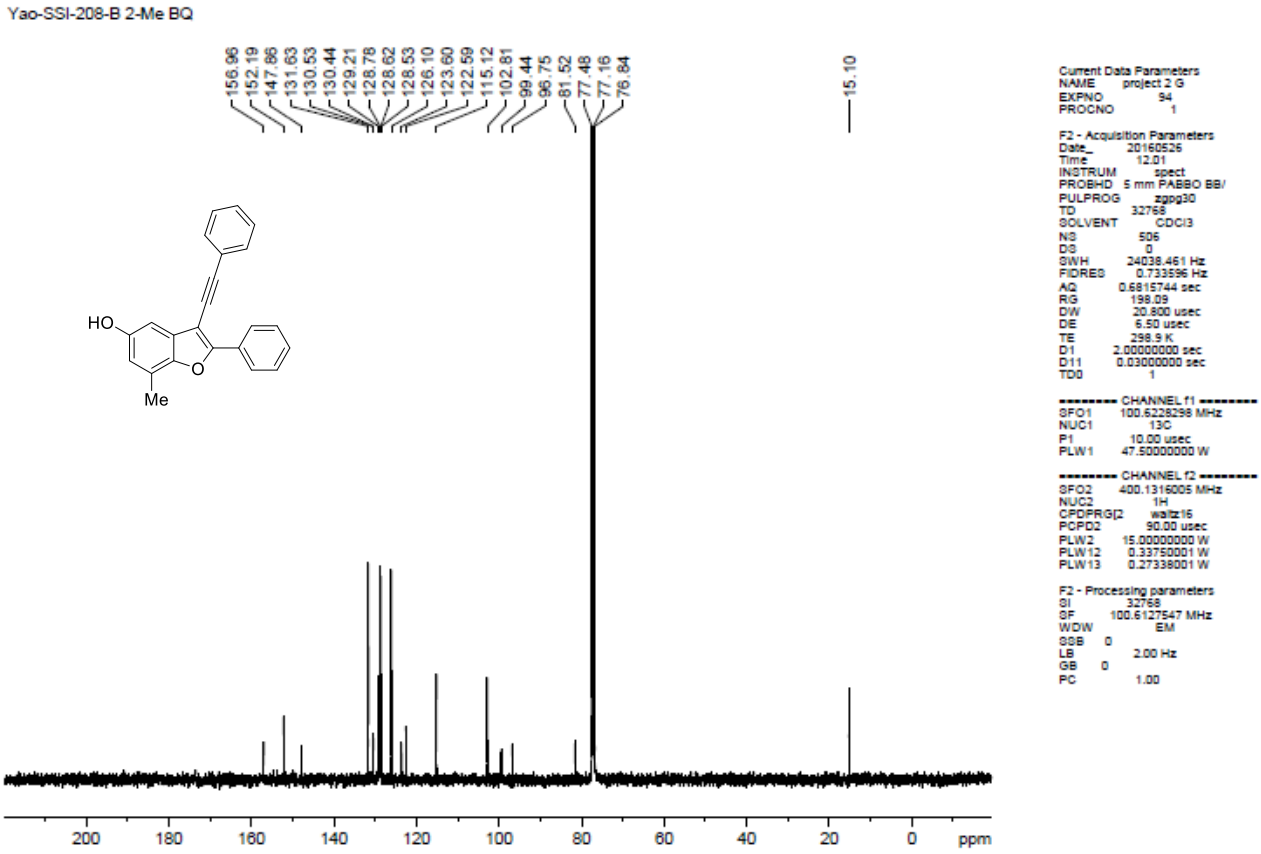
6-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**5a**): ^{13}C NMR (100 MHz, $CDCl_3$)



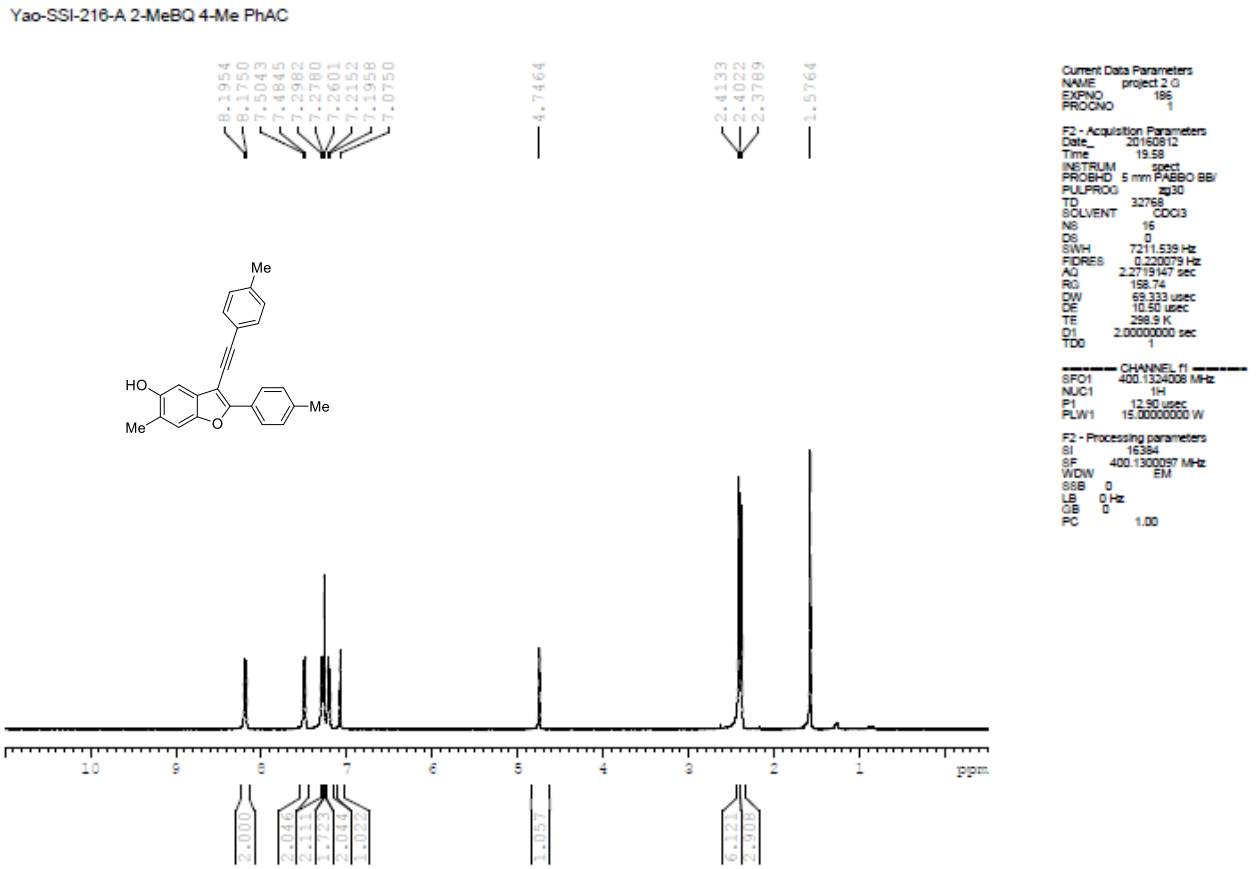
7-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**5a'**): ^{1}H NMR (400 MHz, $CDCl_3$)



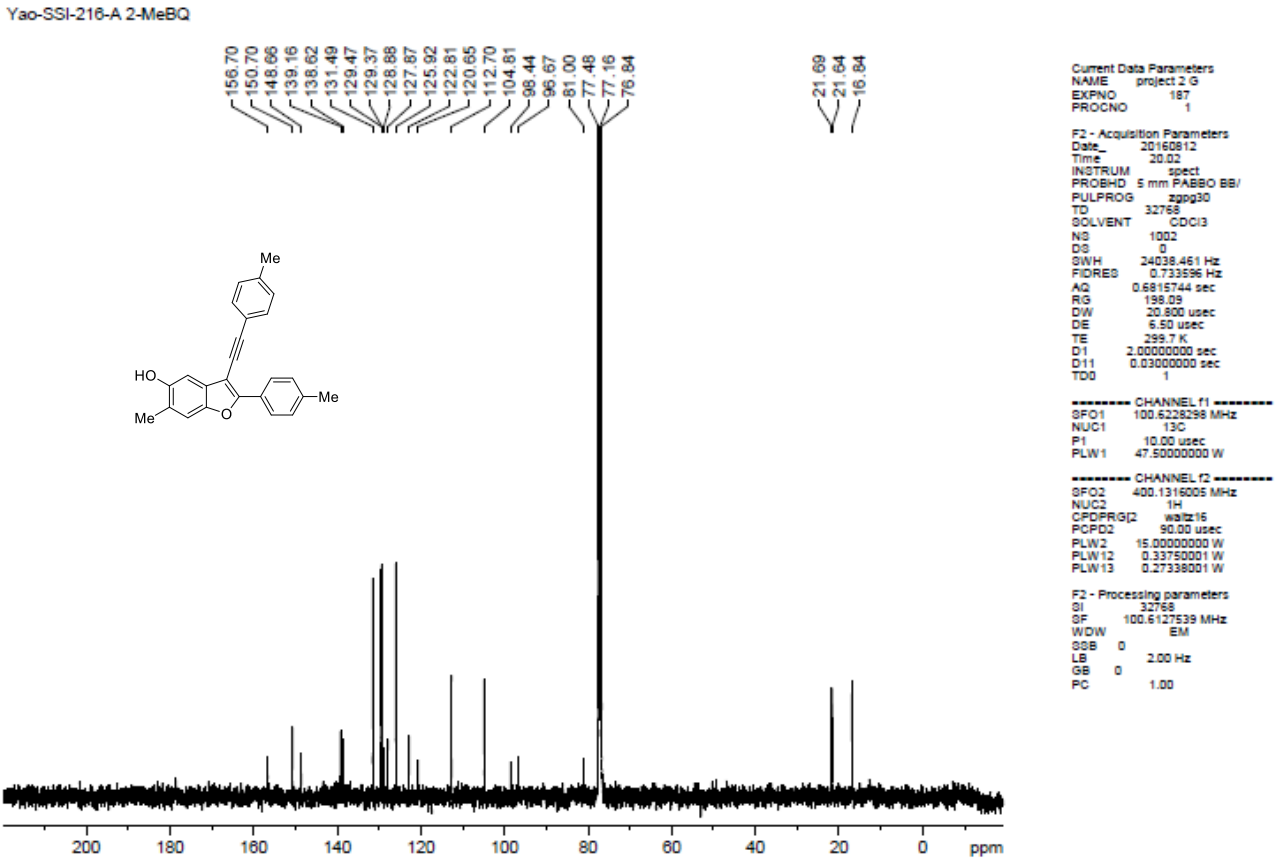
7-methyl-2-phenyl-3-(phenylethynyl)benzofuran-5-ol (**5a'**) ^{13}C NMR (100 MHz, $CDCl_3$)



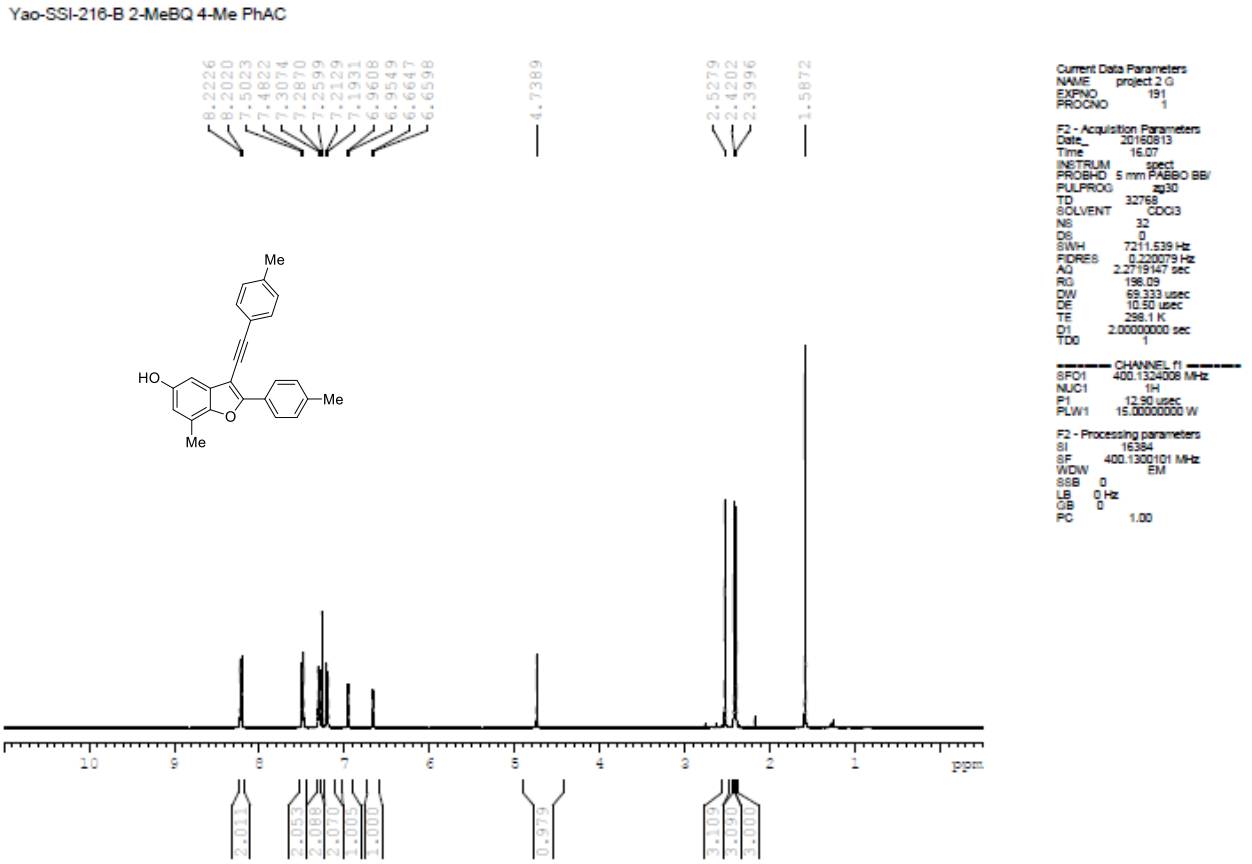
6-methyl-2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**5b**): ^{1}H NMR (400 MHz, $CDCl_3$)



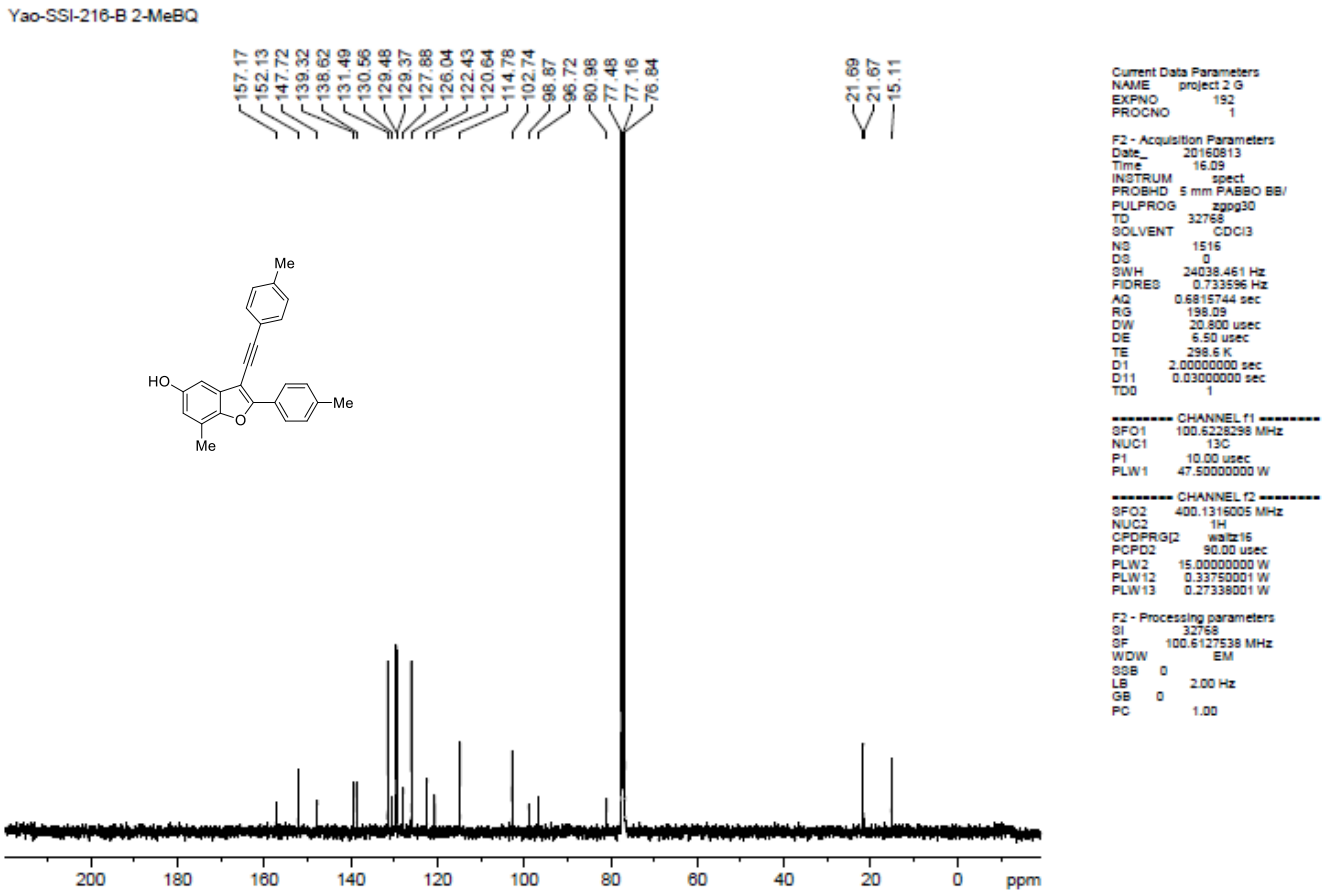
6-methyl-2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**5b**): ^{13}C NMR (100 MHz, $CDCl_3$)



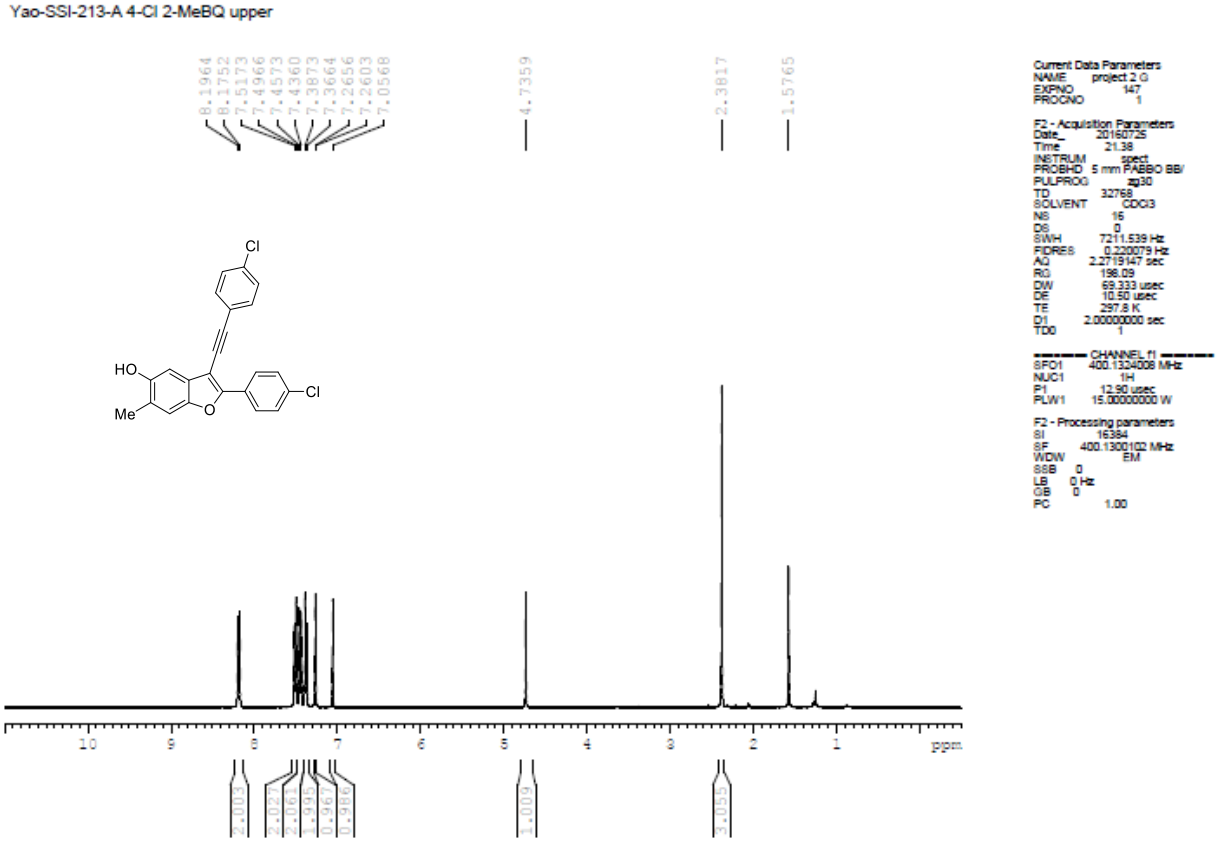
7-methyl-2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**5b'**): ^{1}H NMR (400 MHz, $CDCl_3$)



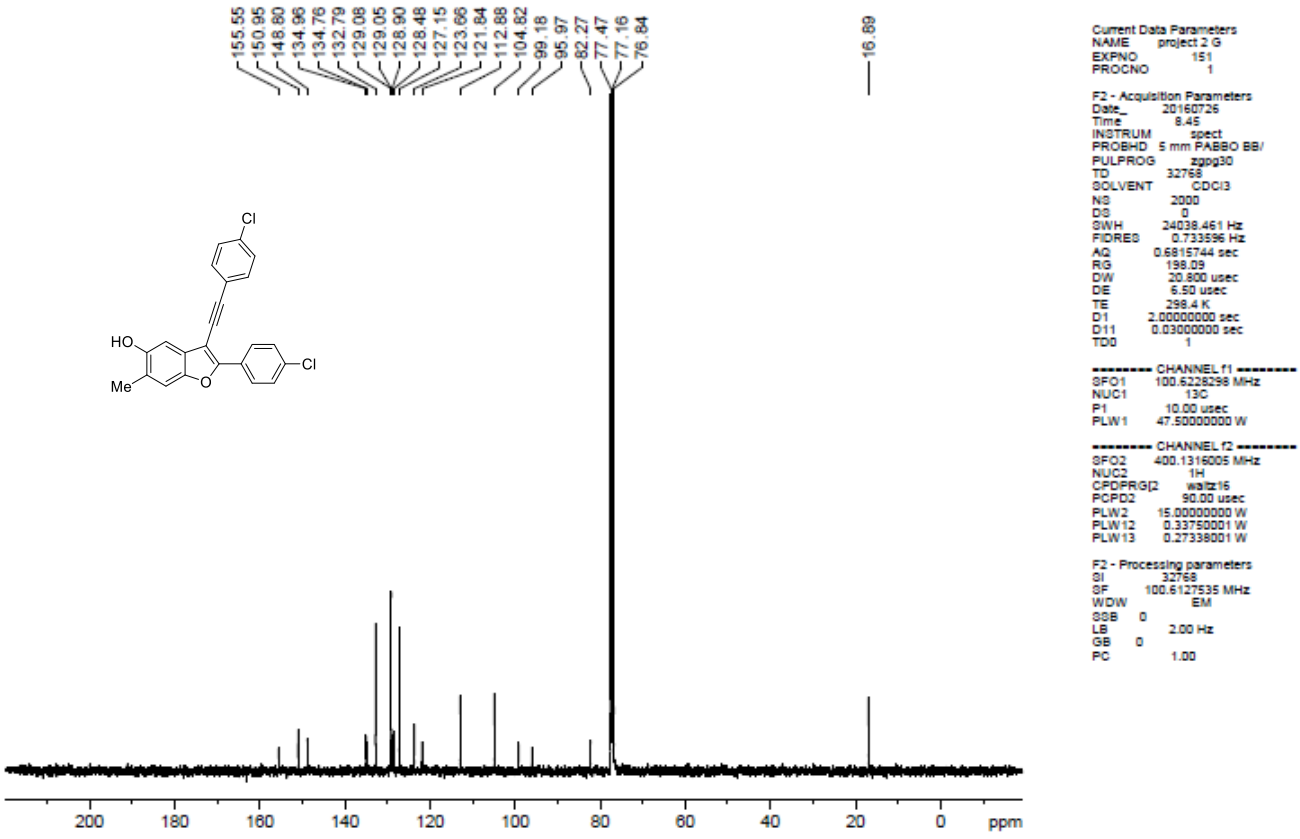
7-methyl-2-(p-tolyl)-3-(p-tolylethynyl)benzofuran-5-ol (**5b'**): ^{13}C NMR (100 MHz, $CDCl_3$)



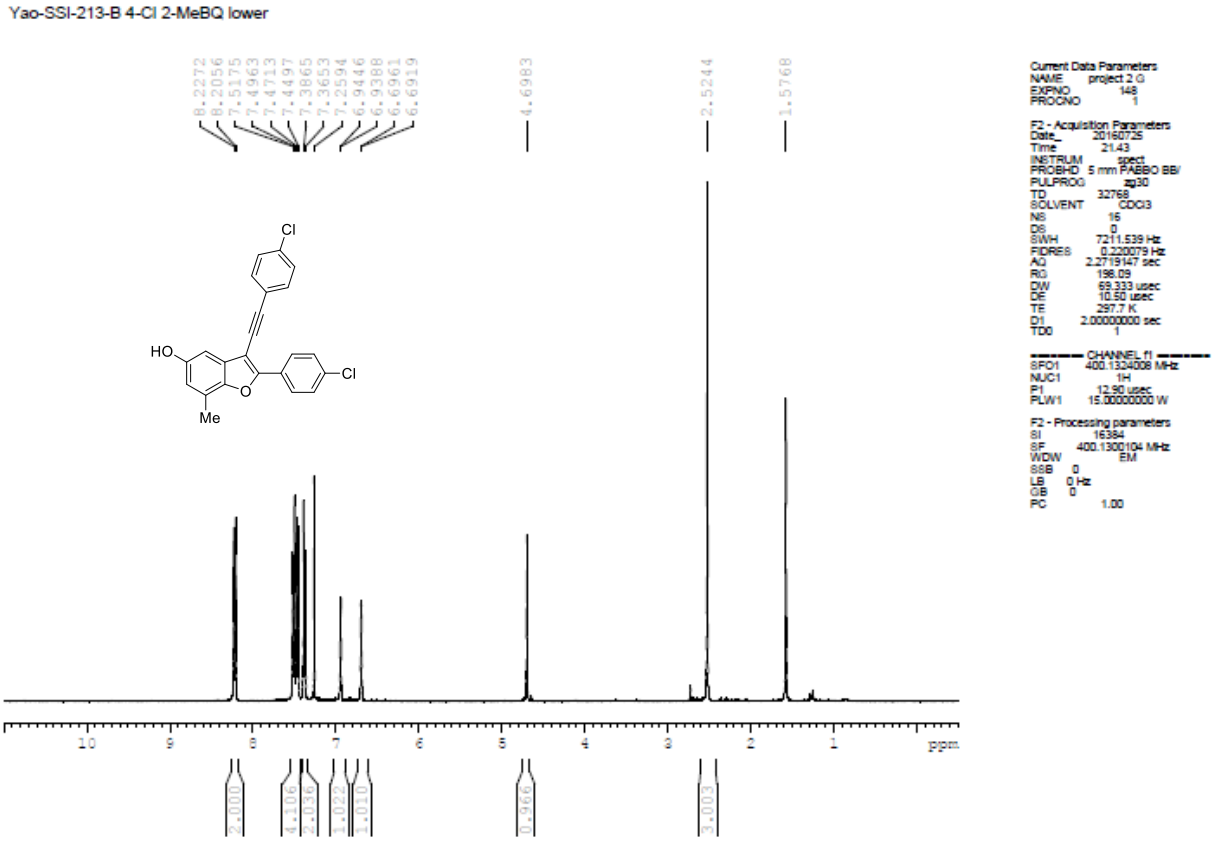
2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)-6-methylbenzofuran-5-ol (**5c**): ^{1}H NMR (400 MHz, $CDCl_3$)



2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)-6-methylbenzofuran-5-ol (**5c**): ^{13}C NMR (100 MHz, $CDCl_3$)



2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)-7-methylbenzofuran-5-ol (**5c'**): ^{1}H NMR (400 MHz, $CDCl_3$)



2-(4-chlorophenyl)-3-((4-chlorophenyl)ethynyl)-7-methylbenzofuran-5-ol (**5c'**): ^{13}C NMR (100 MHz, $CDCl_3$)