Unusual participation of *O*-propargyl group during cyclization of 6-hydroxy-2-propargyl ethers of aryl chalcones: One-pot synthesis of 2-acyl-3-styrylbenzofuran and 7-aryldibenzo[*b,d*]furan-1,7-diols

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Content

4. Scanned copies of spectra (^{1}H and ^{13}C NMR, DEPT-135, FTIR, HRMS)

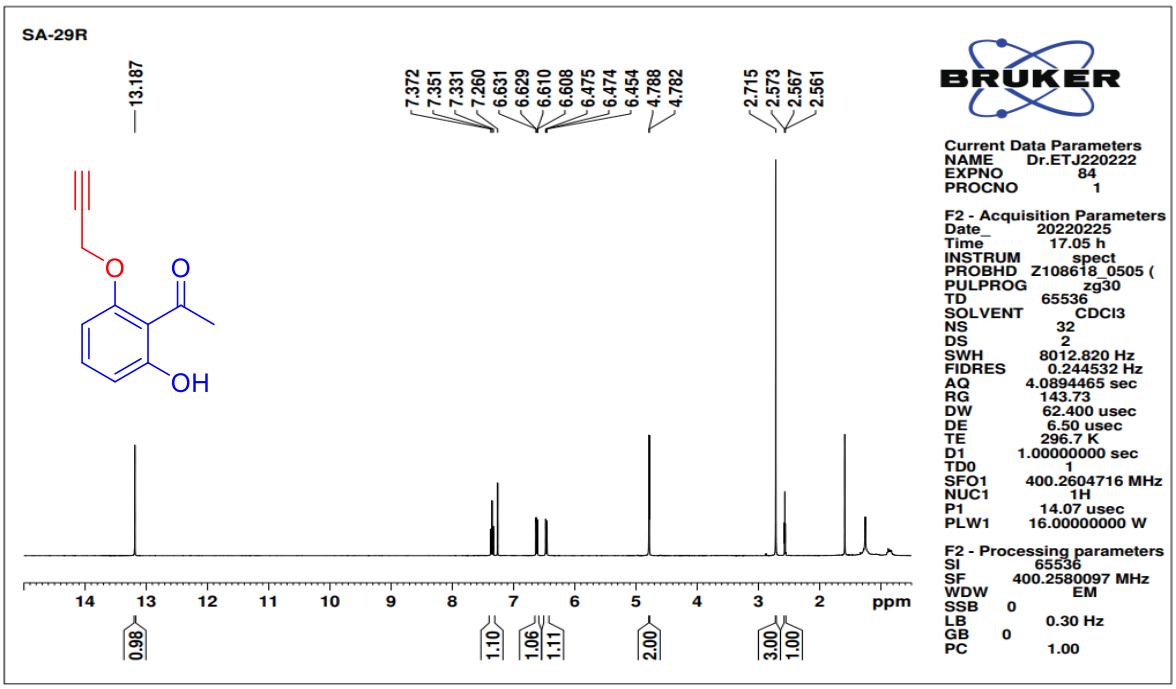


Figure 1: ^{1}H NMR spectrum of compound **3**

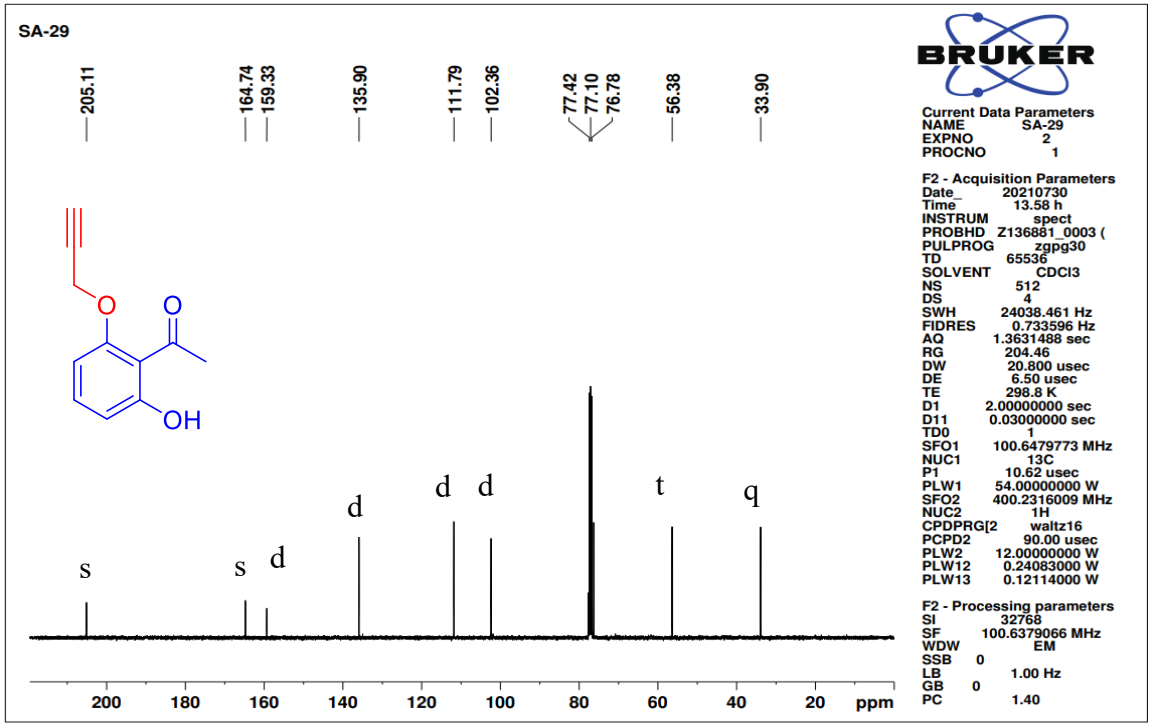


Figure 2: ^{13}C NMR spectrum of compound **3**

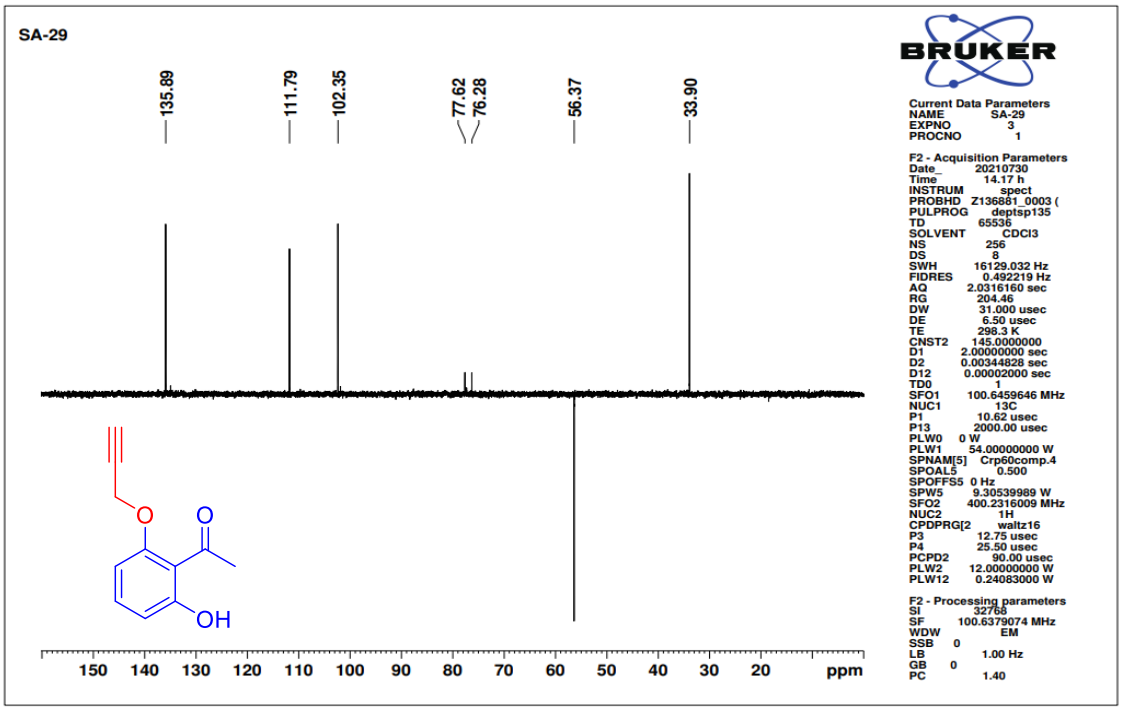


Figure 3: DEPT-135 NMR spectrum of compound **3**

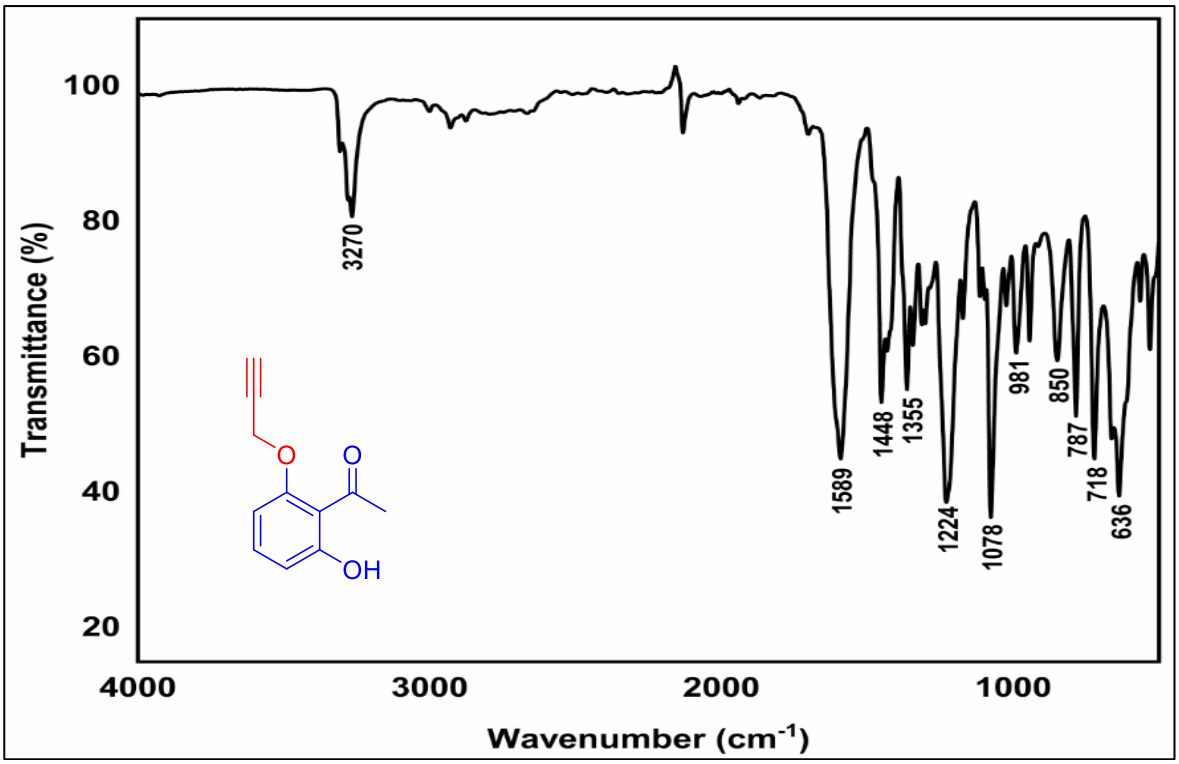


Figure 4: FT-IR spectrum of compound **3**

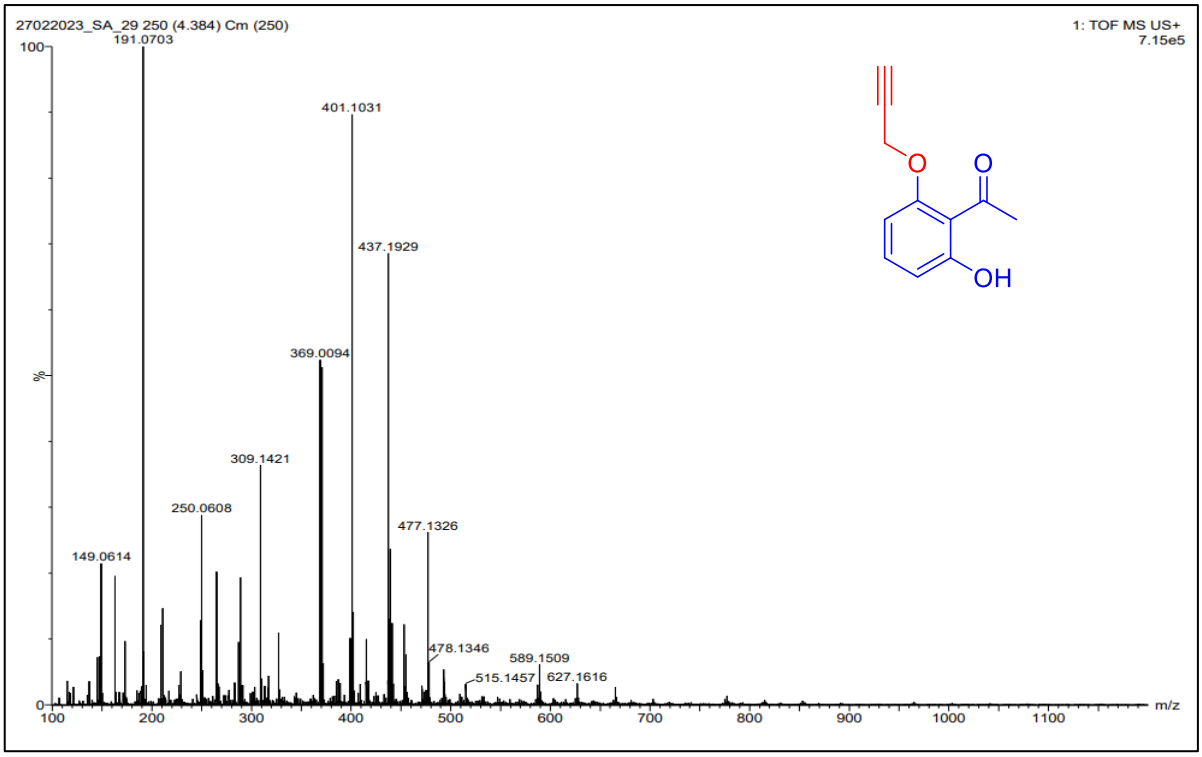


Figure 5: HRMS spectrum of compound **3**

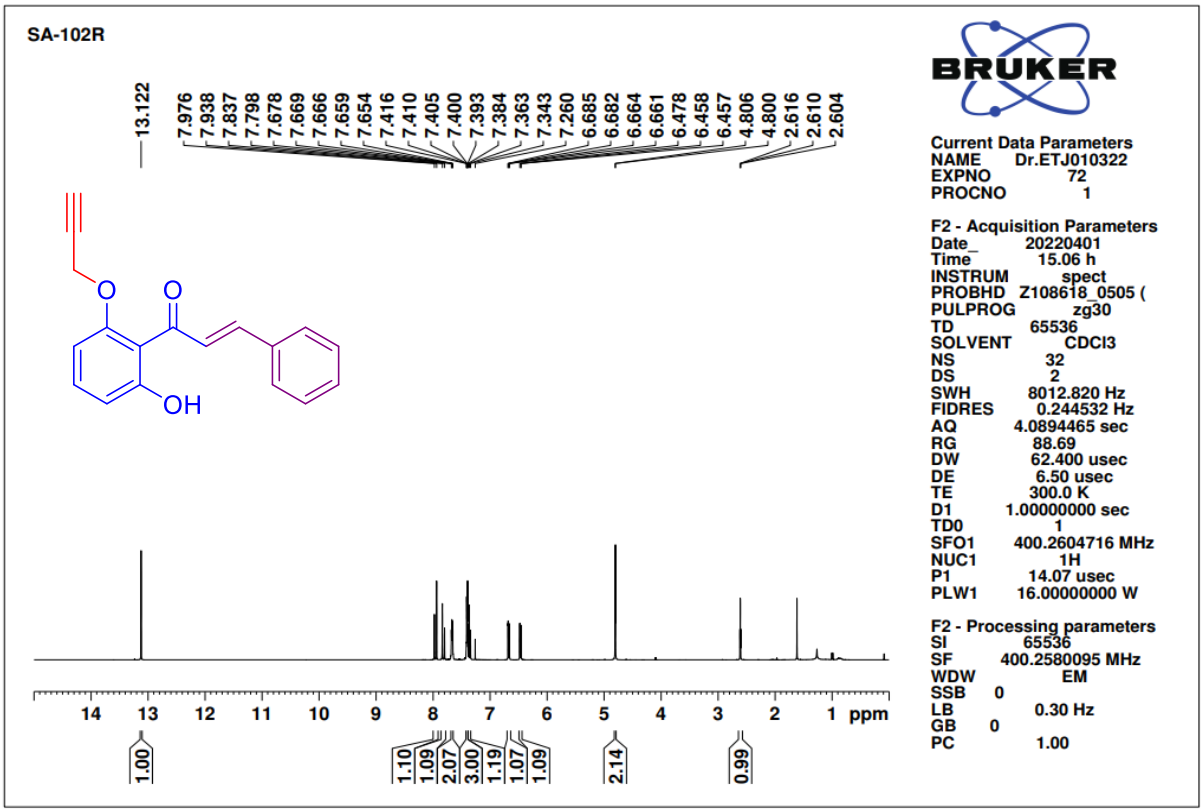


Figure 6: ^{1}H NMR spectrum of compound **5a**

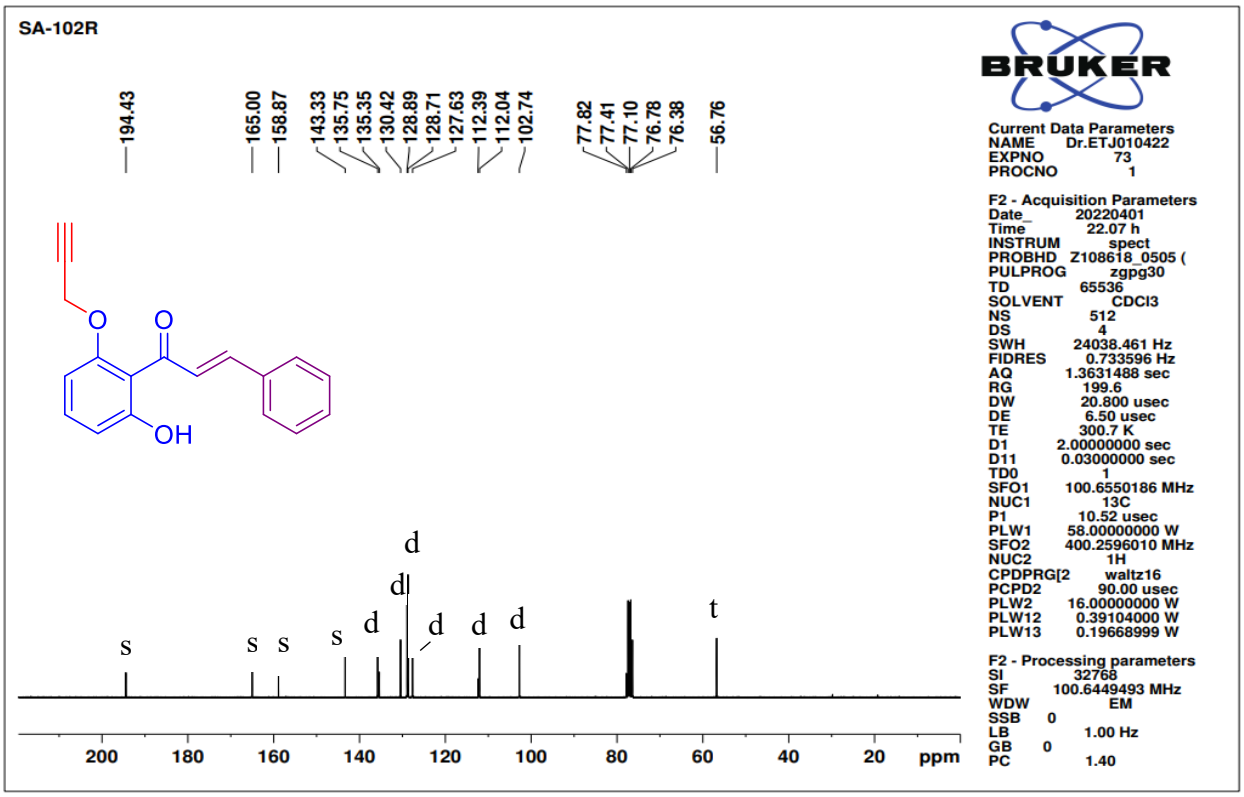


Figure 7: ^{13}C NMR spectrum of compound **5a**

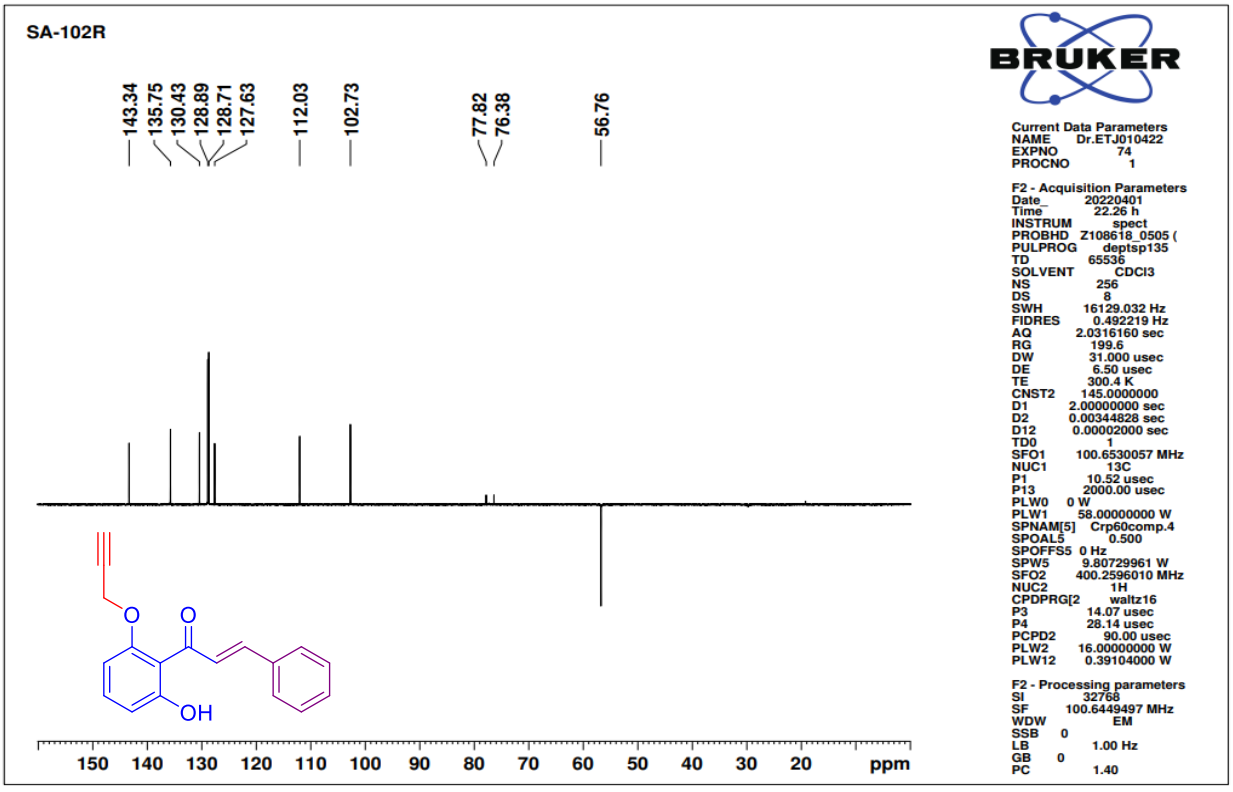


Figure 8: DEPT-135 NMR spectrum of compound **5a**

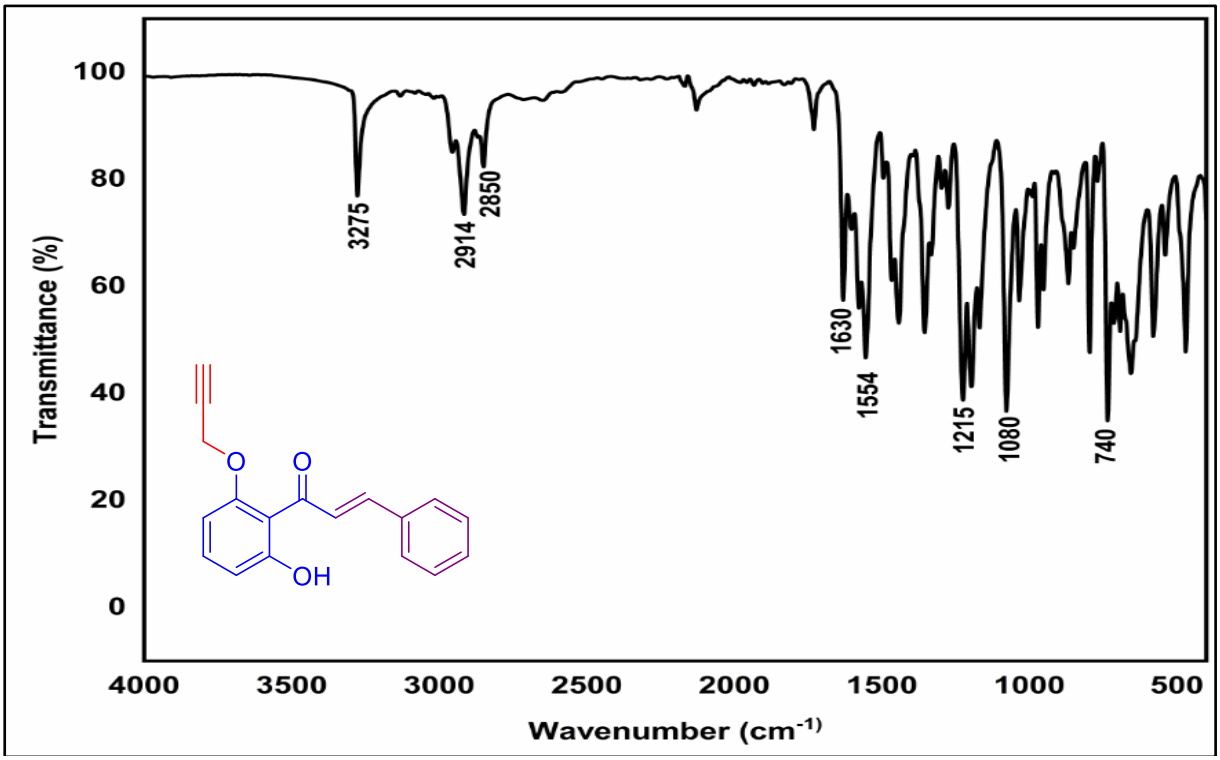


Figure 9: FT-IR spectrum of compound **5a**

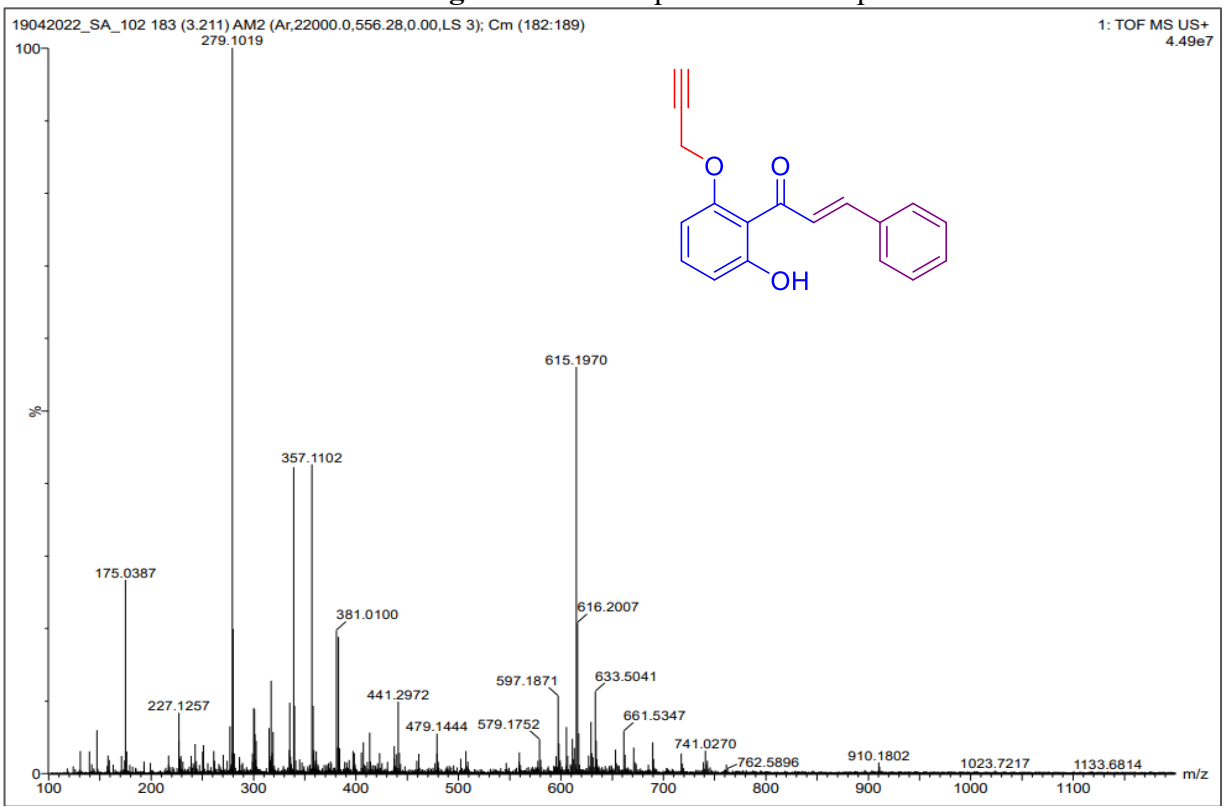


Figure 10: HRMS spectrum of compound **5a**

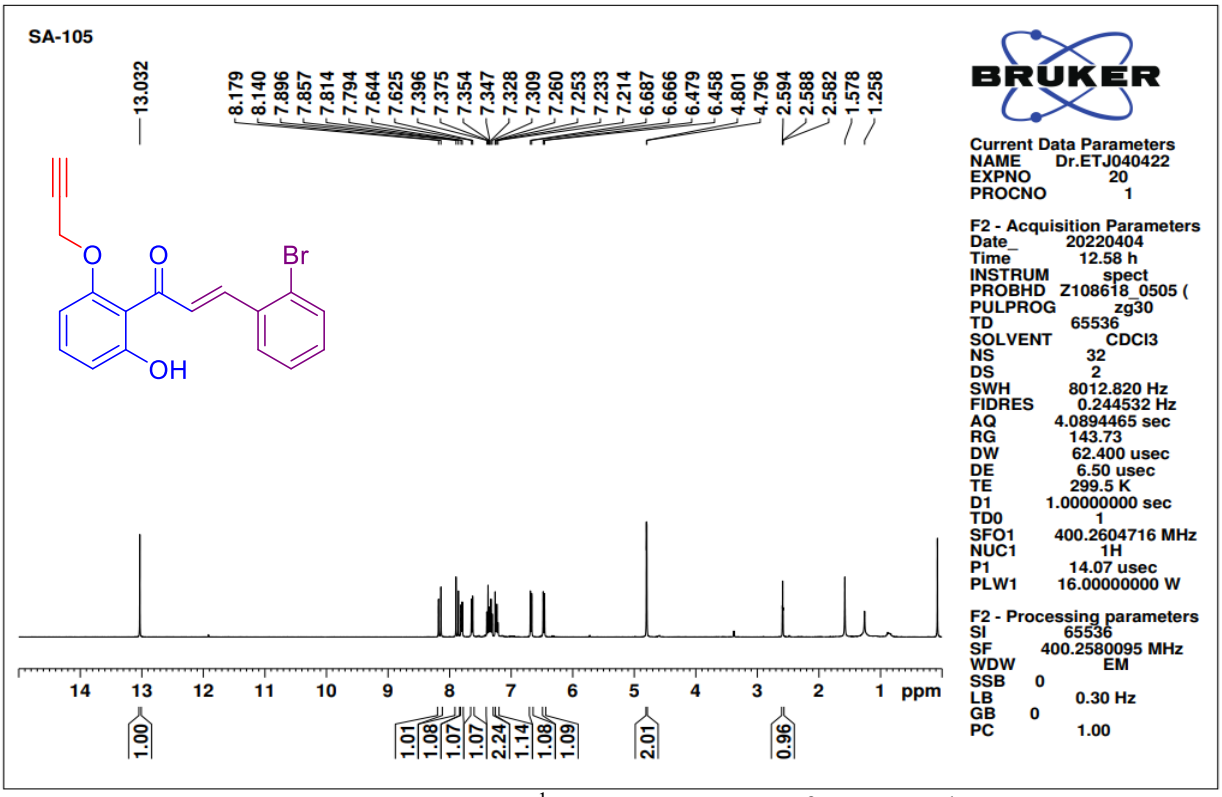


Figure 11: ^{1}H NMR spectrum of compound **5b**

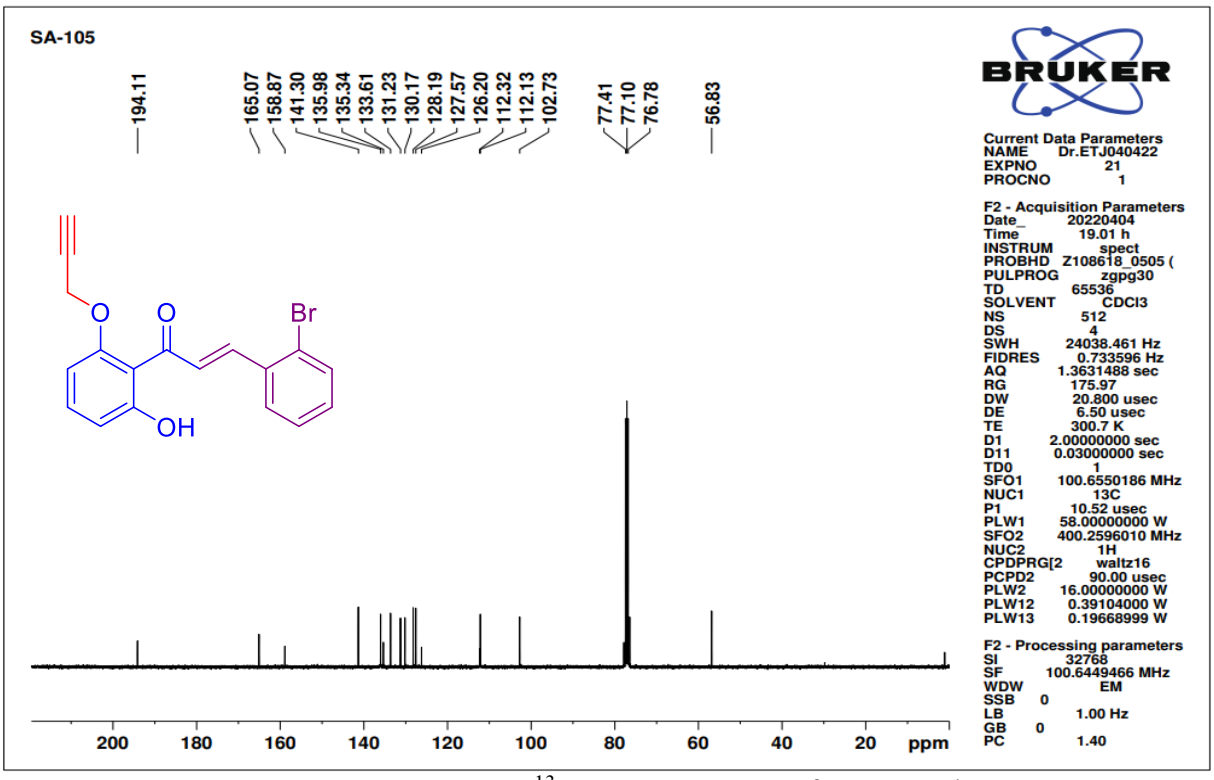


Figure 12: ^{13}C NMR spectrum of compound **5b**

Figure 13: DEPT-135 NMR spectrum of compound **5b**

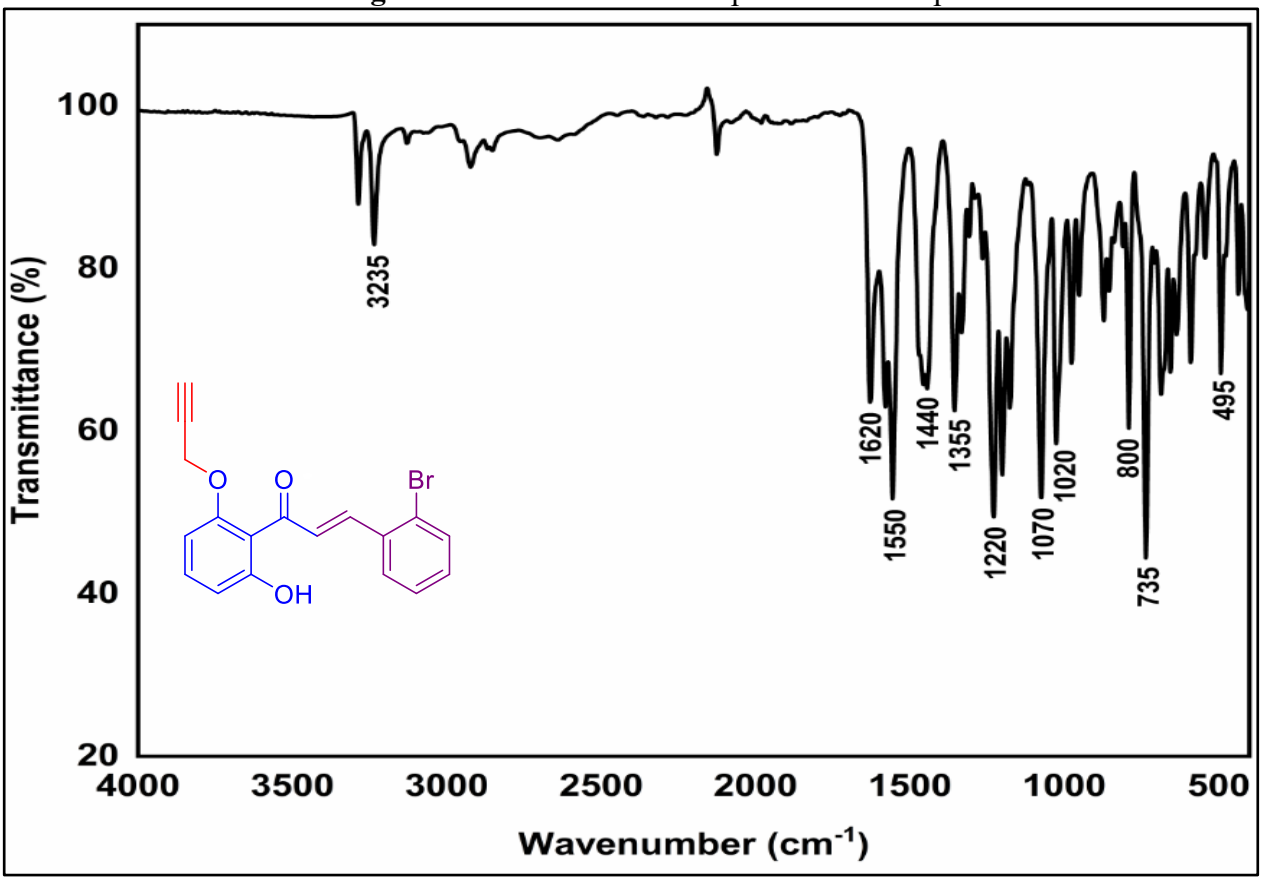


Figure 14: FT-IR spectrum of compound **5b**

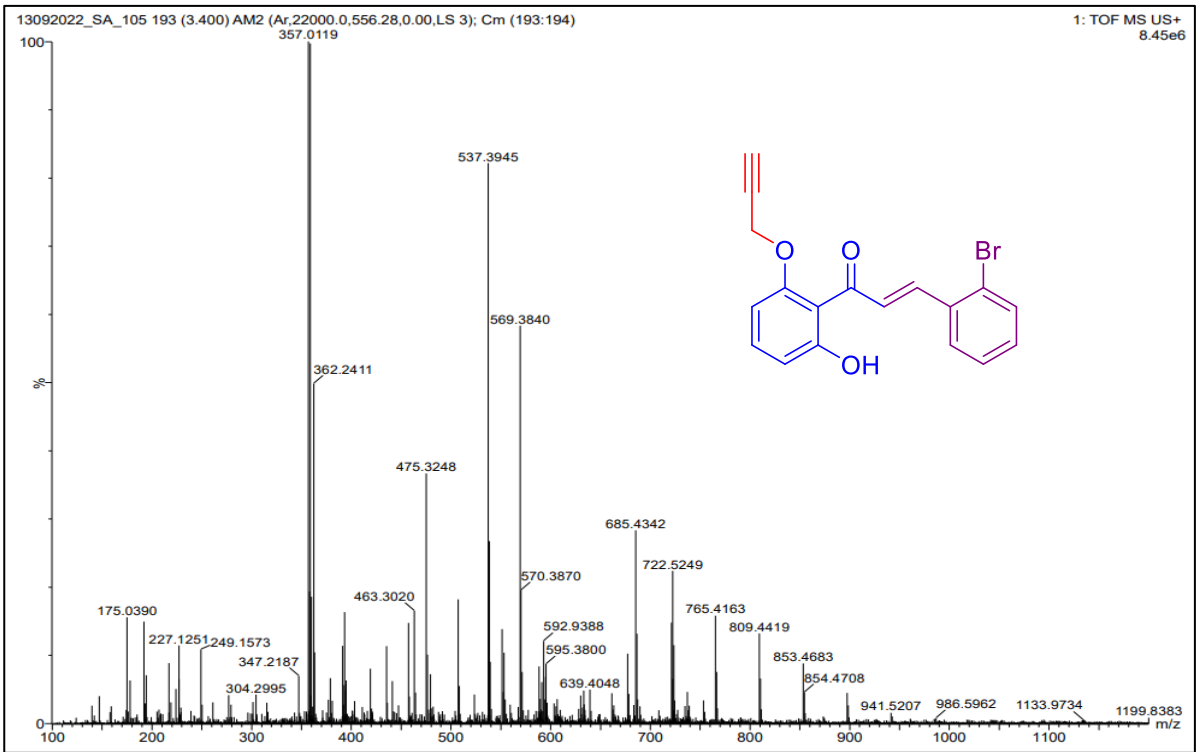


Figure 15: HRMS spectrum of compound **5b**

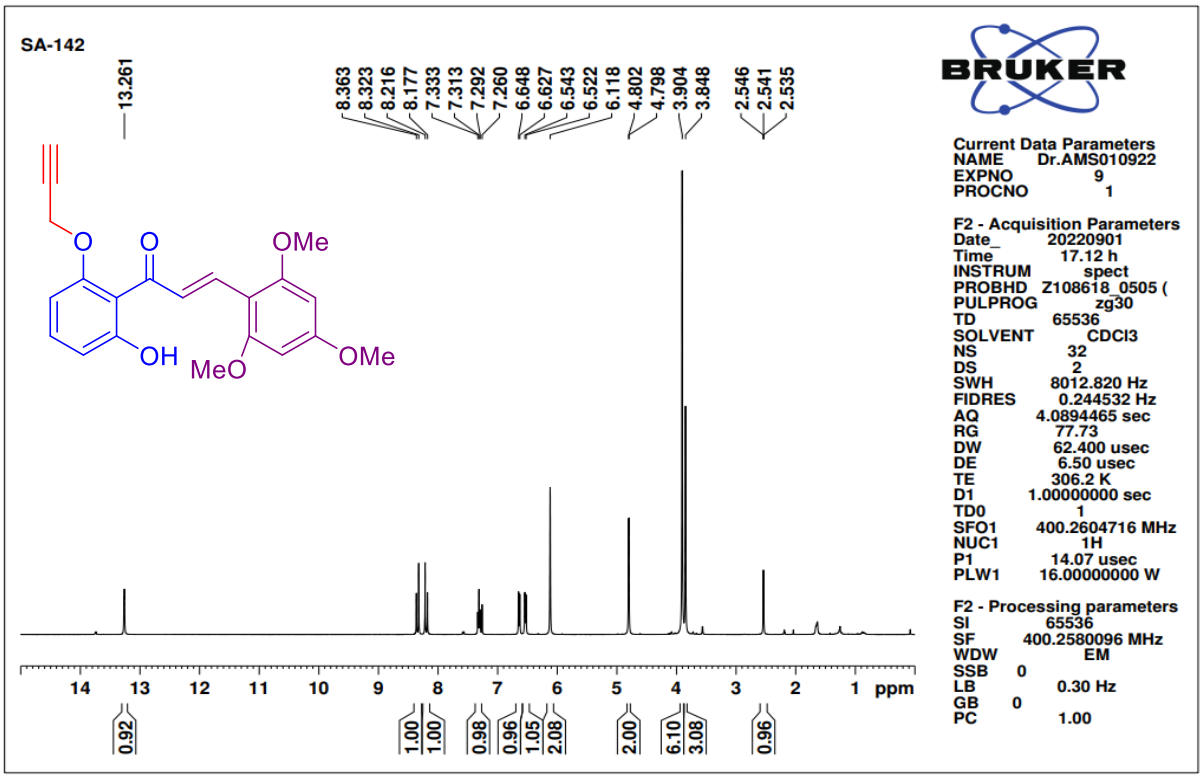


Figure 16: ^{1}H NMR spectrum of compound **5c**

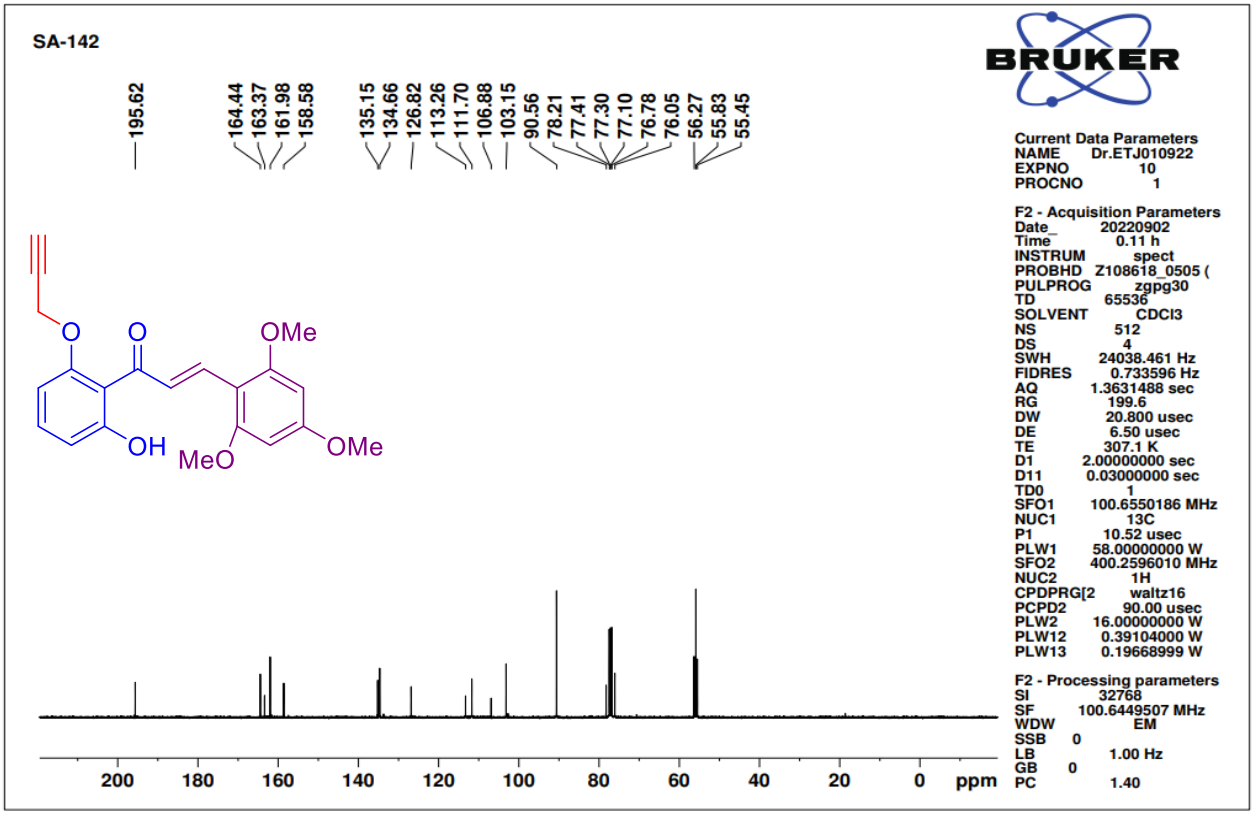


Figure 17: ^{13}C NMR spectrum of compound **5c**

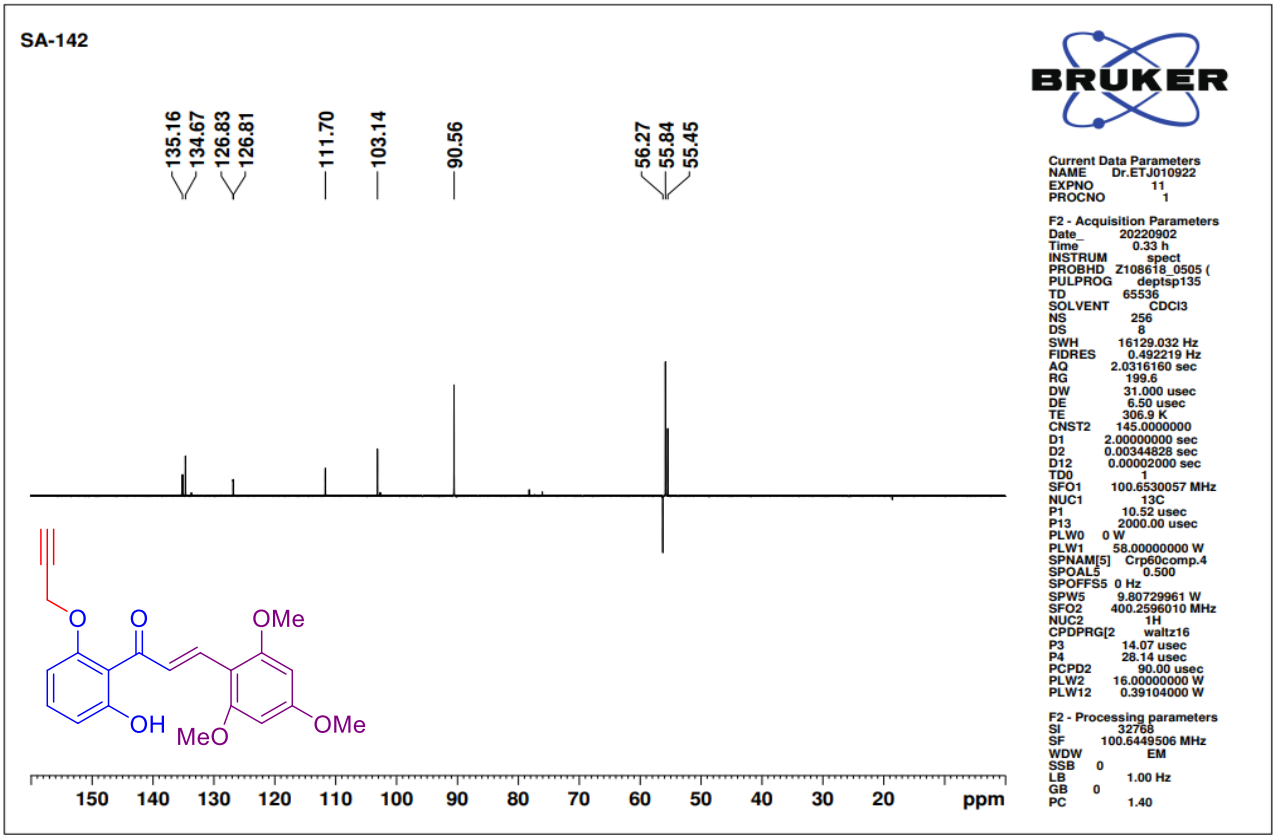


Figure 18: DEPT-135 NMR spectrum of compound **5c**

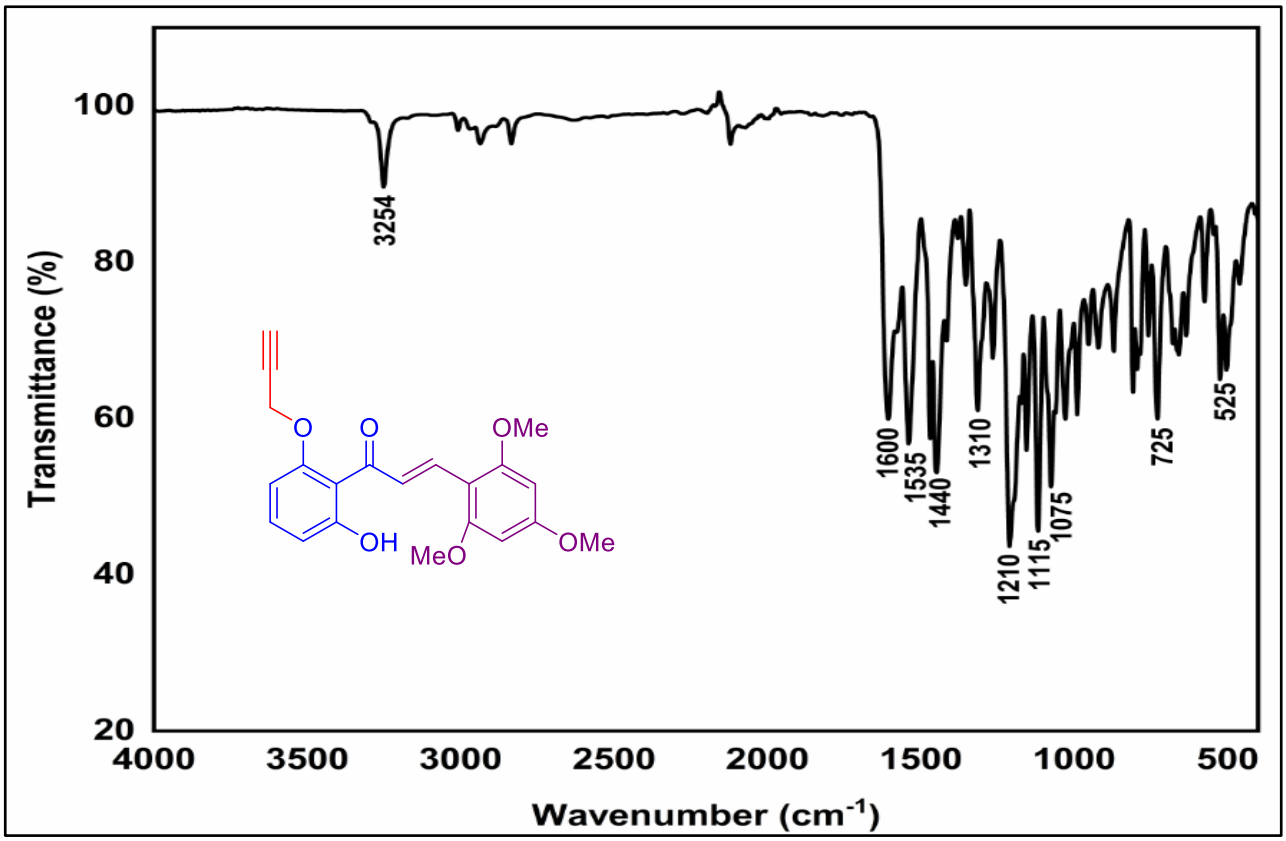


Figure 19: FT-IR spectrum of compound **5c**

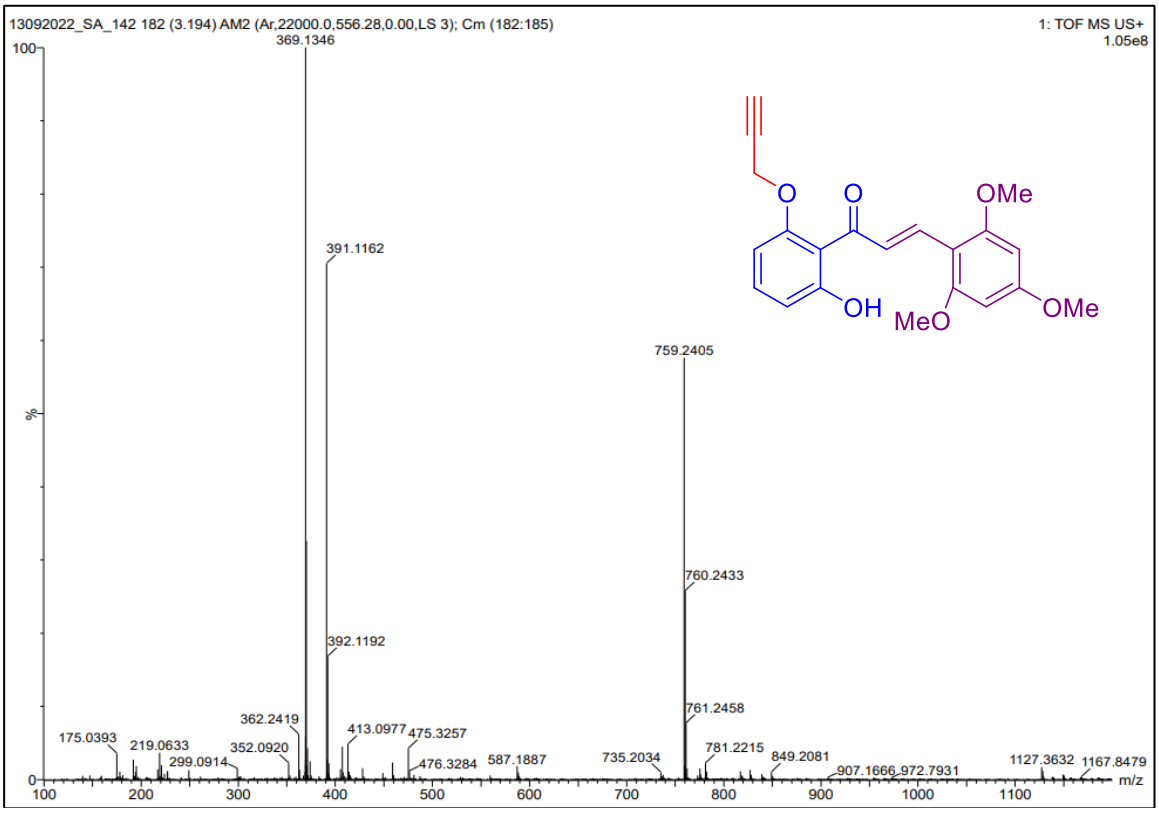


Figure 20: HRMS spectrum of compound **5c**

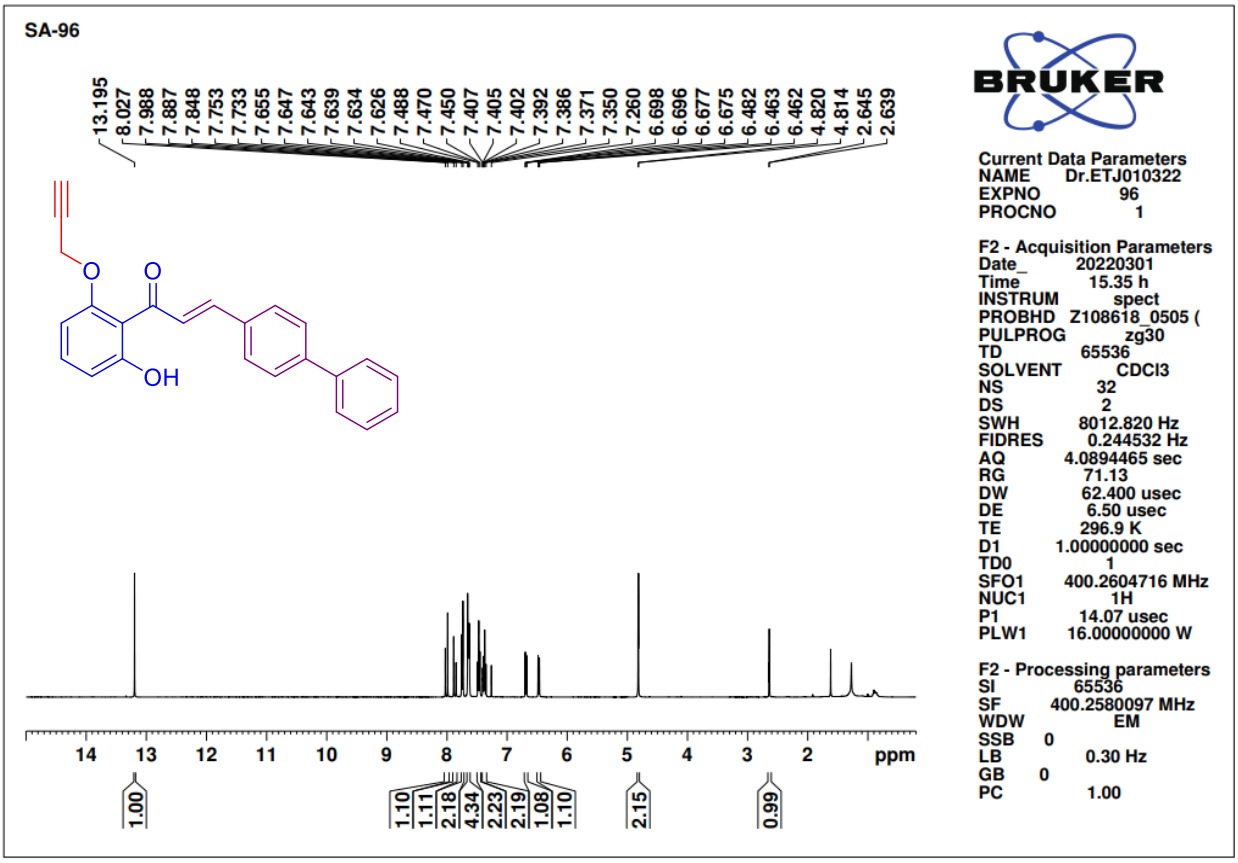


Figure 21: ^{1}H NMR spectrum of compound **5d**

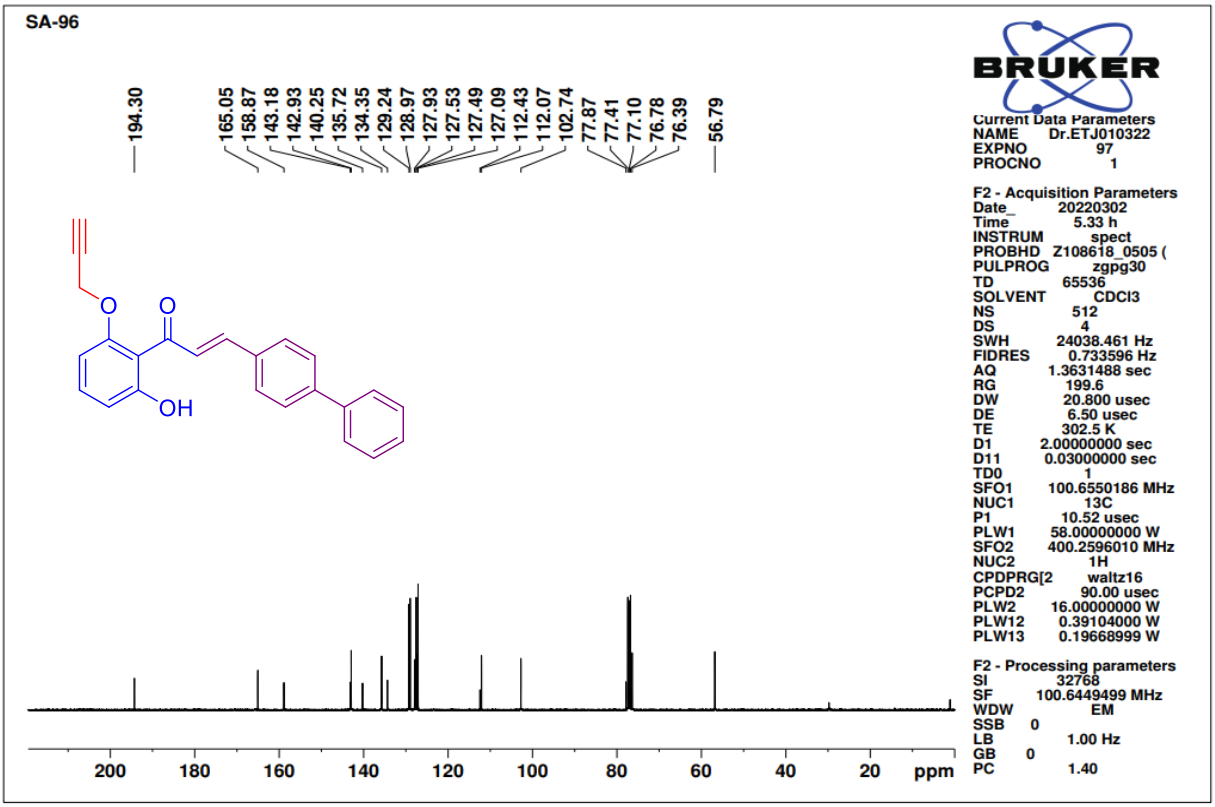


Figure 22: ^{13}C NMR spectrum of compound **5d**

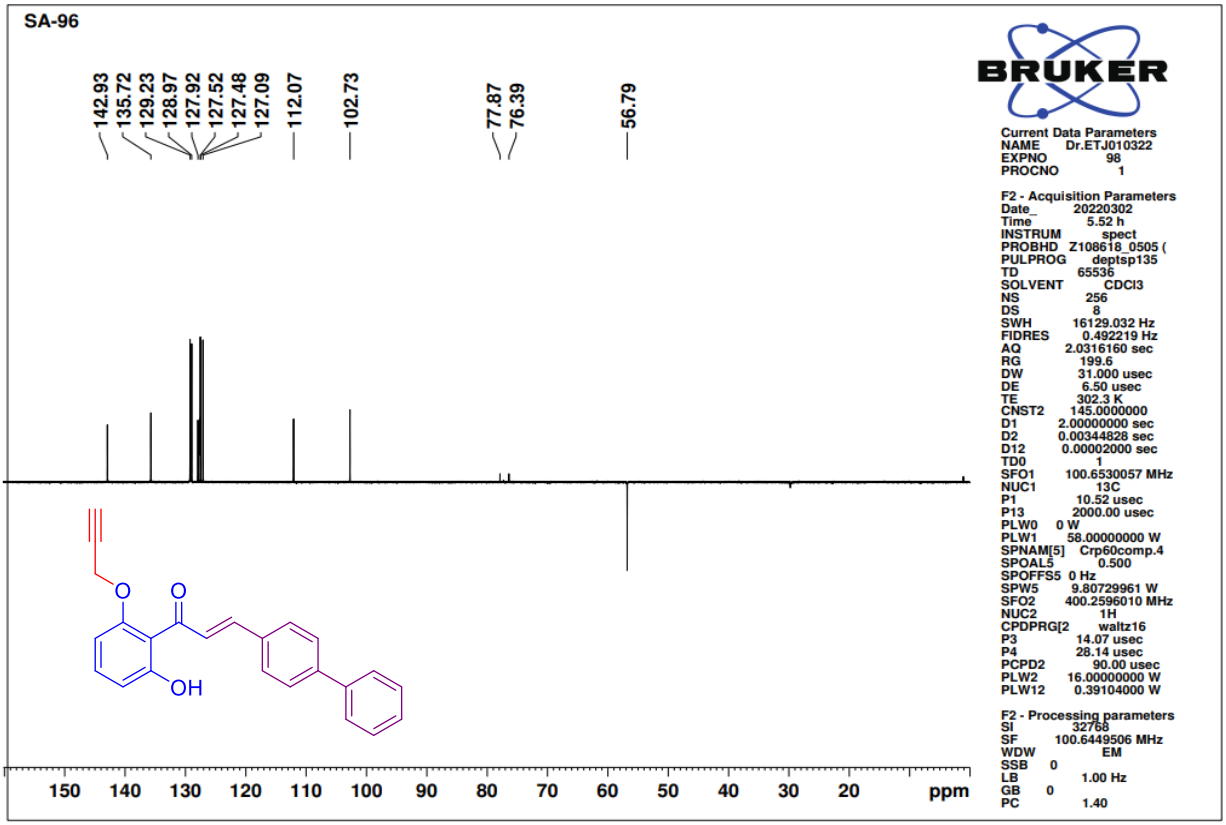


Figure 23: DEPT-135 NMR spectrum of compound **5d**

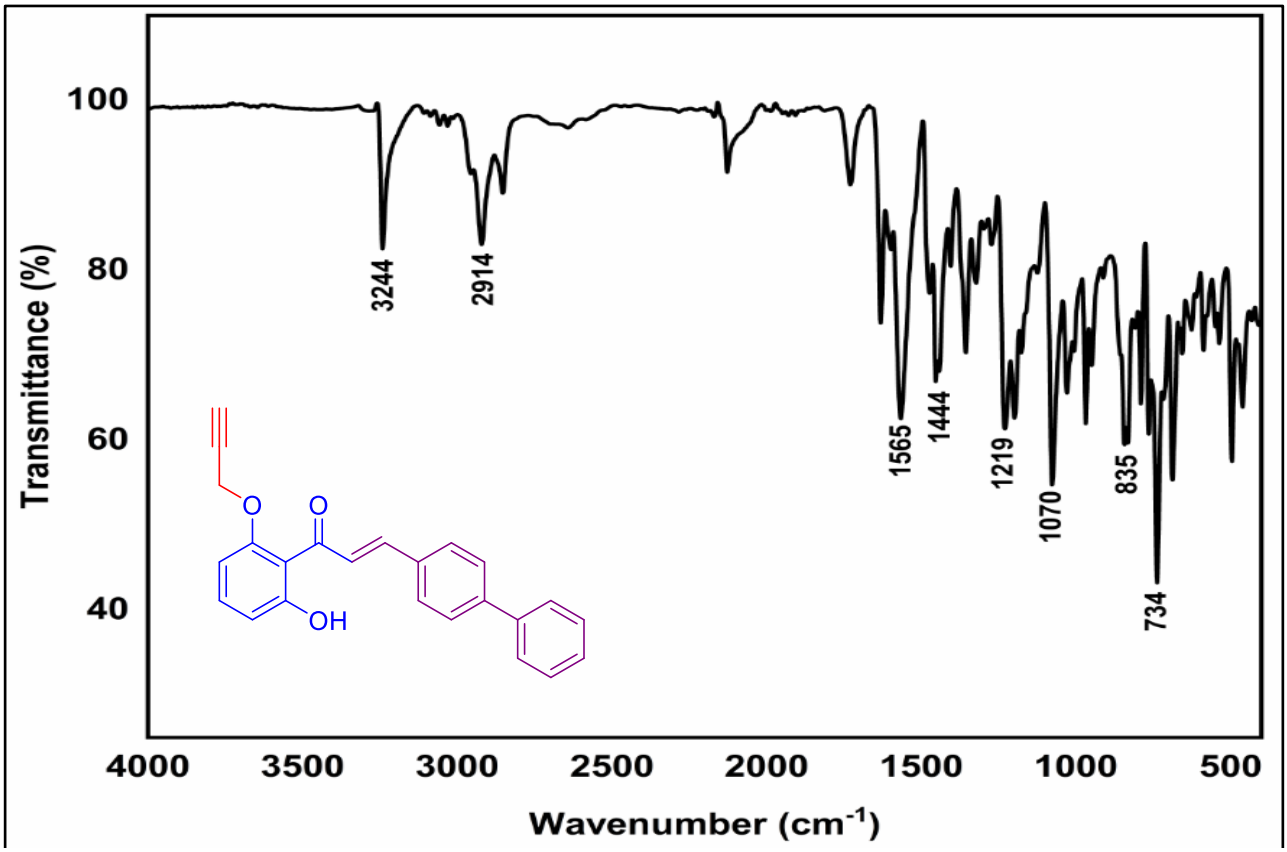


Figure 24: FT-IR spectrum of compound **5d**

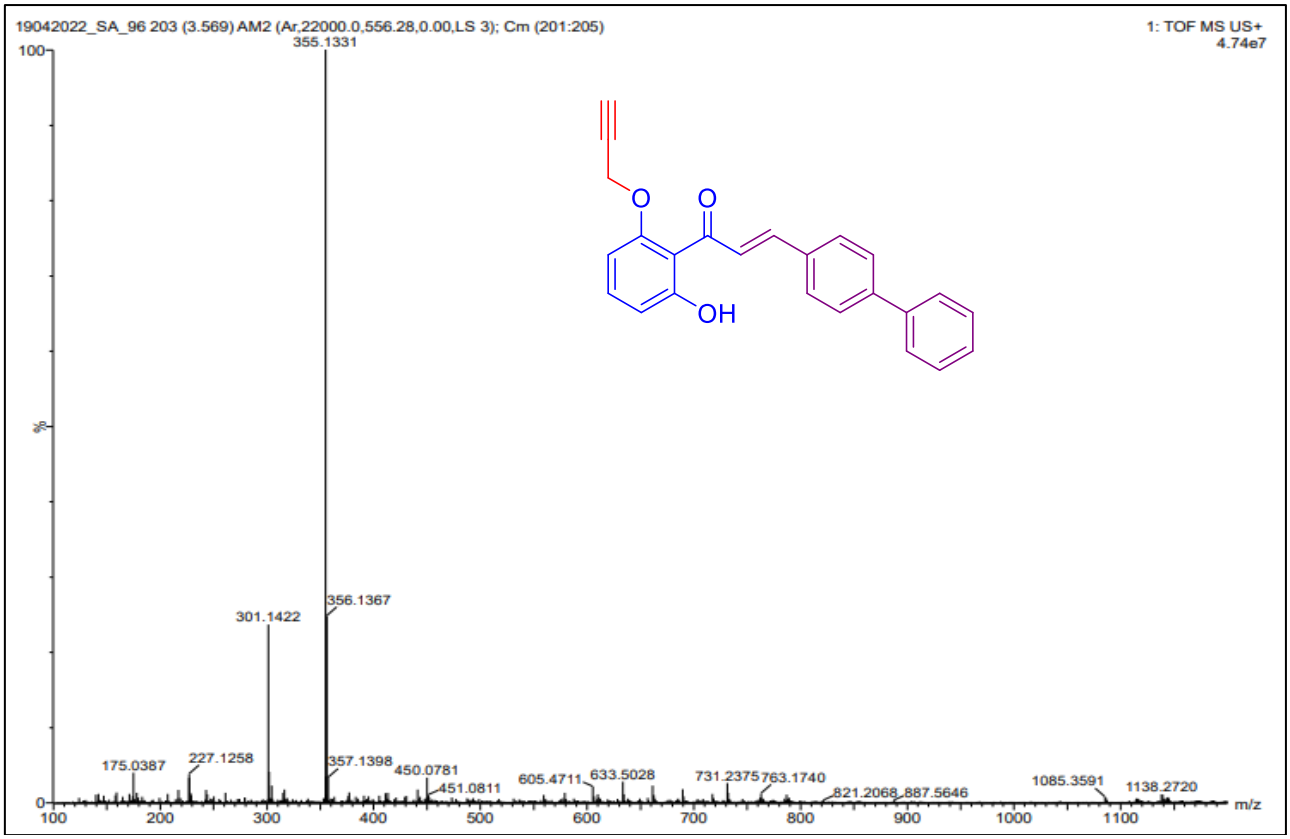


Figure 25: HRMS spectrum of compound **5d**

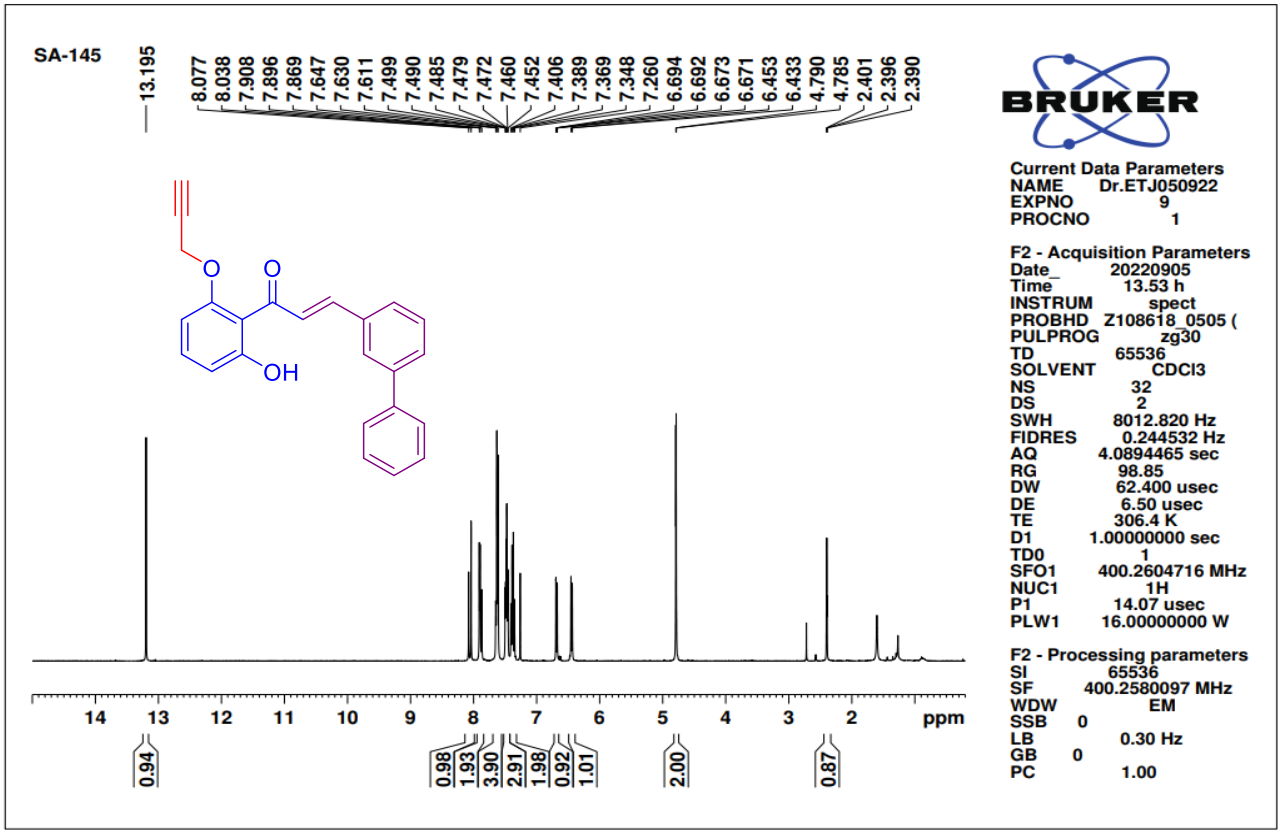


Figure 26: ^{1}H NMR spectrum of compound **5e**

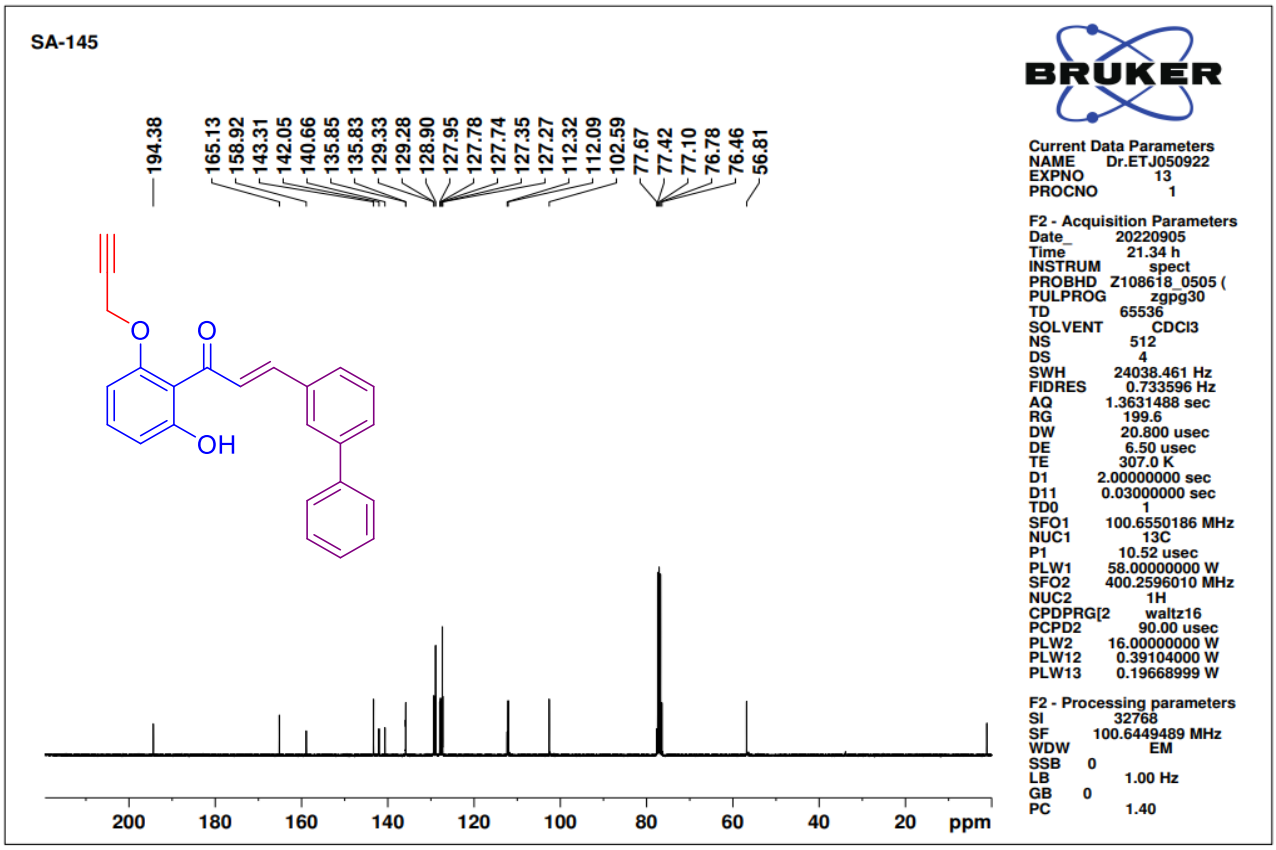


Figure 27: ^{13}C NMR spectrum of compound **5e**

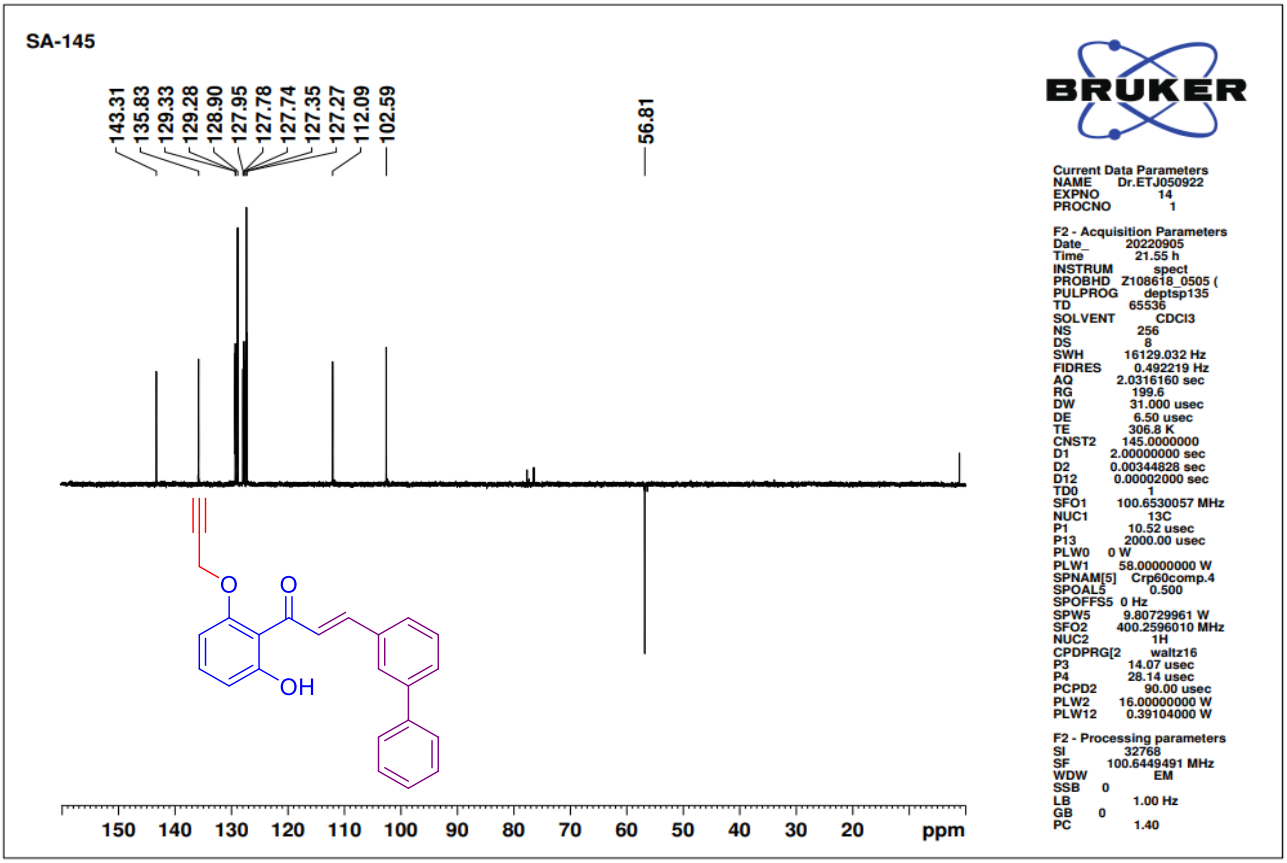


Figure 28: DEPT-135 NMR spectrum of compound **5e**

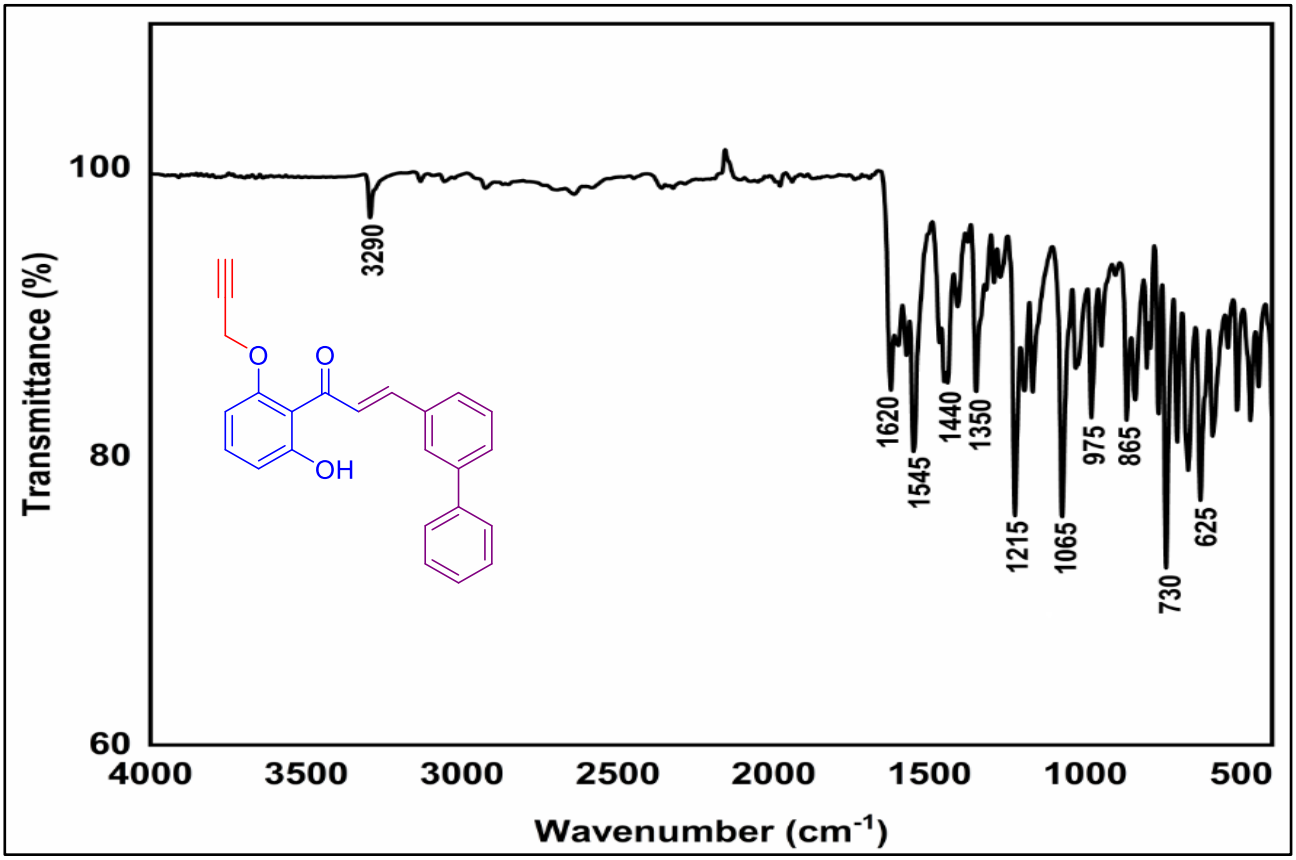


Figure 29: FT-IR spectrum of compound **5e**

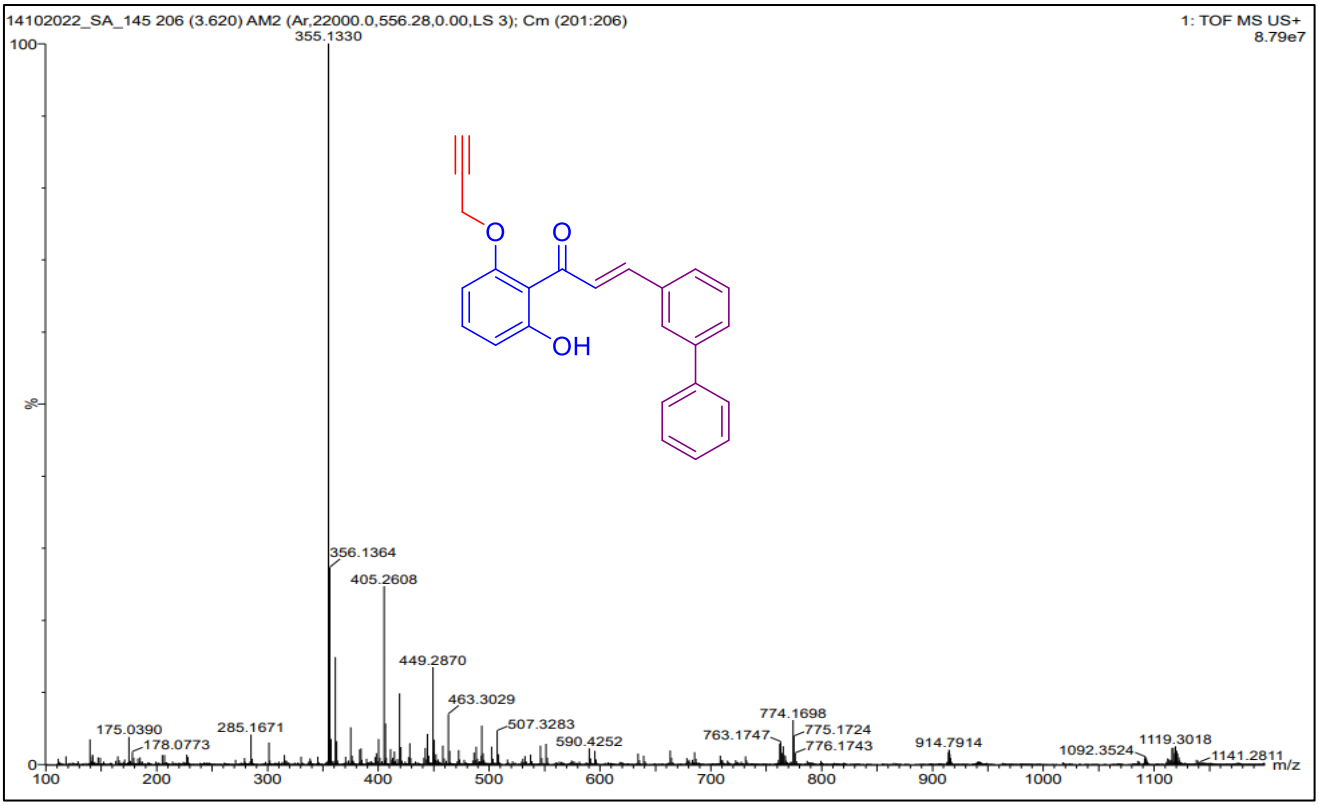


Figure 30: HRMS spectrum of compound **5e**

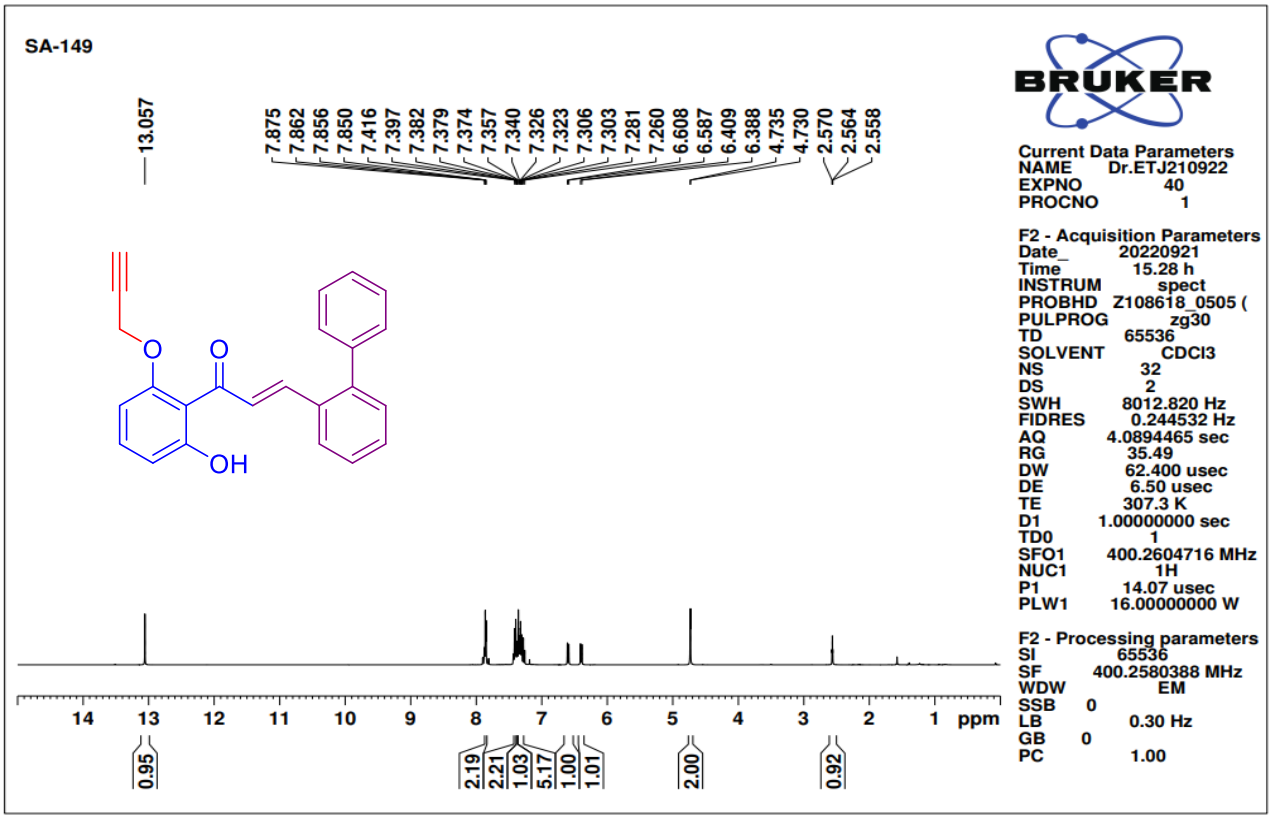


Figure 31: ^{1}H NMR spectrum of compound **5f**

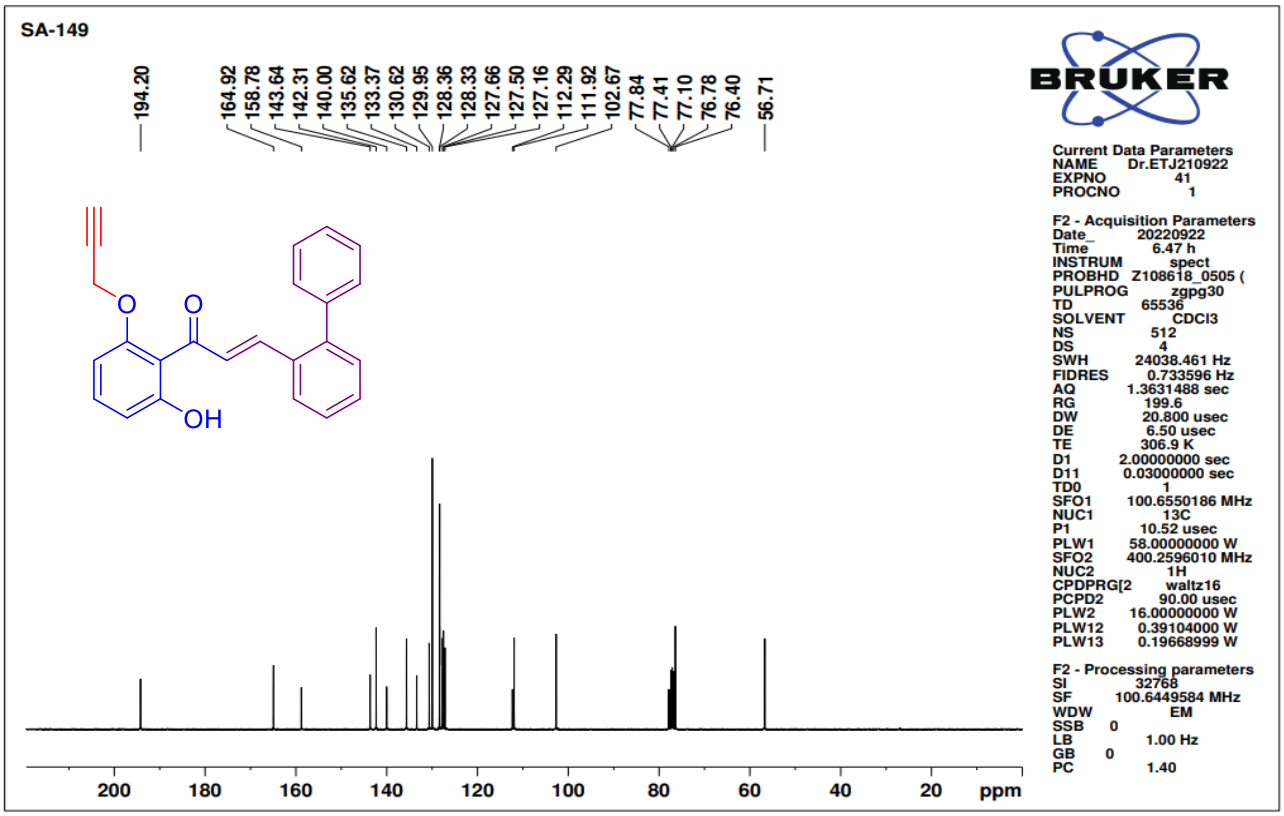


Figure 32: ^{13}C NMR spectrum of compound **5f**

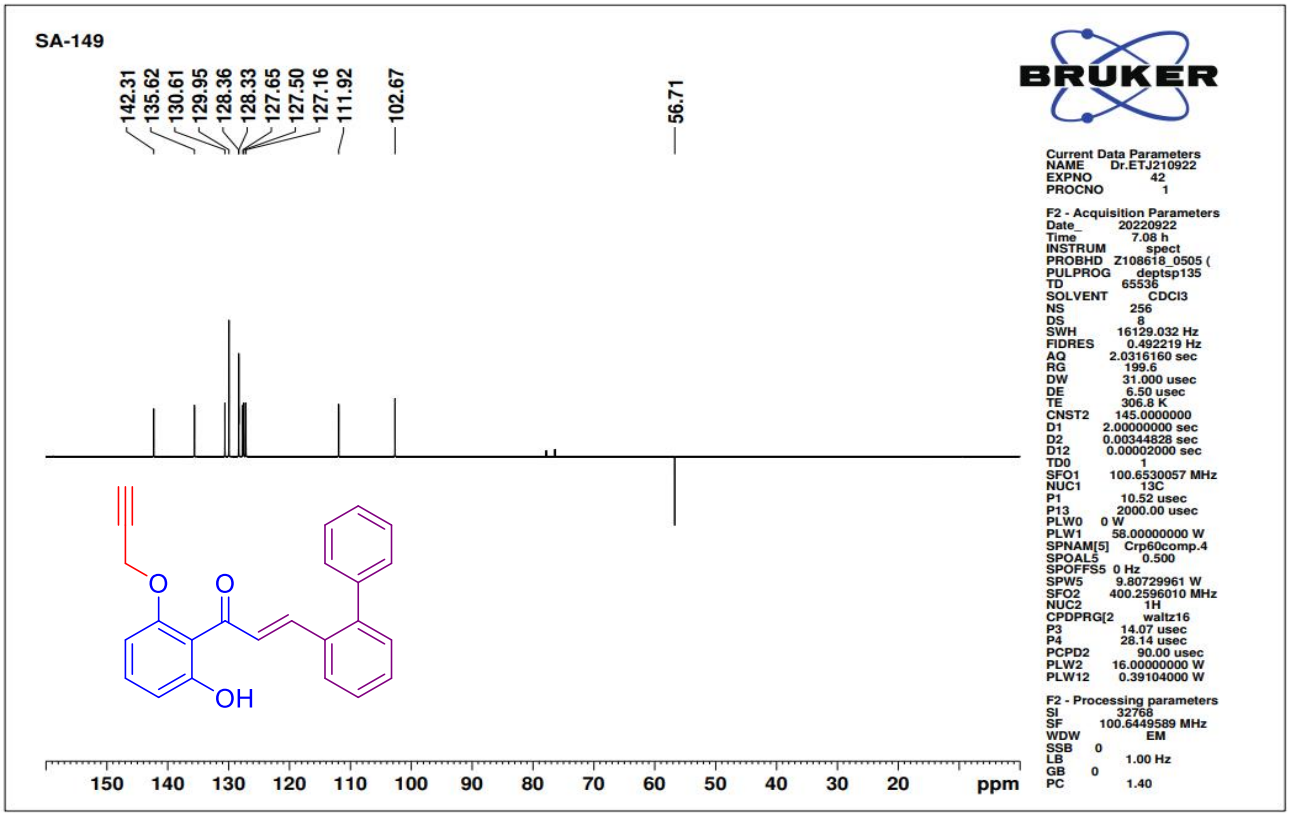


Figure 33: DEPT-135 NMR spectrum of compound **5f**

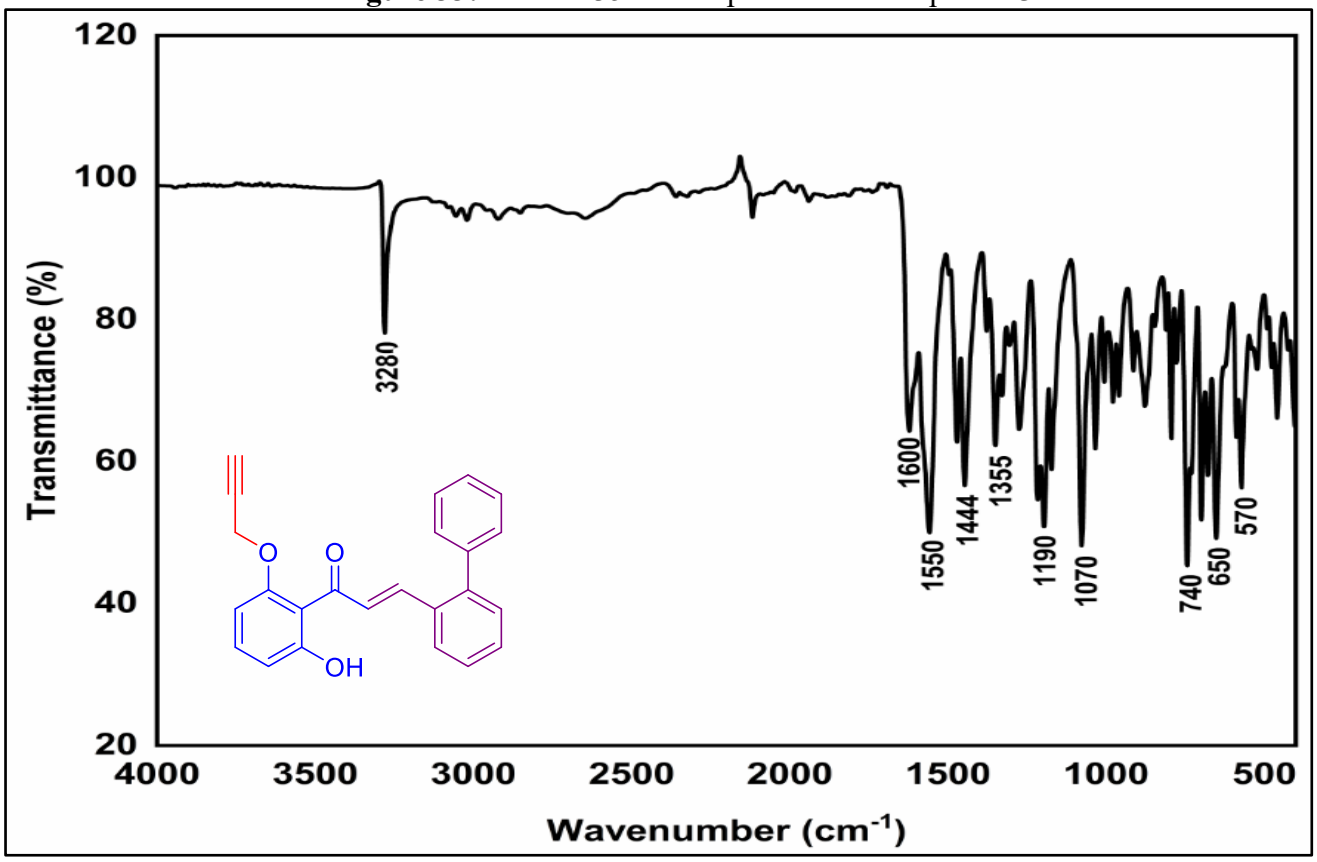


Figure 34: FT-IR spectrum of compound **5f**

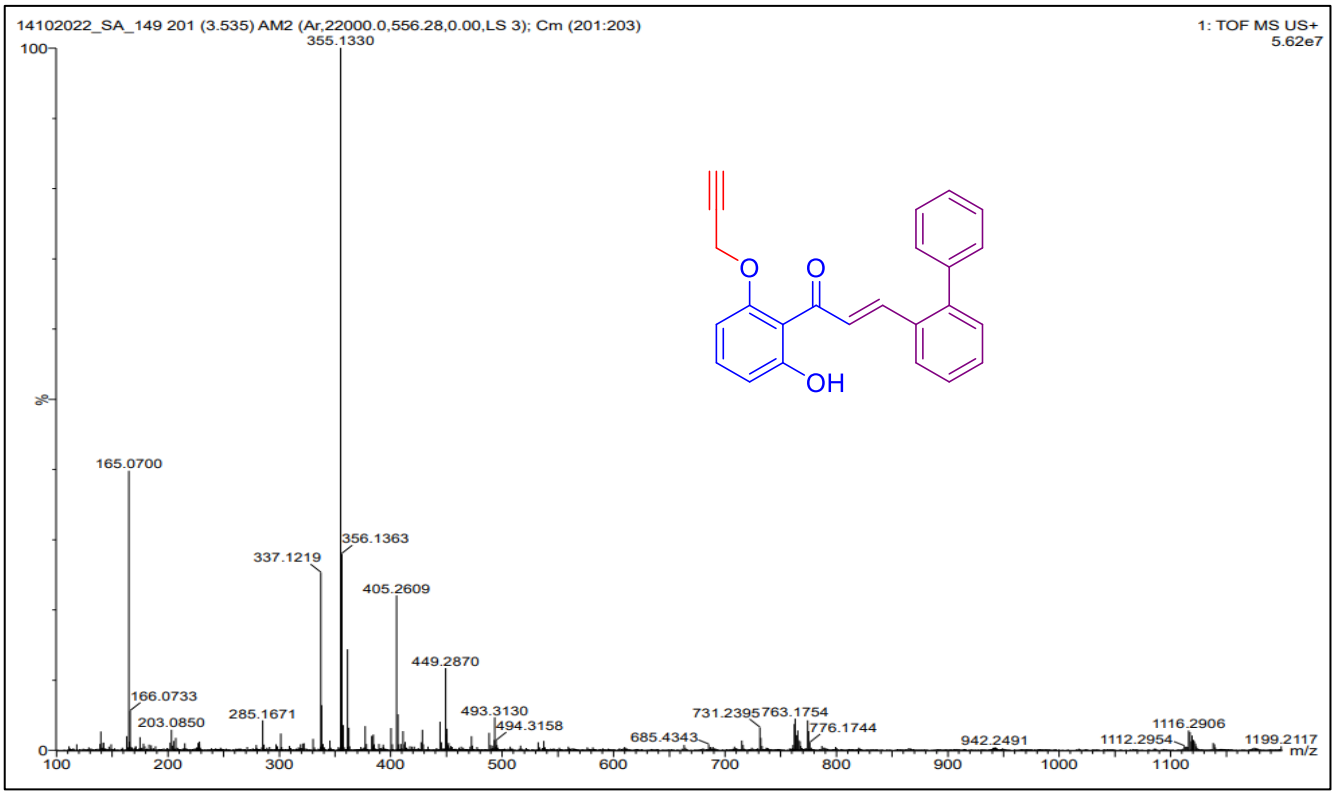


Figure 35: HRMS spectrum of compound **5f**

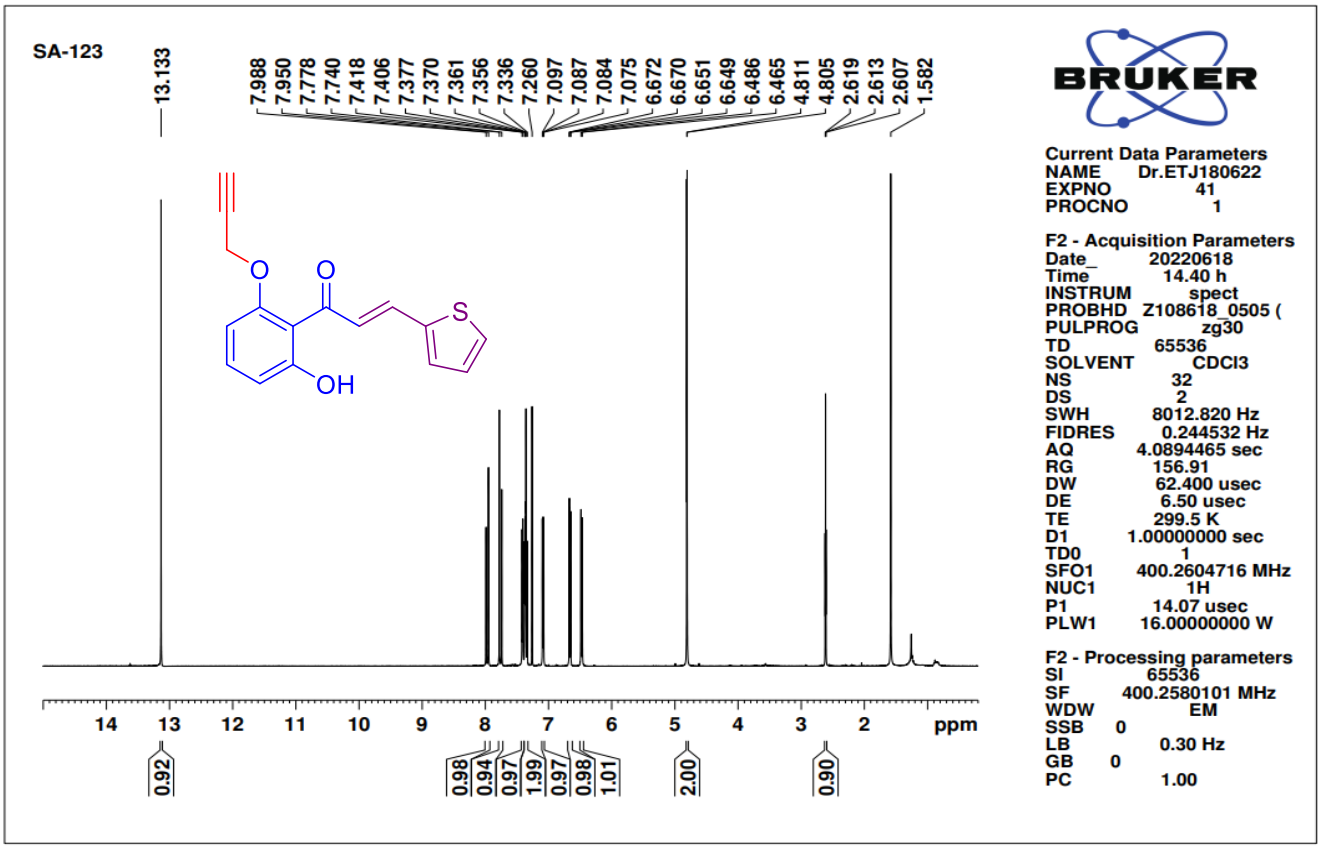


Figure 36: ^{1}H NMR spectrum of compound **5g**

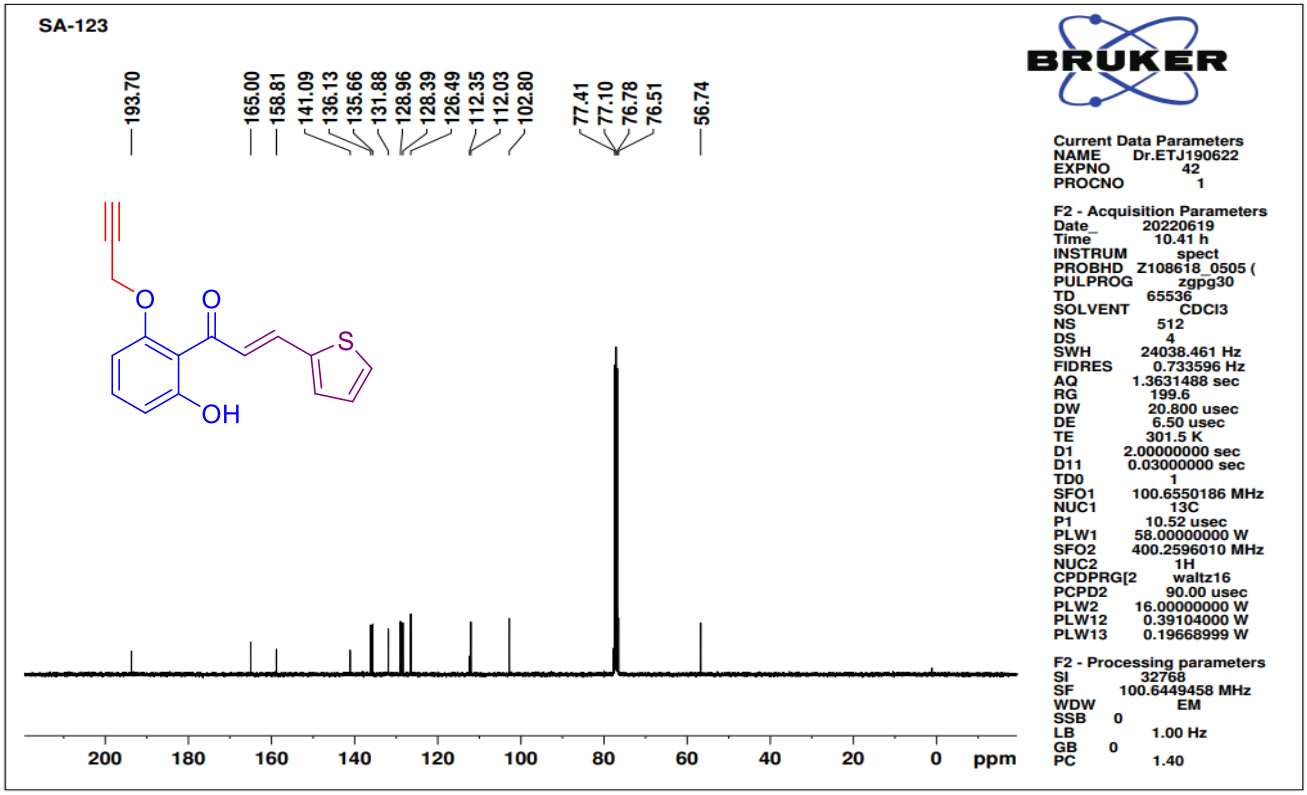


Figure 37: ^{13}C NMR spectrum of compound **5g**

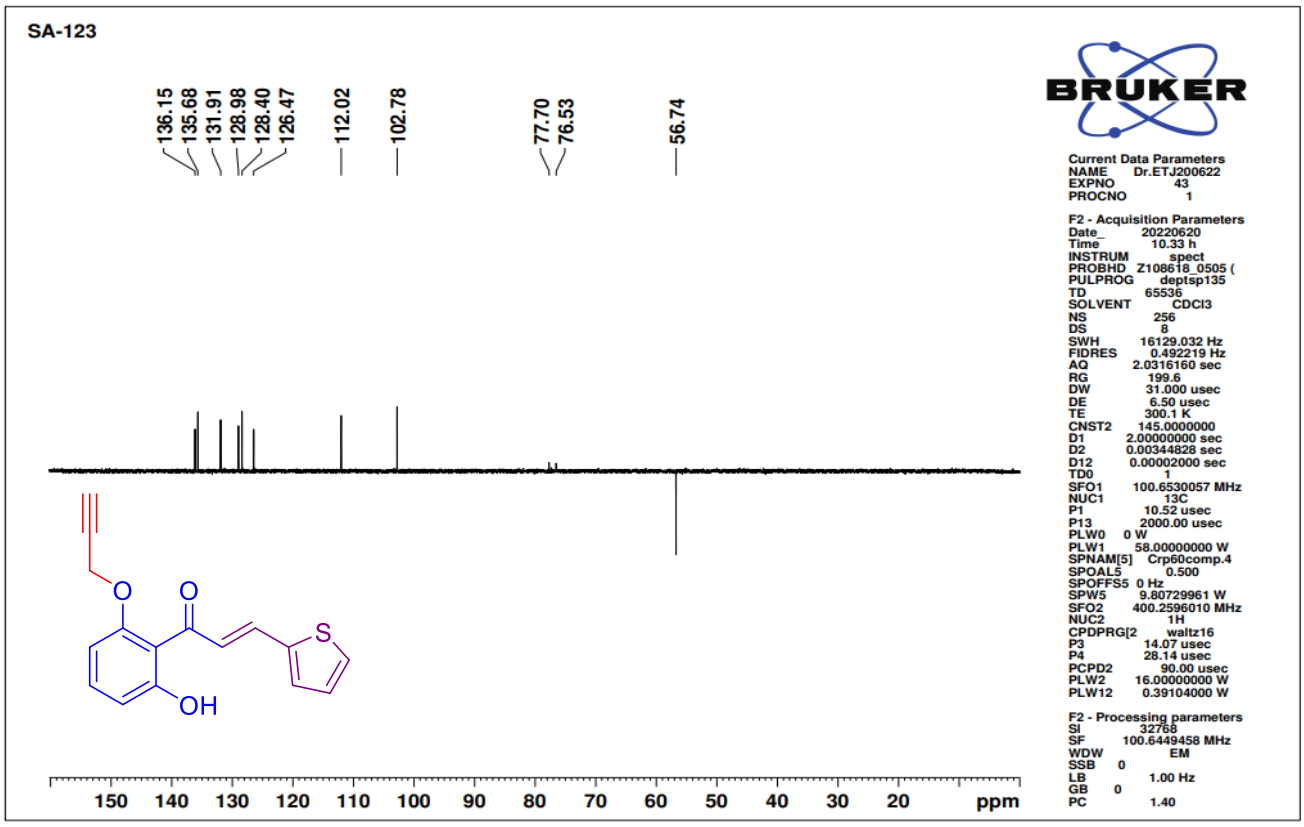


Figure 38: DEPT-135 NMR spectrum of compound **5g**

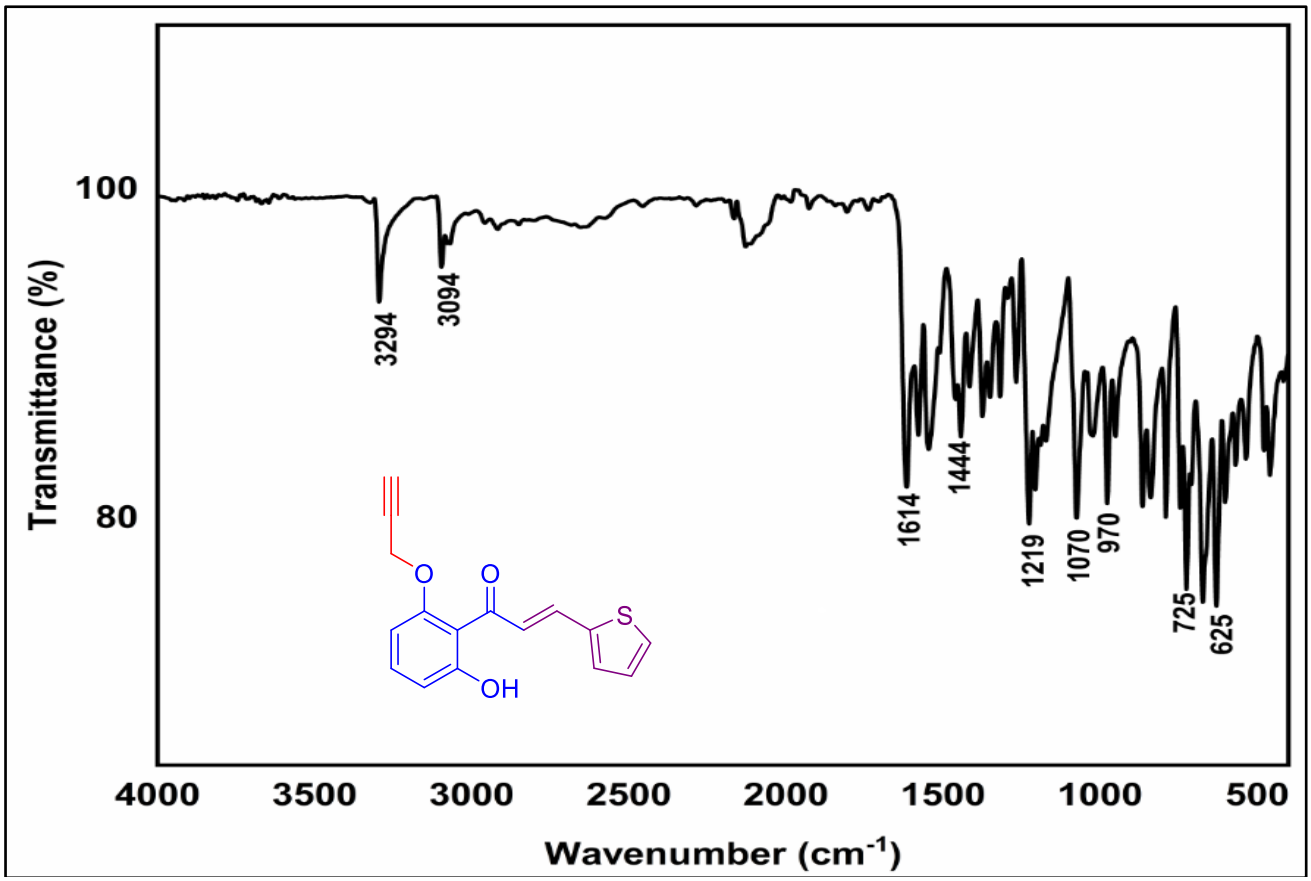


Figure 39: FT-IR spectrum of compound **5g**

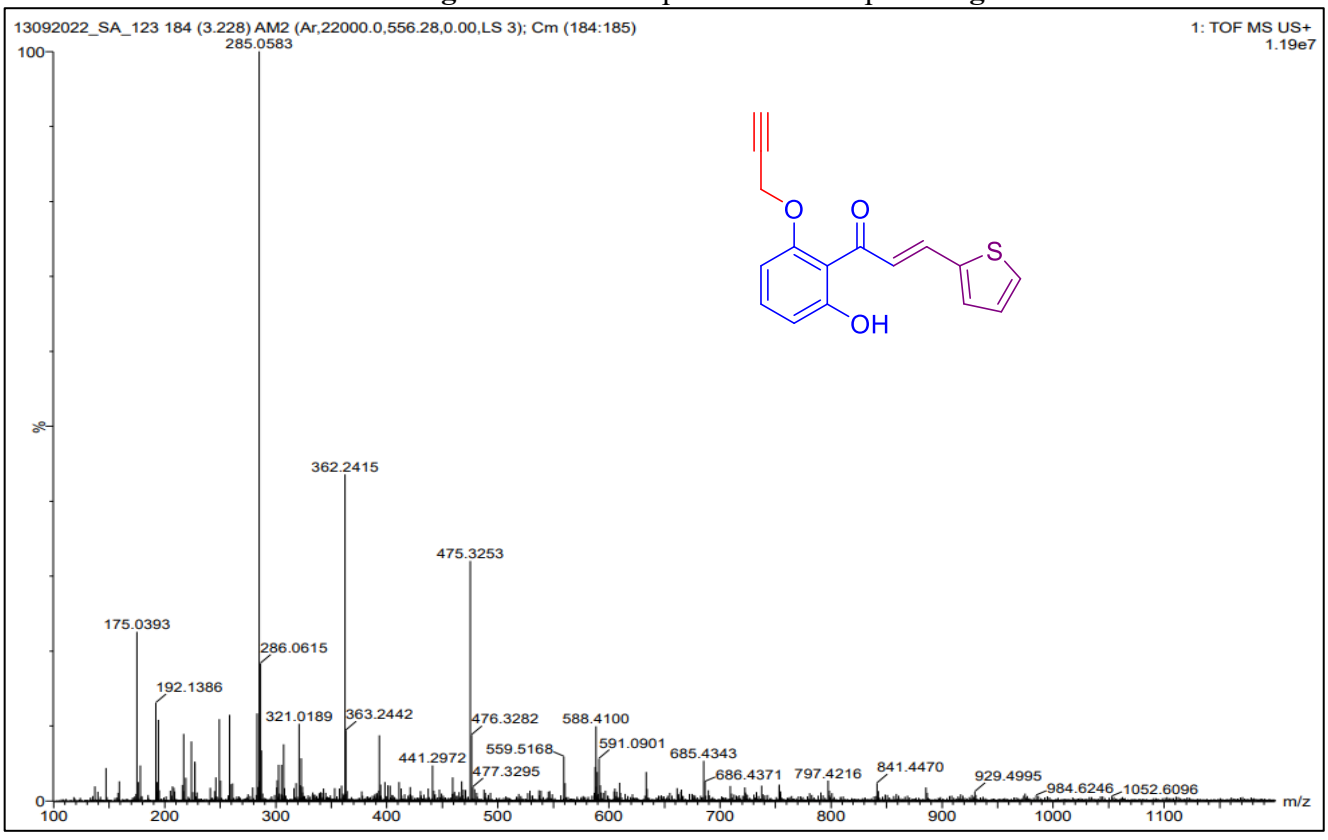


Figure 40: HRMS spectrum of compound **5g**

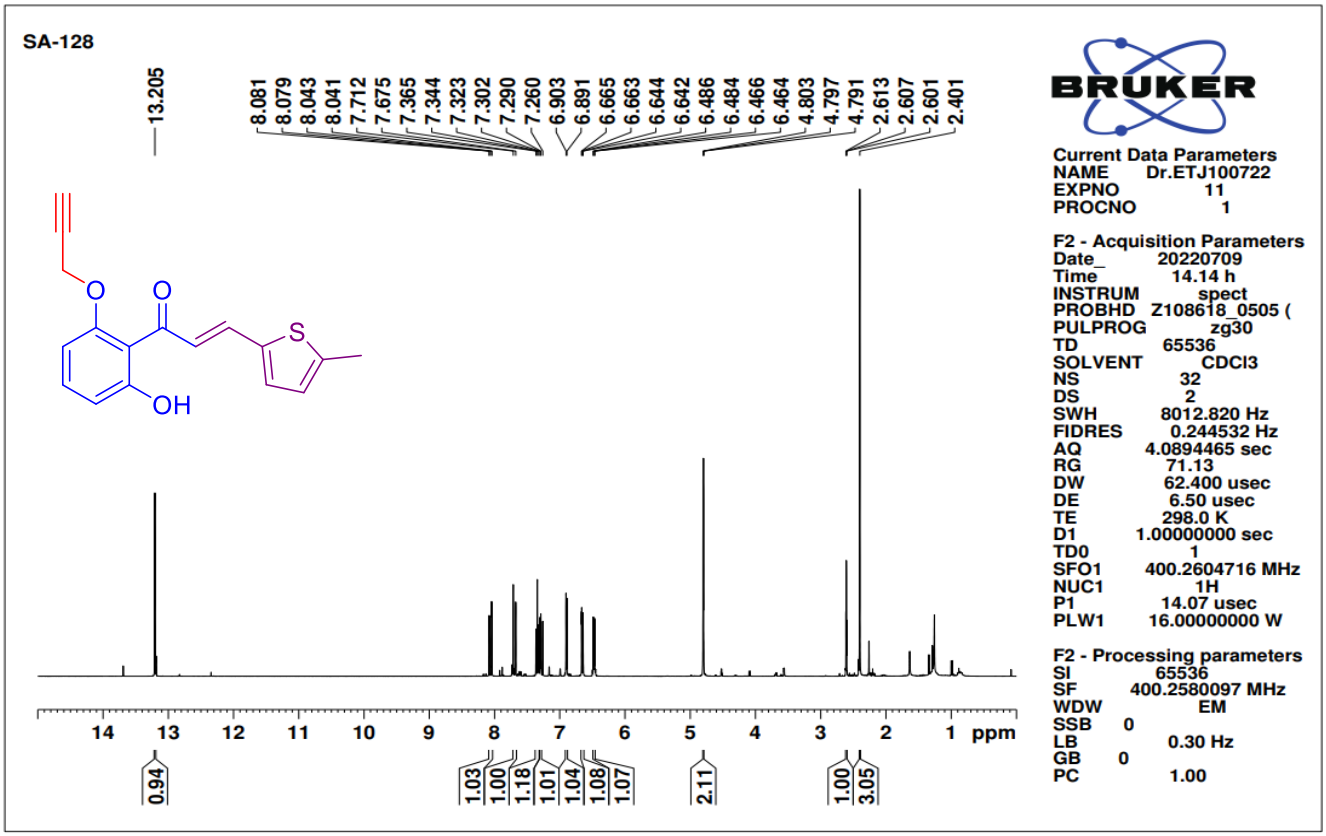


Figure 41: ^{1}H NMR spectrum of compound **5h**

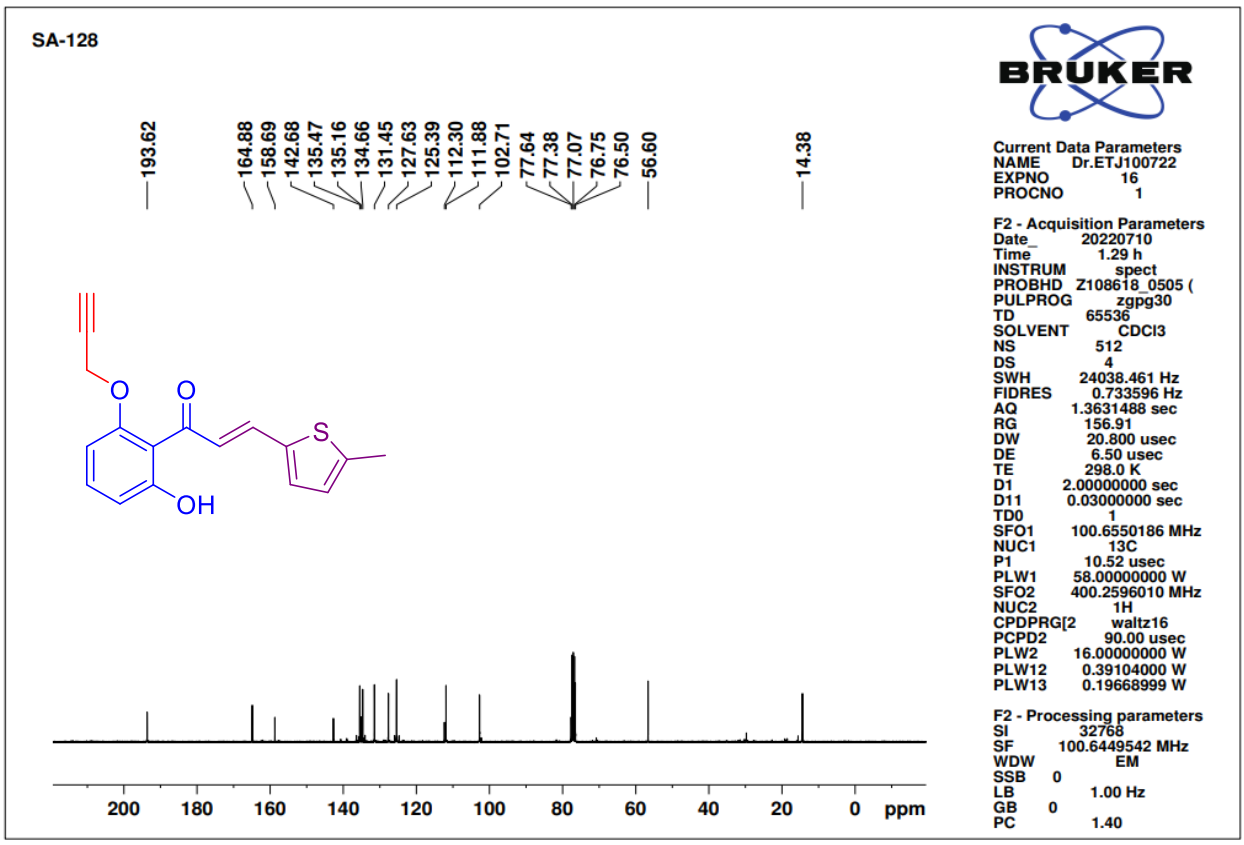


Figure 42: ^{13}C NMR spectrum of compound **5h**

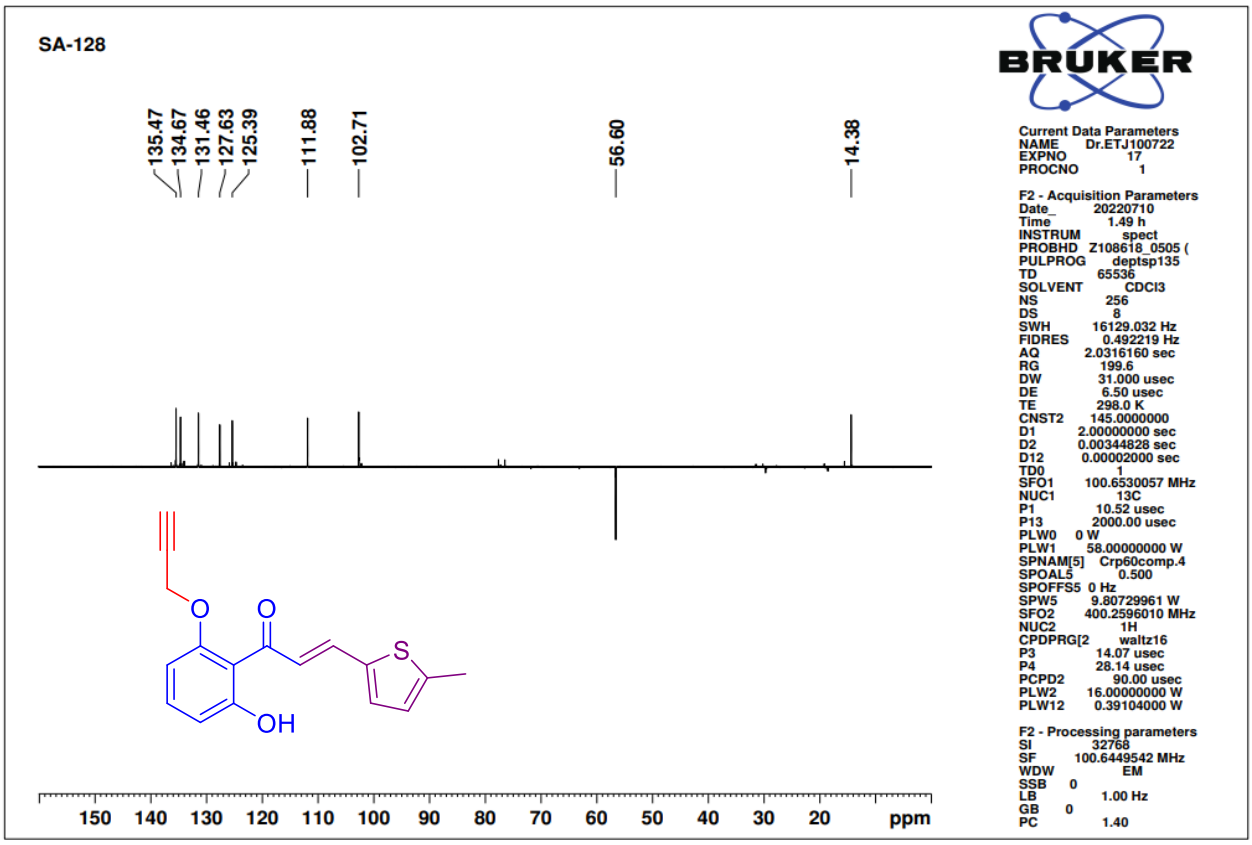


Figure 43: DEPT-135 NMR spectrum of compound **5h**

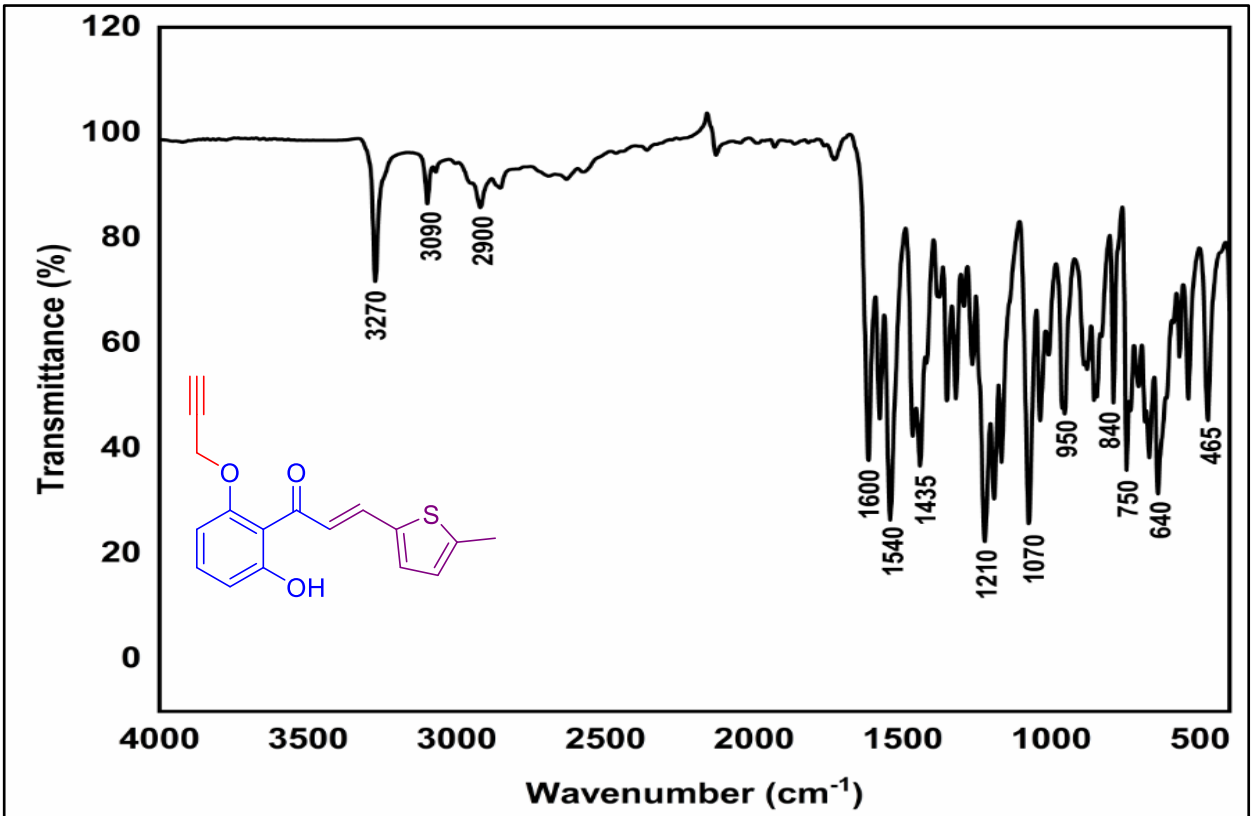


Figure 44: FT-IR spectrum of compound **5h**

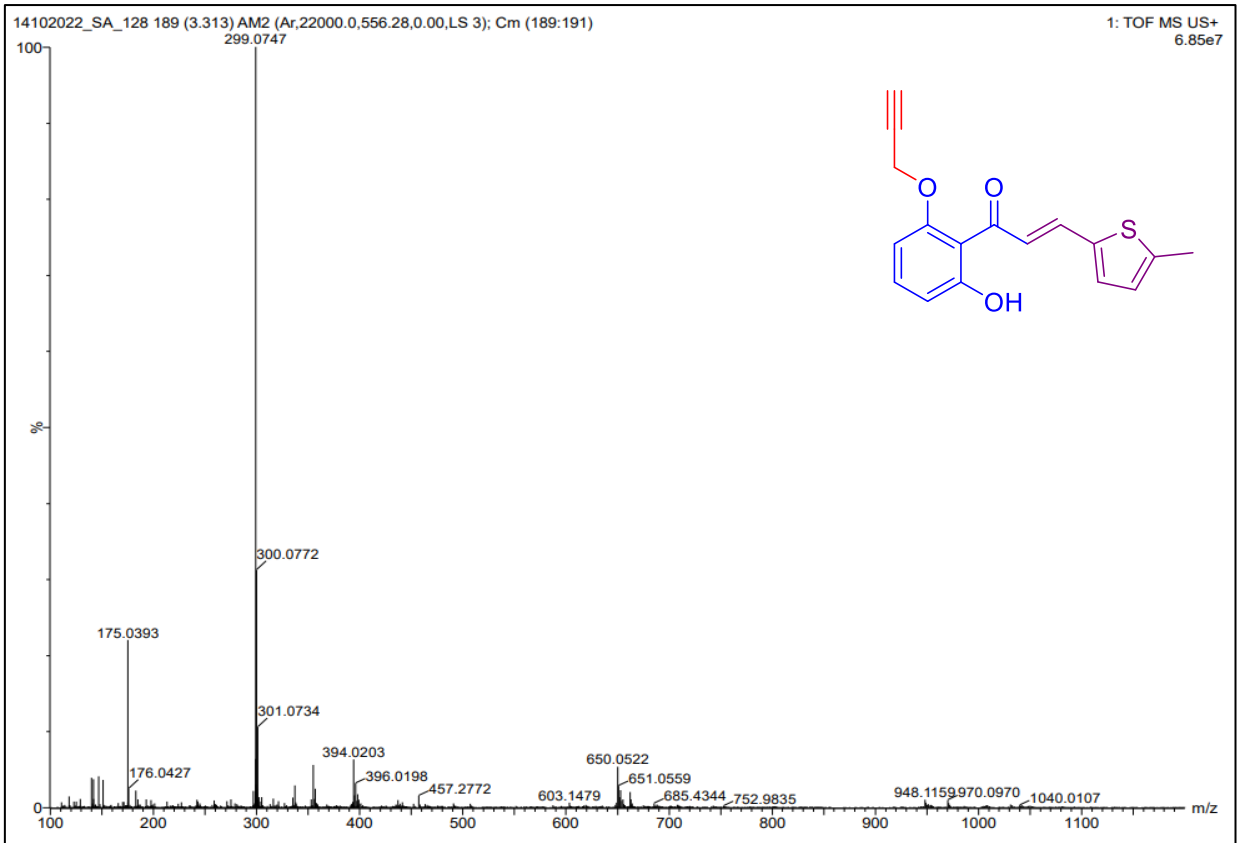


Figure 45: HRMS spectrum of compound **5h**

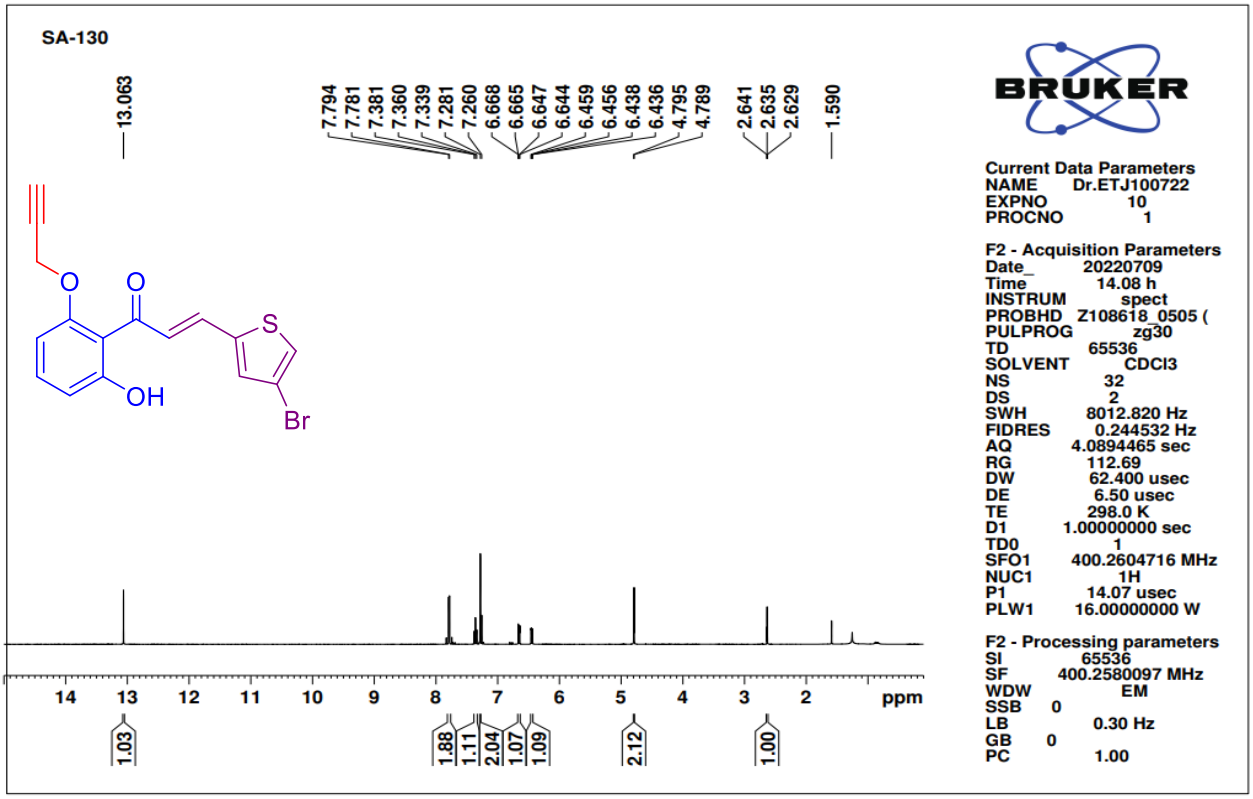


Figure 46: ^{1}H NMR spectrum of compound **5i**

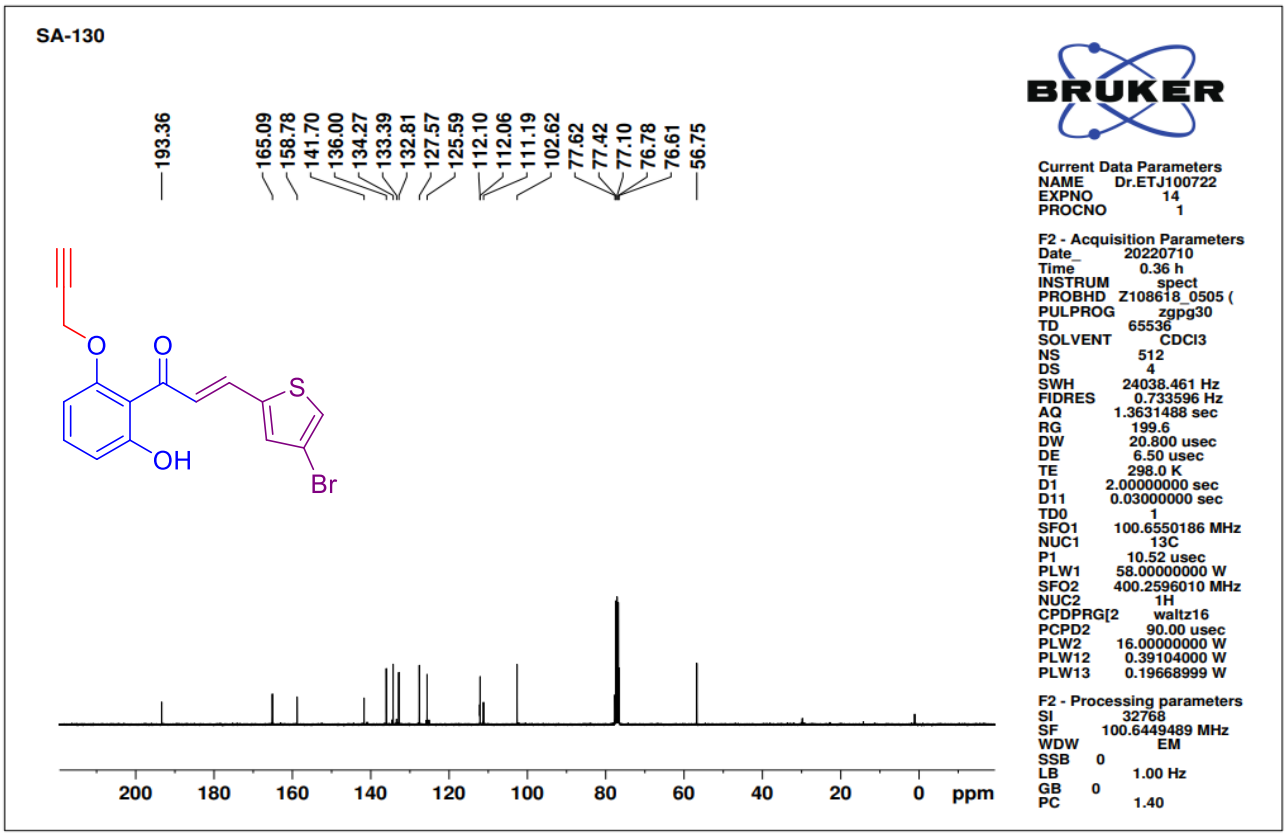


Figure 47: ^{13}C NMR spectrum of compound **5i**

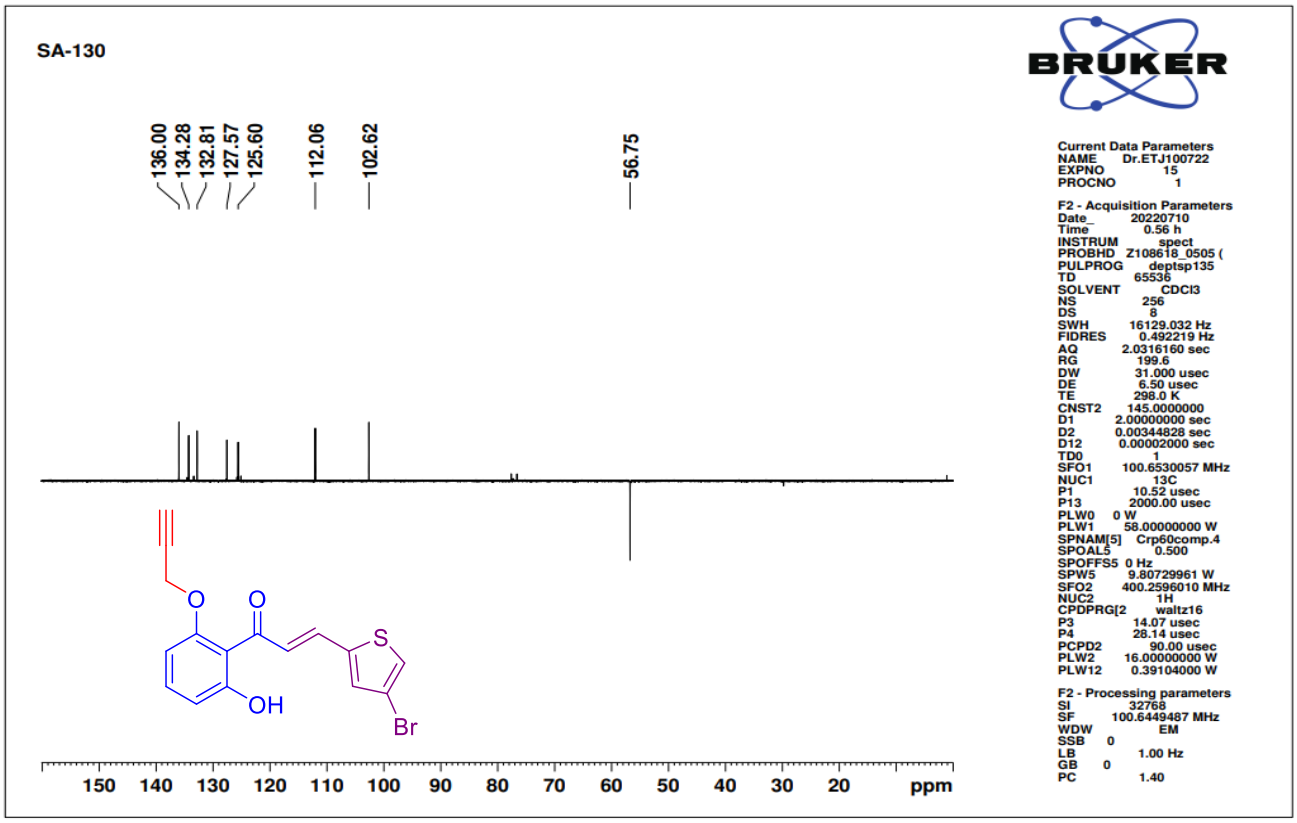


Figure 48: DEPT-135 NMR spectrum of compound **5i**

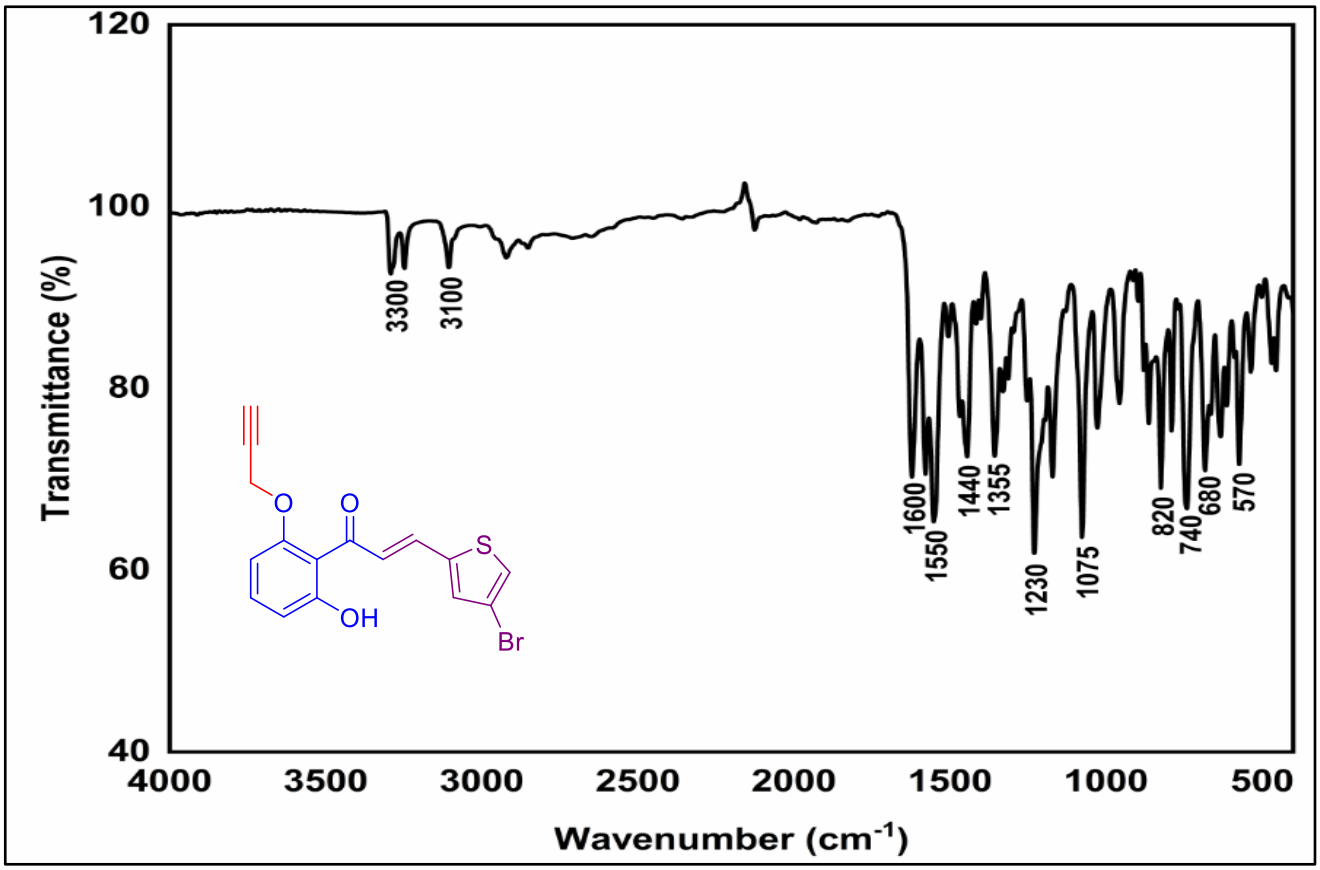


Figure 49: FT-IR spectrum of compound **5i**

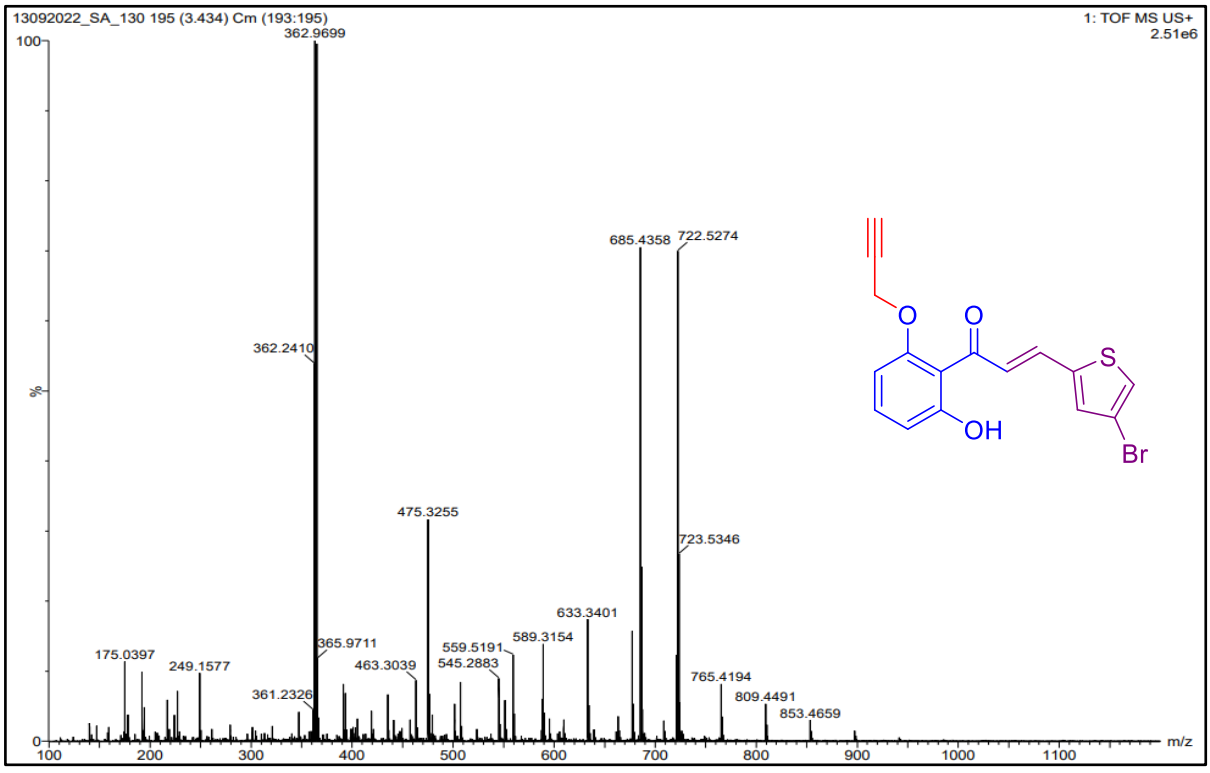


Figure 50: HRMS spectrum of compound **5i**

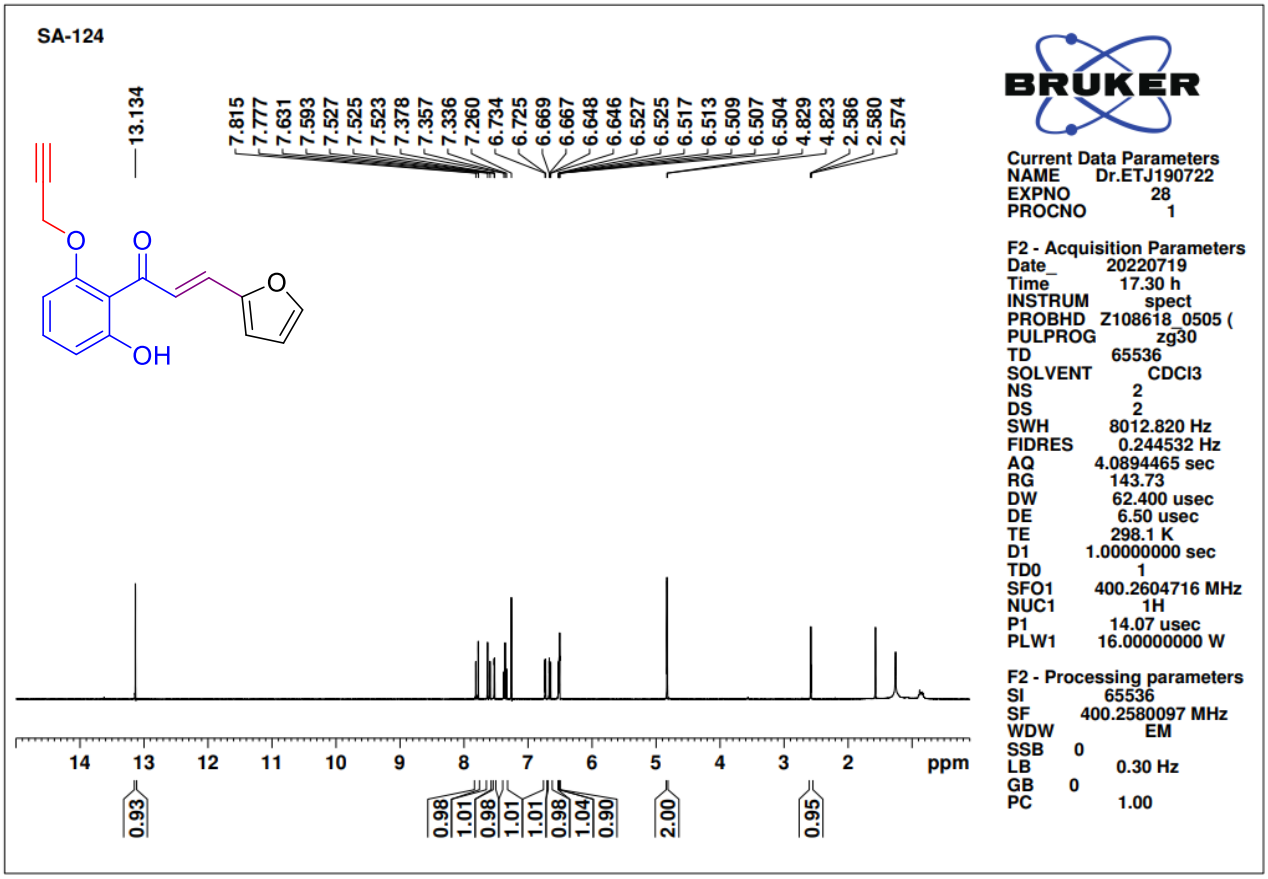


Figure 51: ^{1}H NMR spectrum of compound **5j**

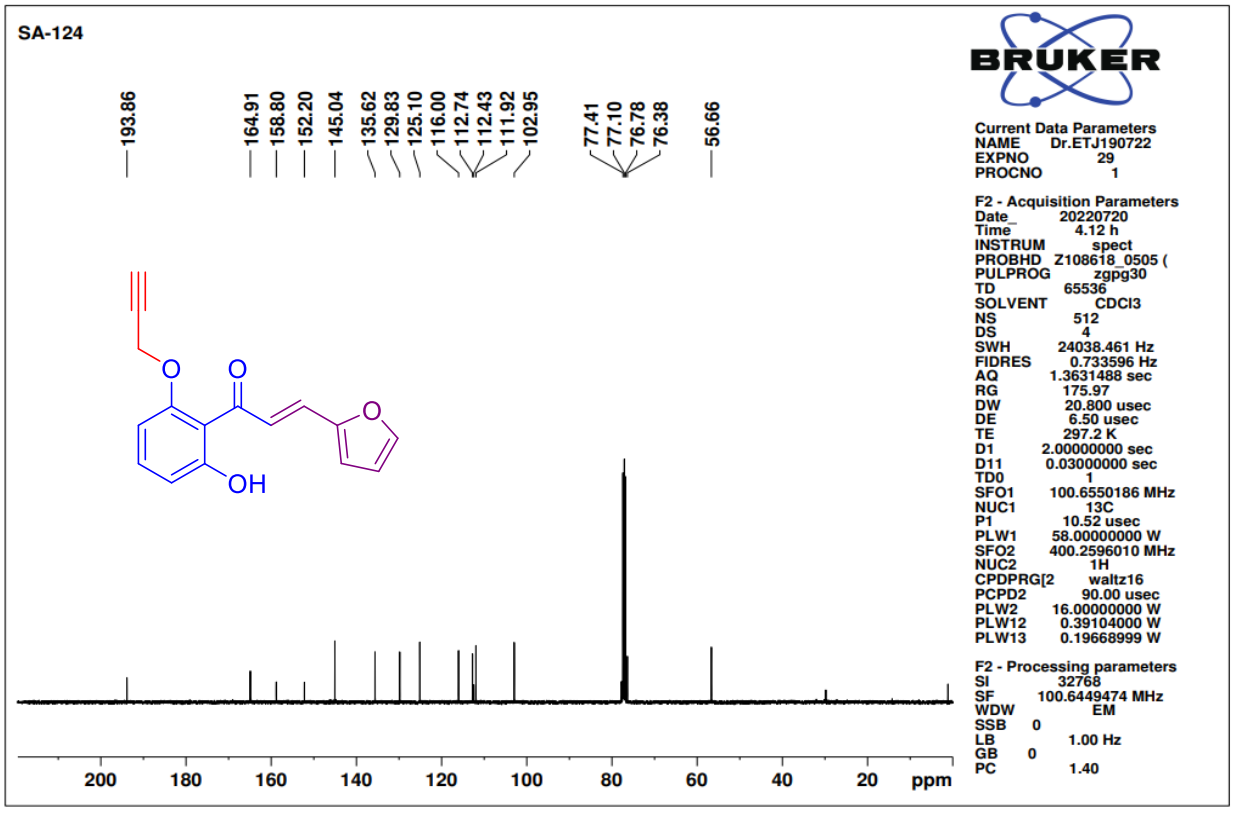


Figure 52: ^{13}C NMR spectrum of compound **5j**

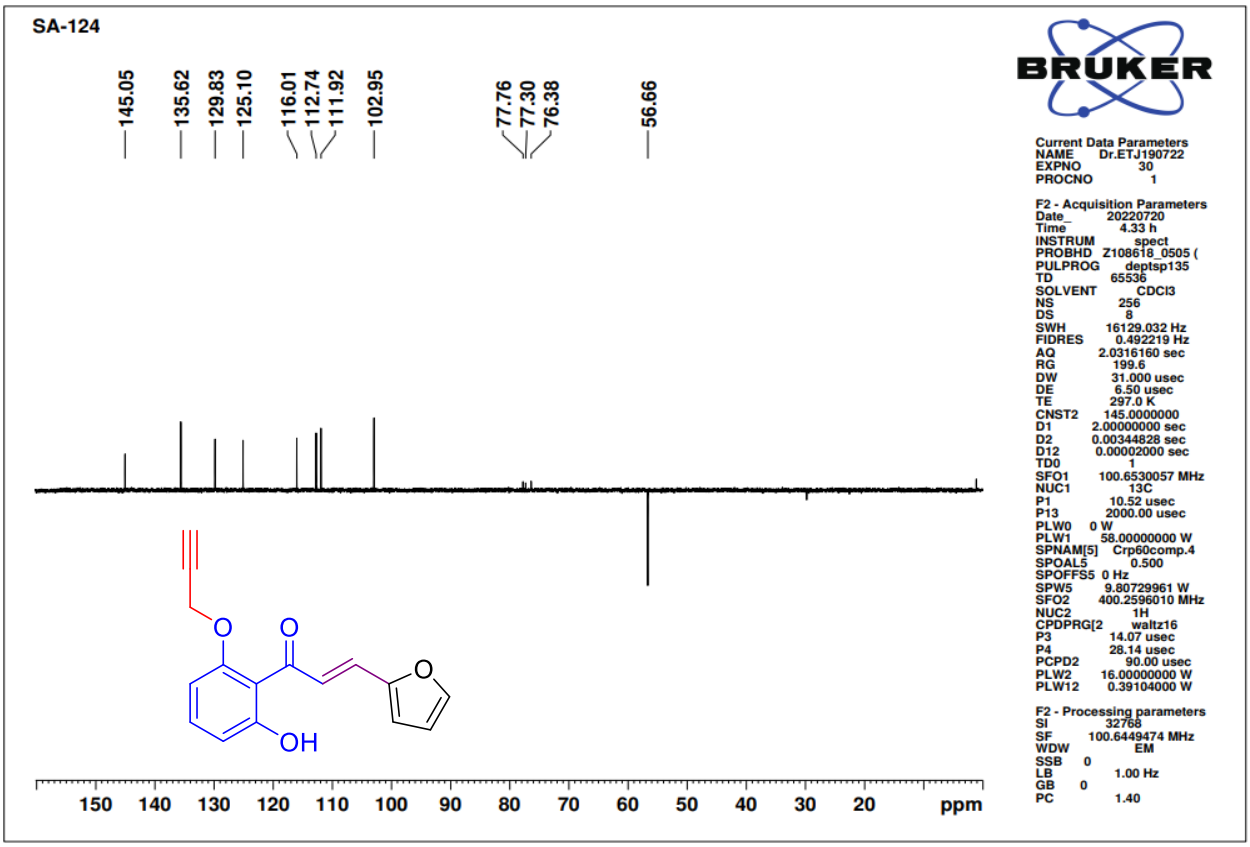


Figure 53: DEPT-135 NMR spectrum of compound **5j**

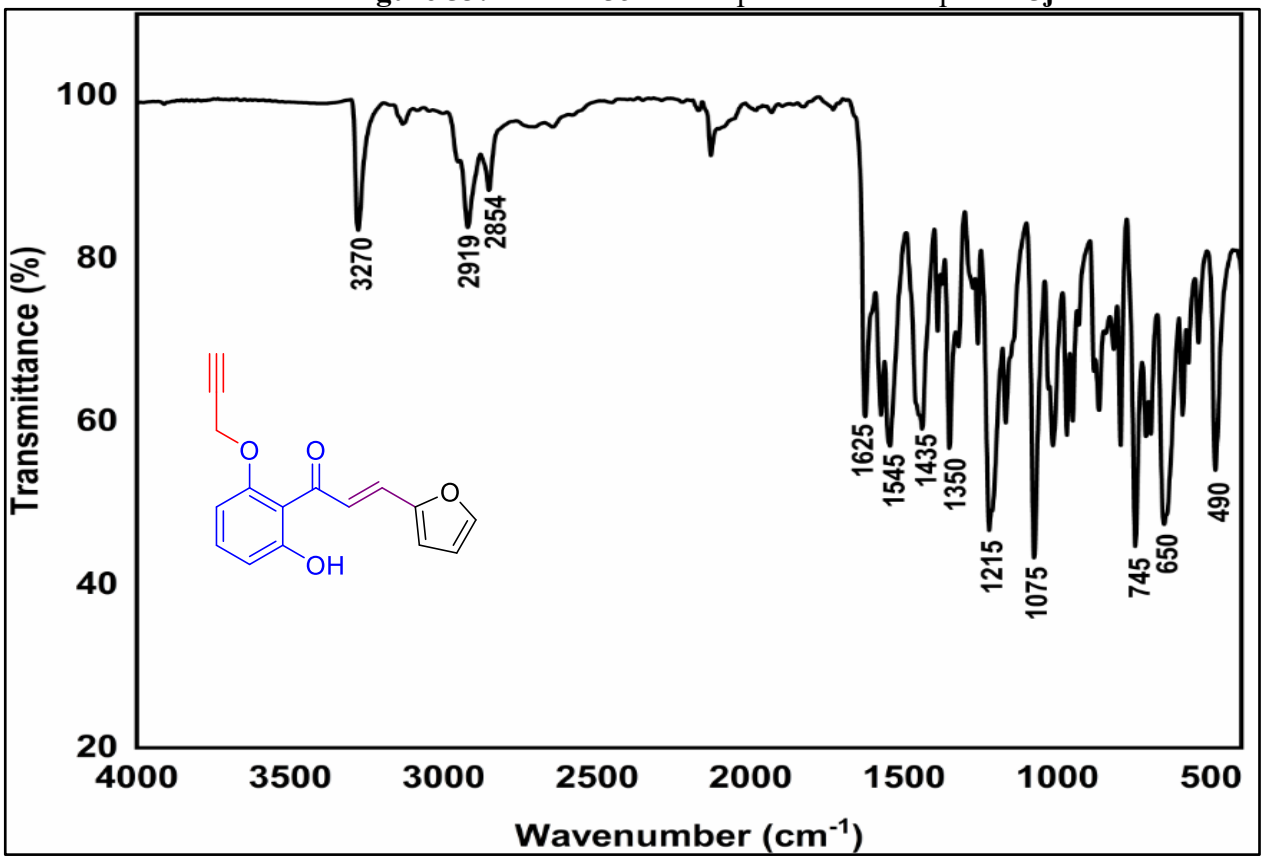


Figure 54: FT-IR spectrum of compound **5j**

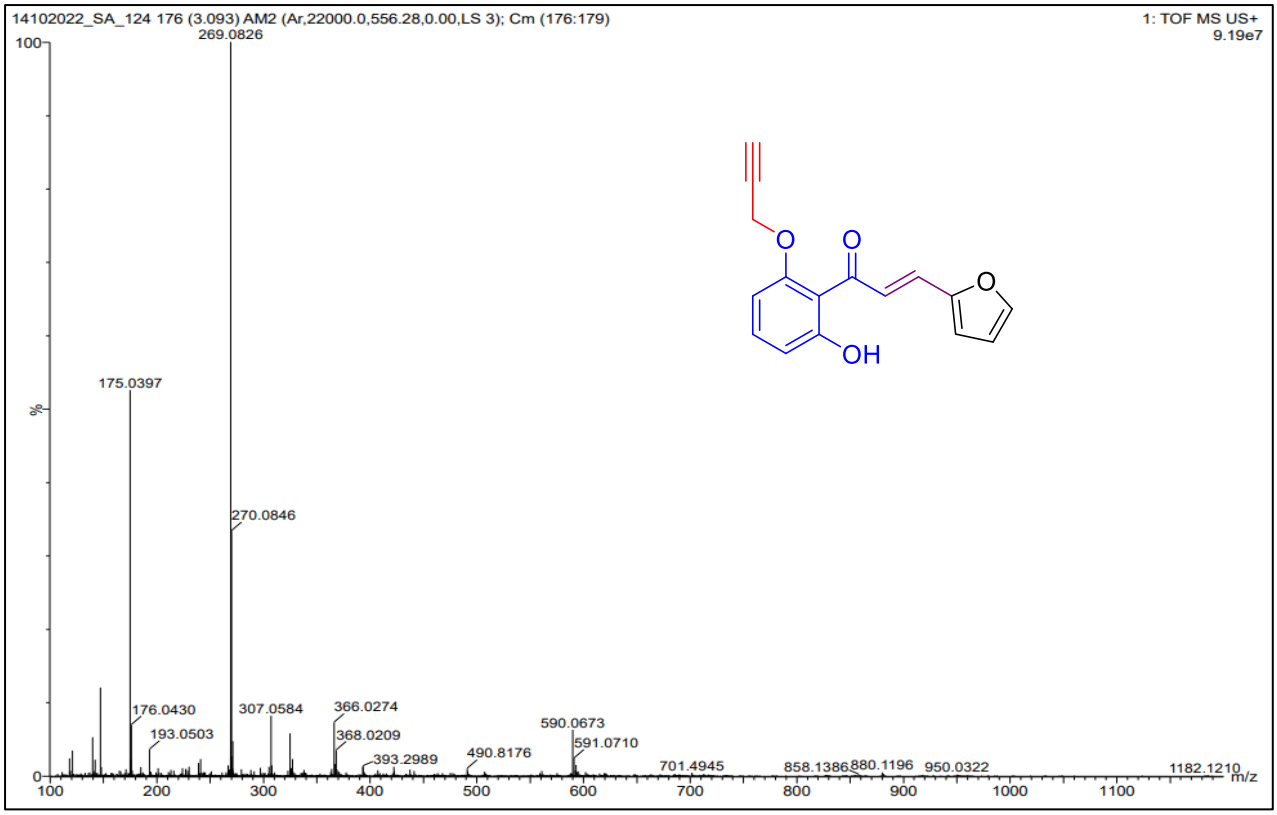


Figure 55: HRMS spectrum of compound **5j**

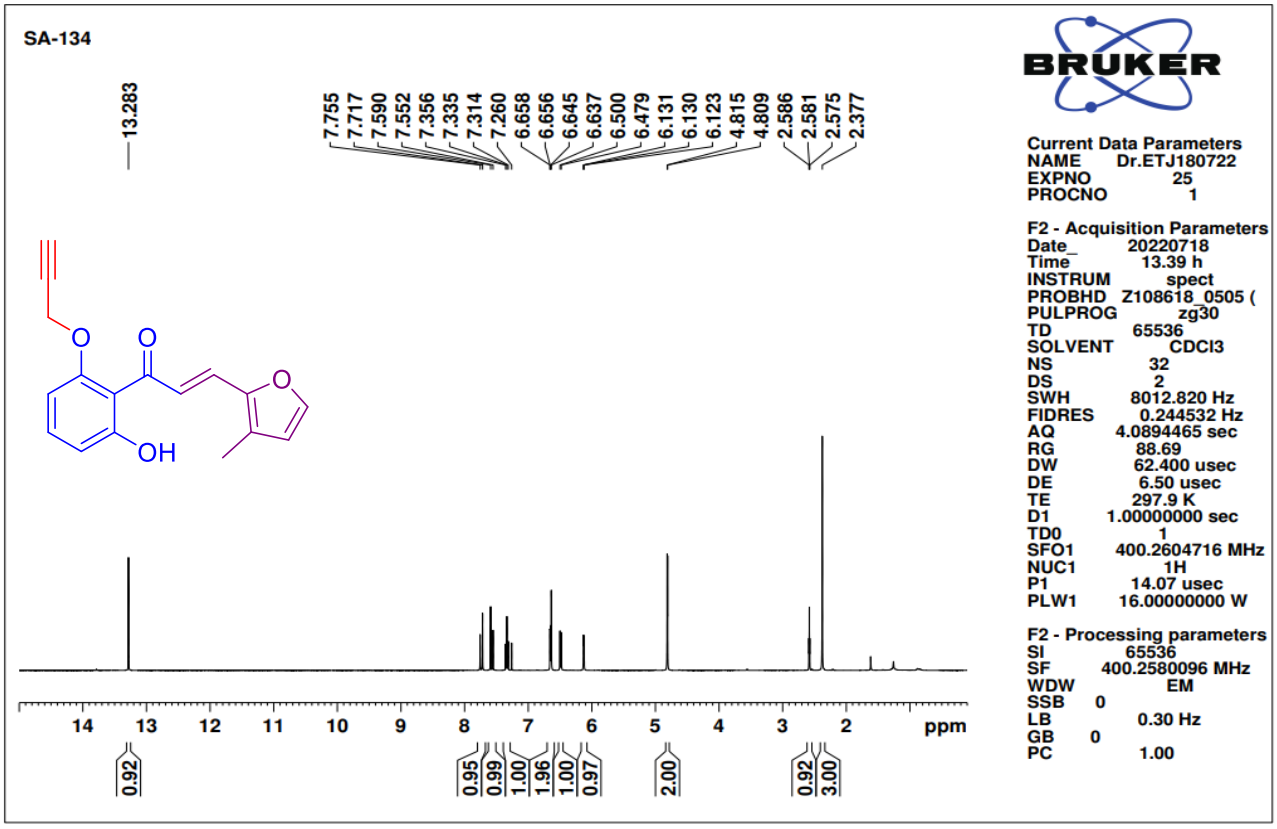


Figure 56: ^{1}H NMR spectrum of compound **5k**

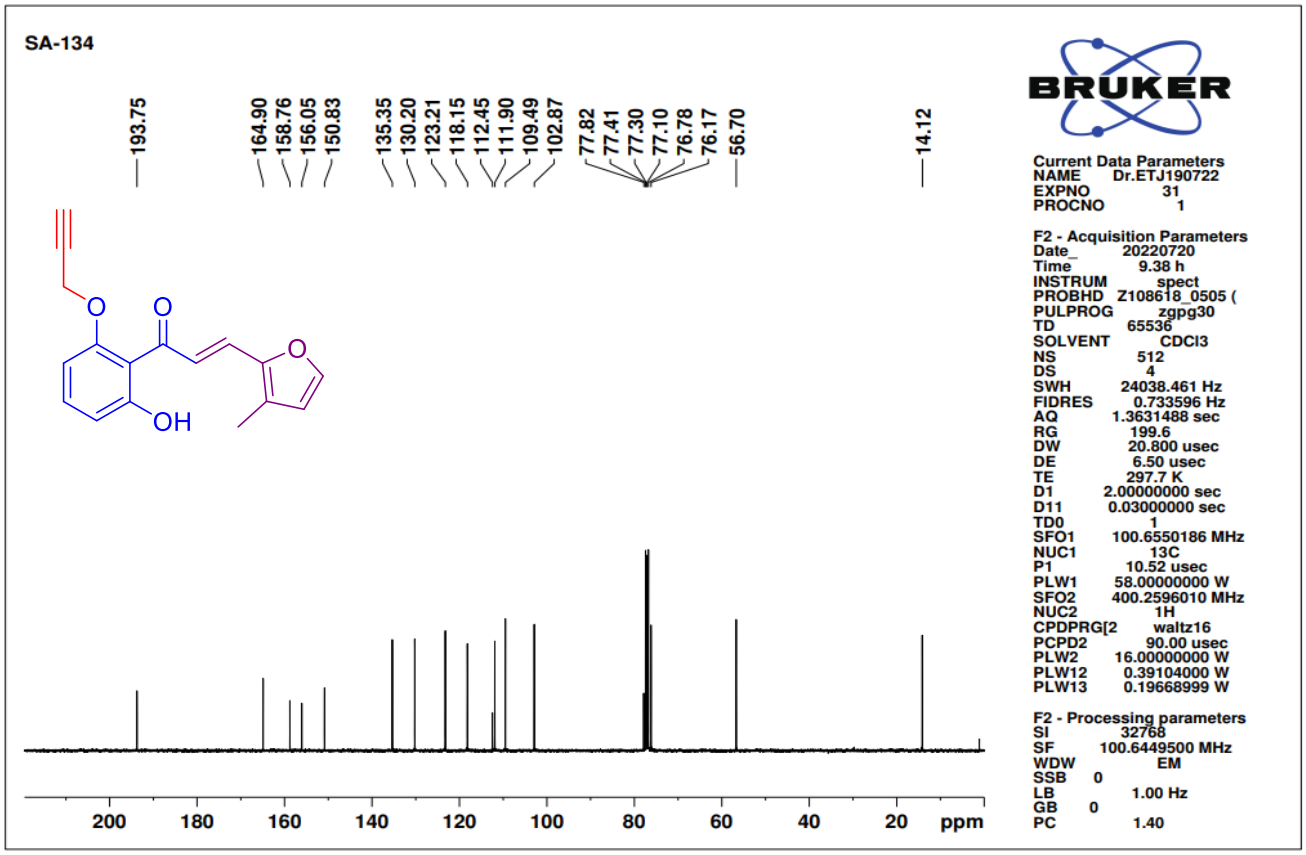


Figure 57: ^{13}C NMR spectrum of compound **5k**

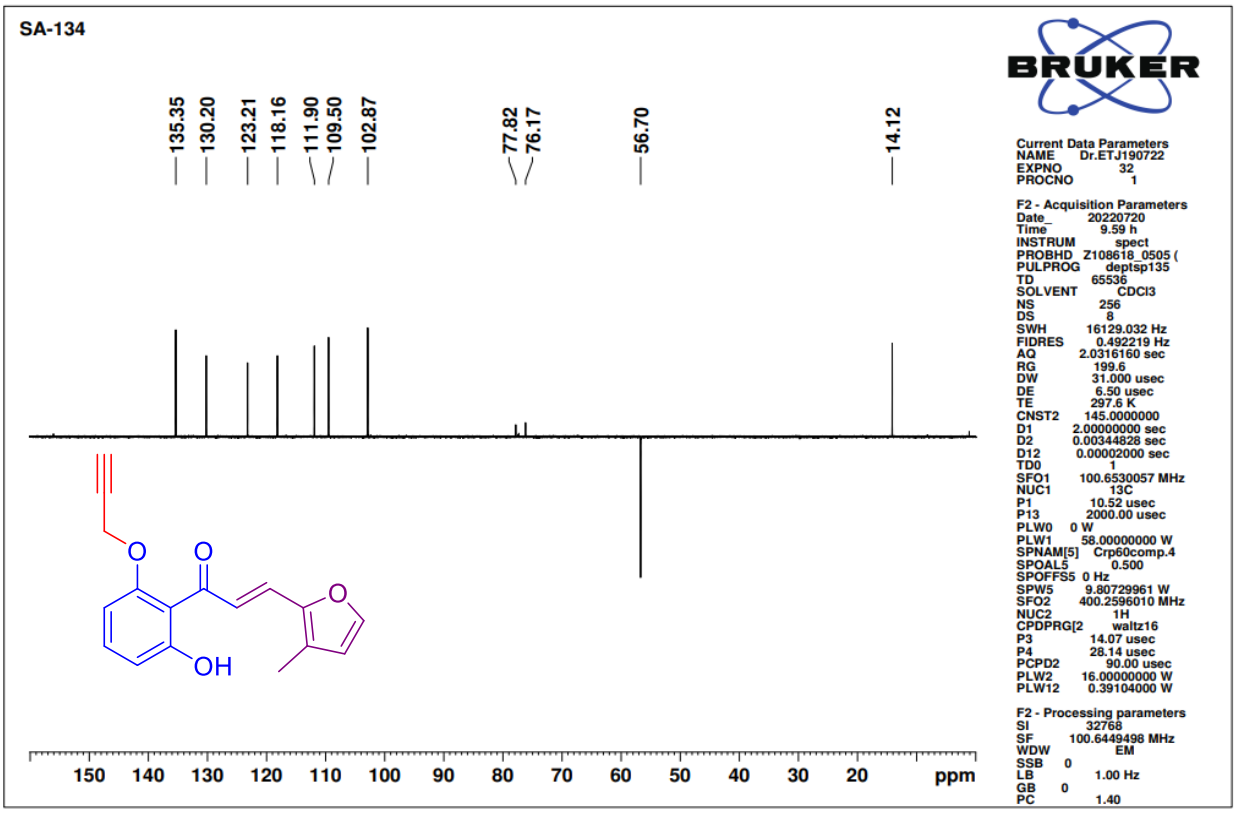


Figure 58: DEPT-135 NMR spectrum of compound **5k**

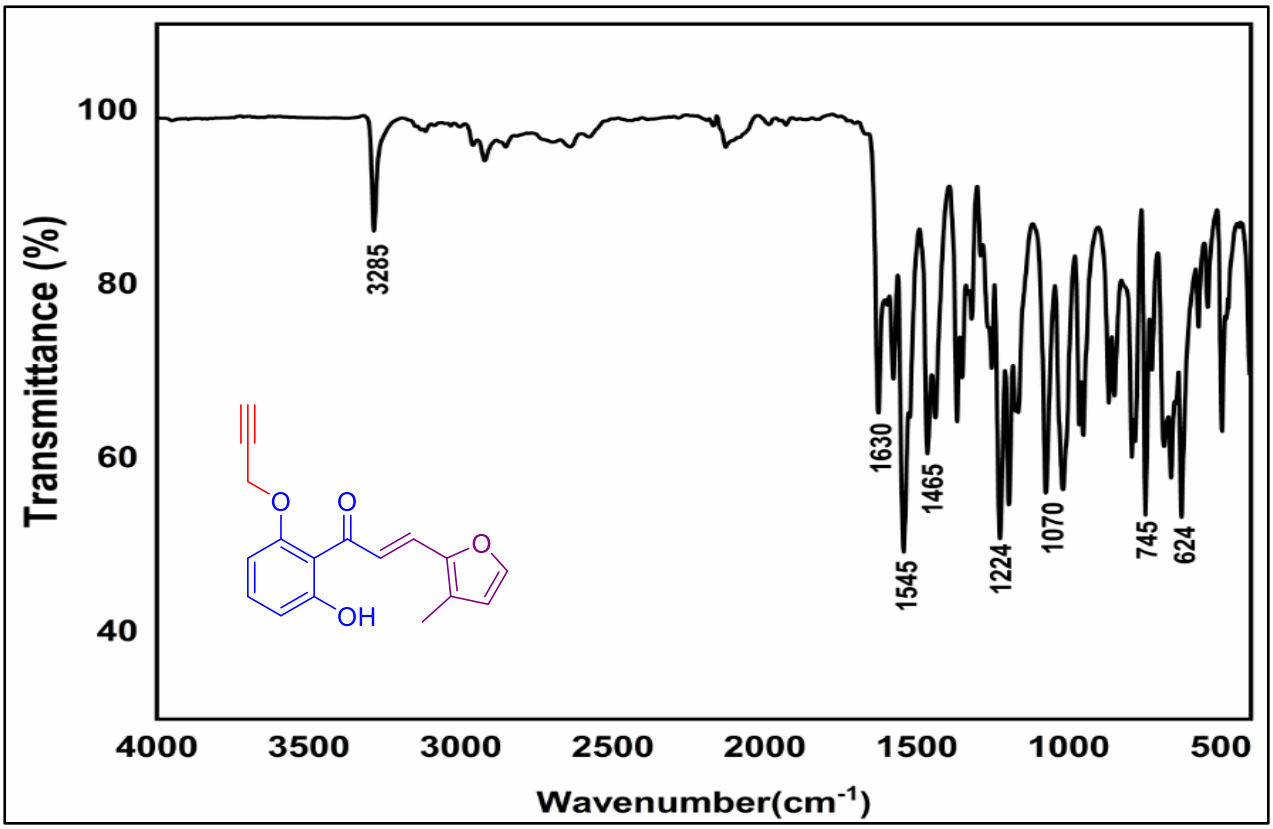


Figure 59: FT-IR spectrum of compound **5k**

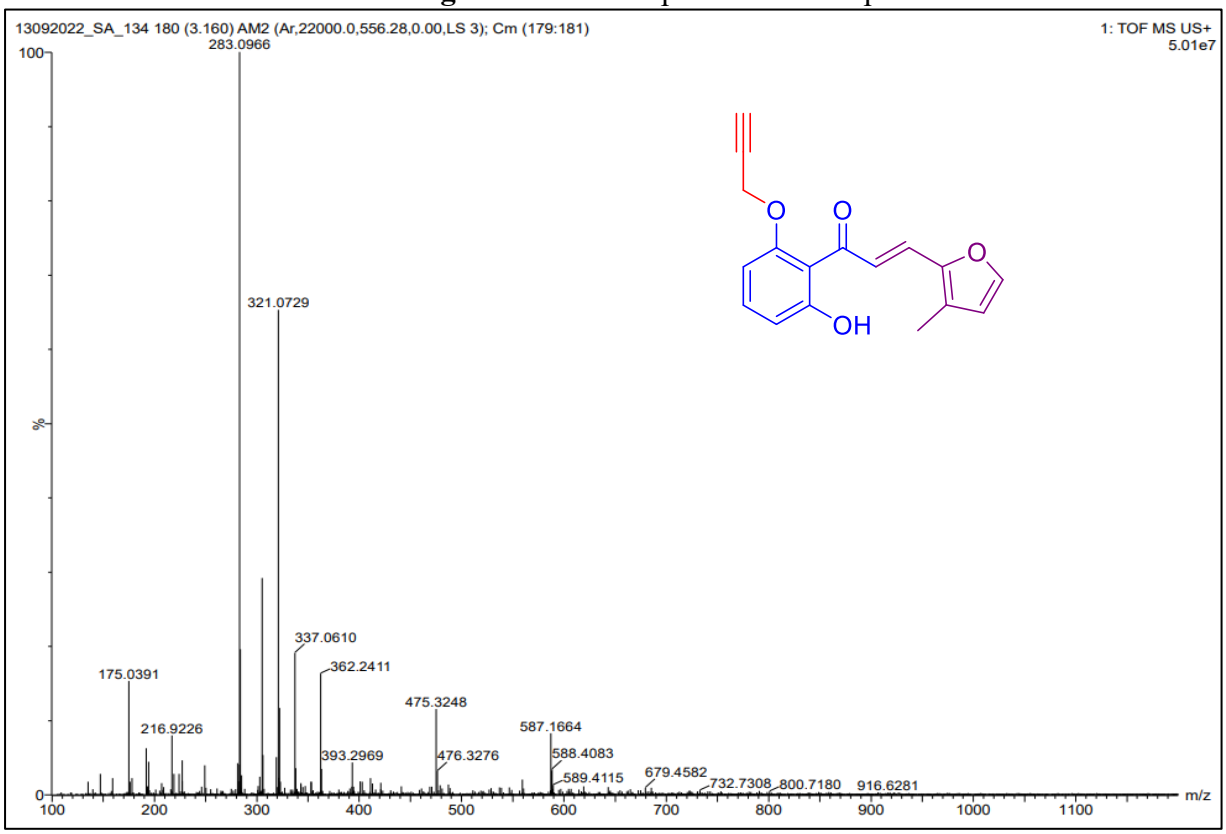


Figure 60: HRMS spectrum of compound **5k**

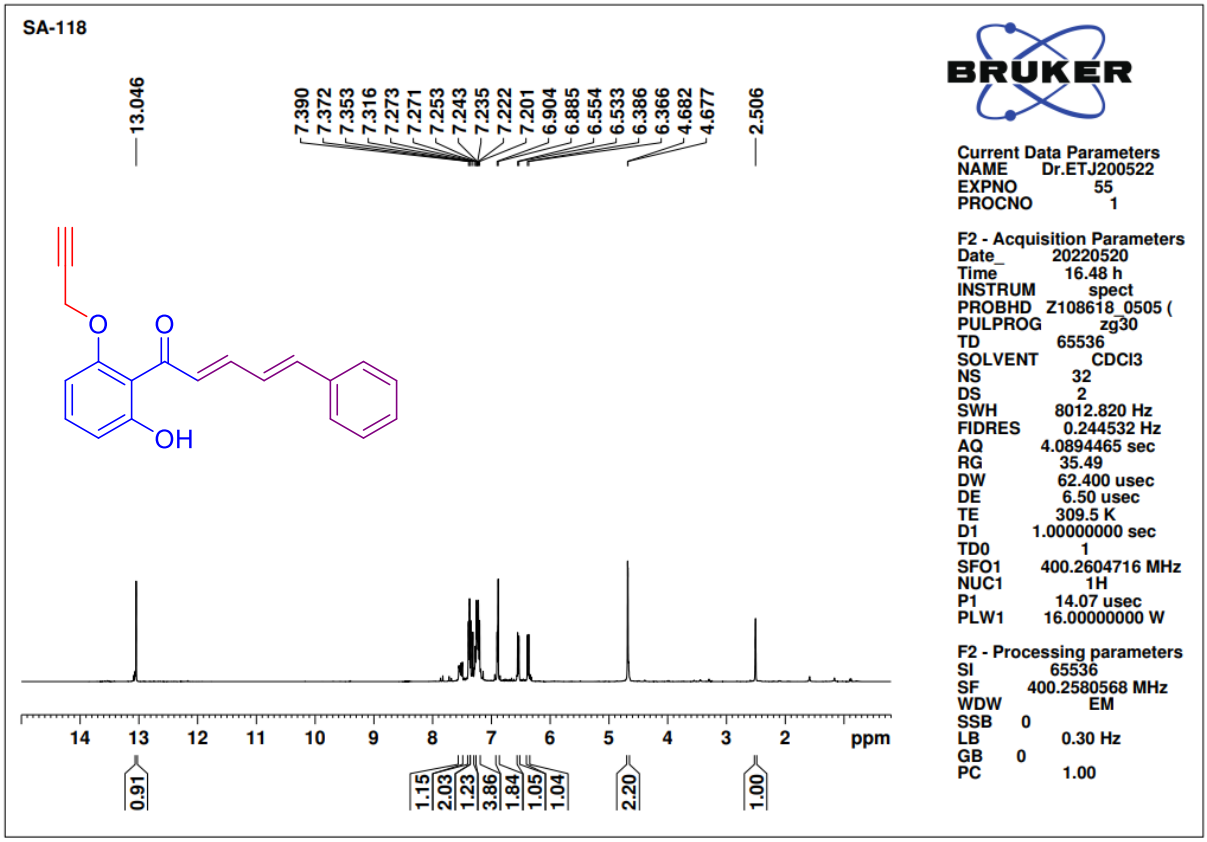


Figure 61: ^{1}H NMR spectrum of compound **5l**

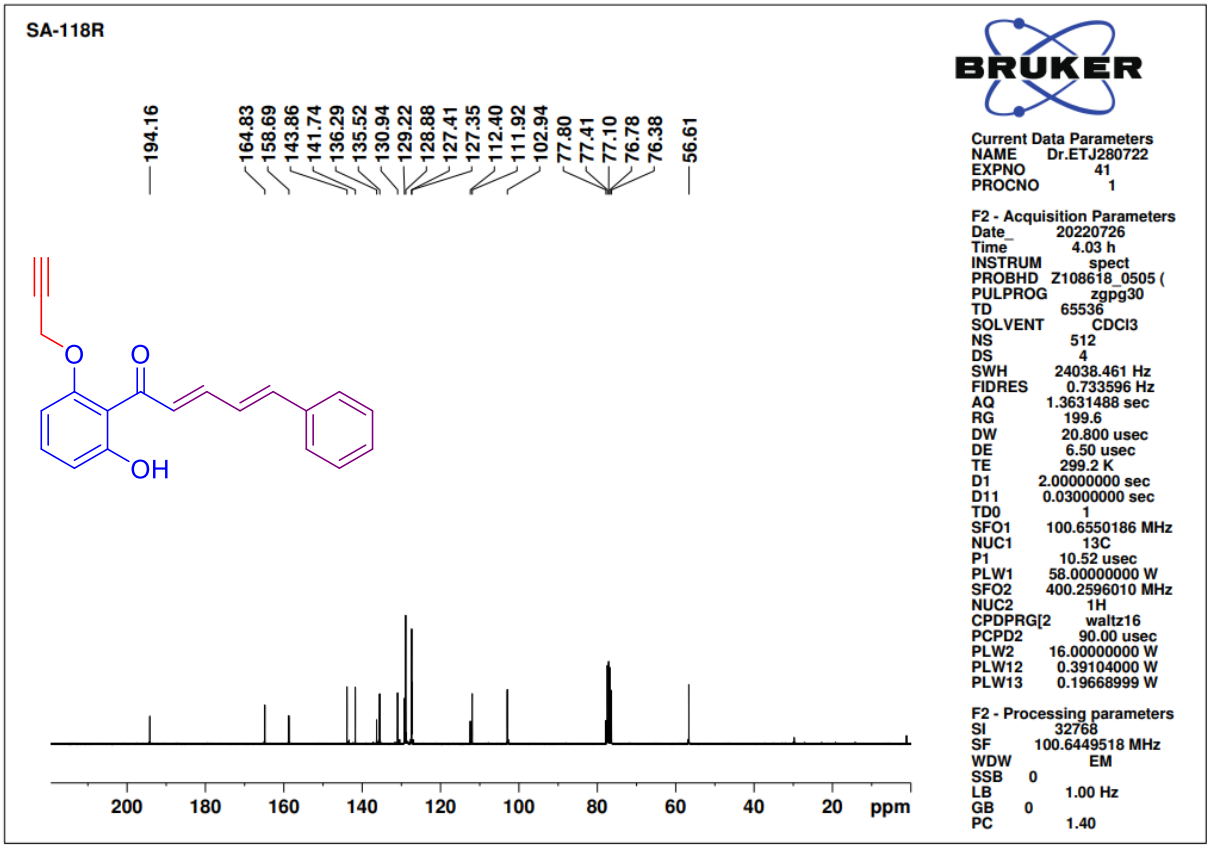


Figure 62: ^{13}C NMR spectrum of compound **5l**

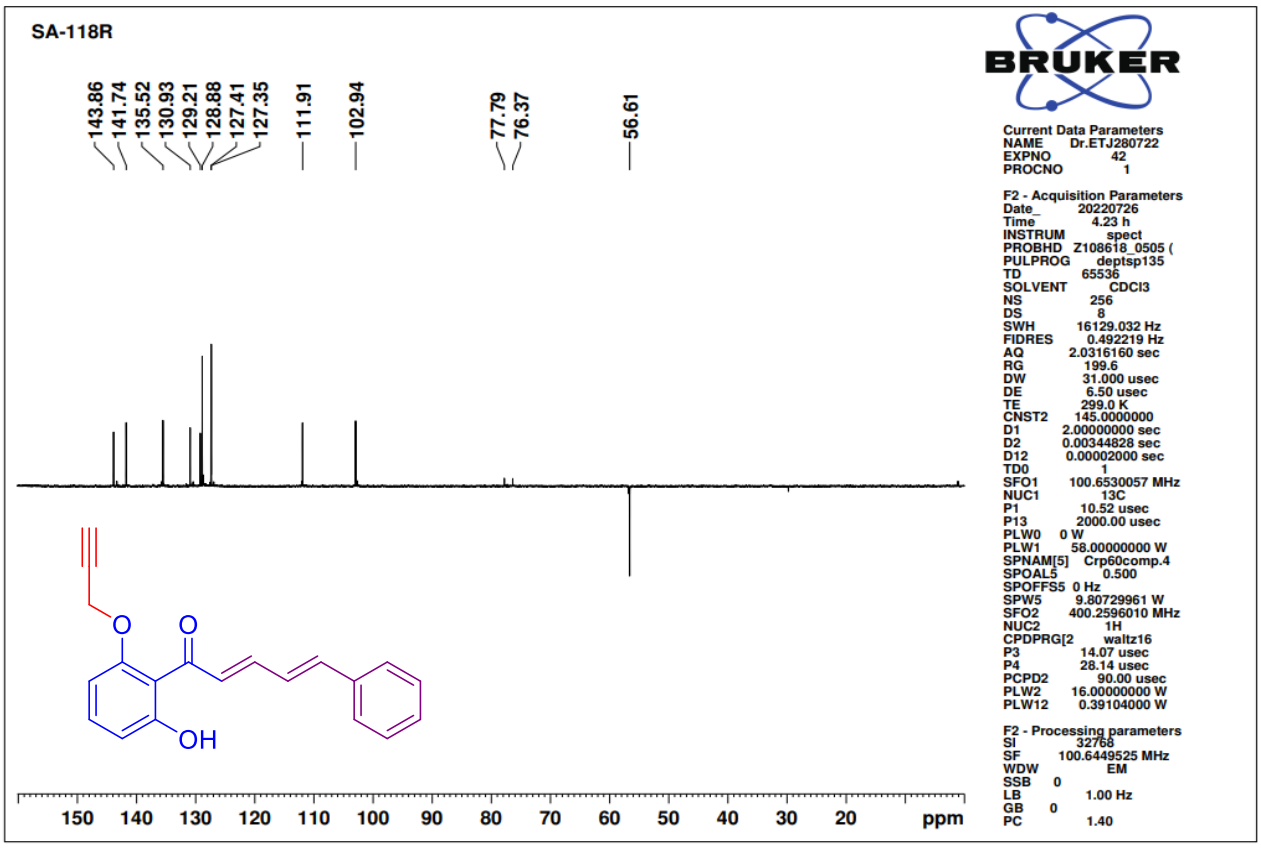


Figure 63: DEPT-135 NMR spectrum of compound **5l**

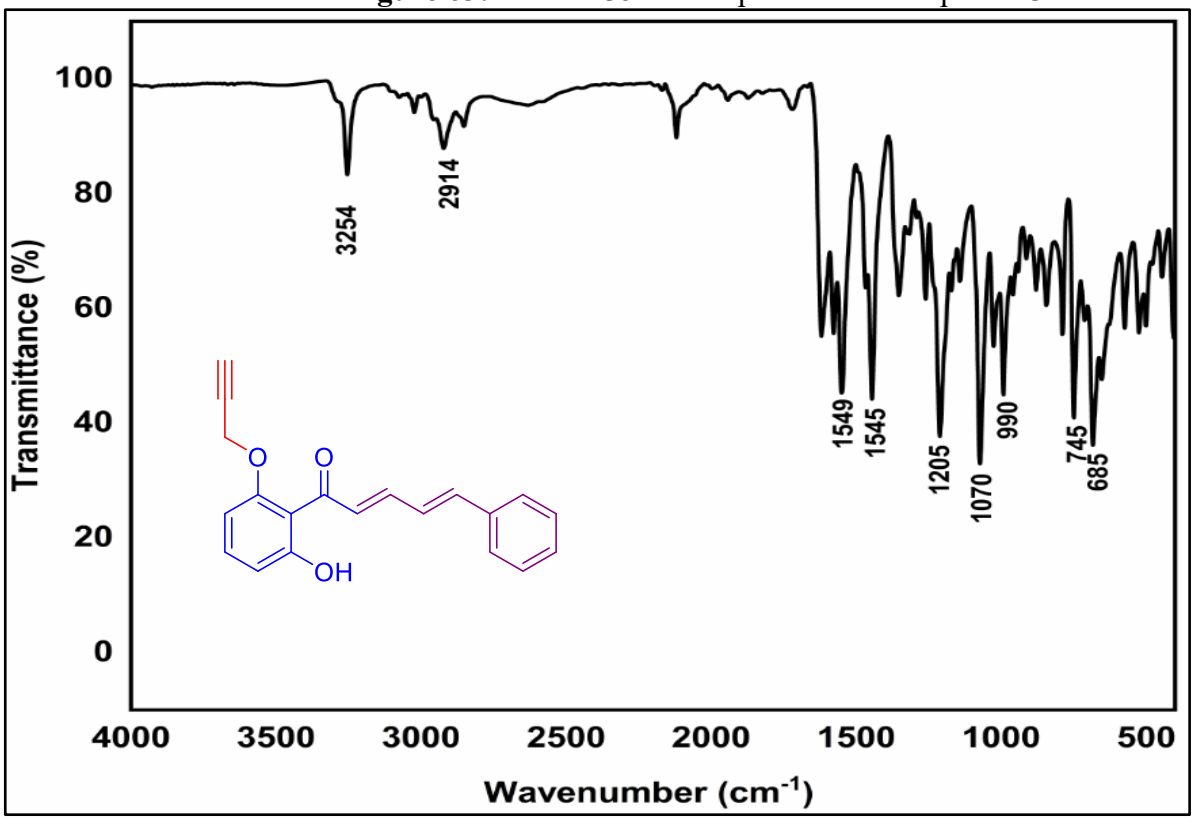


Figure 64: FT-IR spectrum of compound **5l**

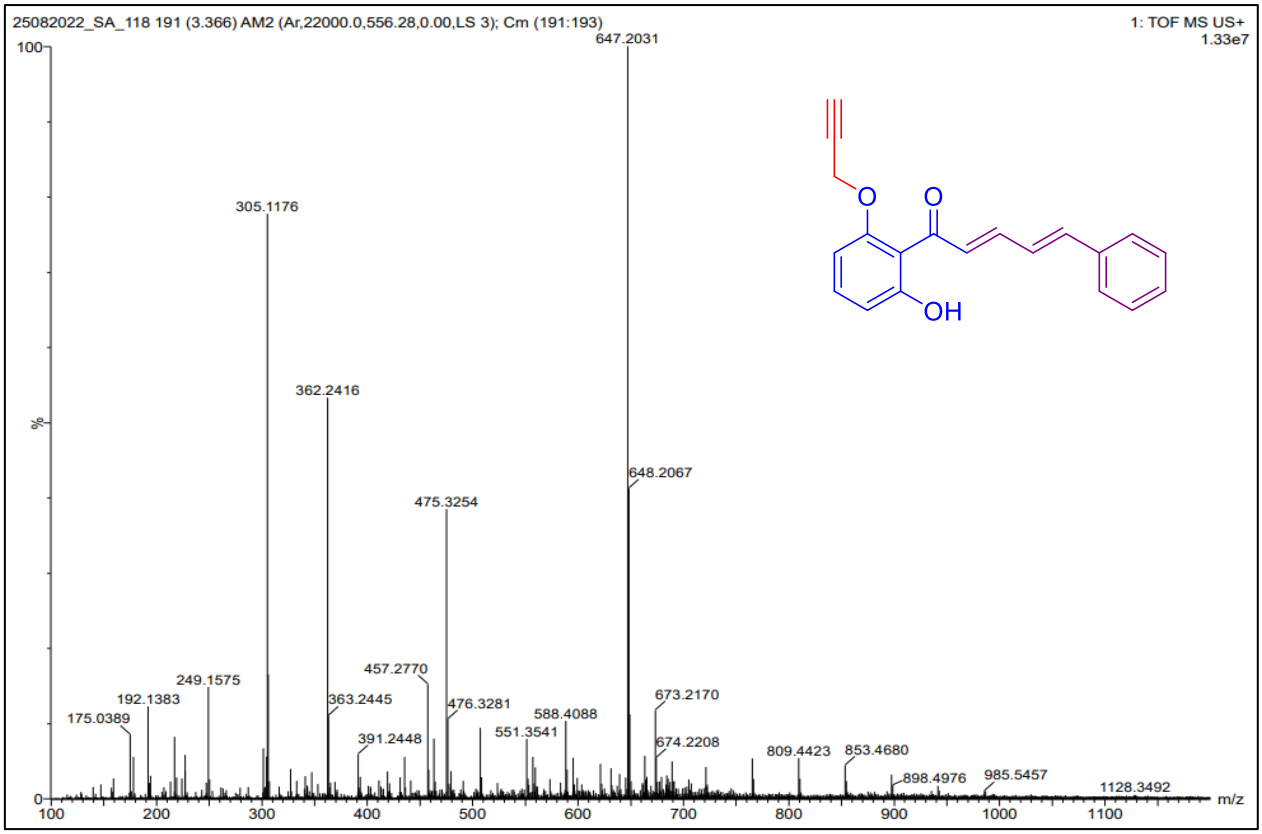


Figure 65: HRMS spectrum of compound **5l**

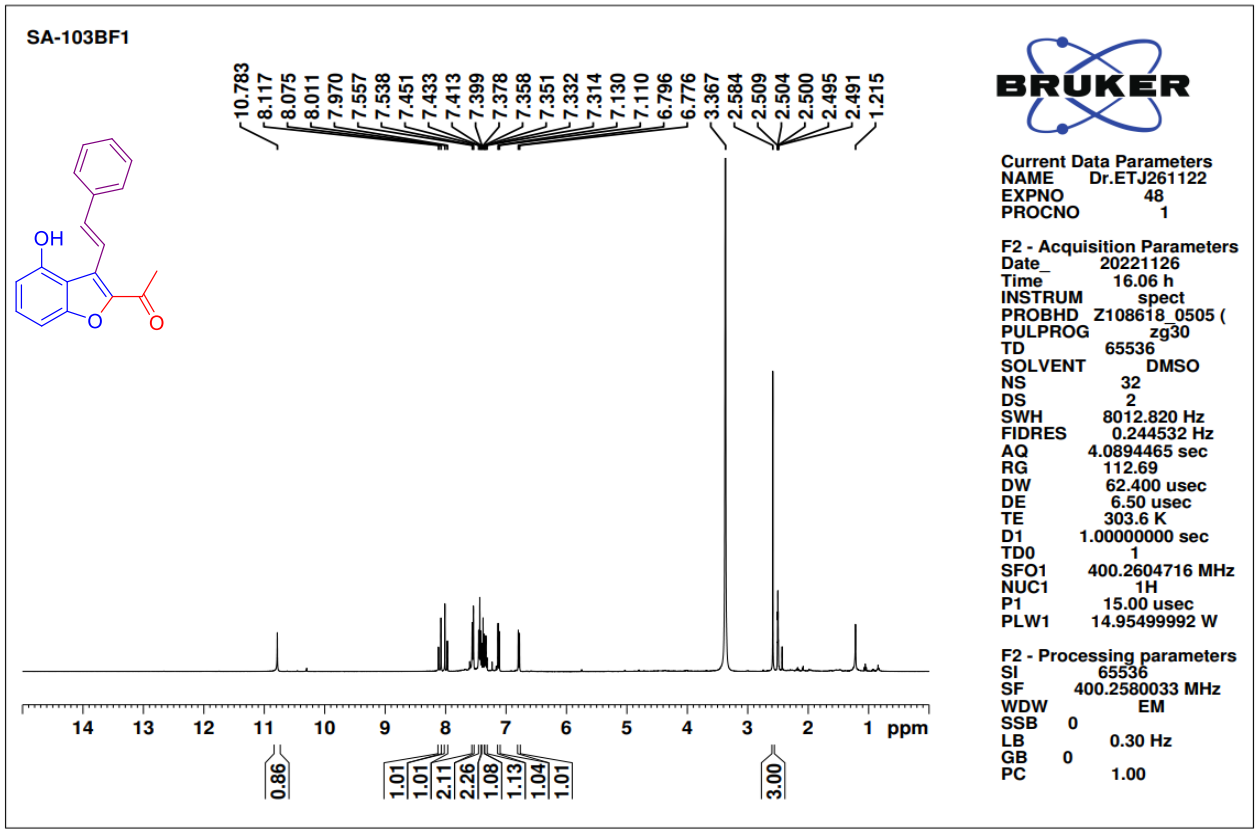


Figure 66: ^{1}H NMR spectrum of compound **6a**

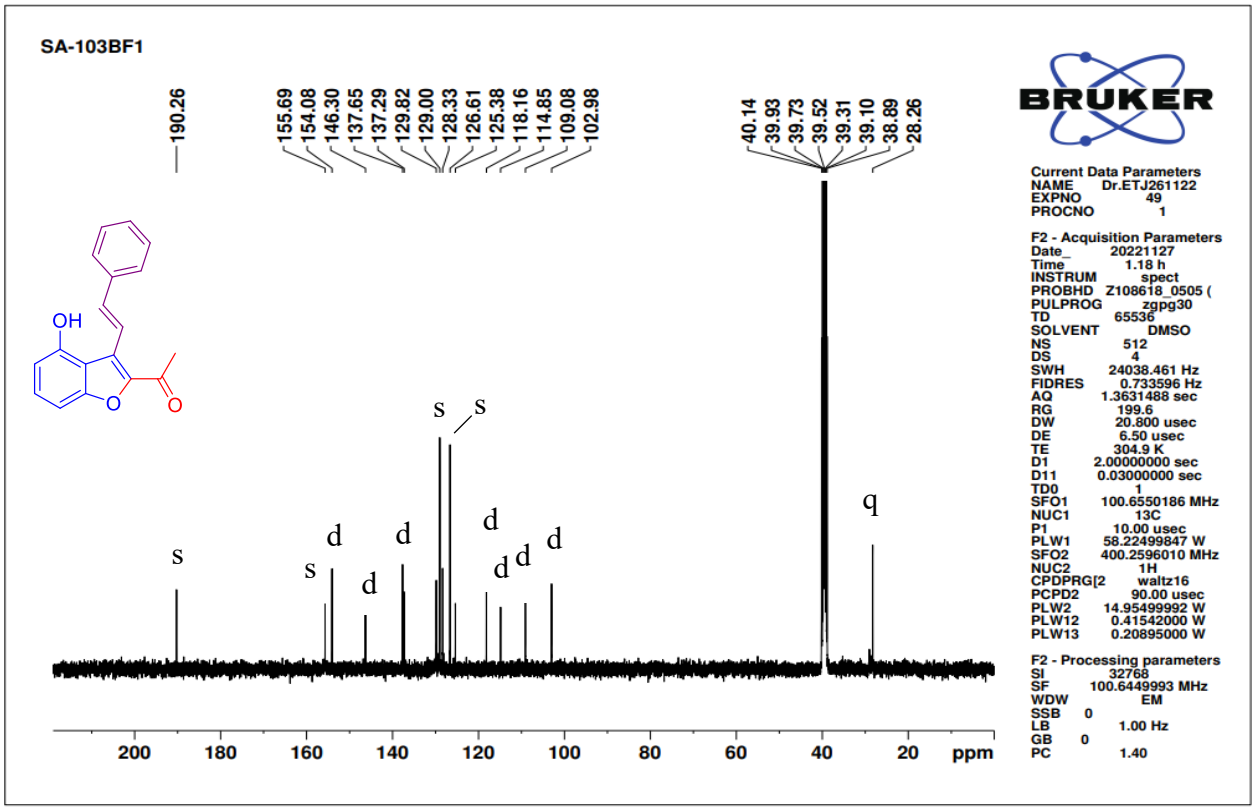


Figure 67: ^{13}C NMR spectrum of compound **6a**

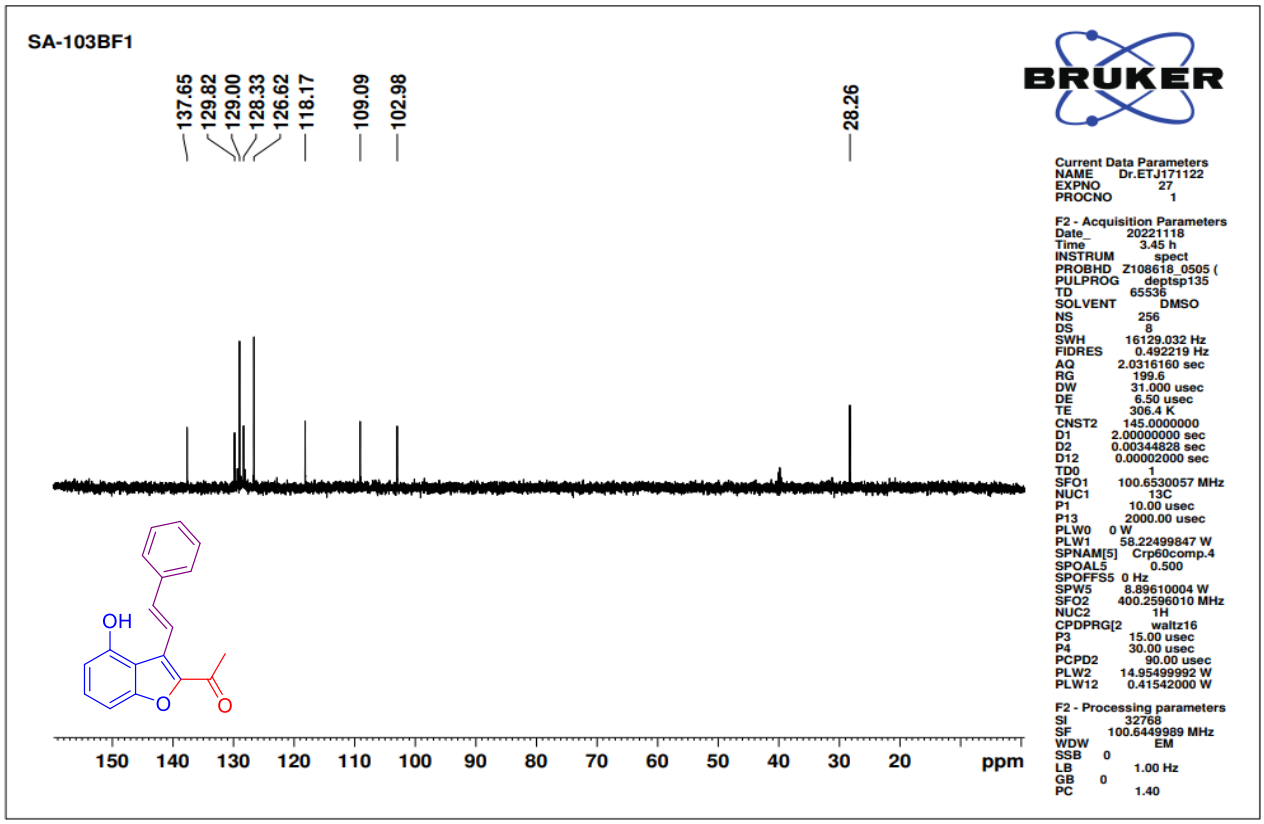


Figure 68: DEPT-135 NMR spectrum of compound **6a**

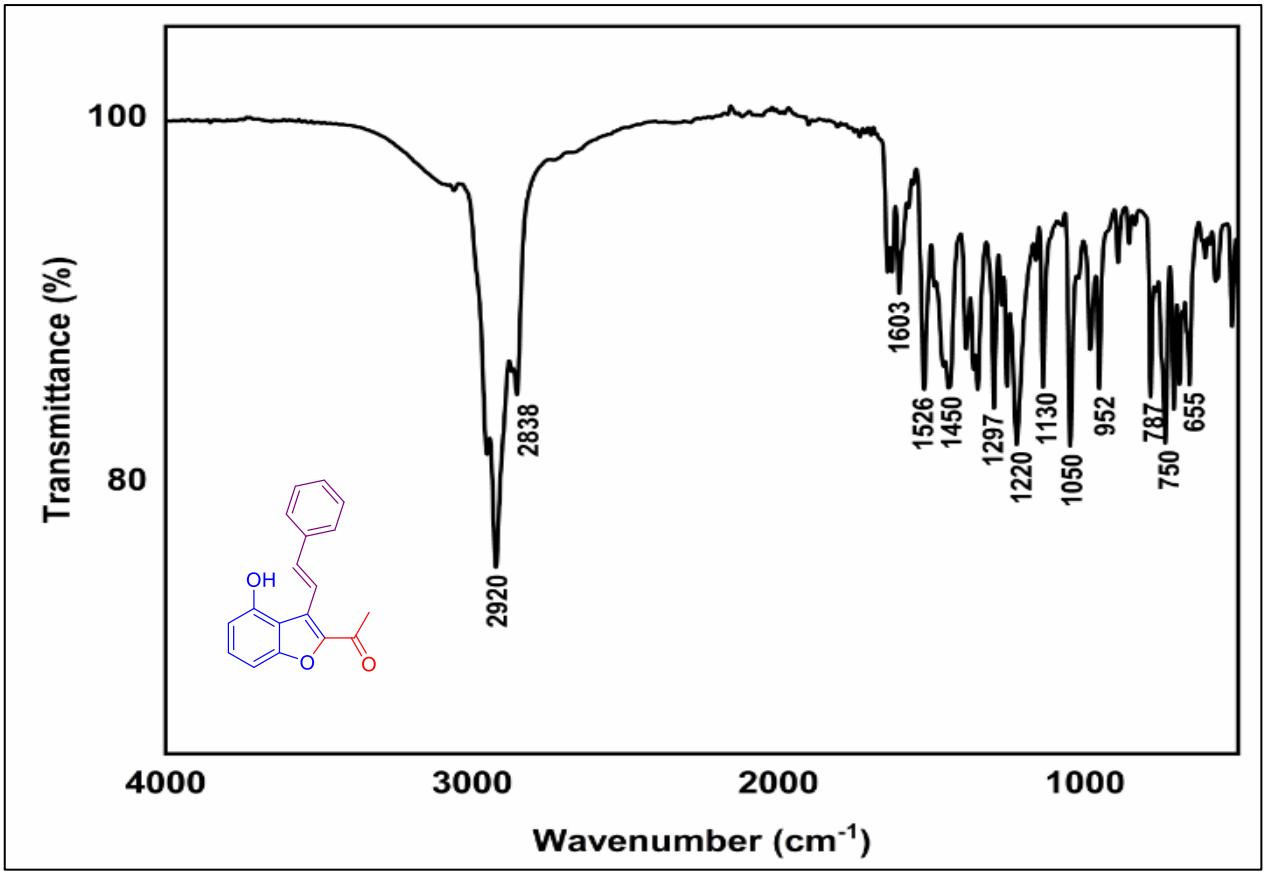


Figure 69: FT-IR spectrum of compound **6a**

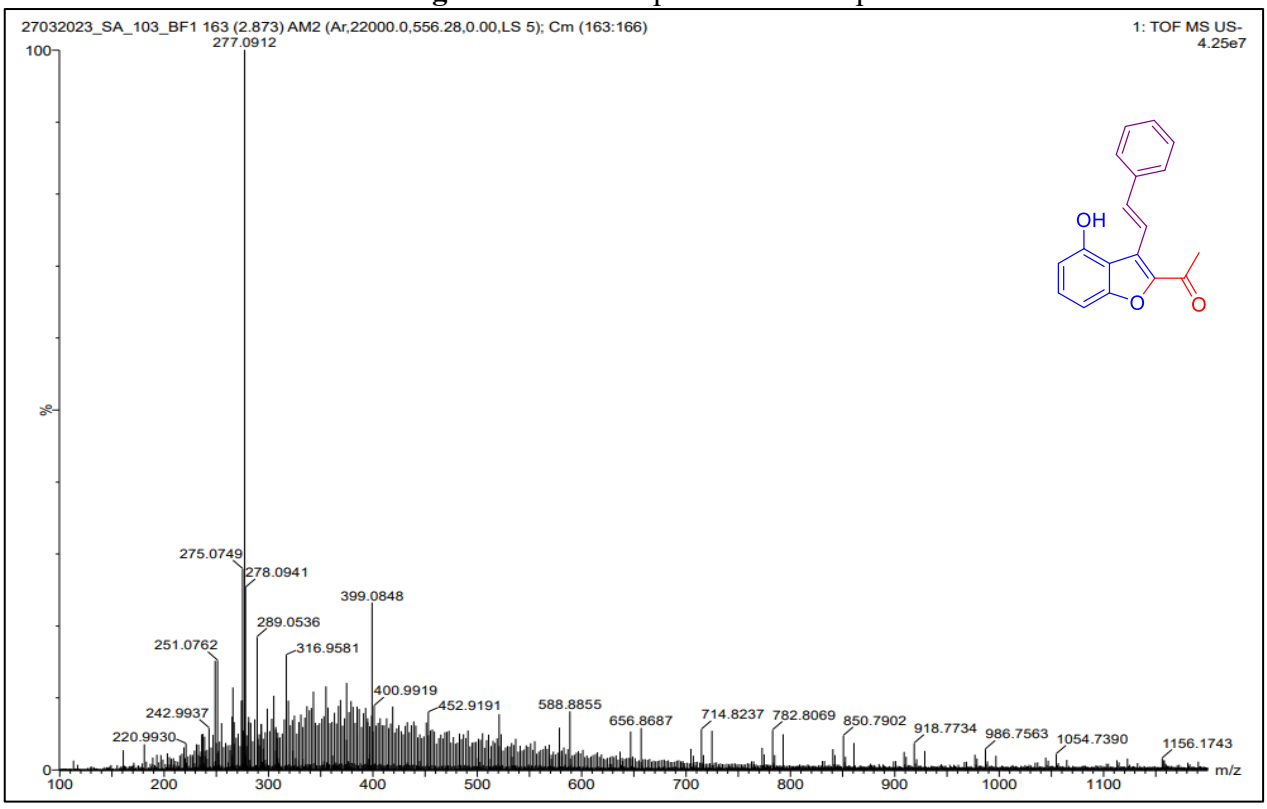


Figure 70: HRMS spectrum of compound **6a**

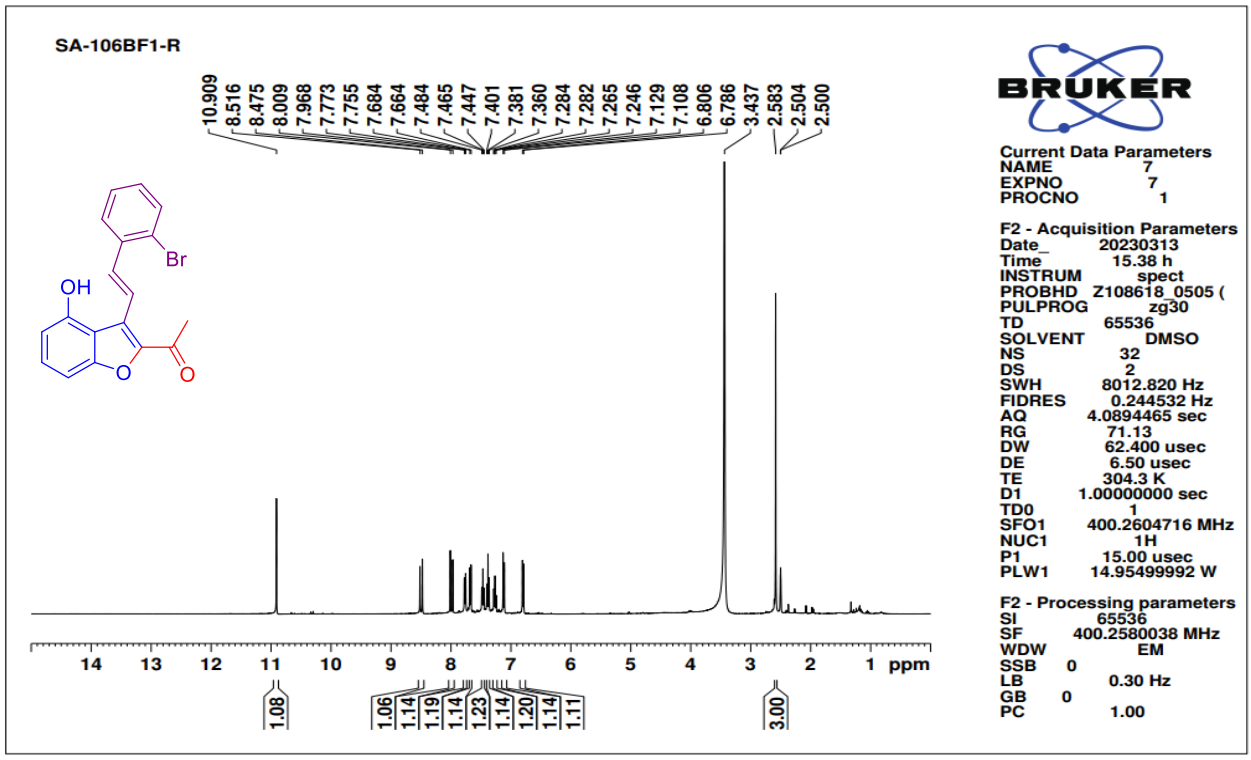


Figure 71: ^{1}H NMR spectrum of compound **6b**

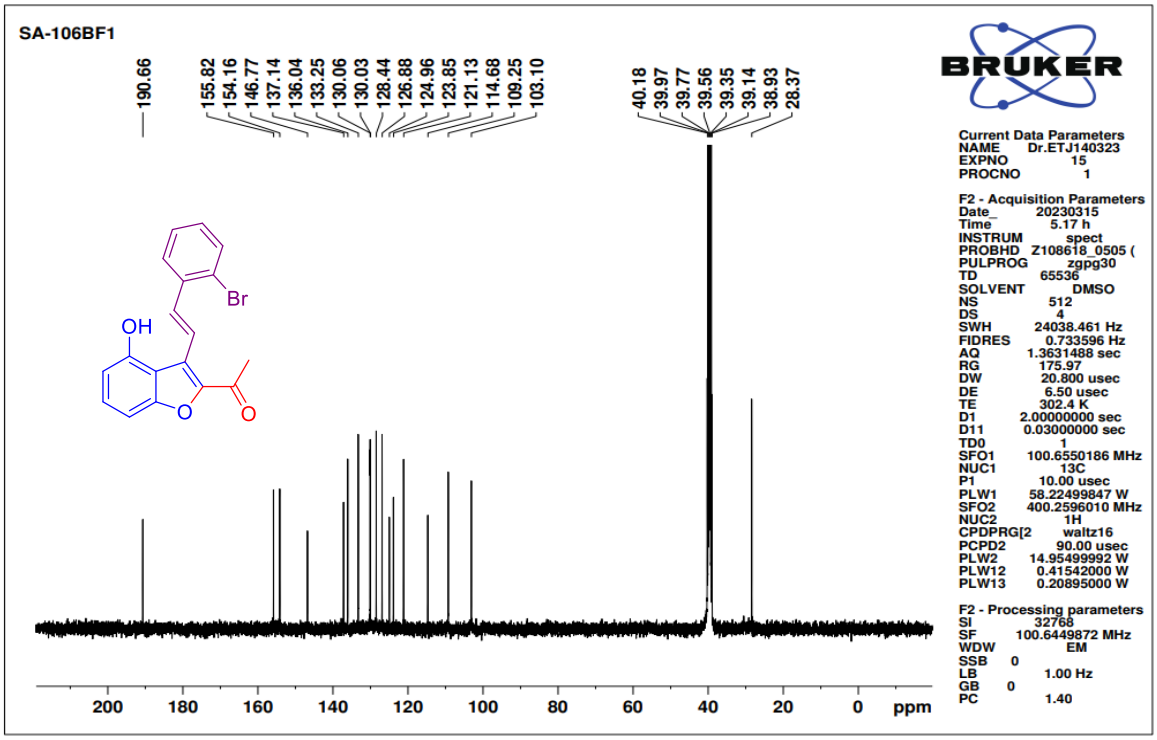


Figure 72: ^{13}C NMR spectrum of compound **6b**

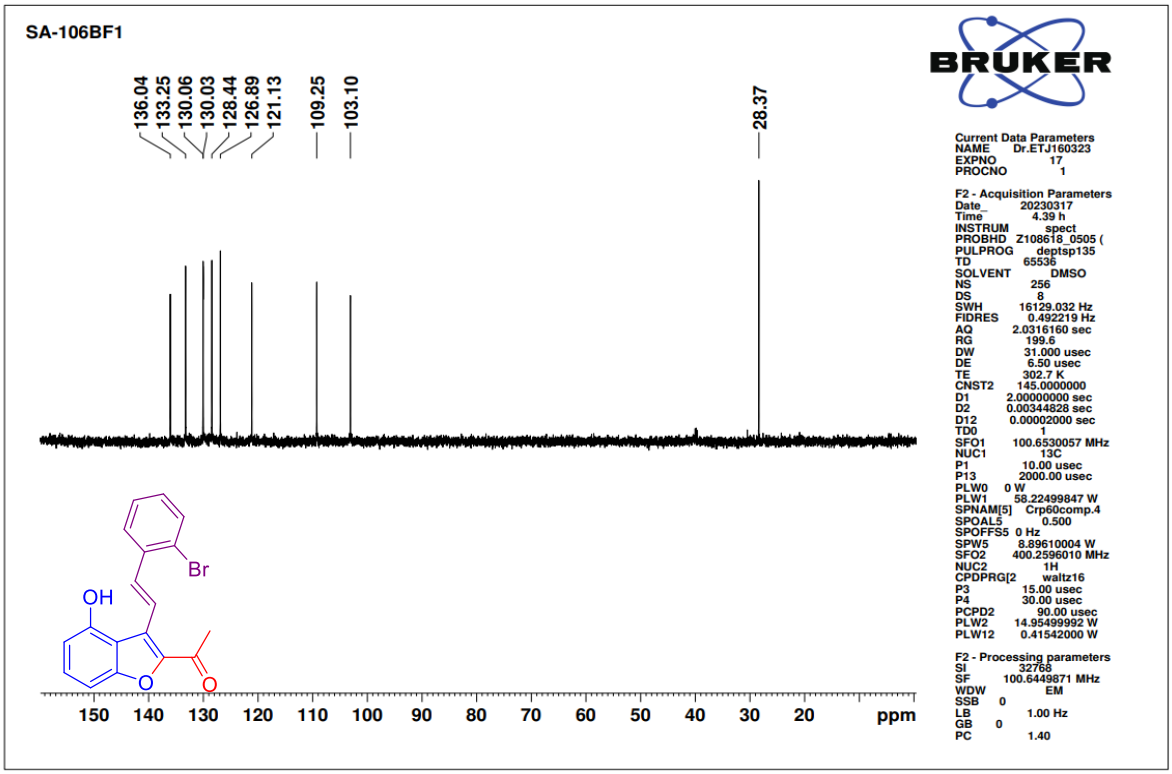


Figure 73: DEPT-135 NMR spectrum of compound **6b**

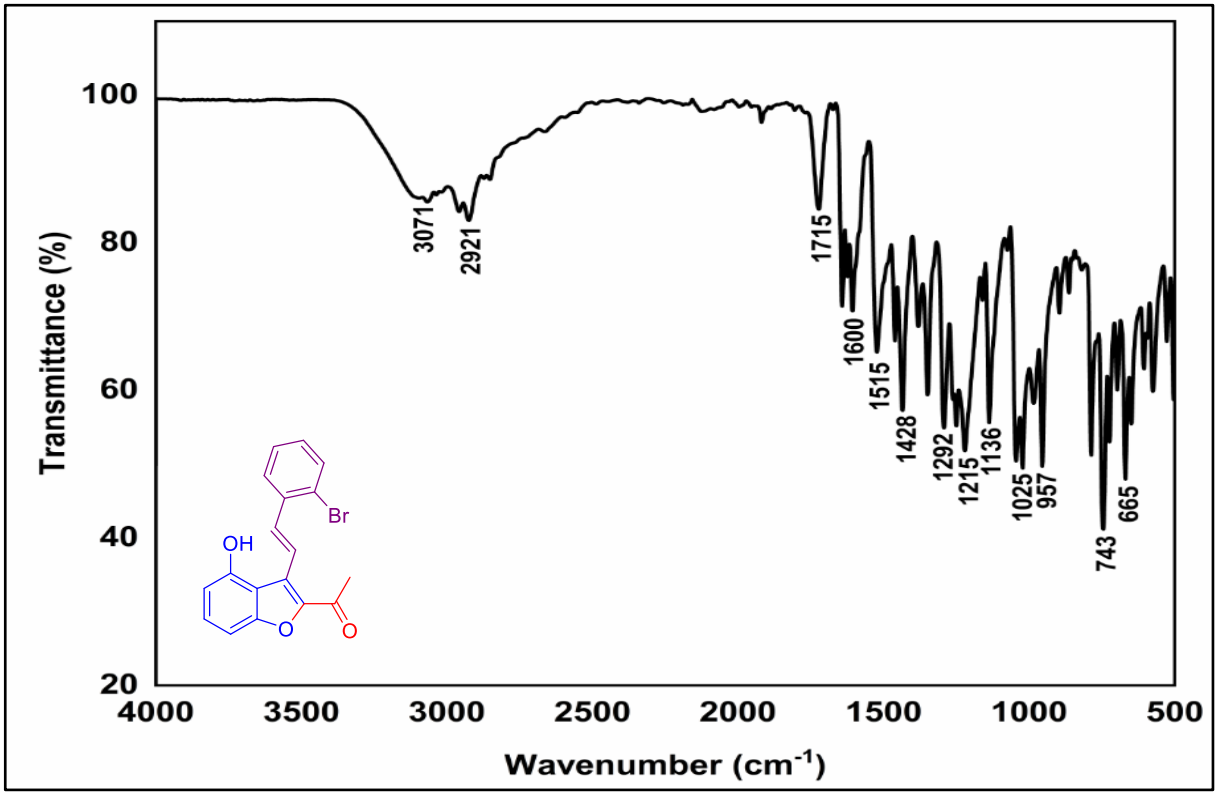


Figure 74: FT-IR spectrum of compound **6b**

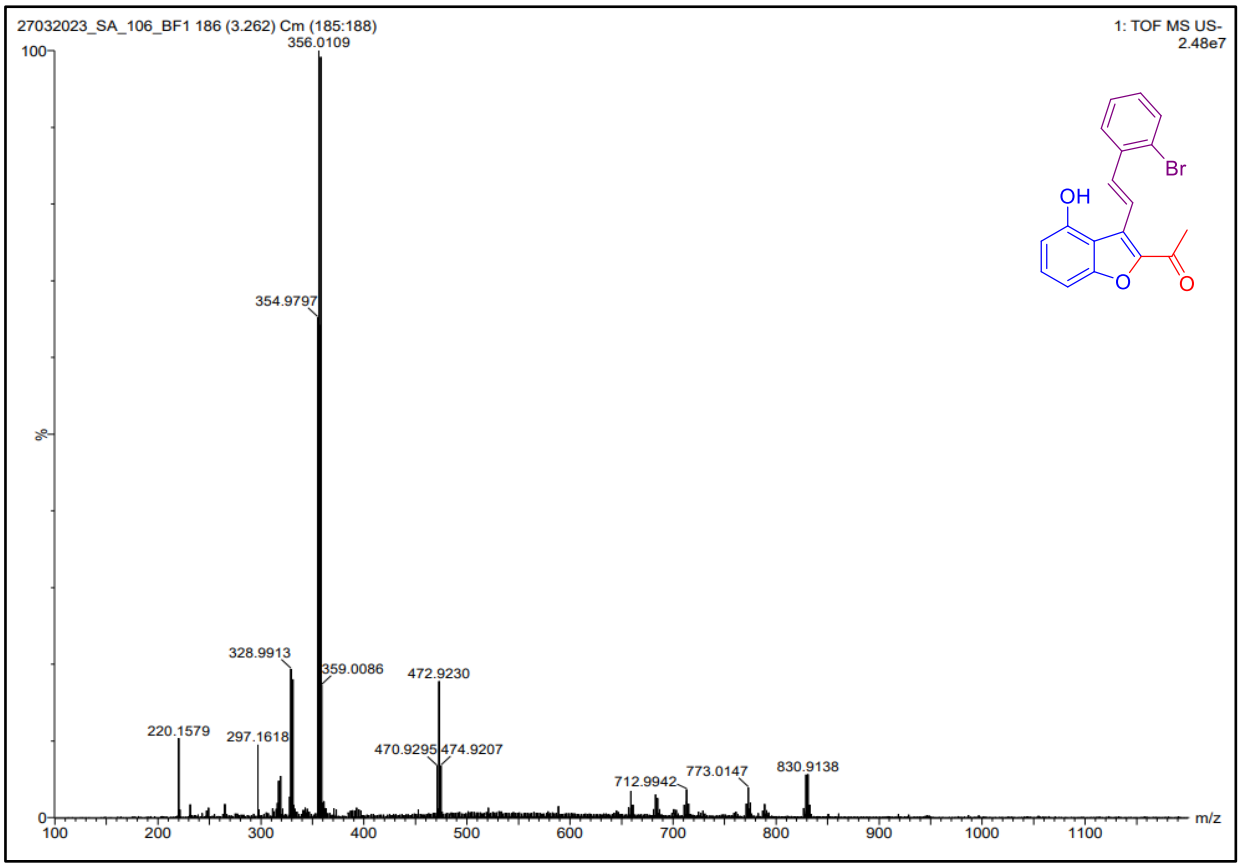


Figure 75: HRMS spectrum of compound **6b**

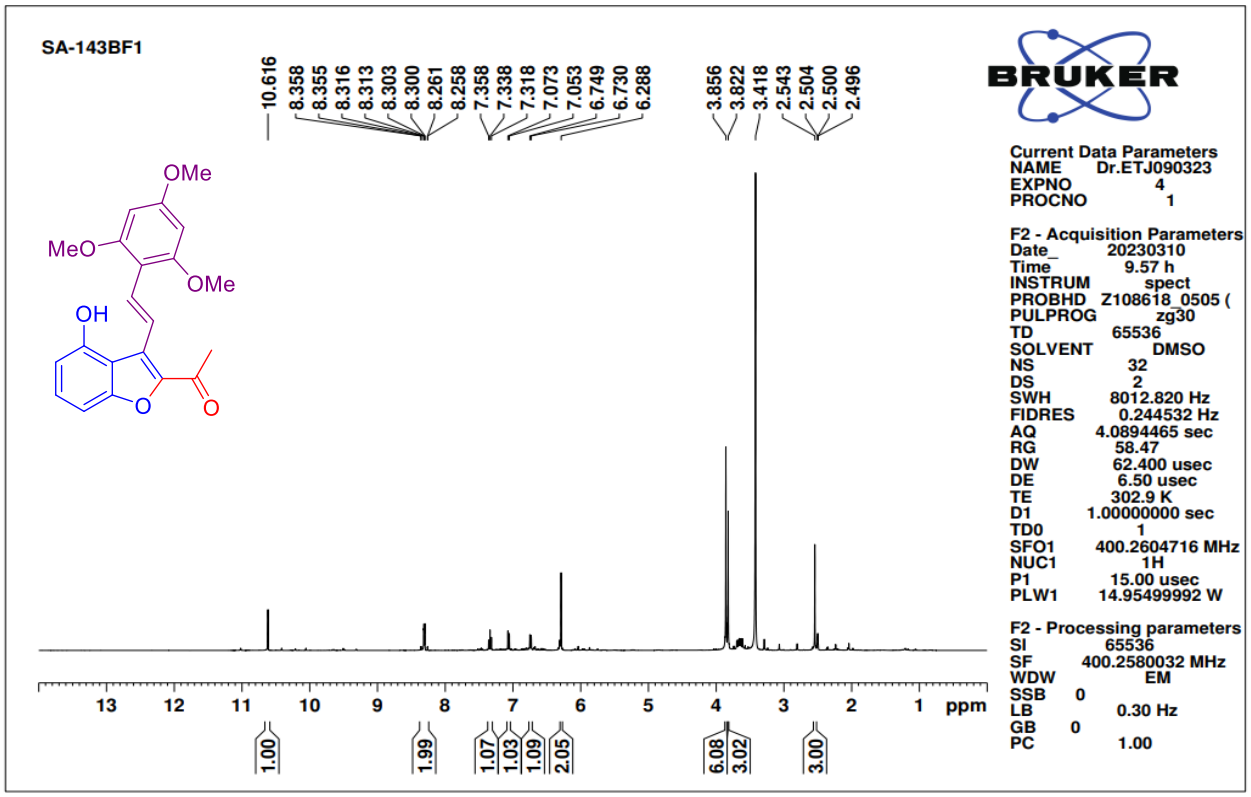


Figure 76: ^{1}H NMR spectrum of compound **6c**

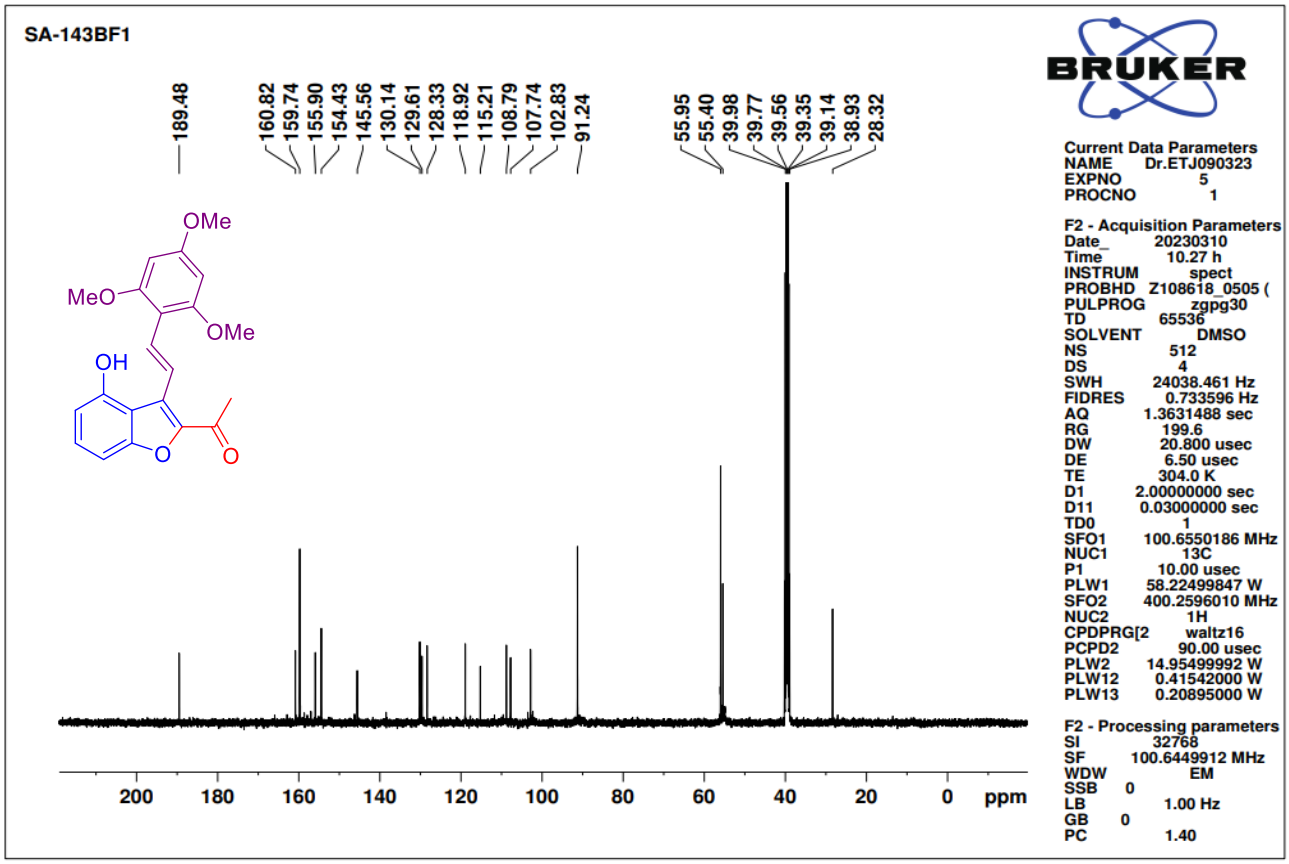


Figure 77: ^{13}C NMR spectrum of compound **6c**

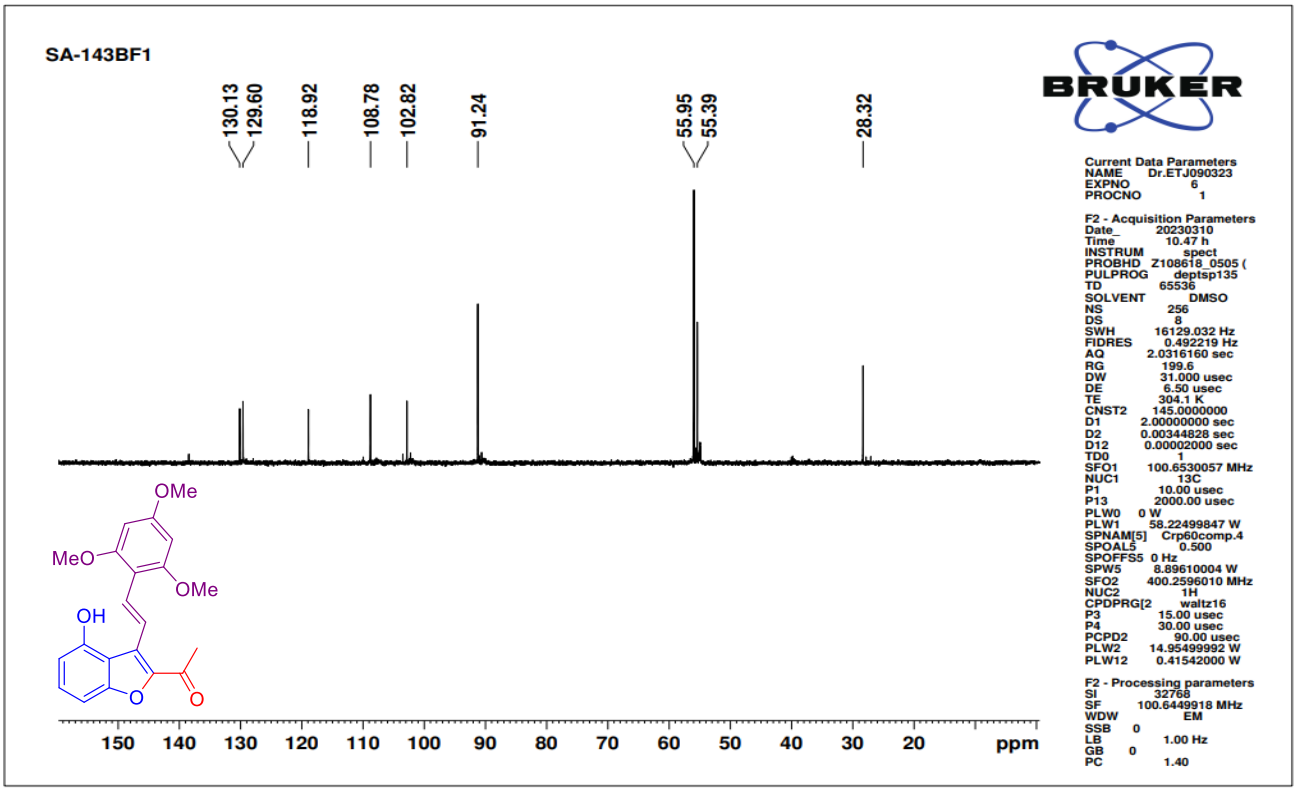


Figure 78: DEPT-135 NMR spectrum of compound **6c**

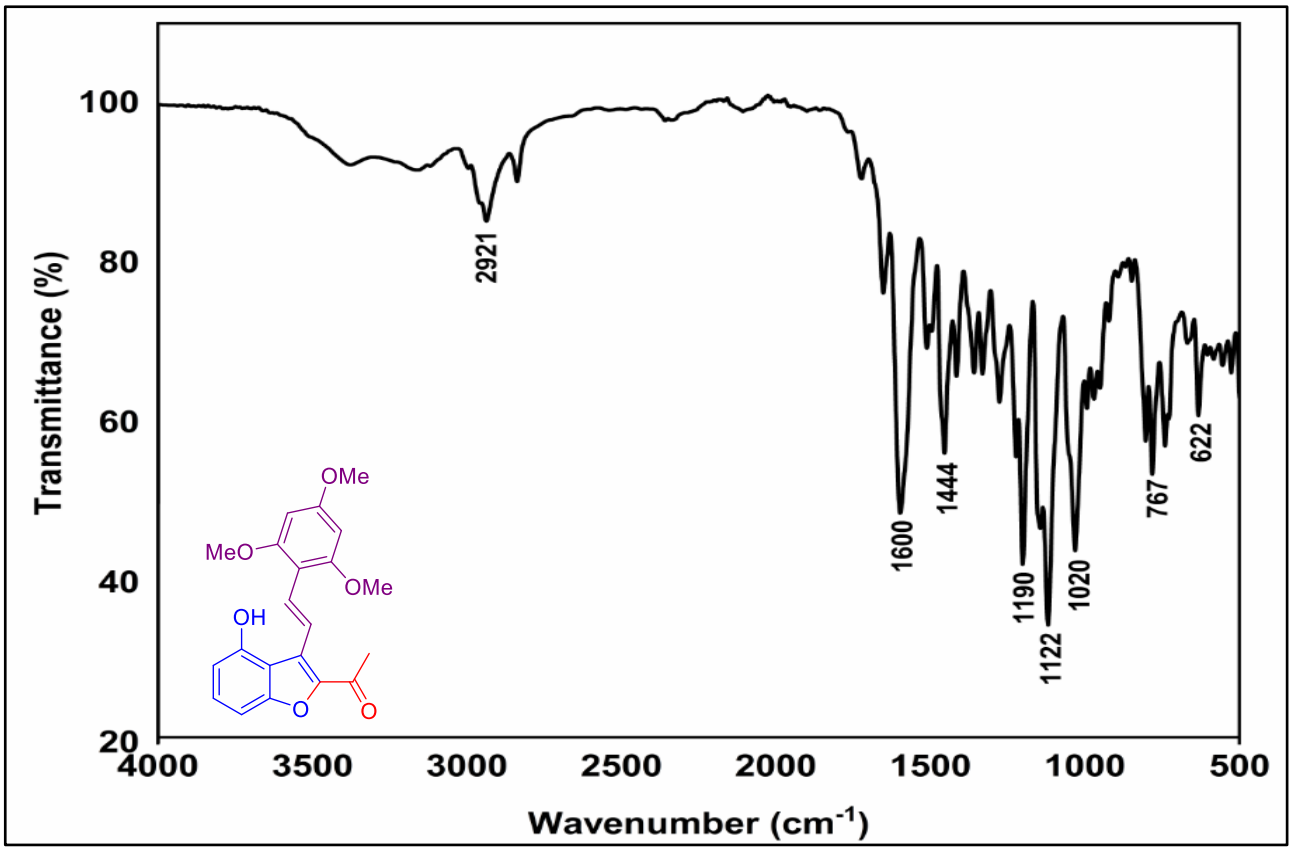


Figure 79: FT-IR spectrum of compound **6c**

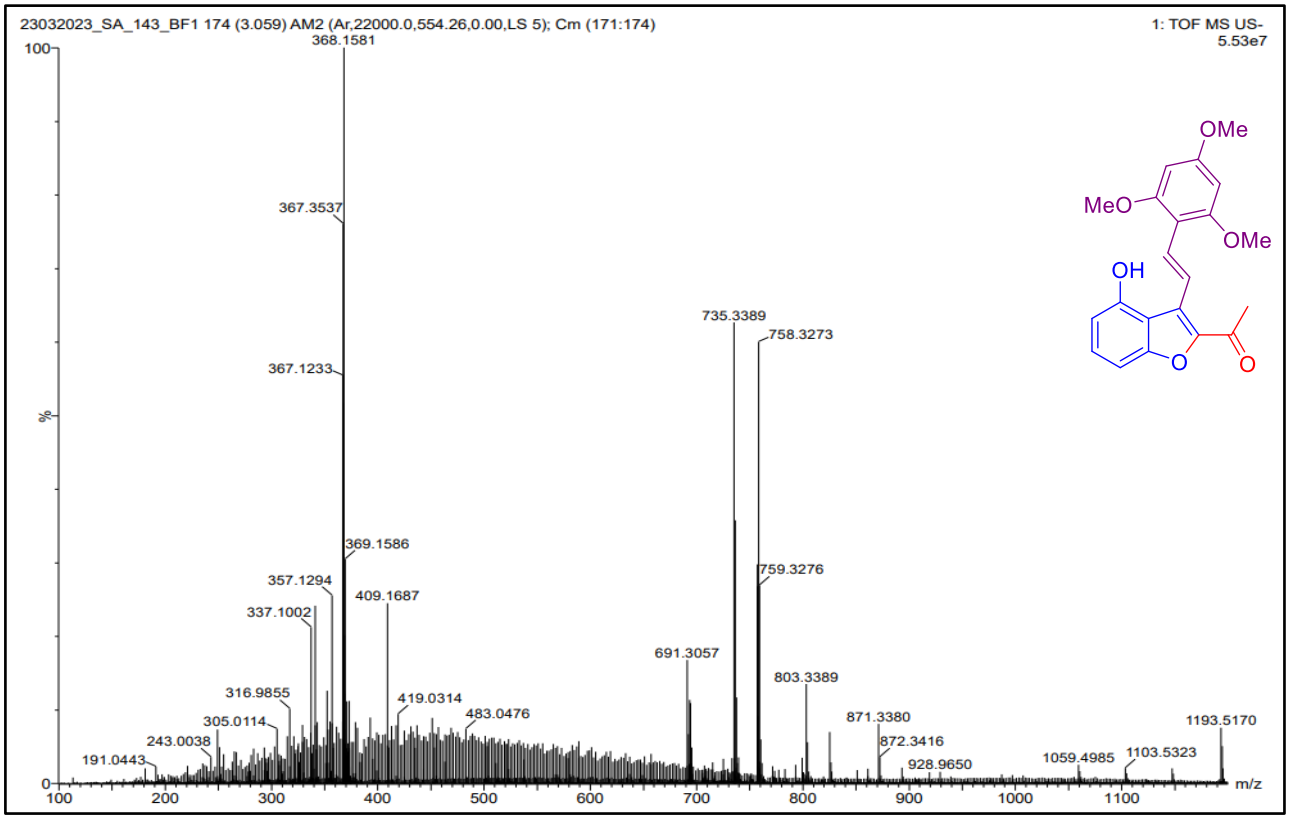


Figure 80: HRMS spectrum of compound **6c**

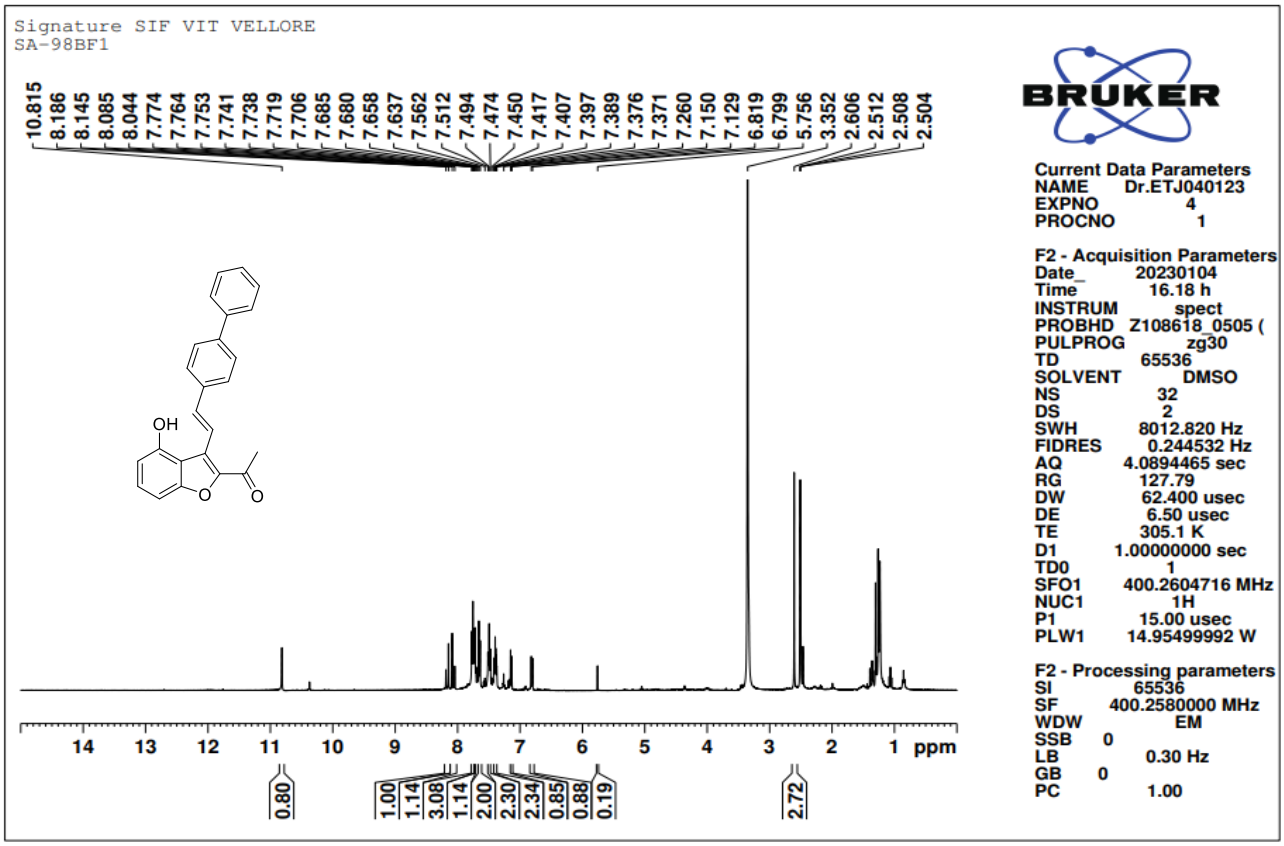


Figure 81: ^{1}H NMR spectrum of compound **6d**

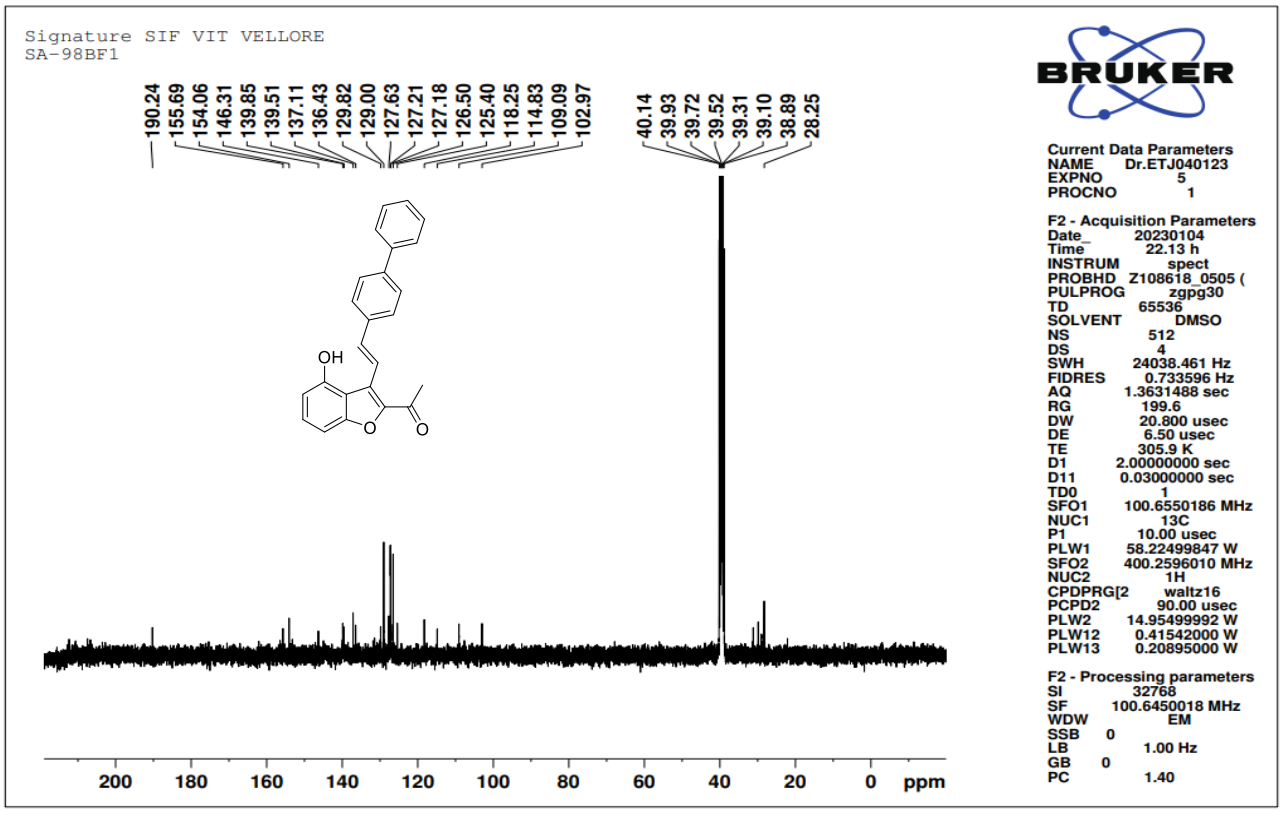


Figure 82: ^{13}C NMR spectrum of compound **6d**

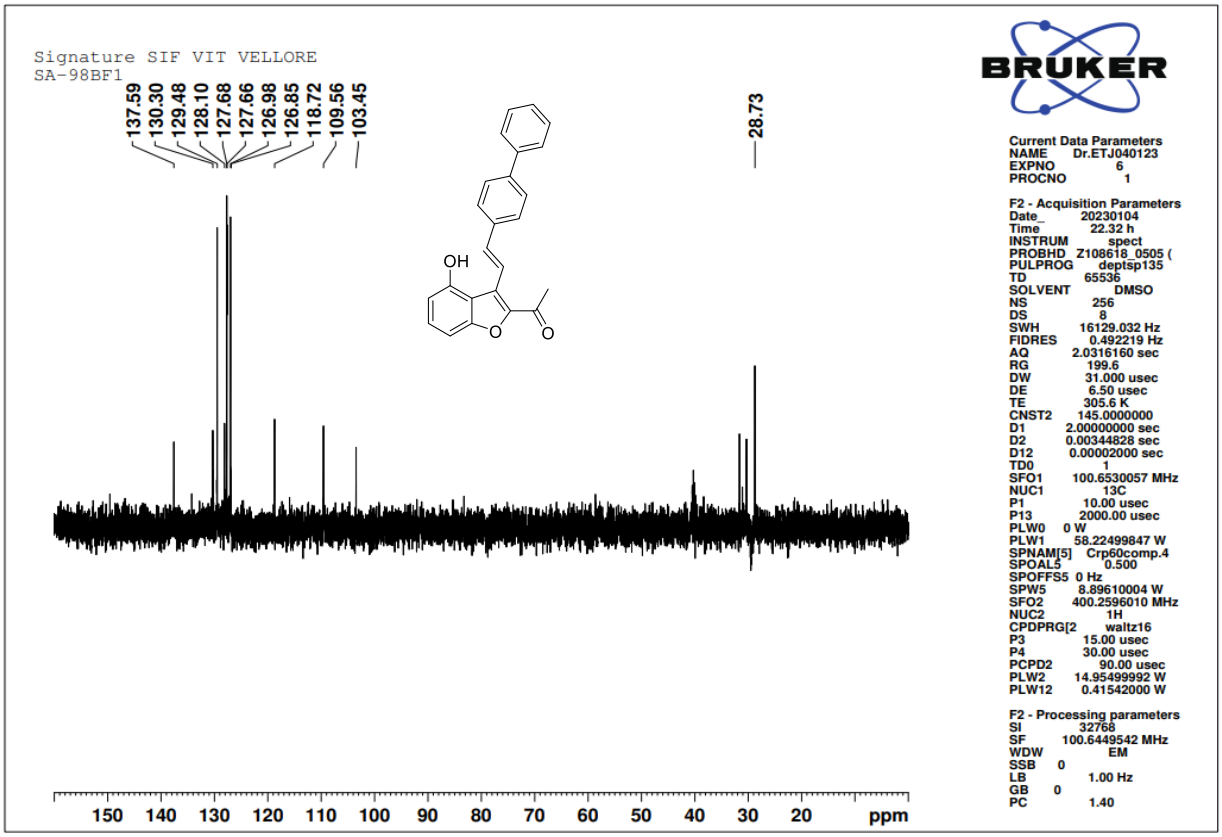


Figure 83: DEPT-135 NMR spectrum of compound **6d**

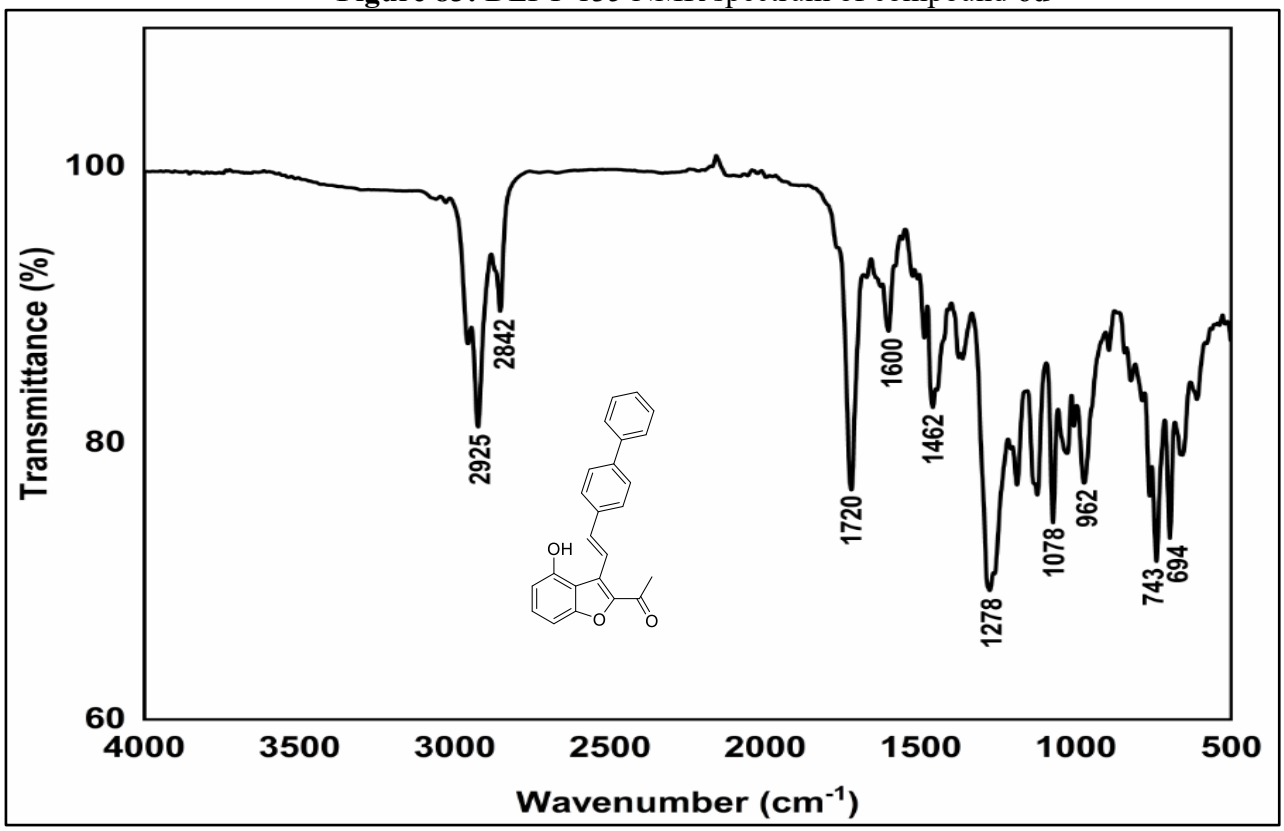


Figure 84: FT-IR spectrum of compound **6d**

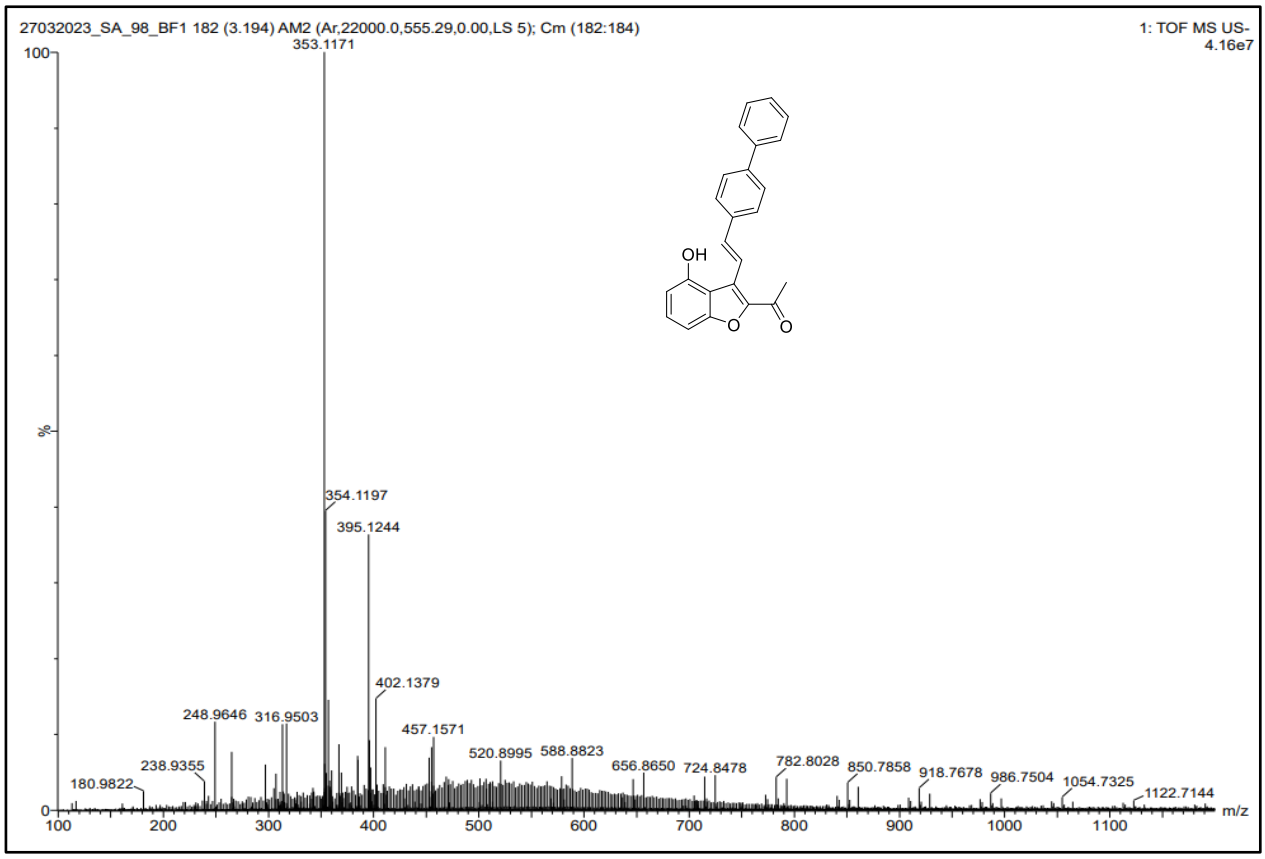


Figure 85: HRMS spectrum of compound **6d**

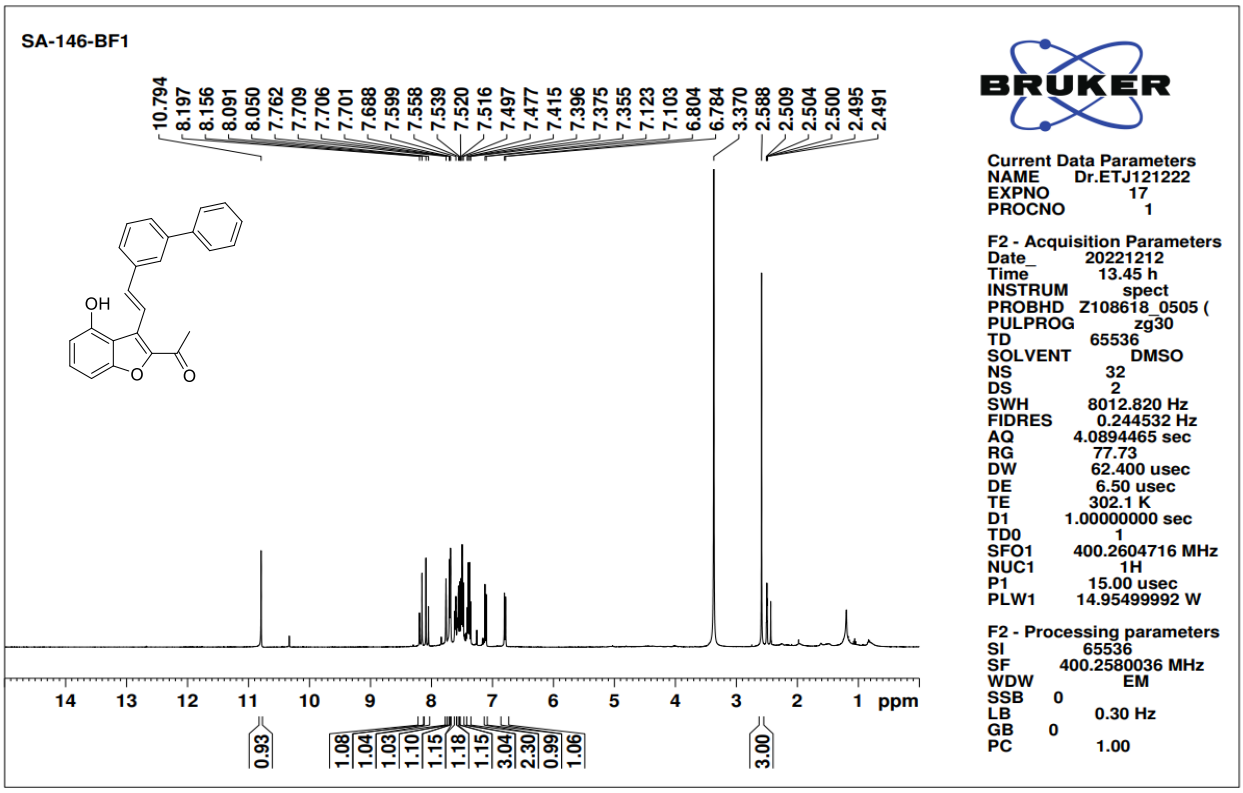


Figure 86: ^{1}H NMR spectrum of compound **6e**

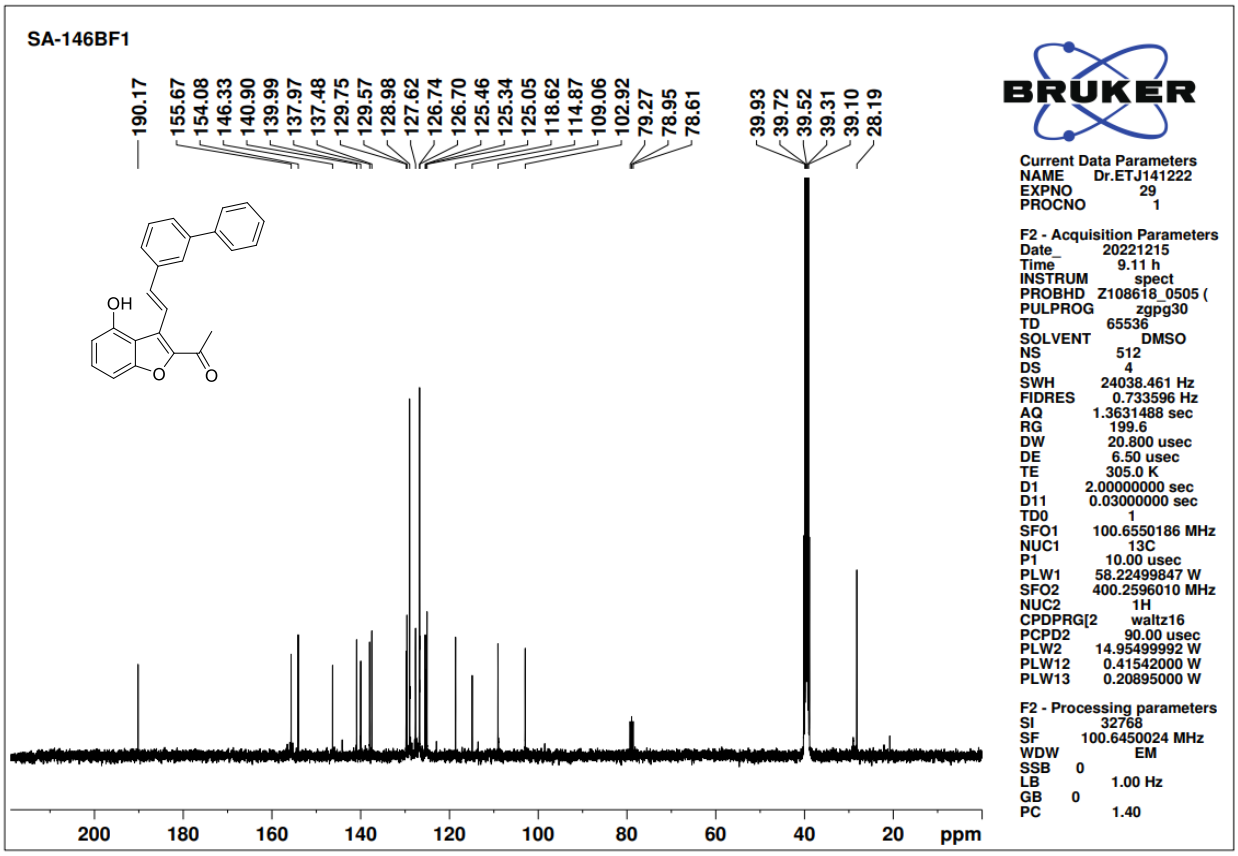


Figure 87: ^{13}C NMR spectrum of compound **6e**

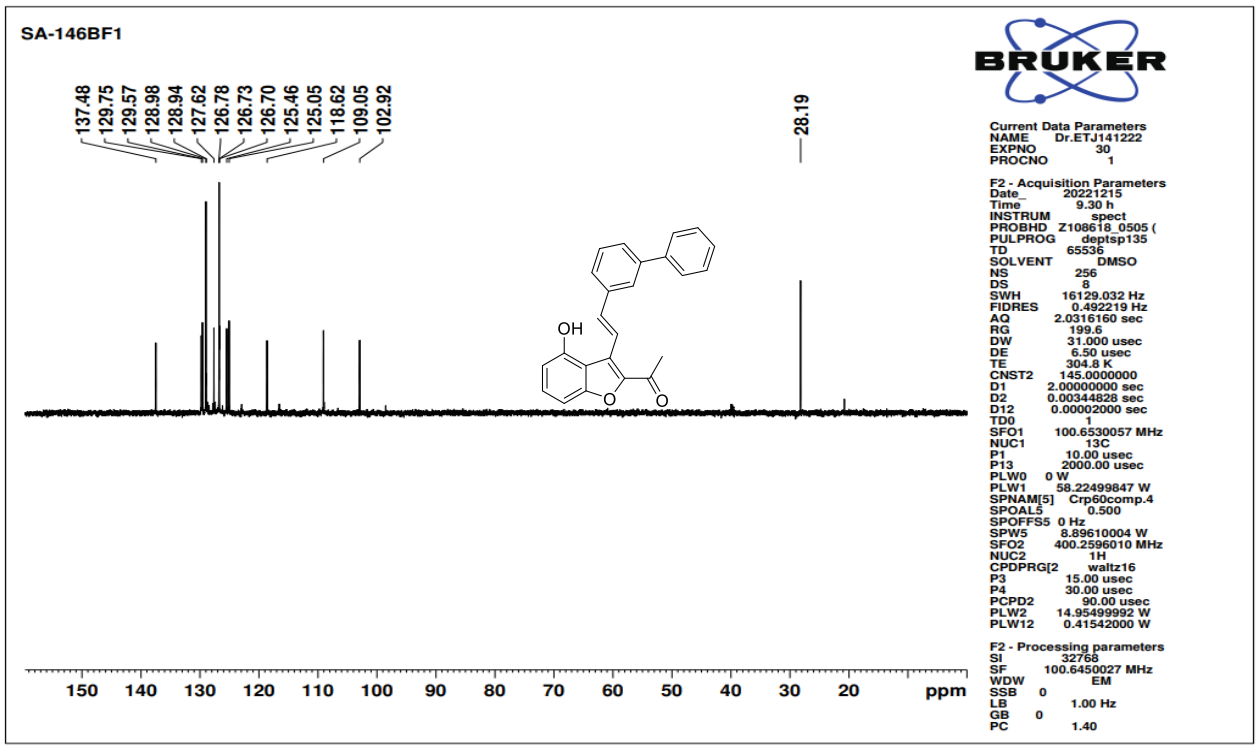


Figure 88: DEPT-135 NMR spectrum of compound **6e**

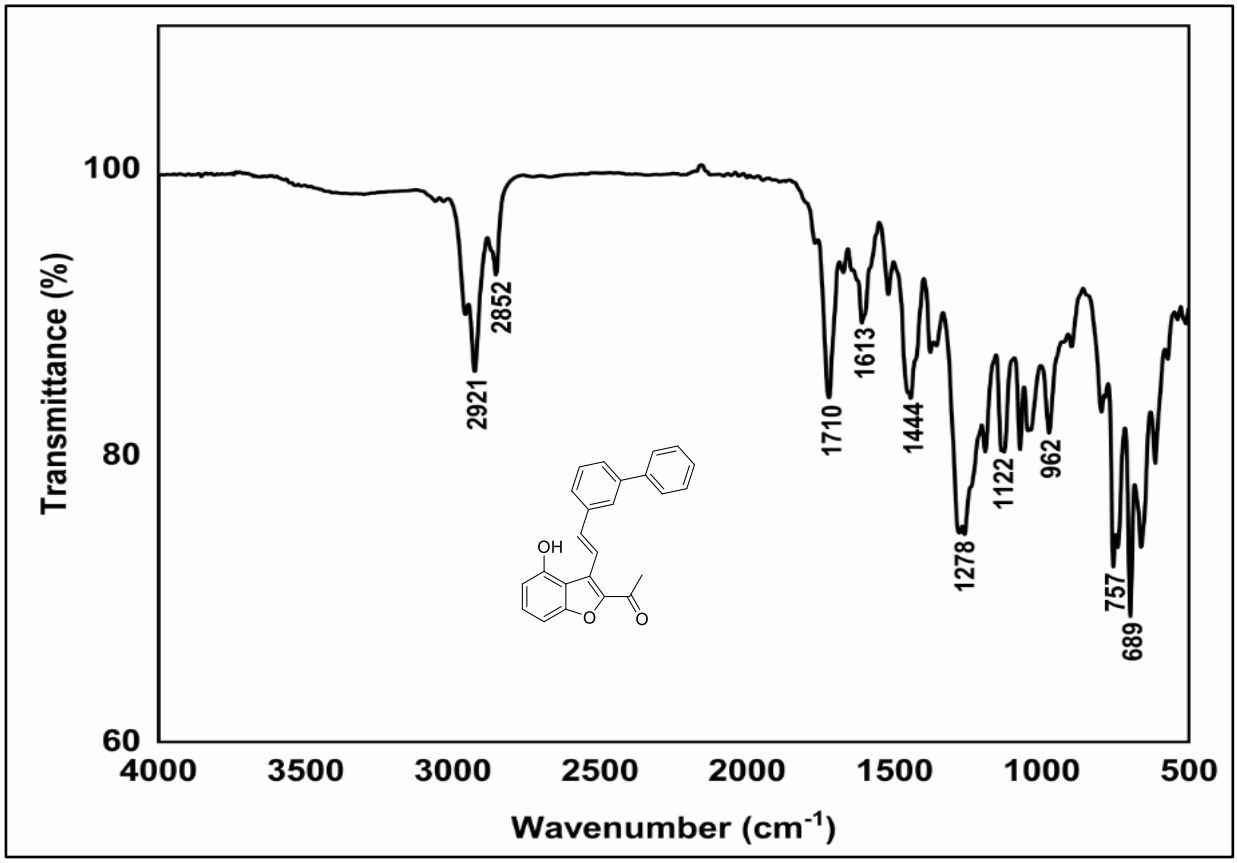


Figure 89: FT-IR spectrum of compound **6e**

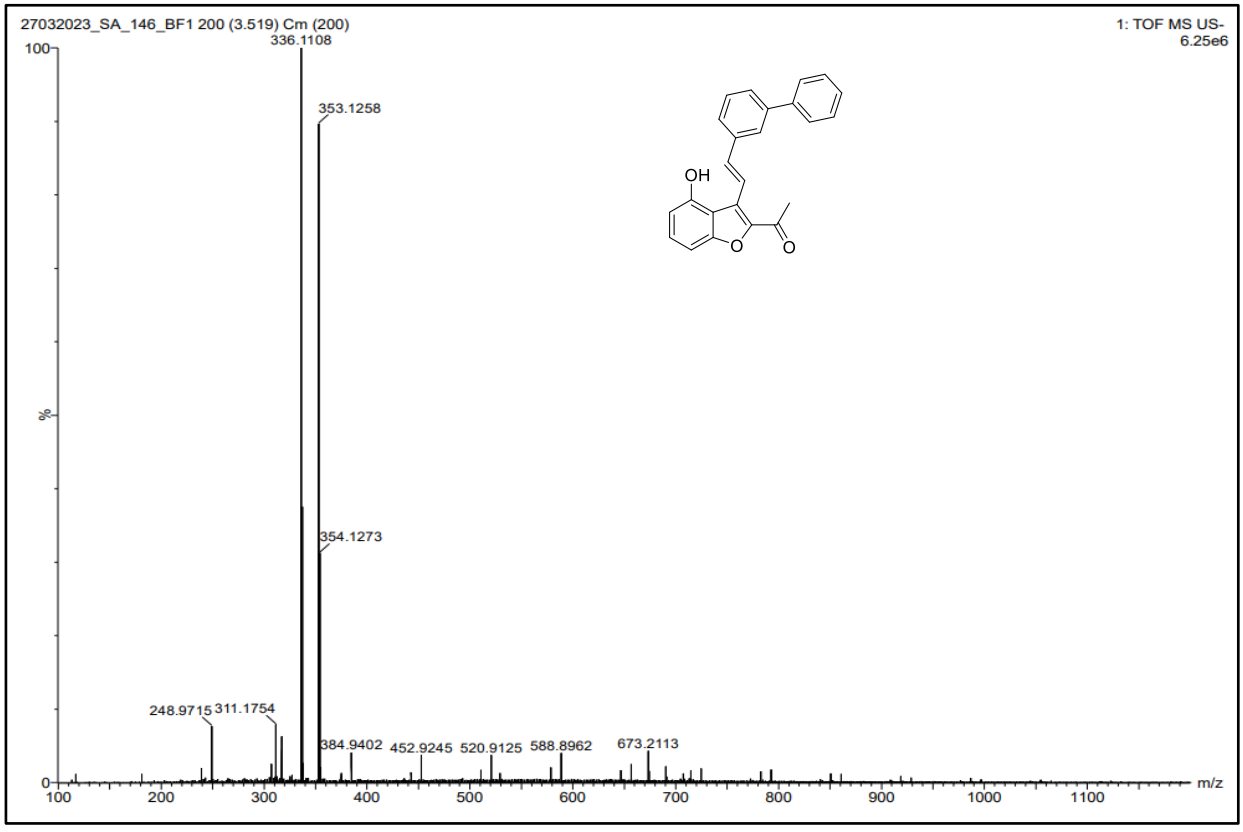


Figure 90: HRMS spectrum of compound **6e**

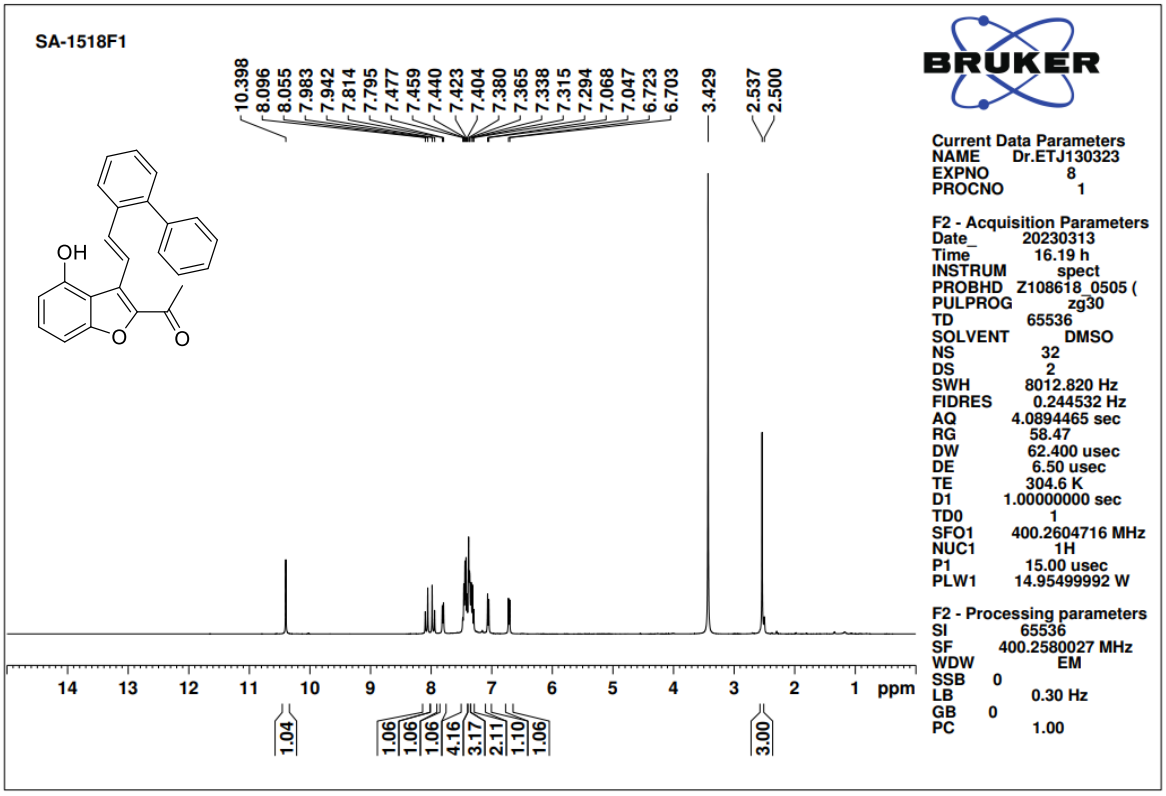


Figure 91: ^{1}H NMR spectrum of compound **6e**

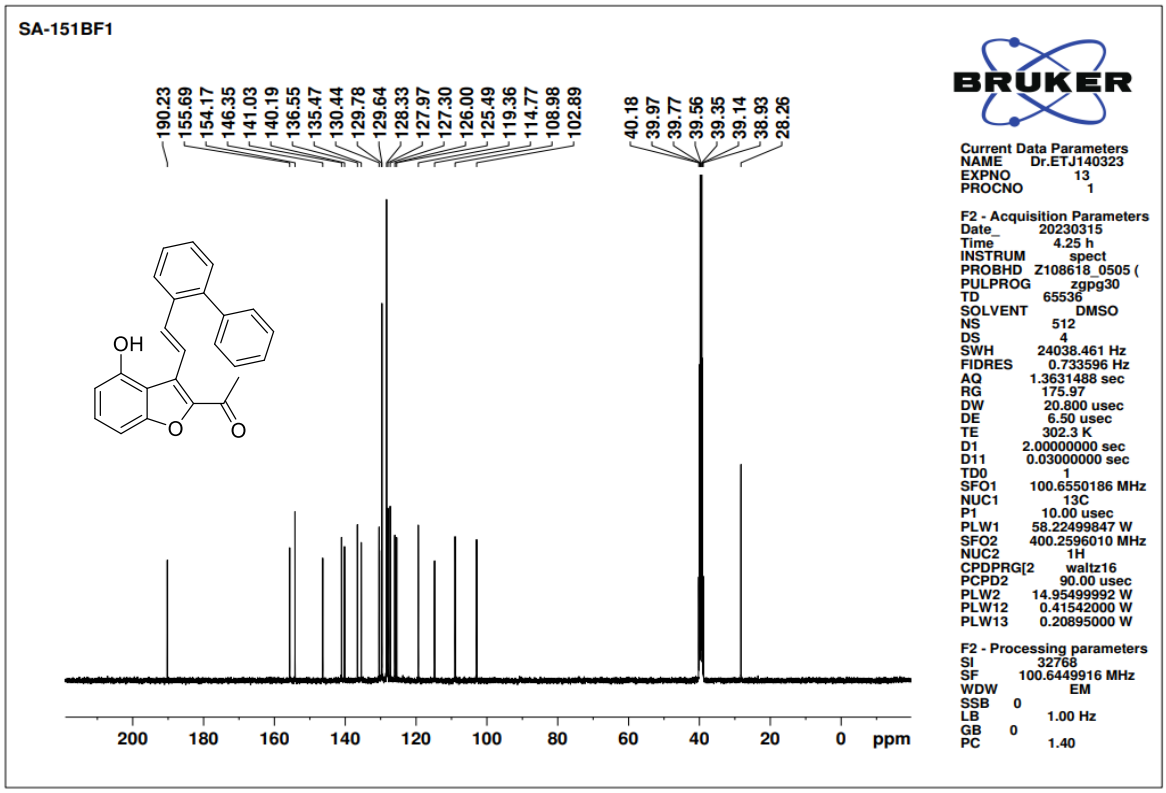


Figure 92: ^{13}C NMR spectrum of compound **6e**

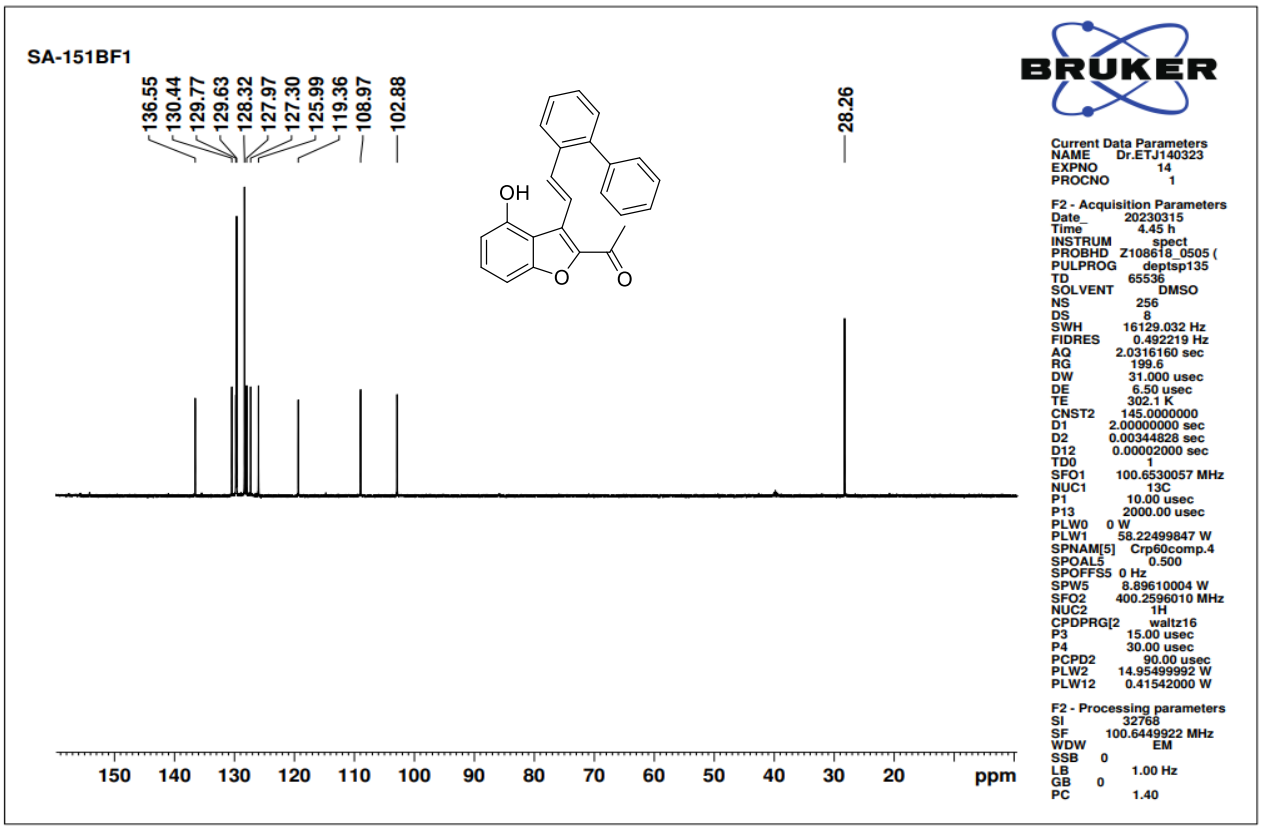


Figure 93: DEPT-135 NMR spectrum of compound **6e**

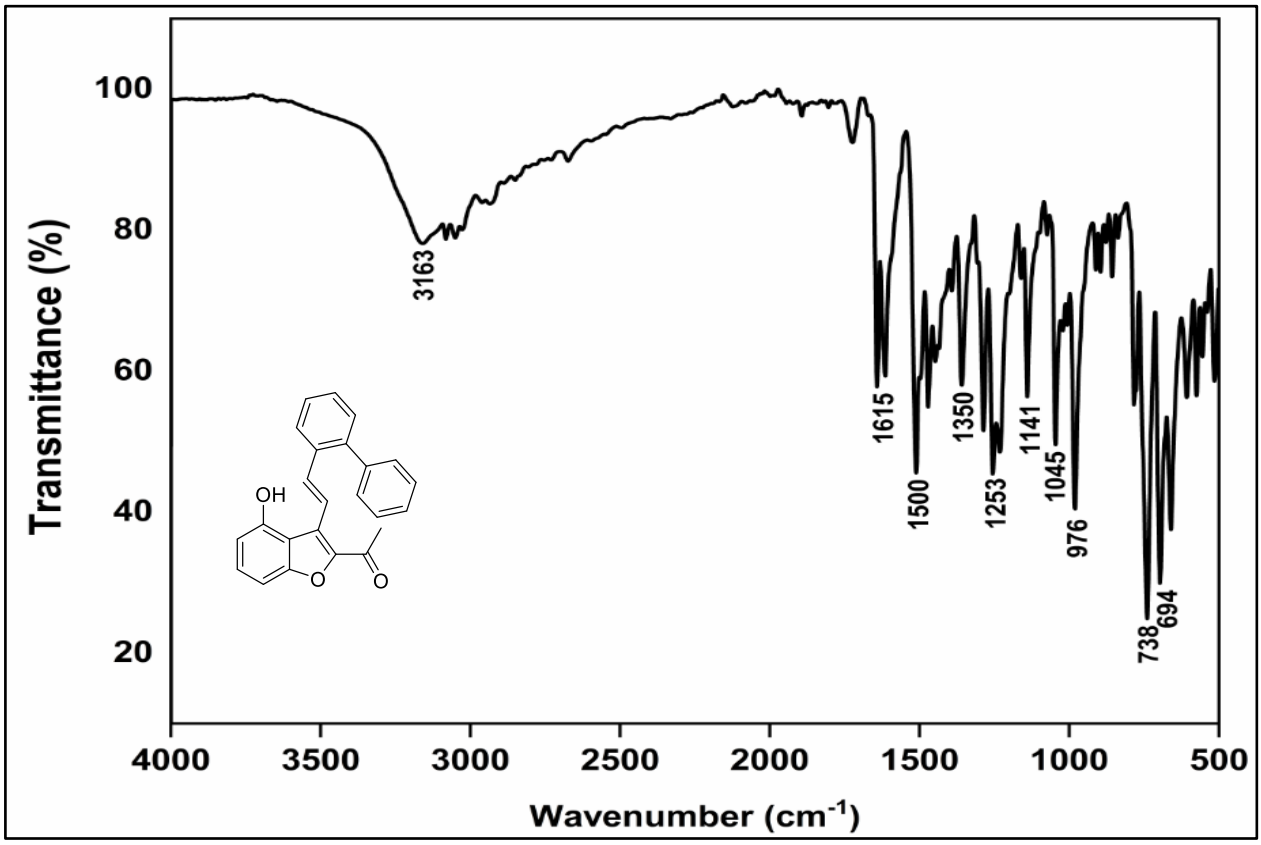


Figure 94: FT-IR spectrum of compound **6e**

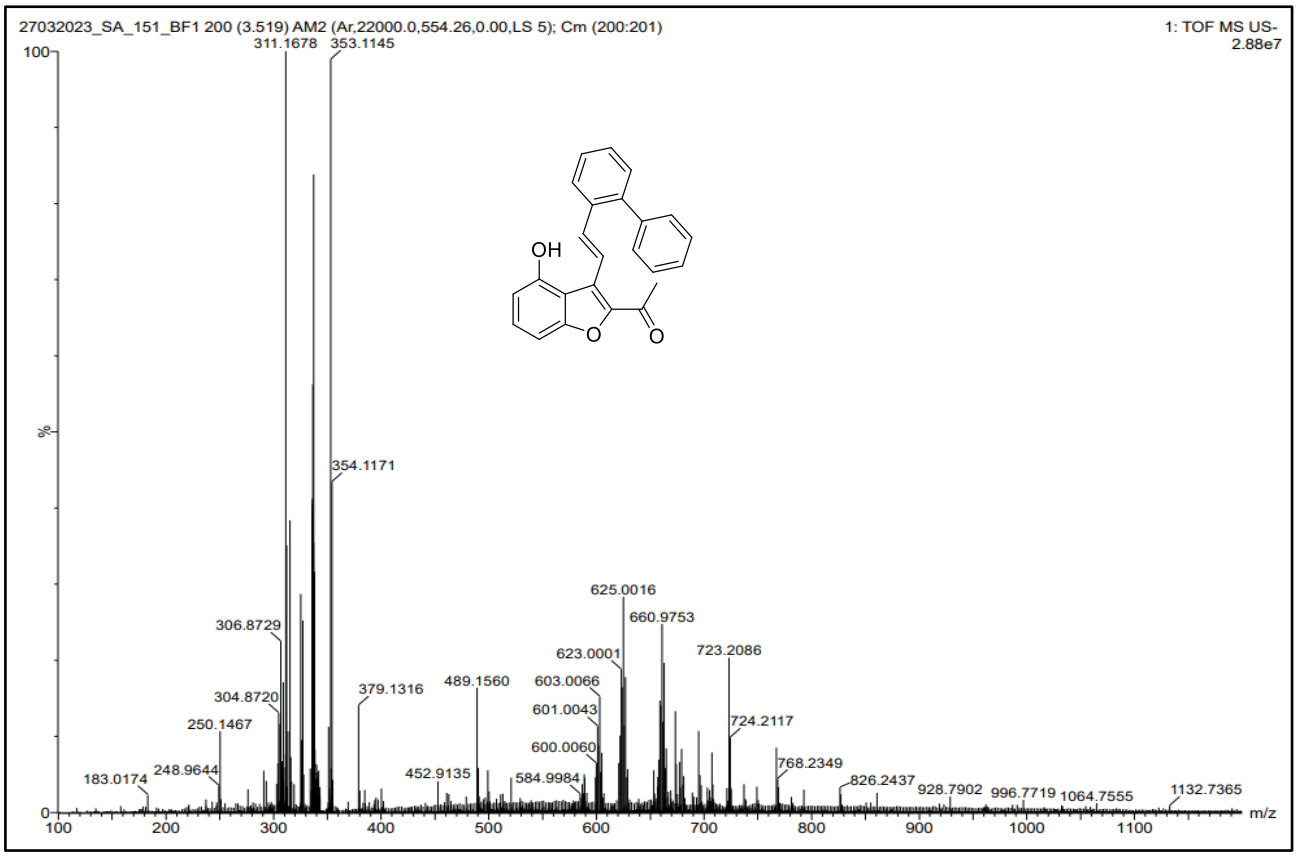


Figure 95: HRMS spectrum of compound **6e**

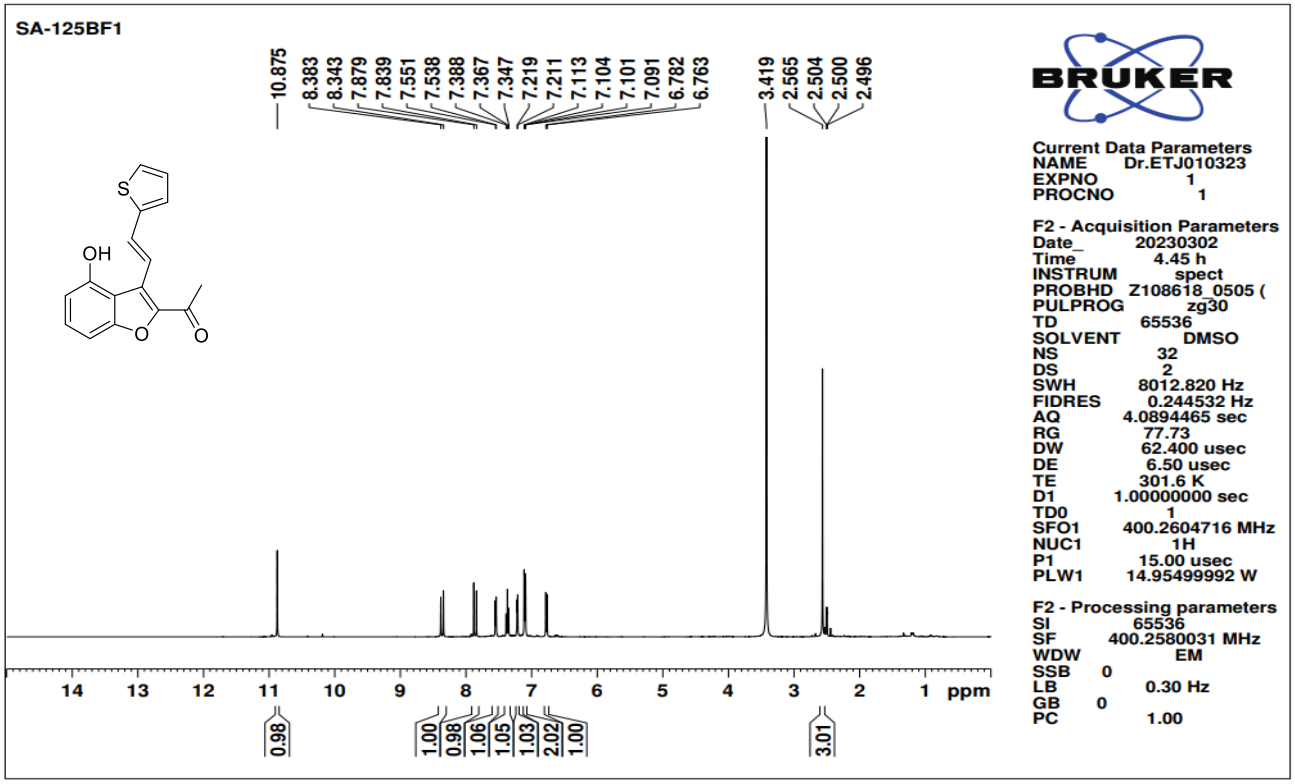


Figure 96: ^{1}H NMR spectrum of compound **6f**

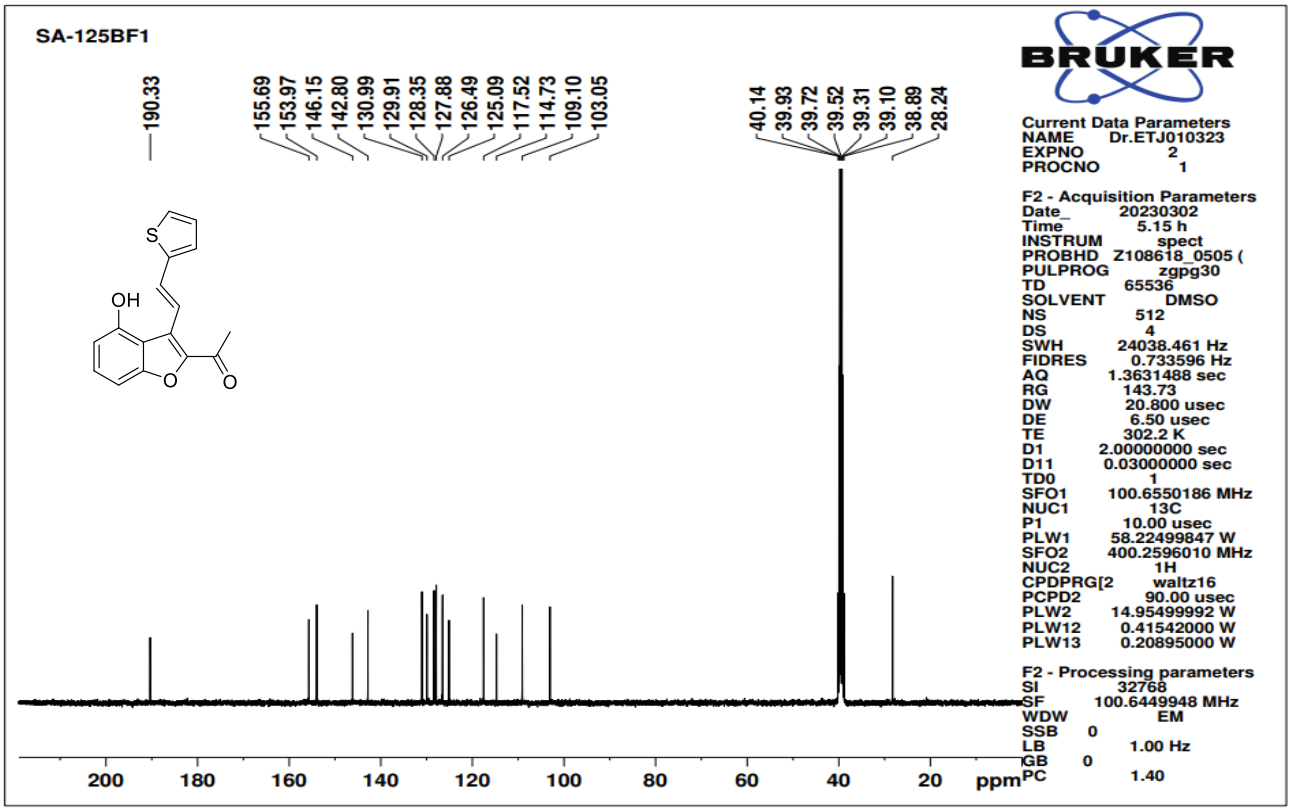


Figure 97: ^{13}C NMR spectrum of compound **6f**

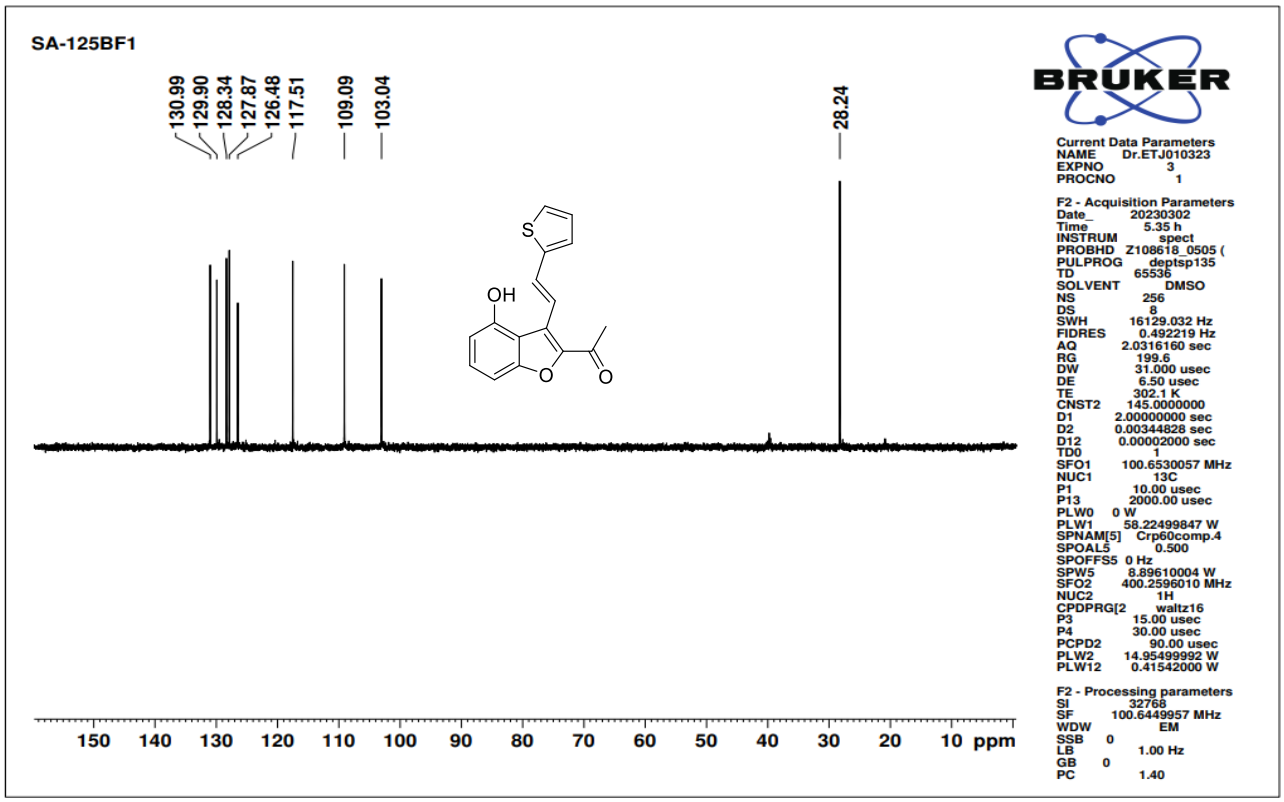


Figure 98: HRMS spectrum of compound **6f**

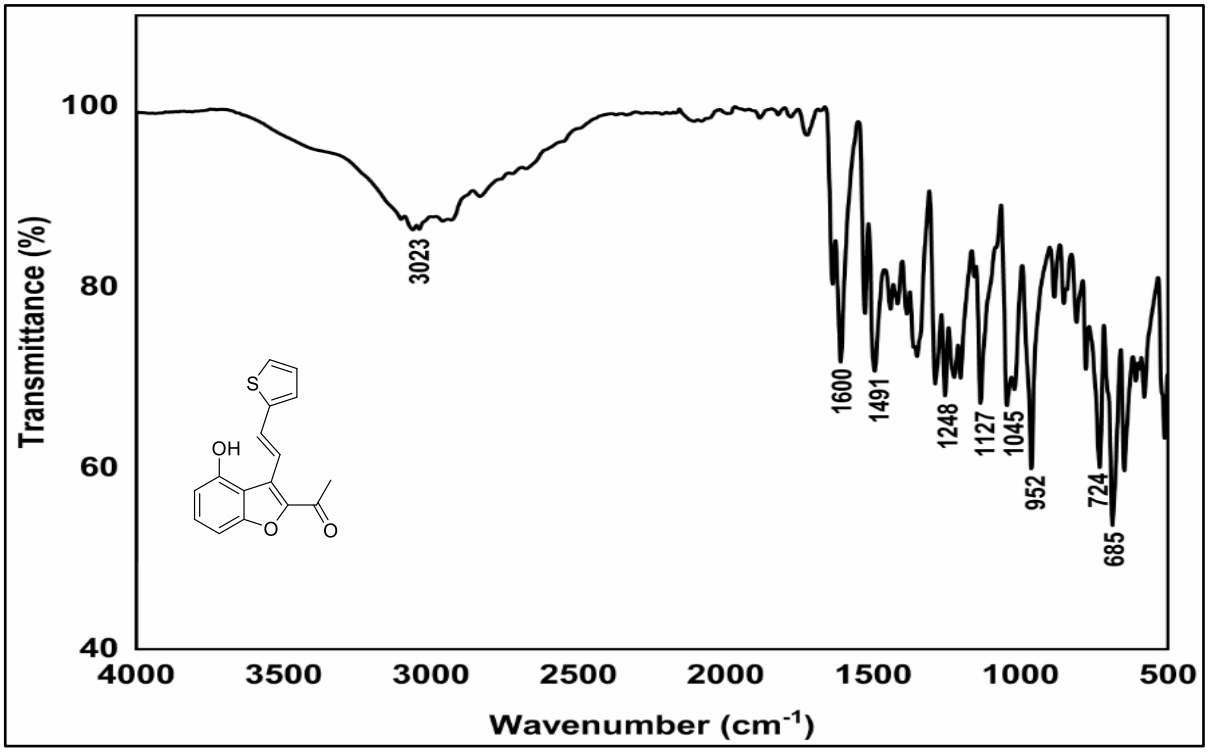


Figure 99: FT-IR spectrum of compound **6f**

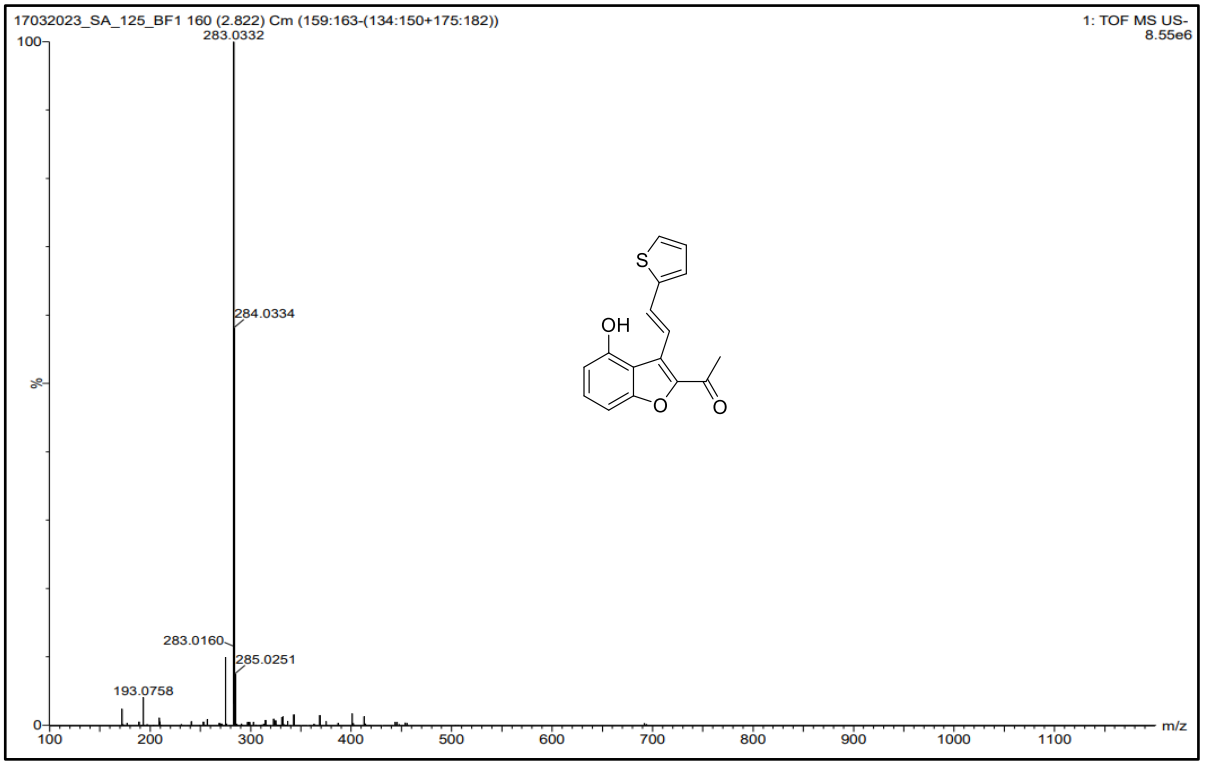


Figure 100: HRMS spectrum of compound **6g**

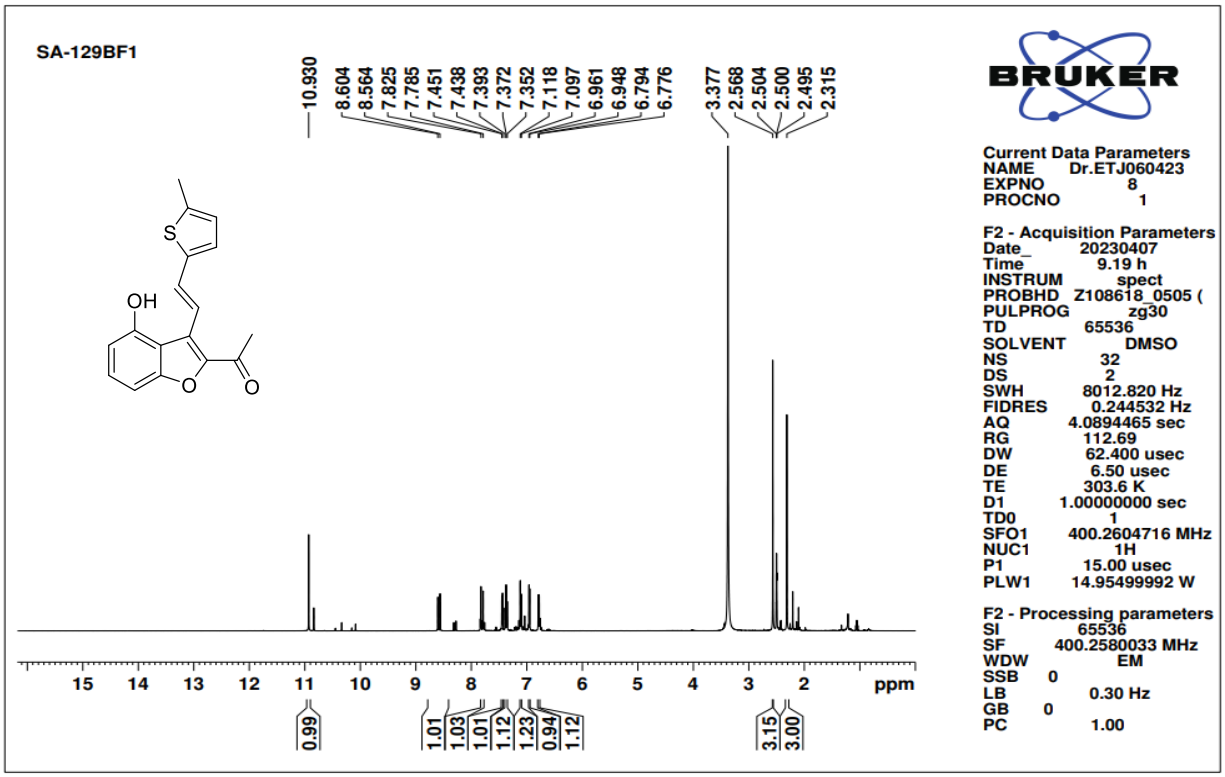


Figure 101: ^{1}H NMR spectrum of compound **6h**

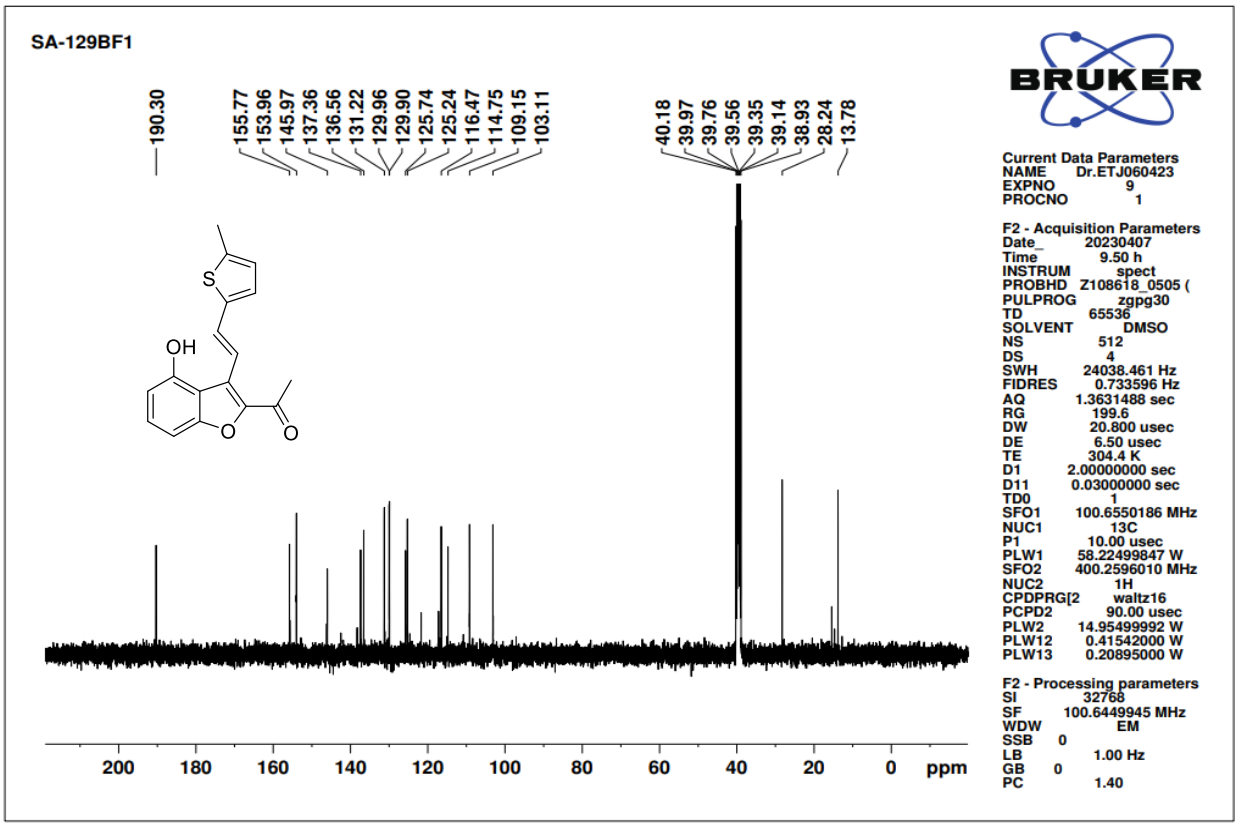


Figure 102: ^{13}C NMR spectrum of compound **6h**

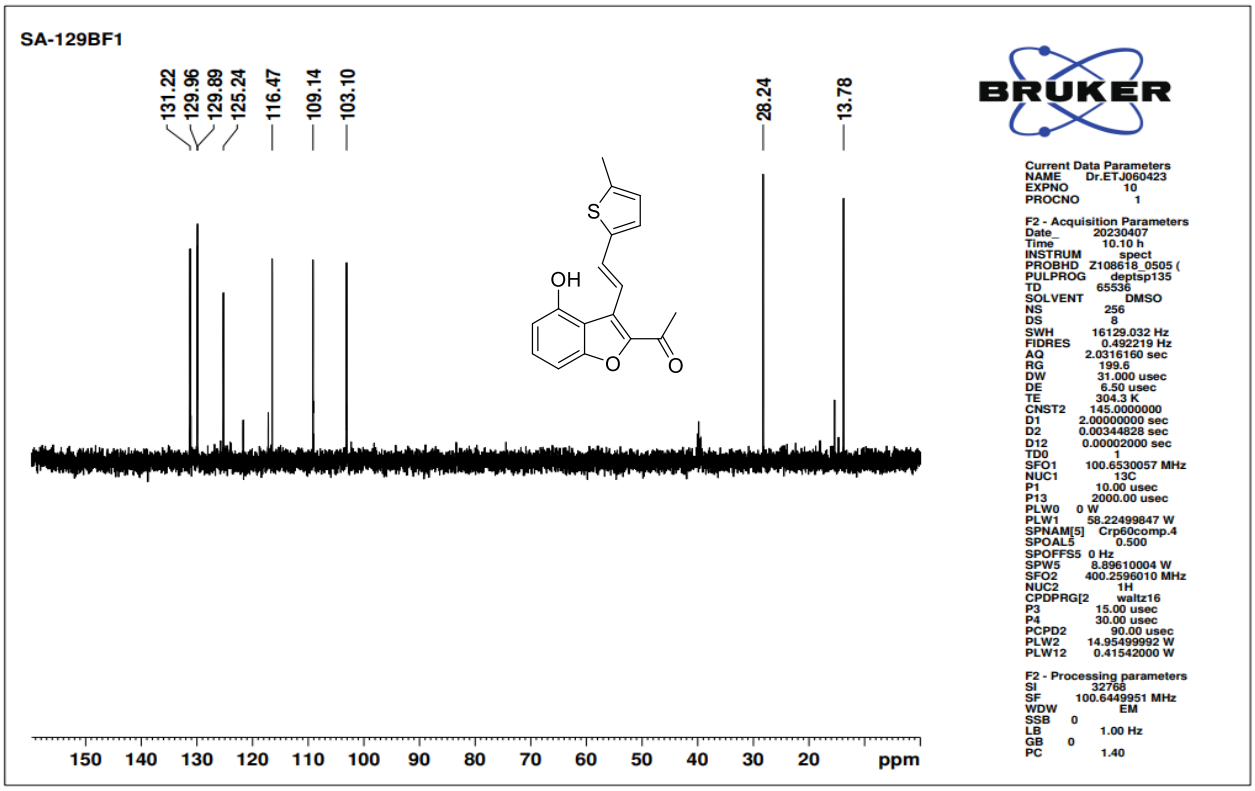


Figure 103: DEPT-135 NMR spectrum of compound **6h**

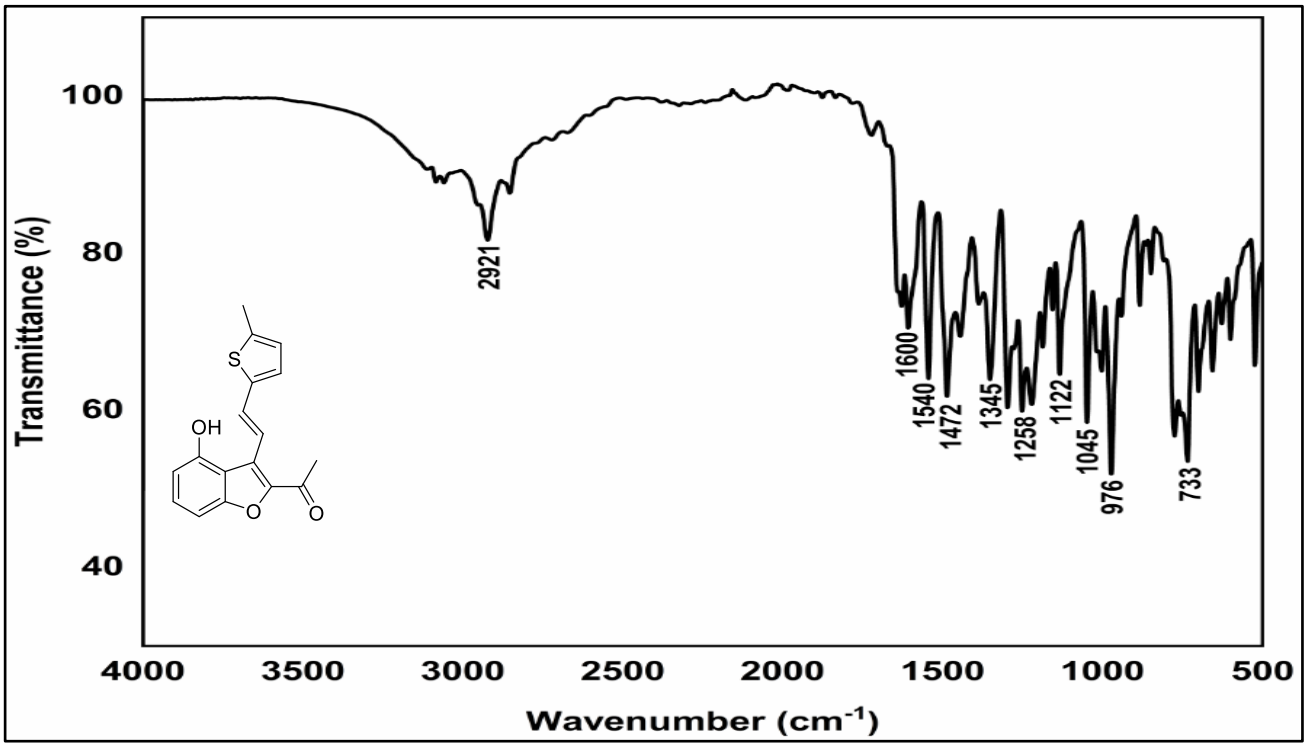


Figure 104: FT-IR spectrum of compound **6h**

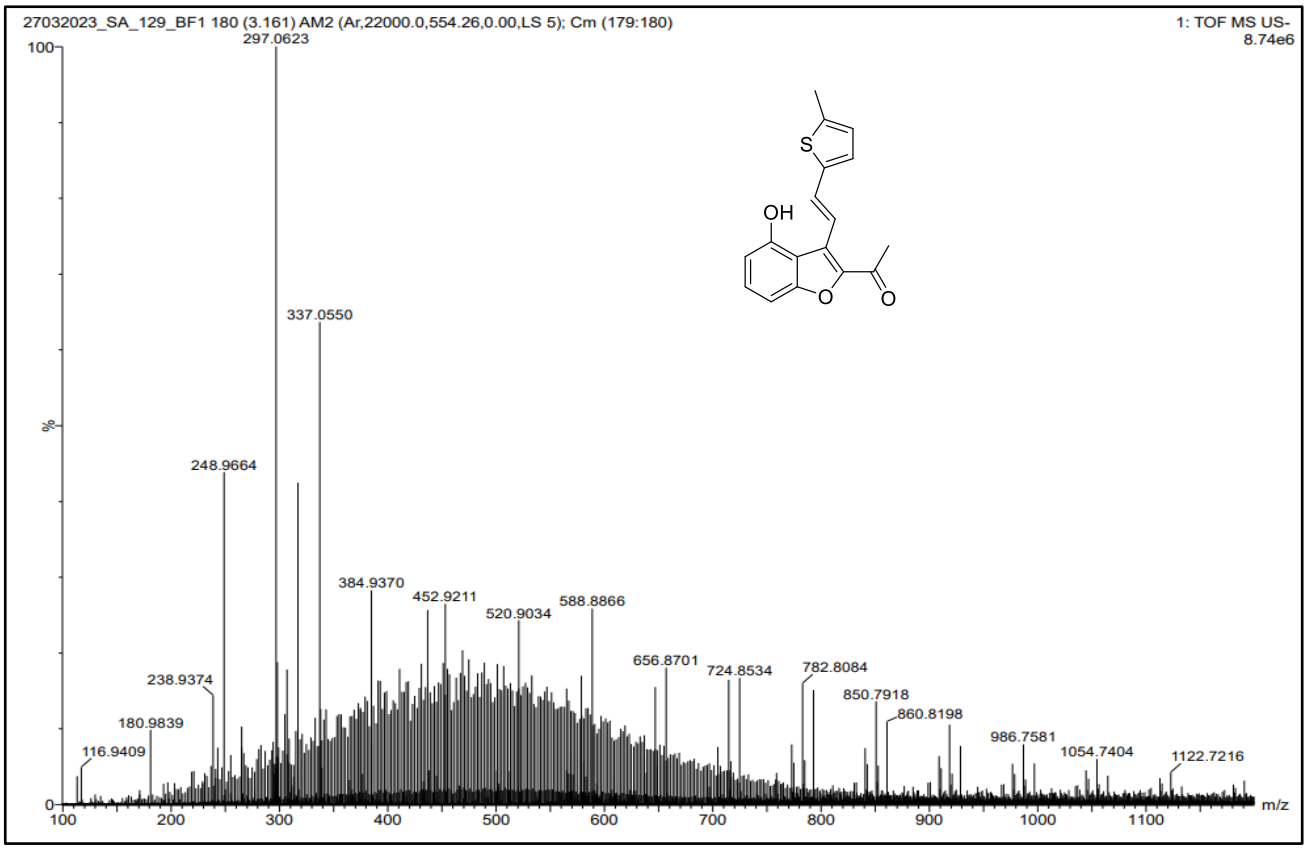


Figure 105: HRMS spectrum of compound **6h**

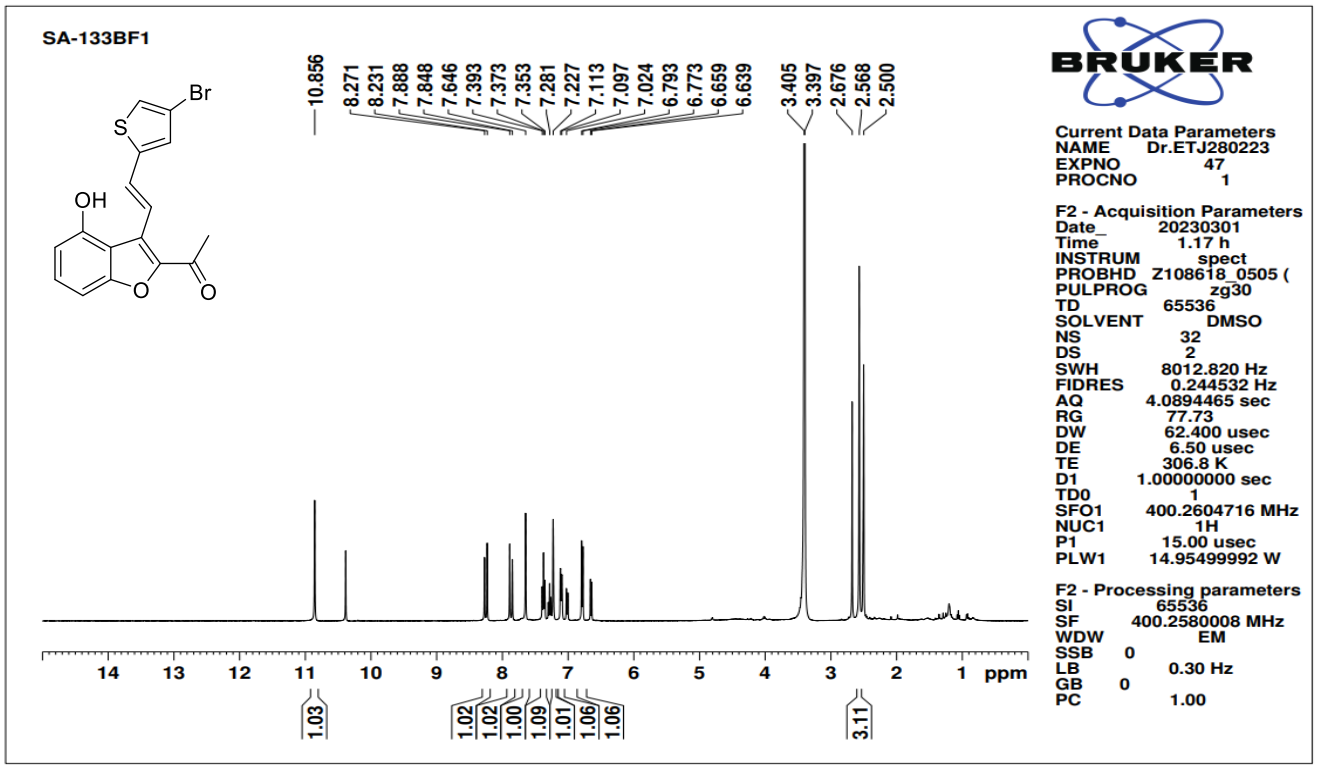


Figure 106: ^{1}H NMR spectrum of compound **6i**

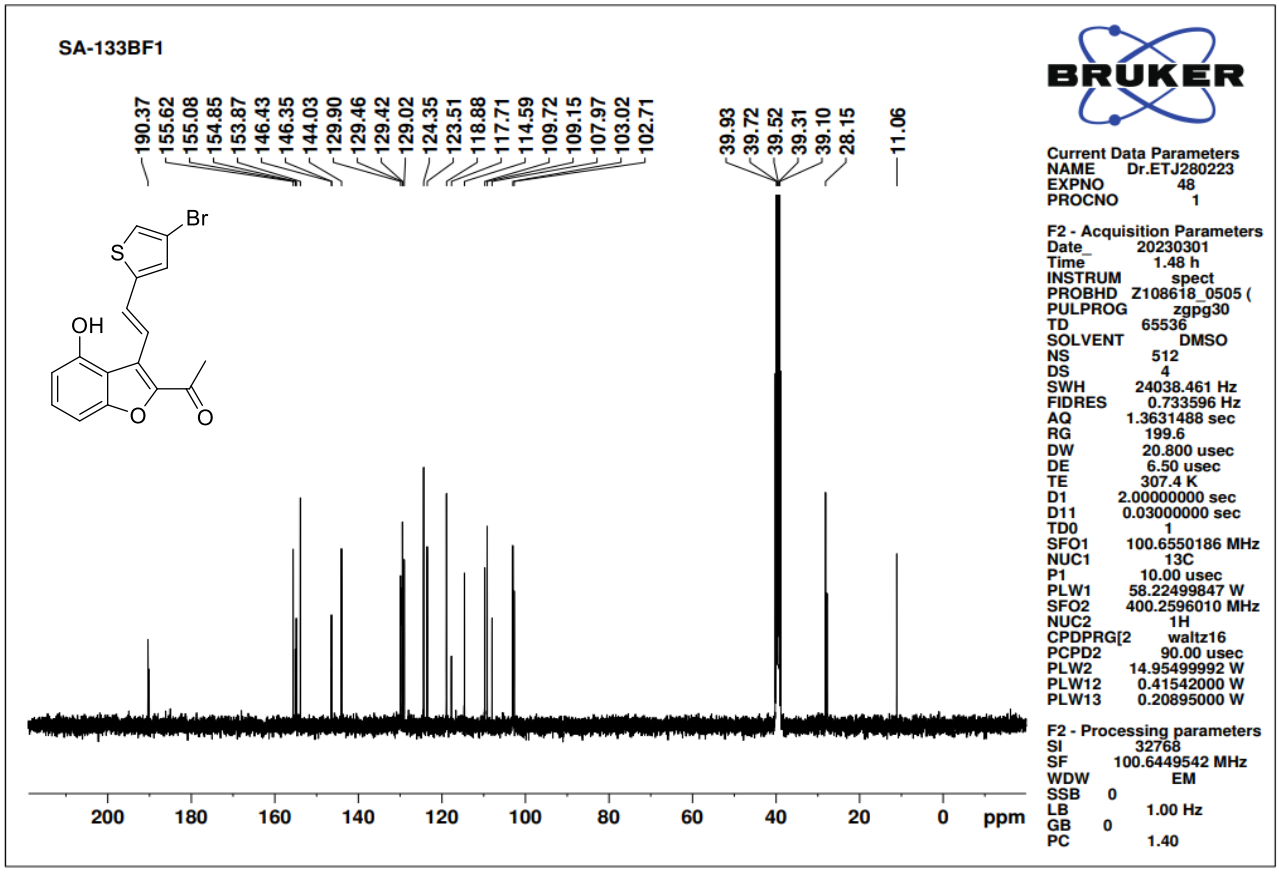


Figure 107: ^{13}C NMR spectrum of compound **6i**

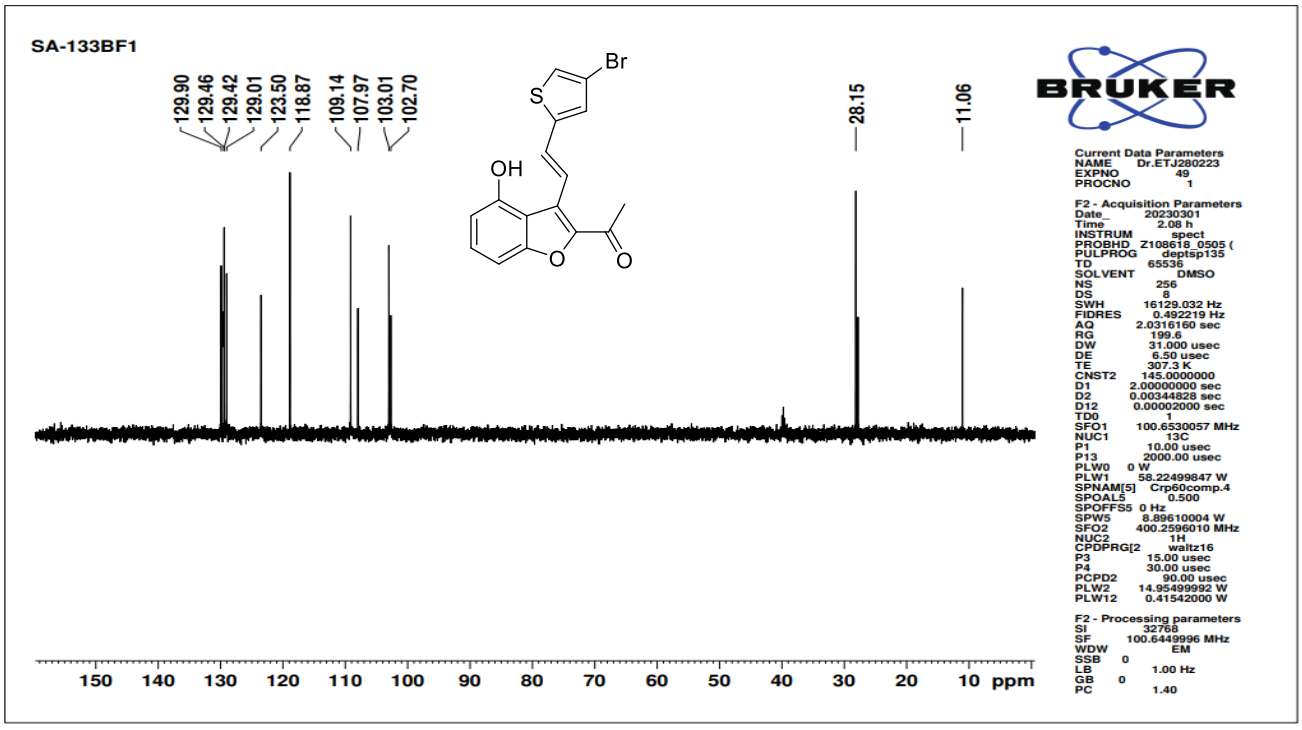


Figure 108: DEPT-135 NMR spectrum of compound **6i**

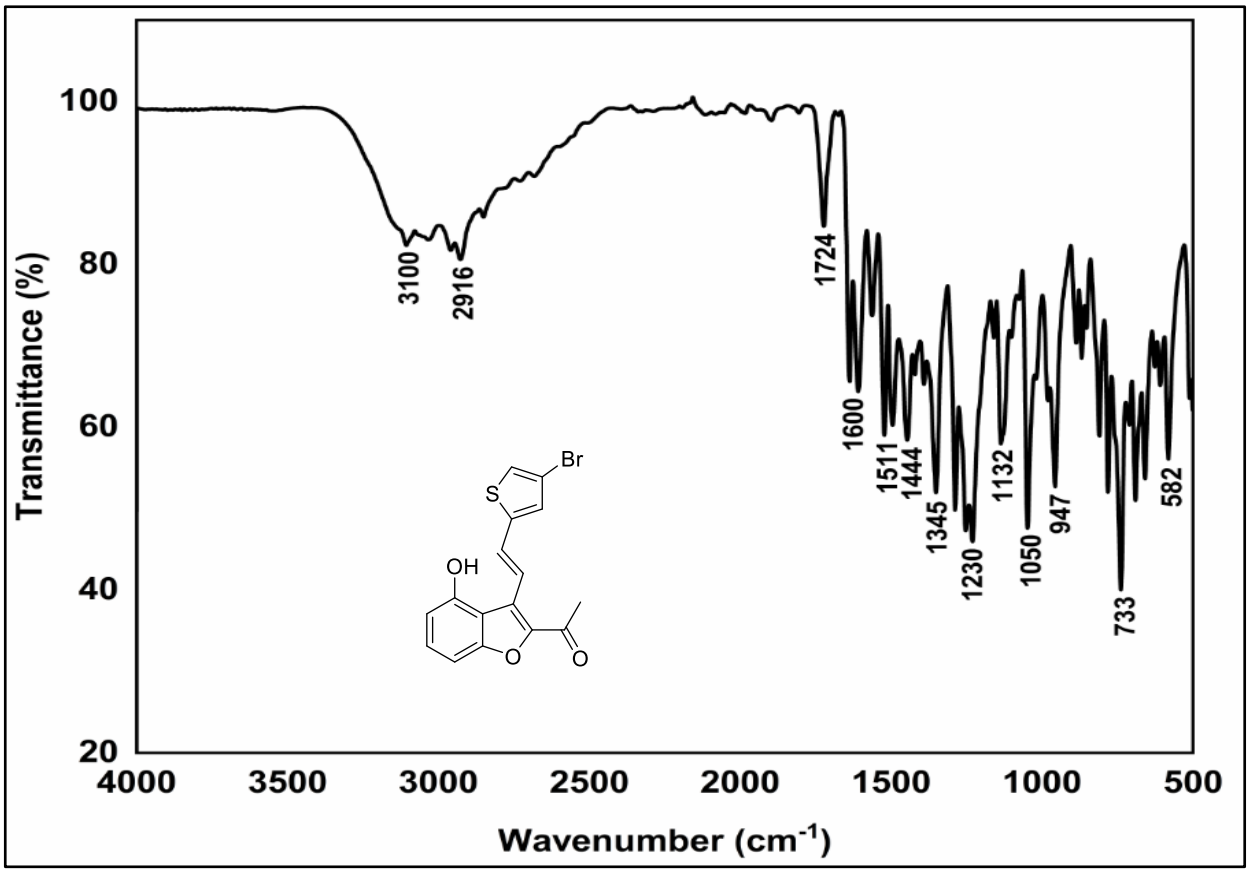


Figure 108: FT-IR spectrum of compound **6i**

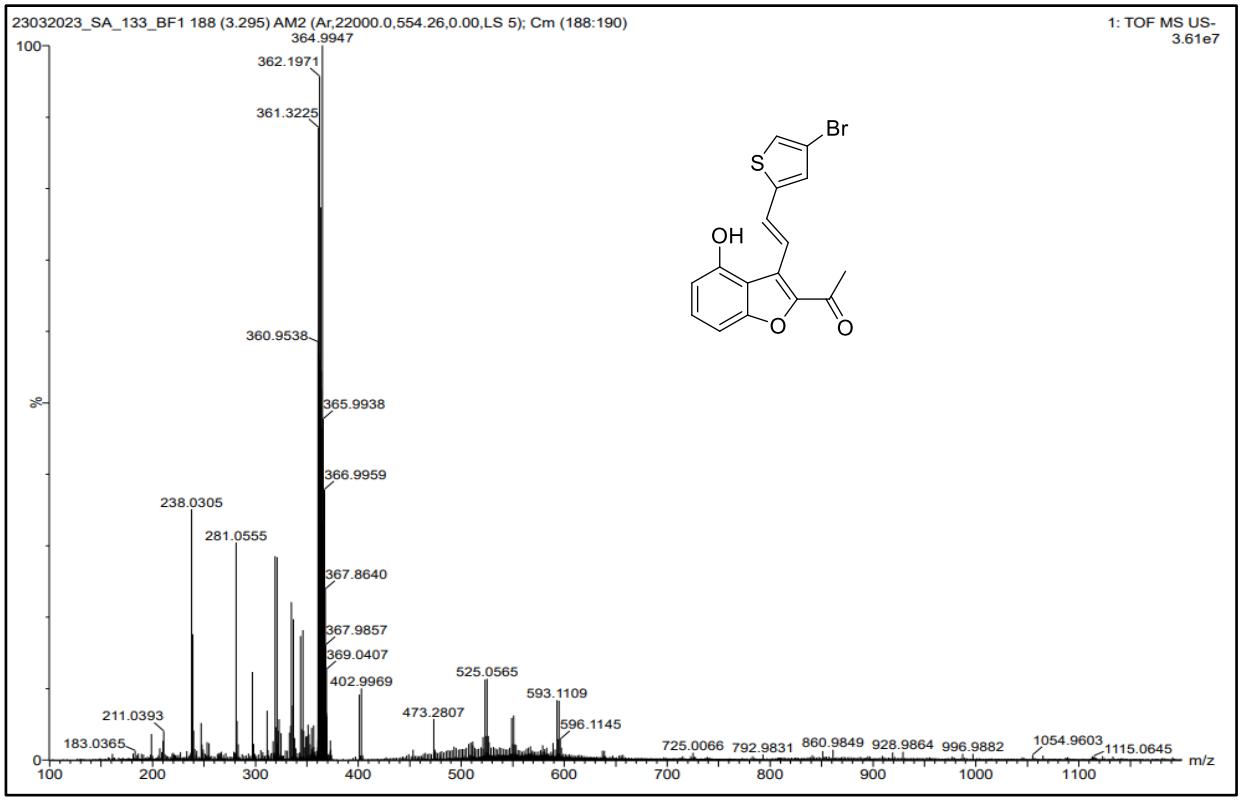


Figure 109: HRMS spectrum of compound **6i**

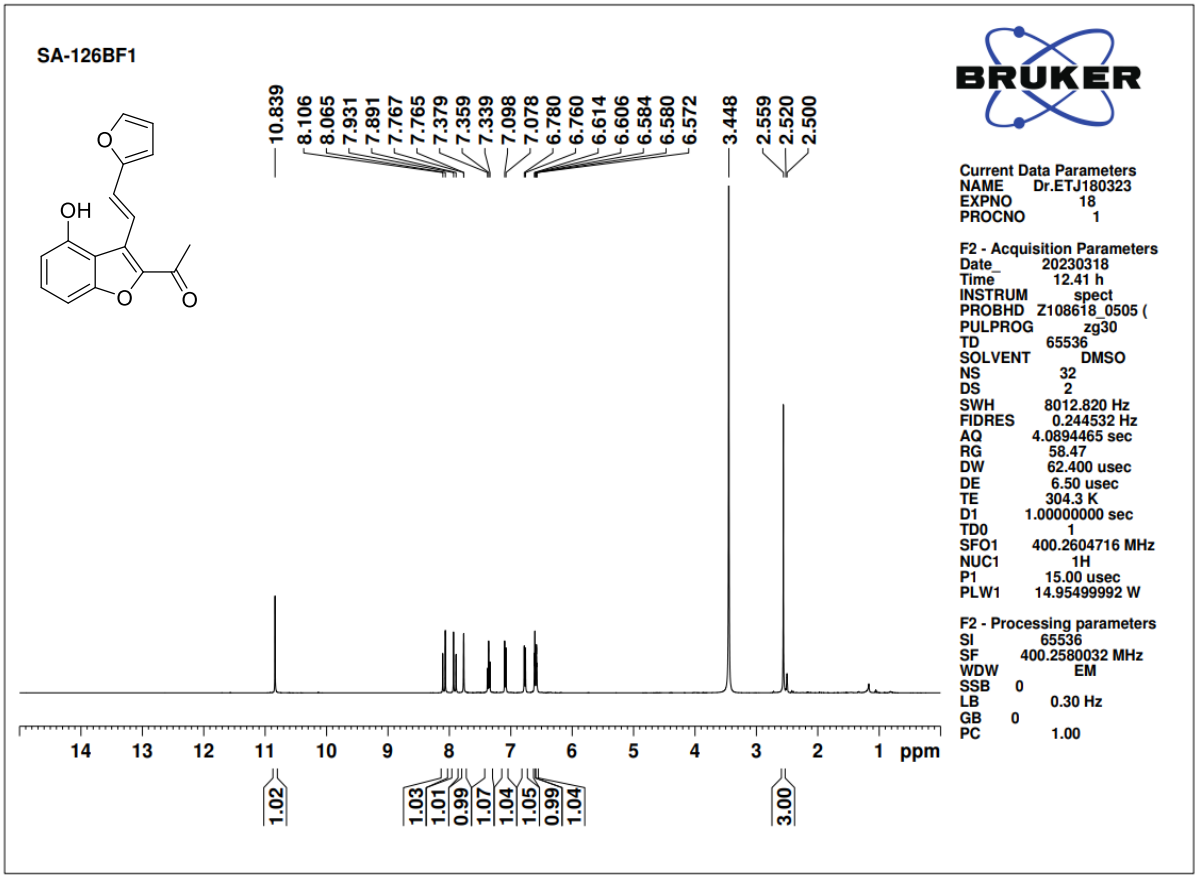


Figure 110: ^{1}H NMR spectrum of compound **6j**

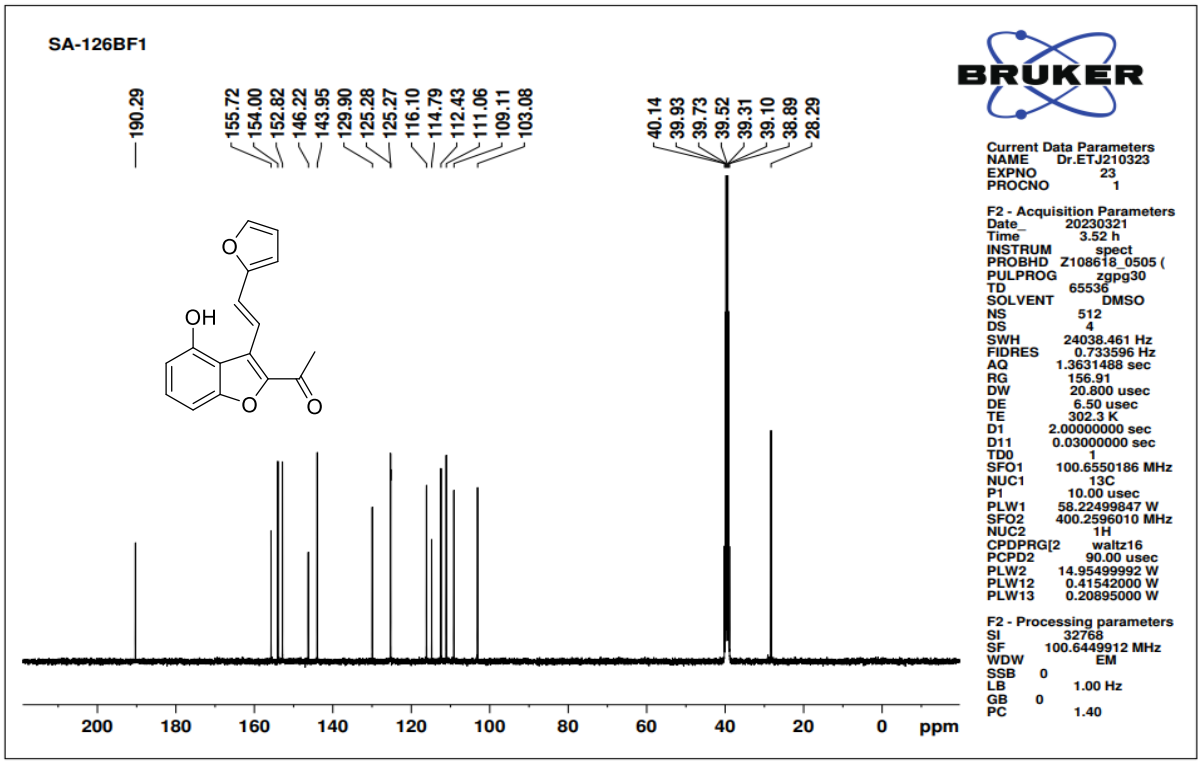


Figure 111: ^{13}C NMR spectrum of compound **6j**

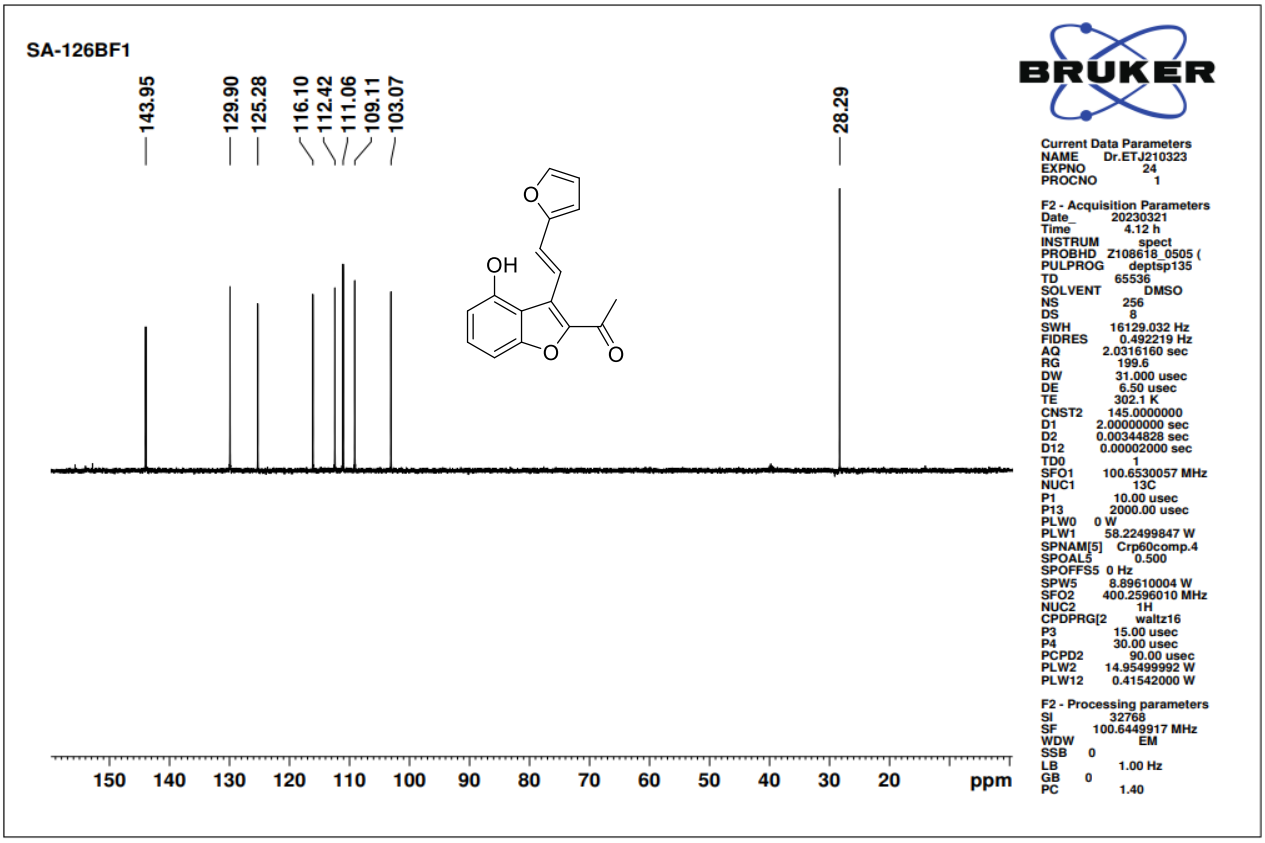


Figure 112: DEPT-135 NMR spectrum of compound **6j**

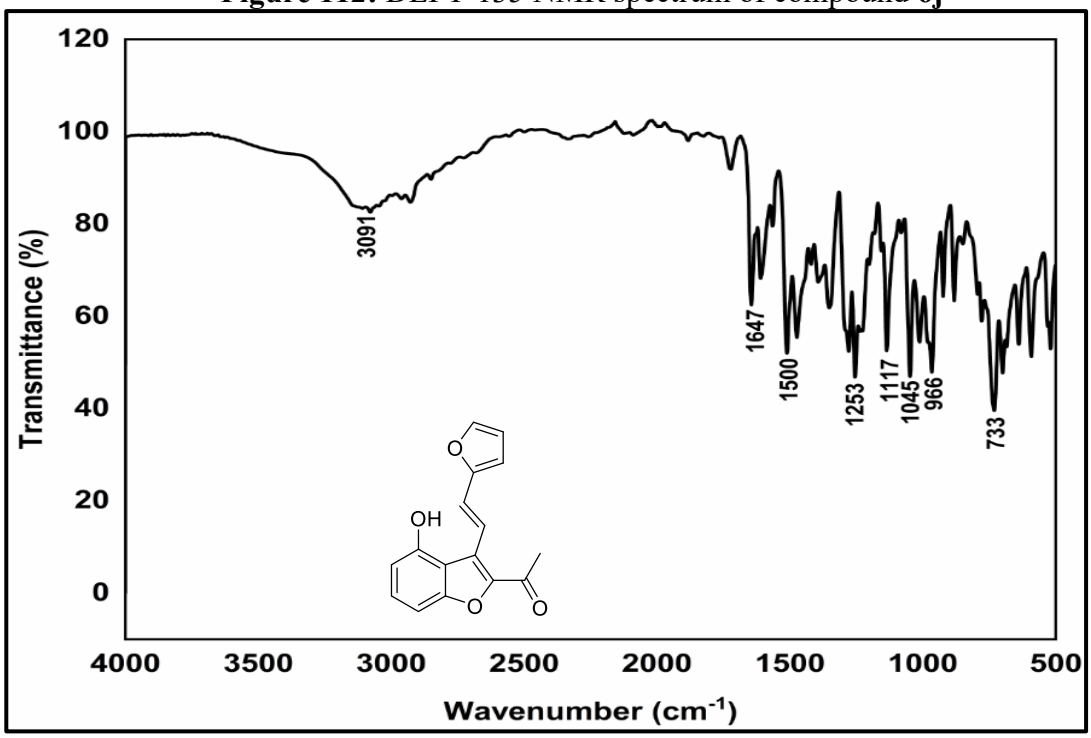


Figure 113: FT-IR spectrum of compound **6j**

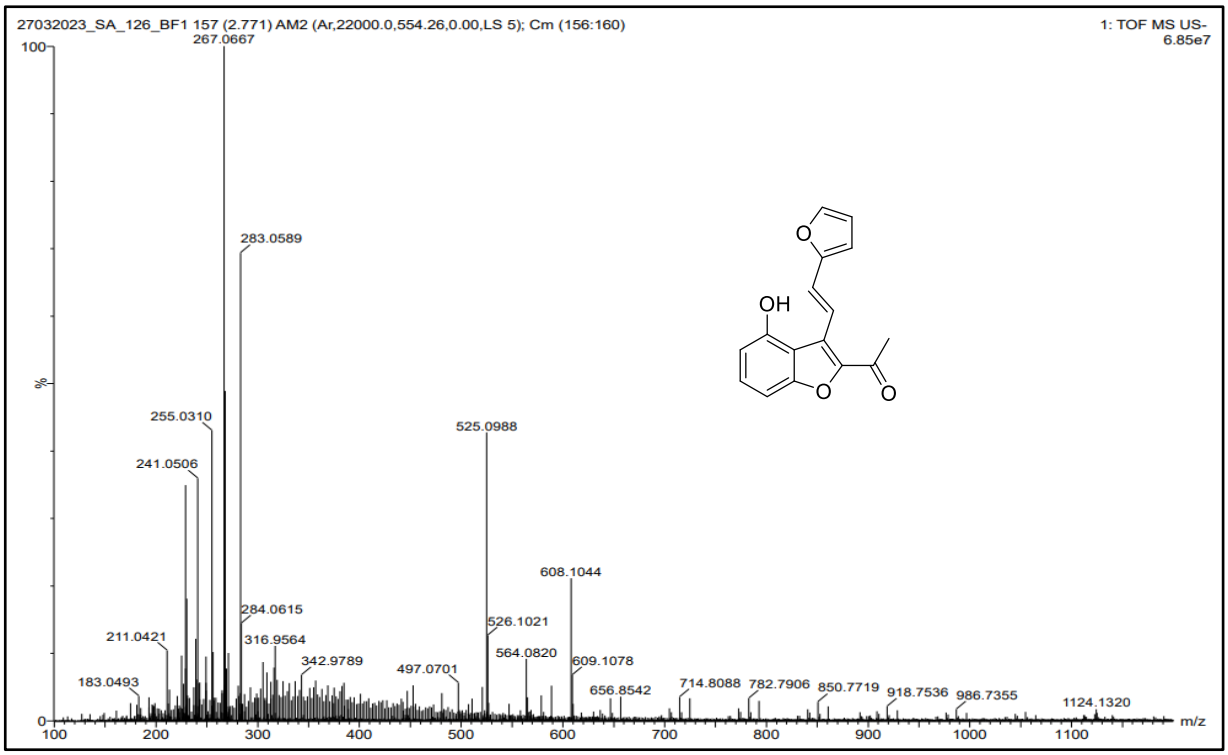


Figure 114: HRMS spectrum of compound **6j**

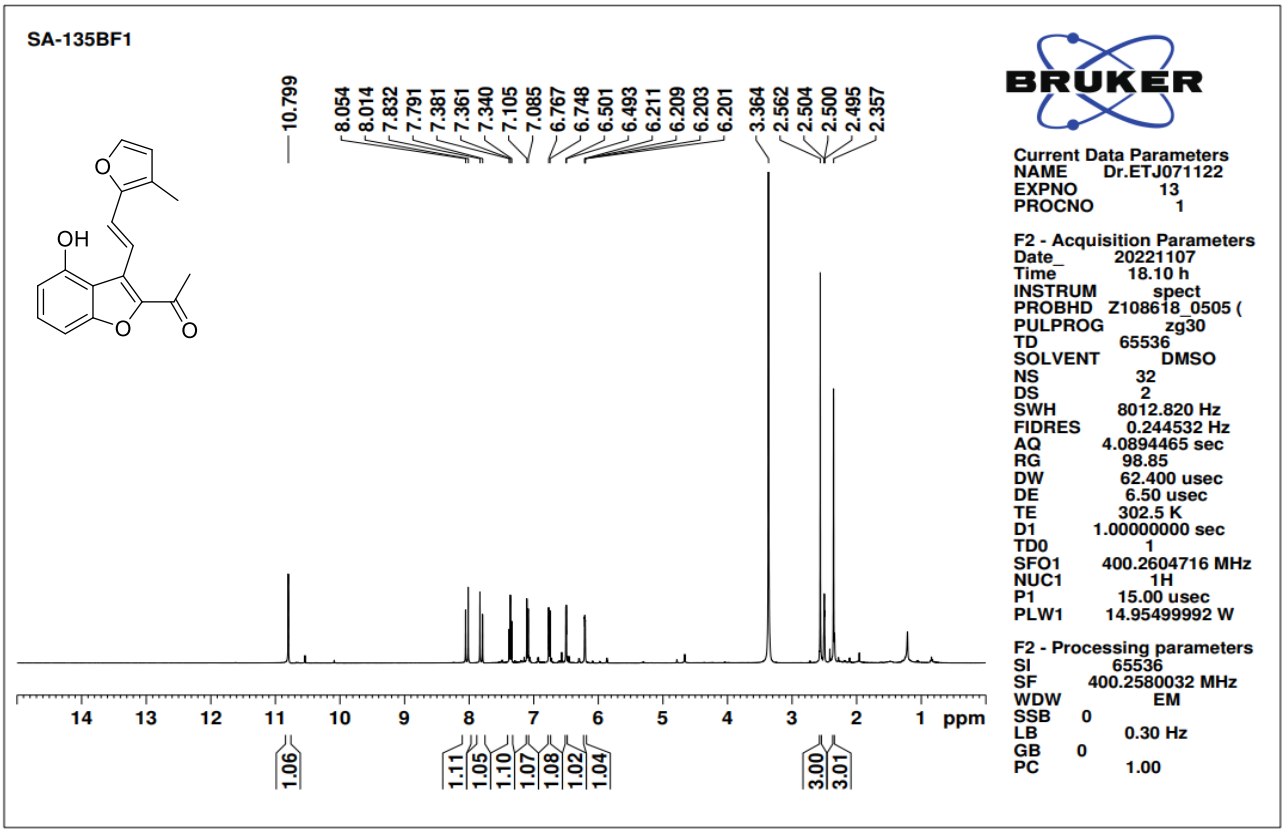


Figure 115: ^{1}H NMR spectrum of compound **6k**

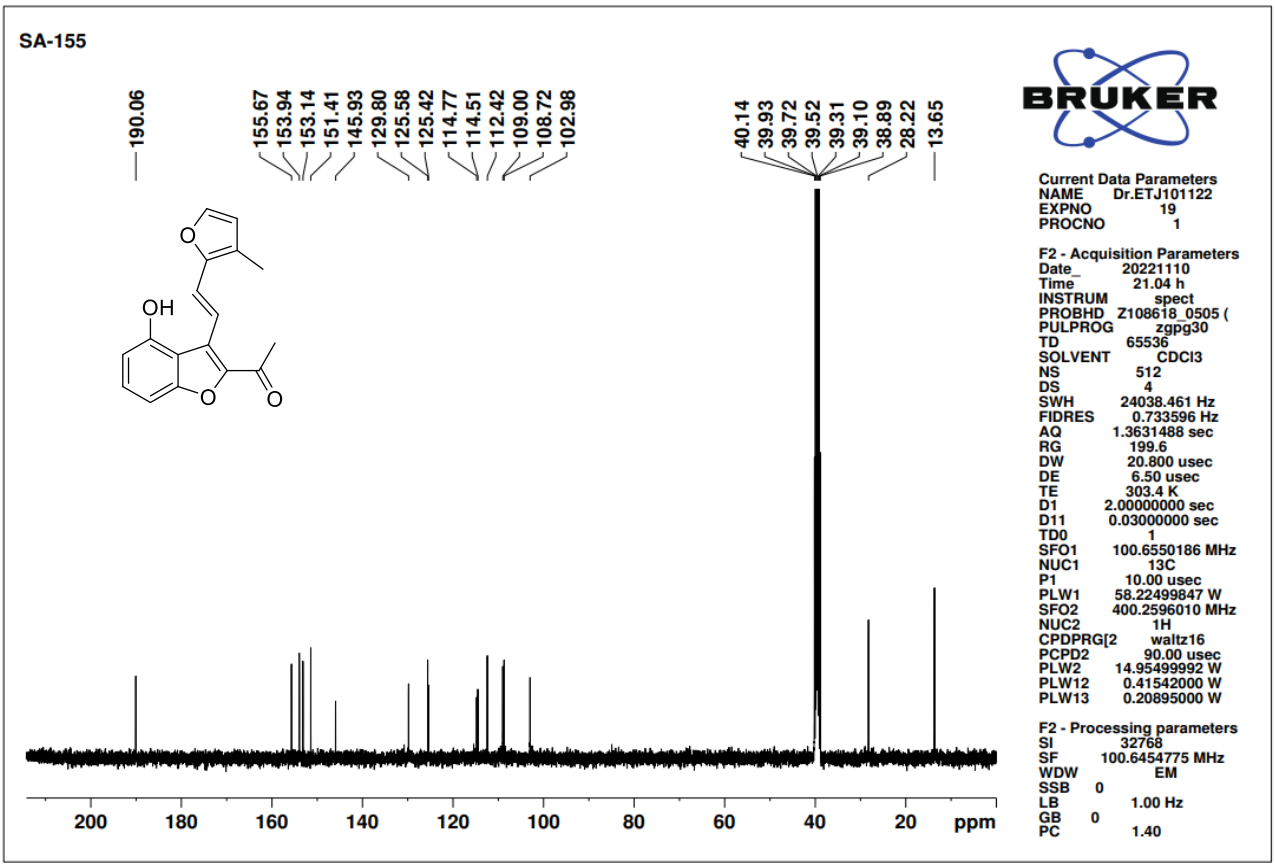


Figure 116: ^{13}C NMR spectrum of compound **6k**

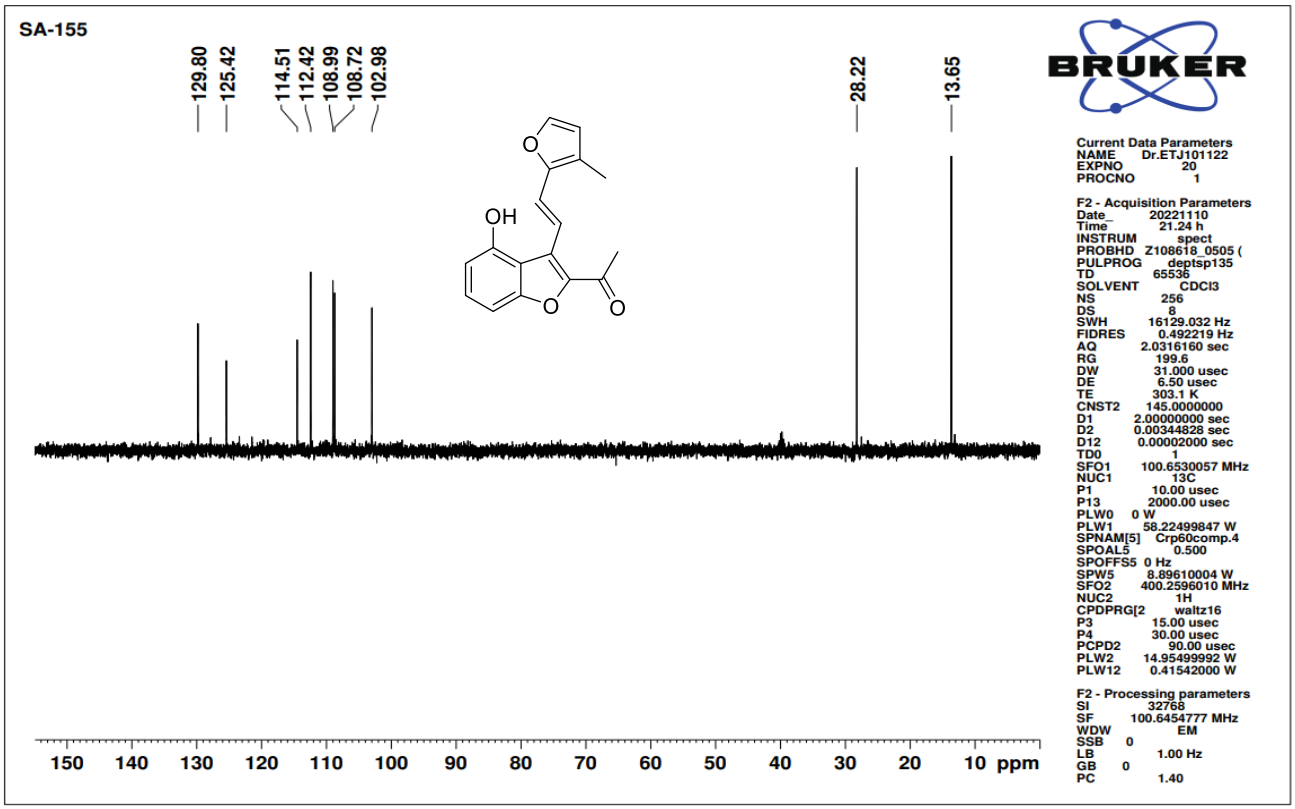


Figure 117: DEPT-135 NMR spectrum of compound **6k**

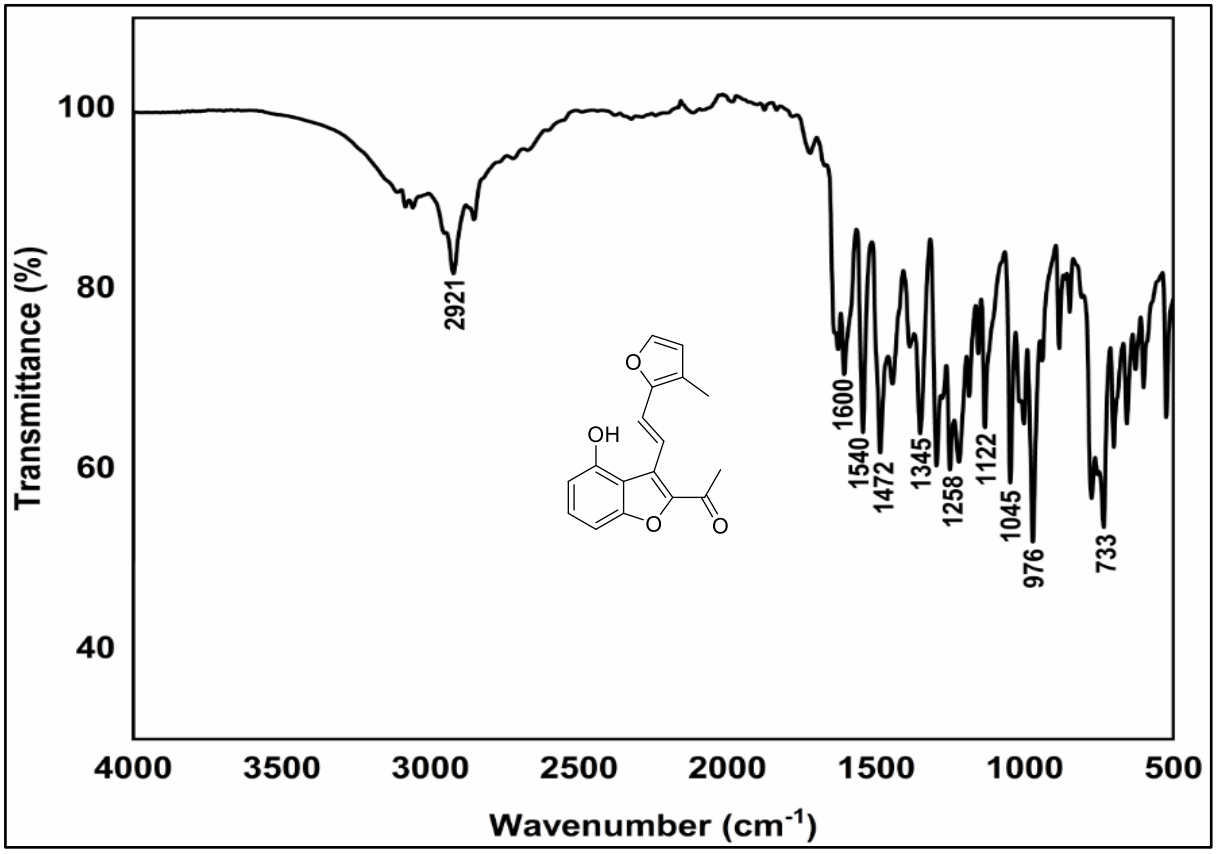


Figure 118: FT-IR spectrum of compound **6k**

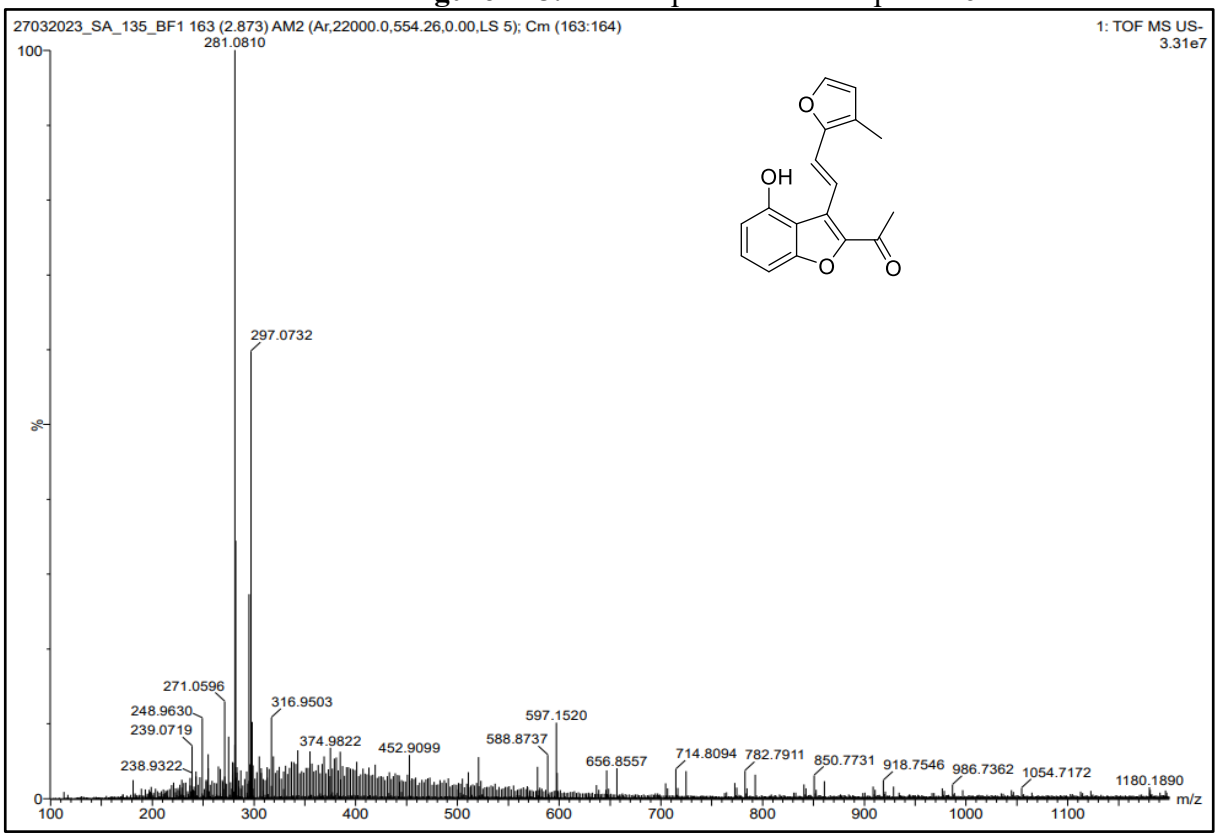


Figure 119: HRMS spectrum of compound **6k**

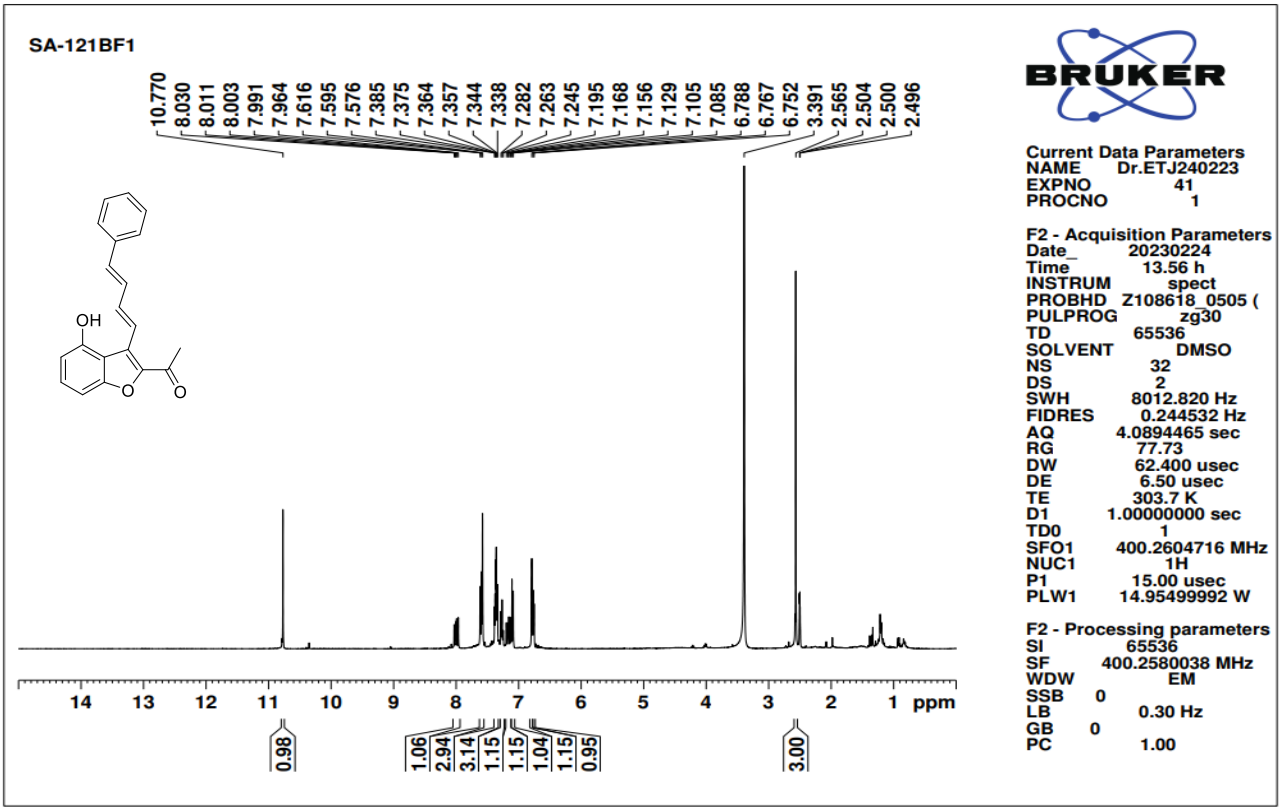


Figure 120: ^{1}H NMR spectrum of compound **6l**

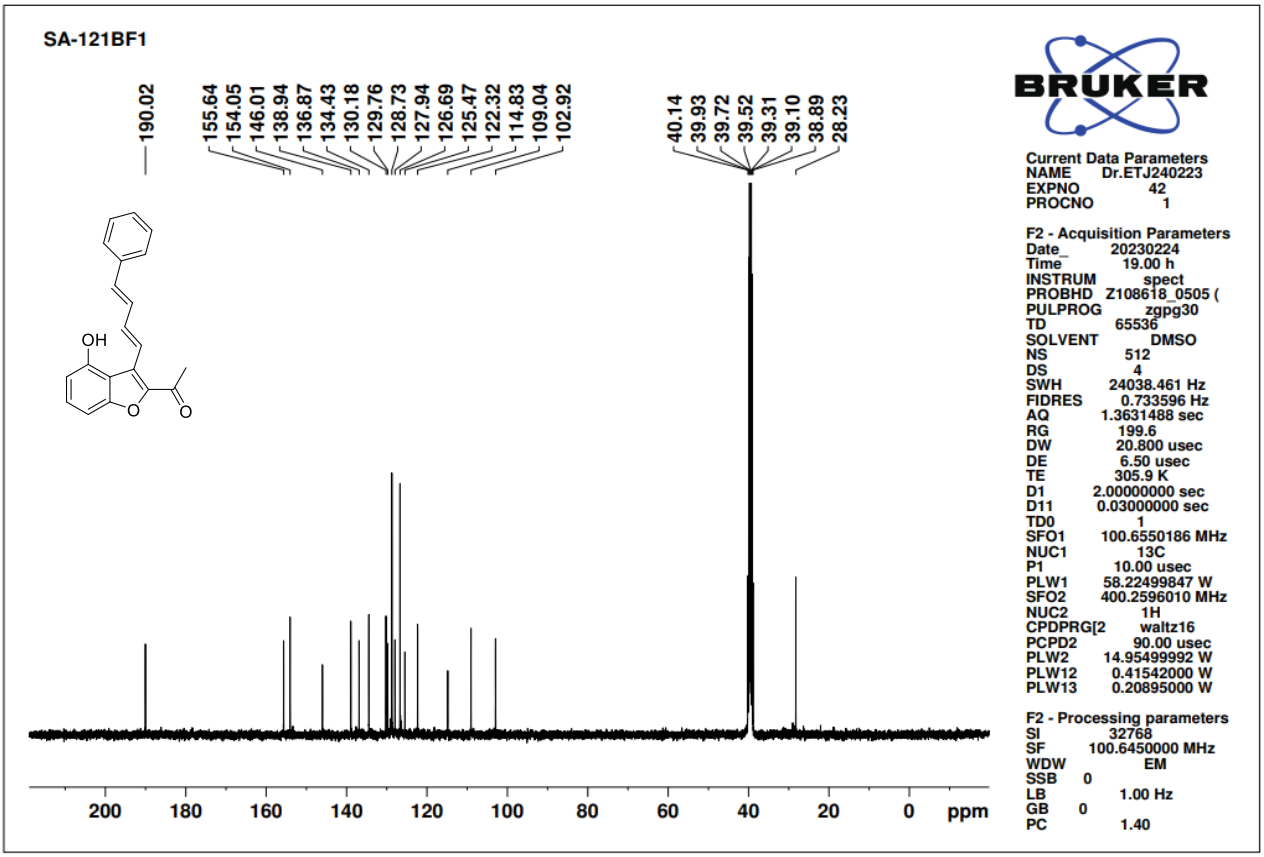


Figure 121: ^{13}C NMR spectrum of compound **6l**

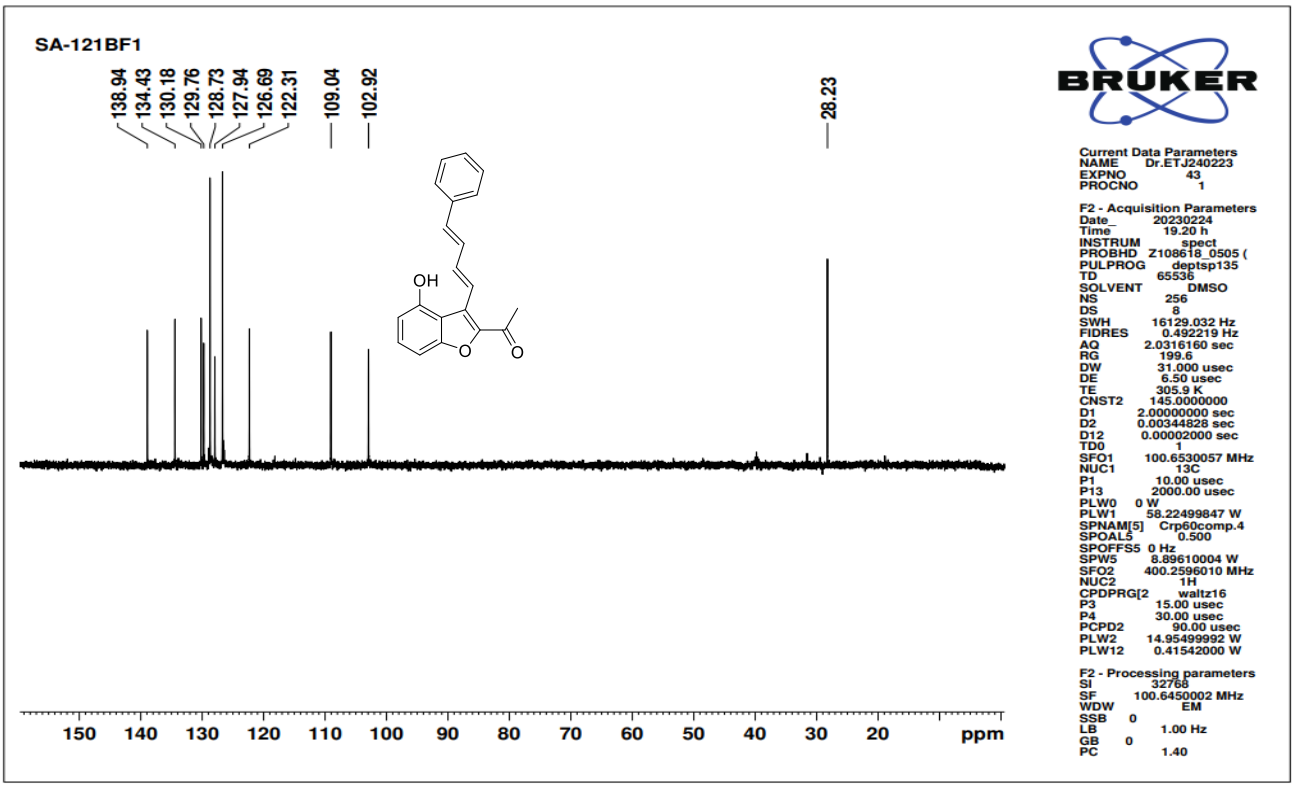


Figure 122: DEPT-135 NMR spectrum of compound **6l**

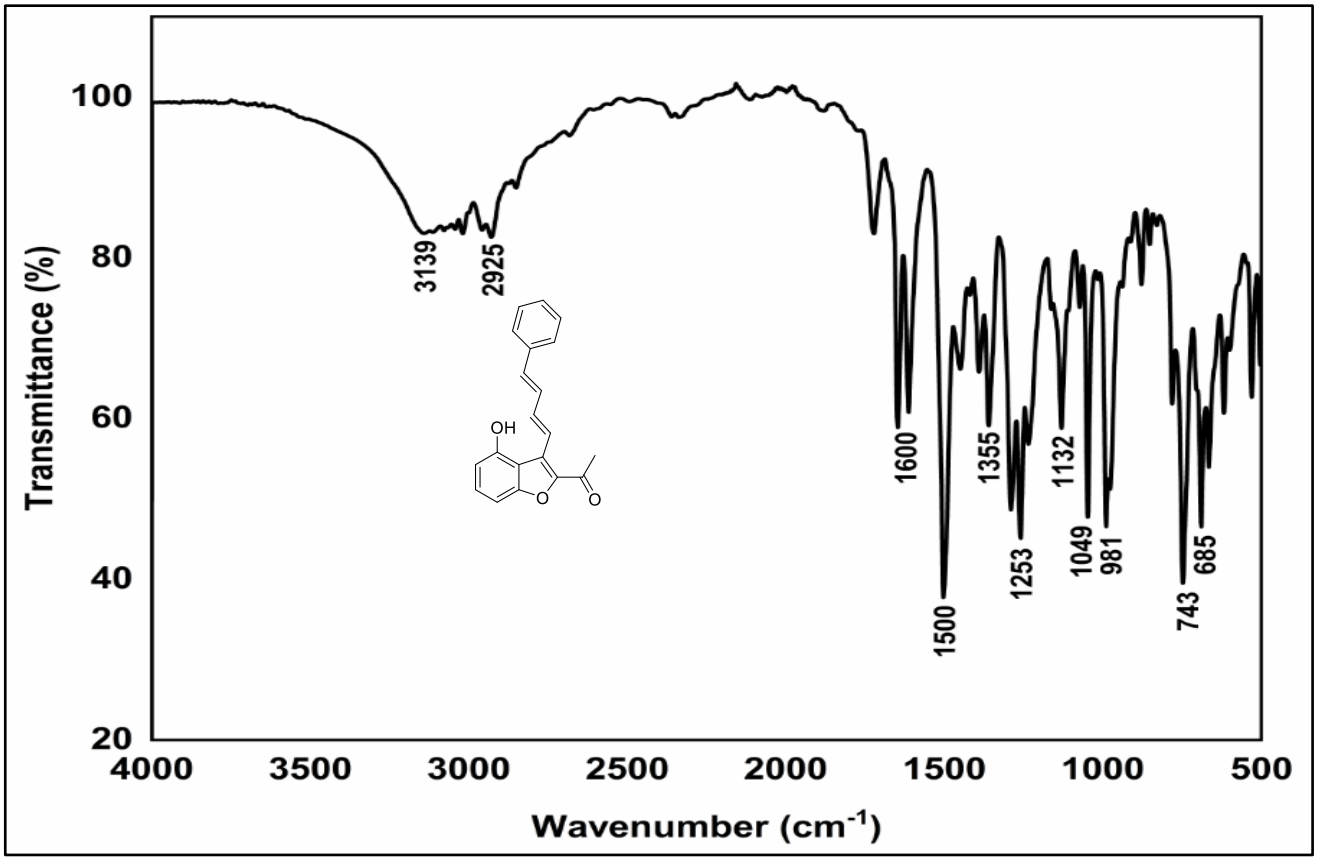


Figure 123: FT-IR spectrum of compound **6l**

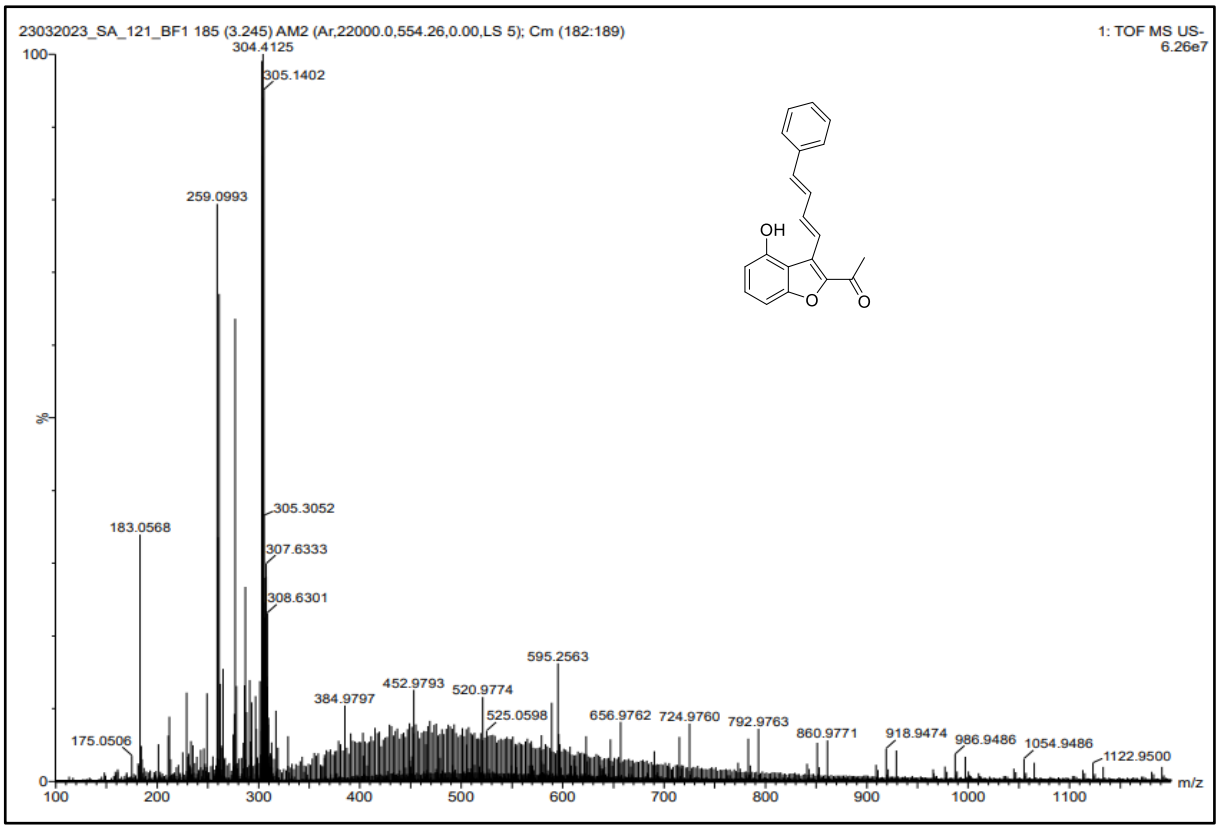


Figure 124: HRMS spectrum of compound **6l**

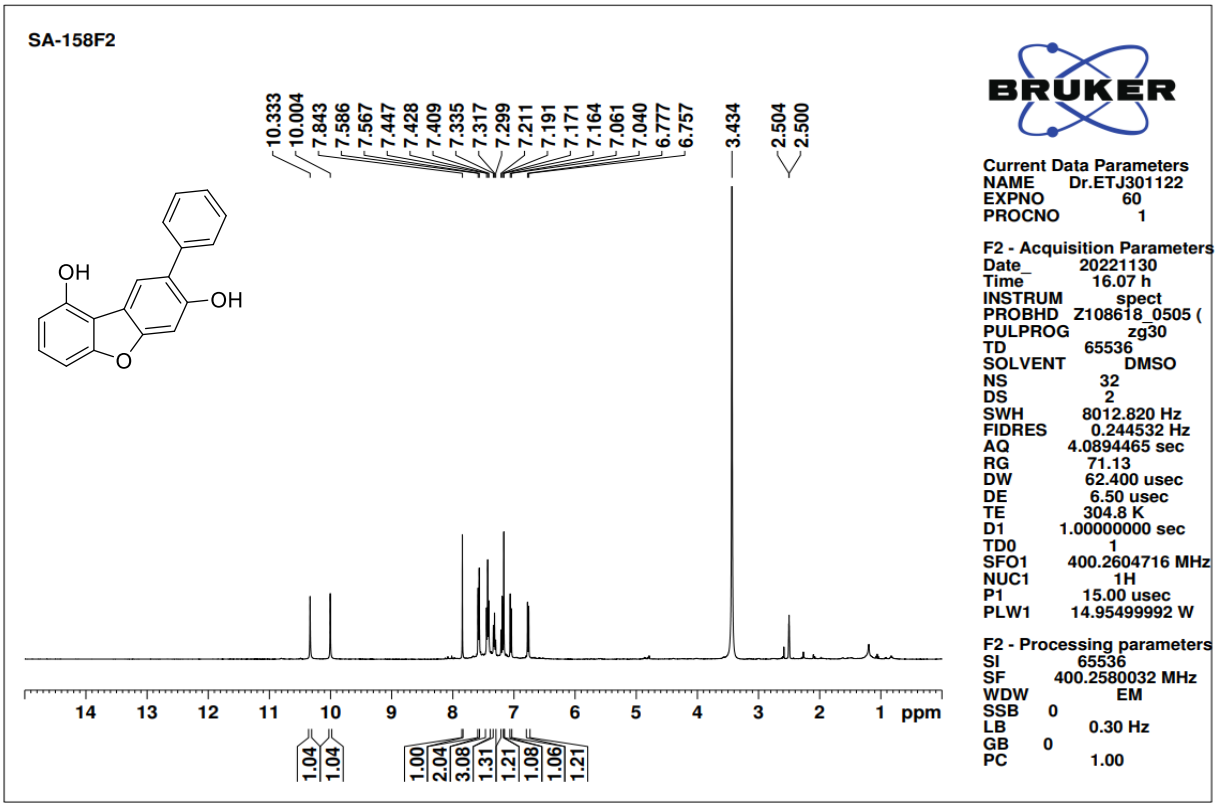


Figure 125: ^{1}H NMR spectrum of compound **7a**

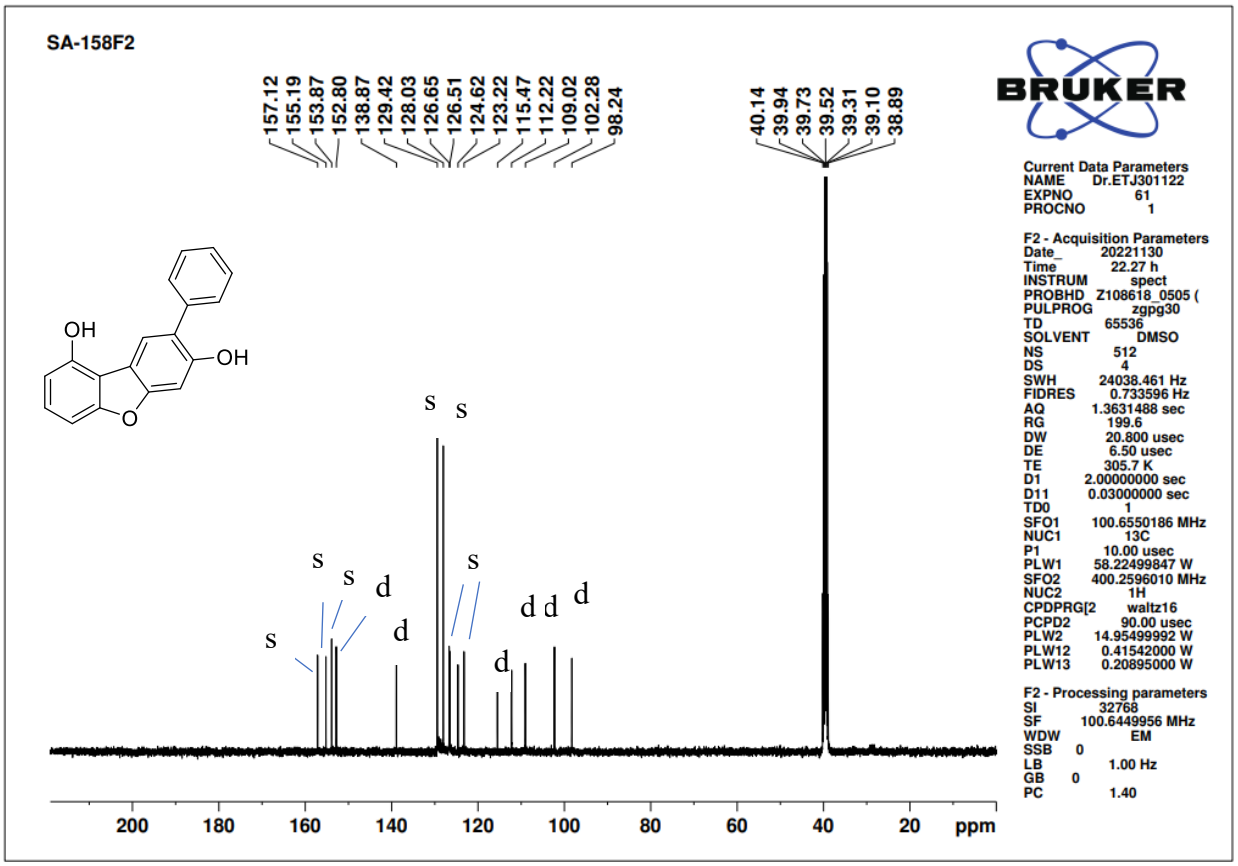


Figure 126: ^{13}C NMR spectrum of compound **7a**

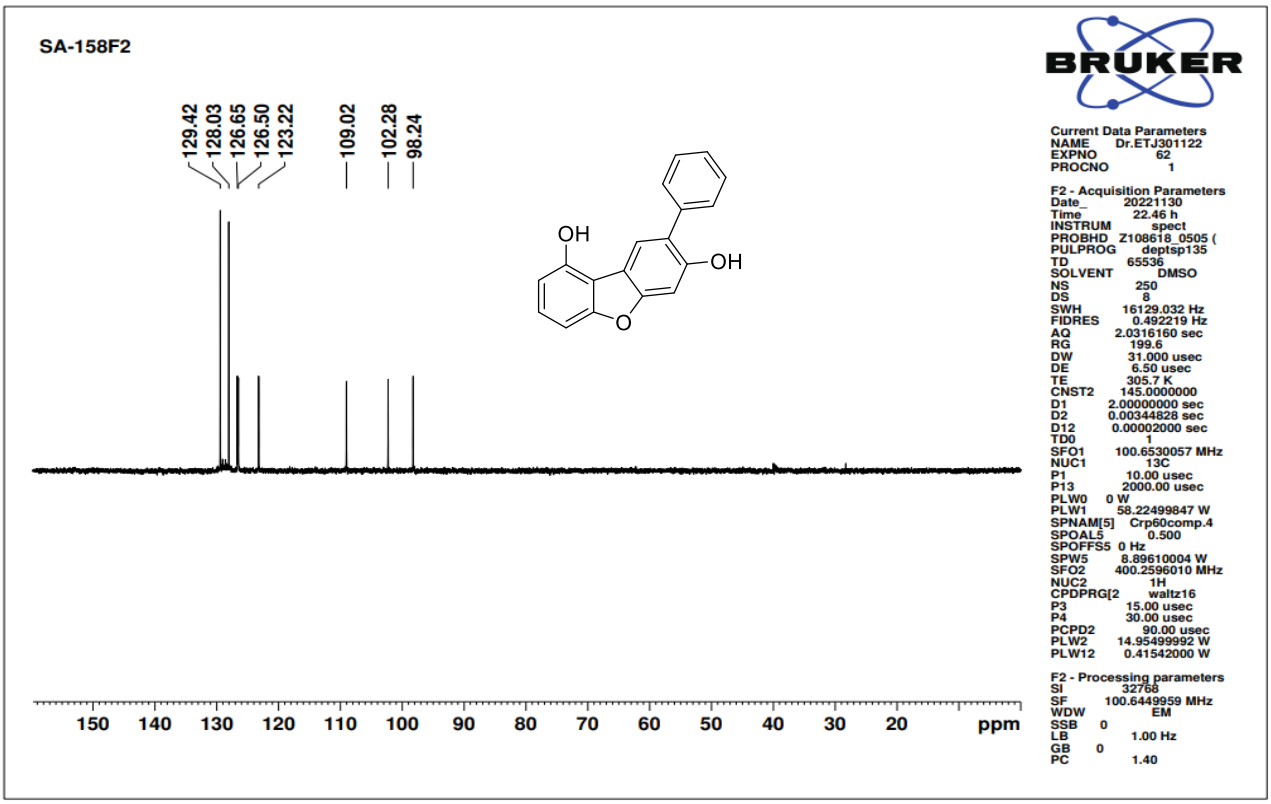


Figure 127: DEPT-135 NMR spectrum of compound **7a**

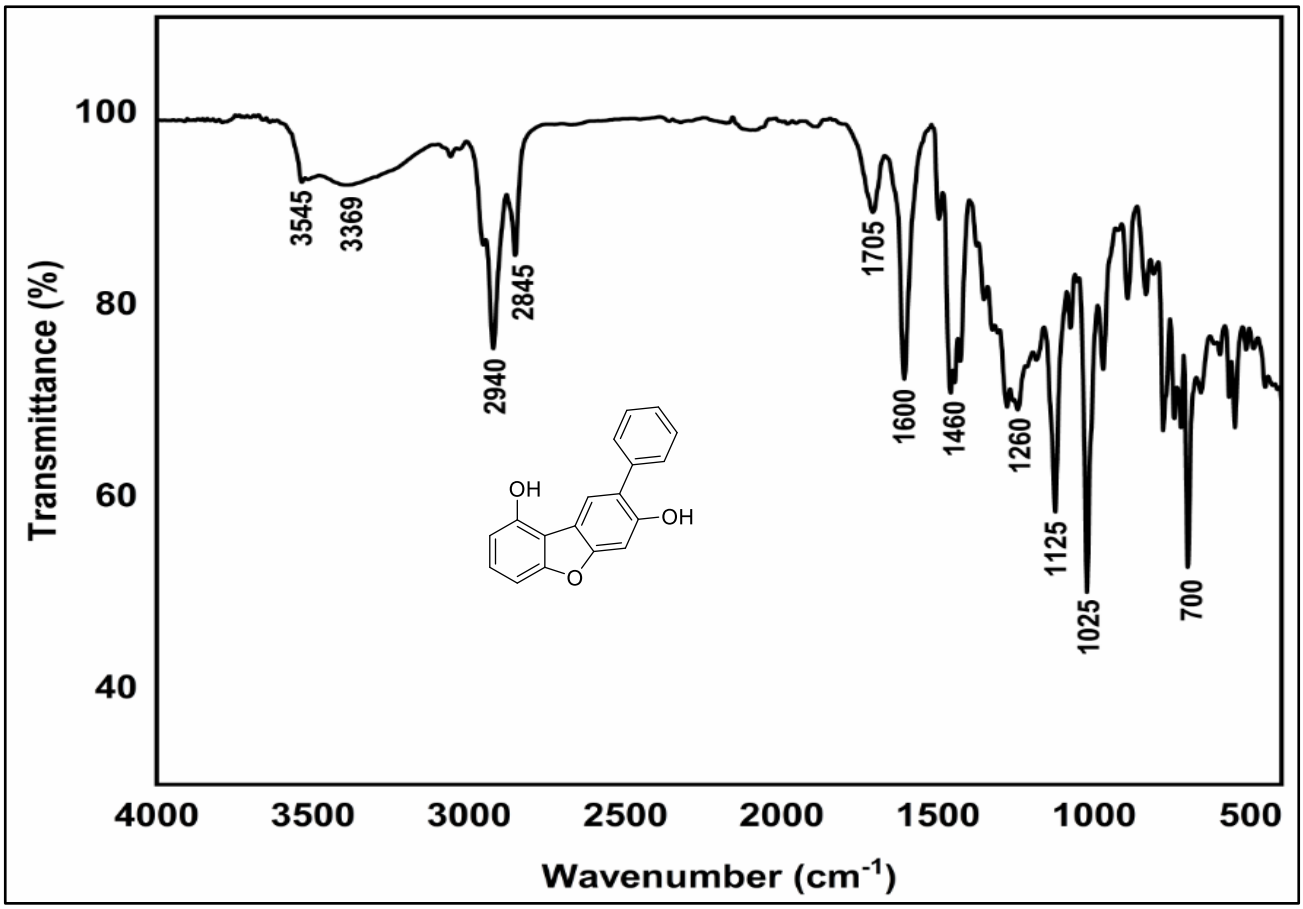


Figure 128: FT-IR spectrum of compound **7a**

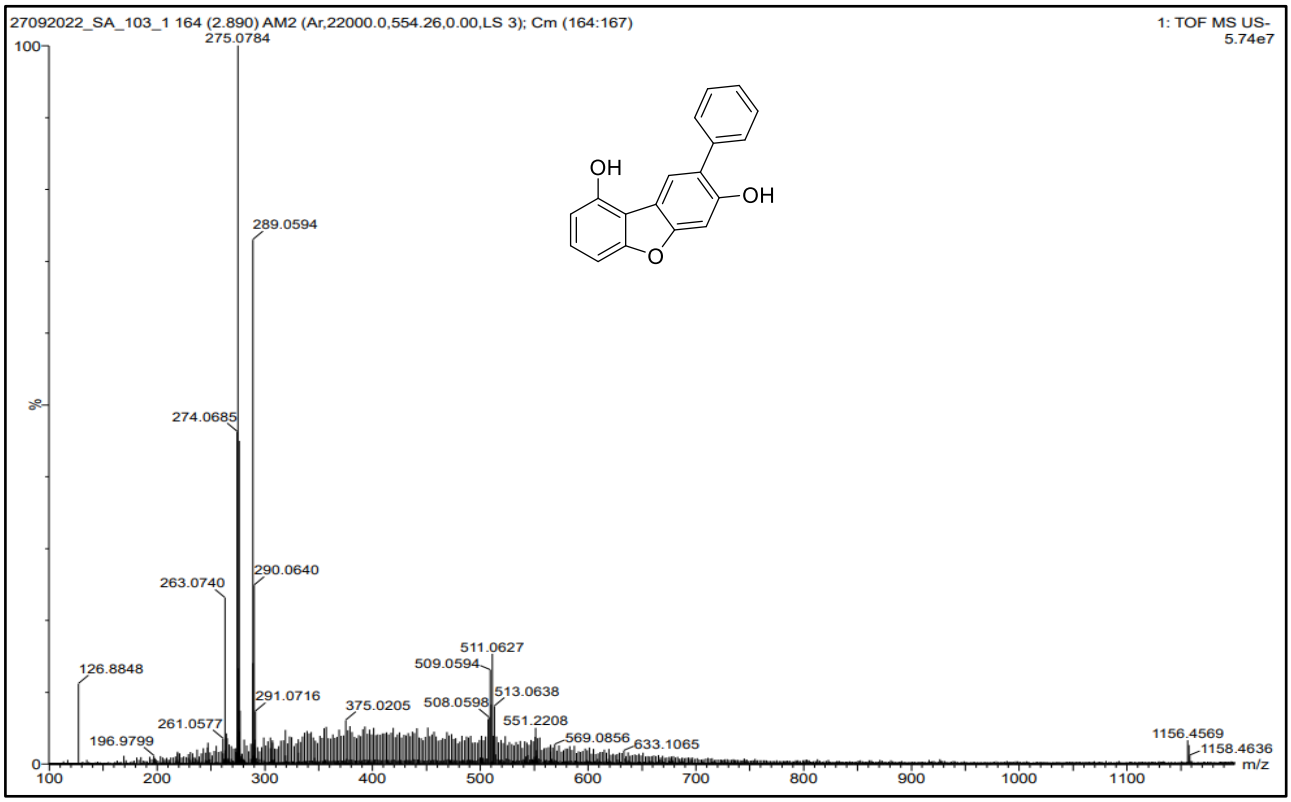


Figure 129: HRMS spectrum of compound **7a**

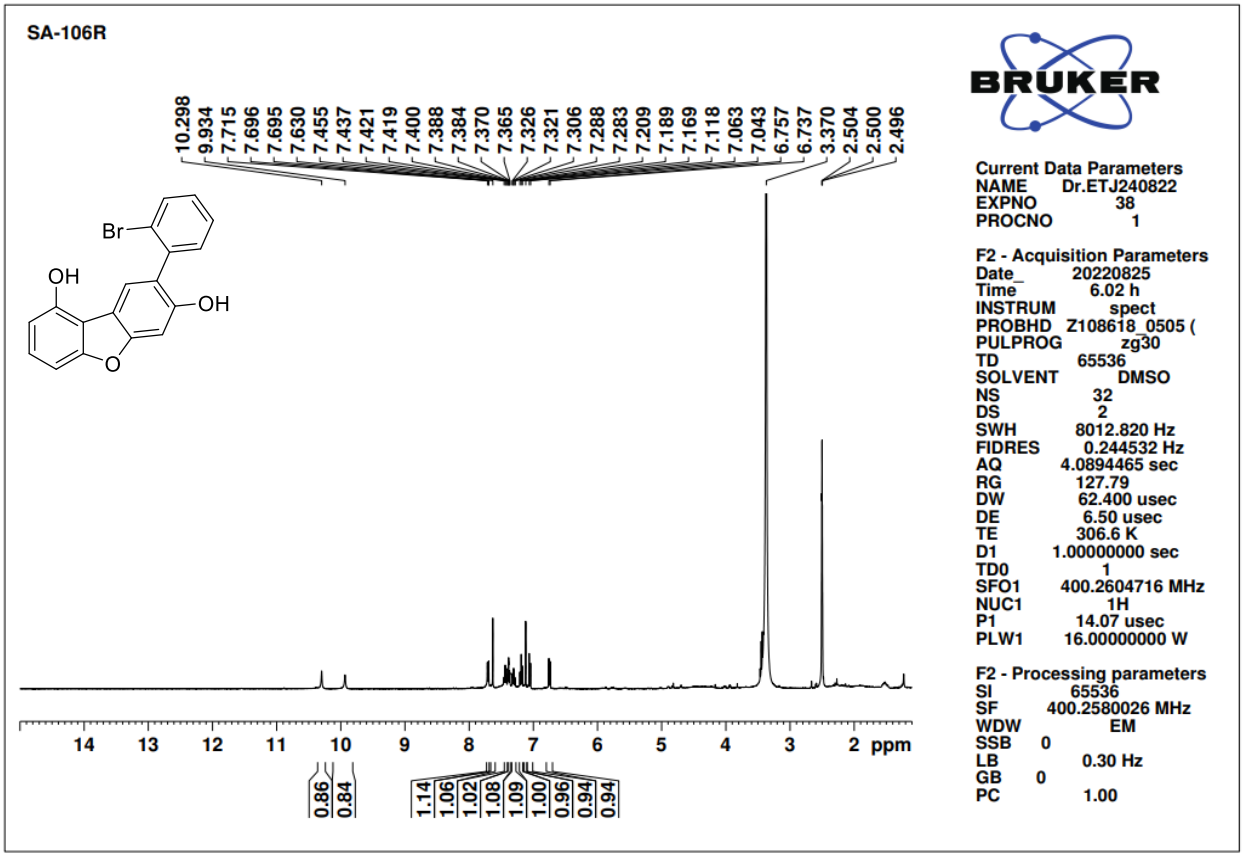


Figure 130: ^{1}H NMR spectrum of compound **7b**

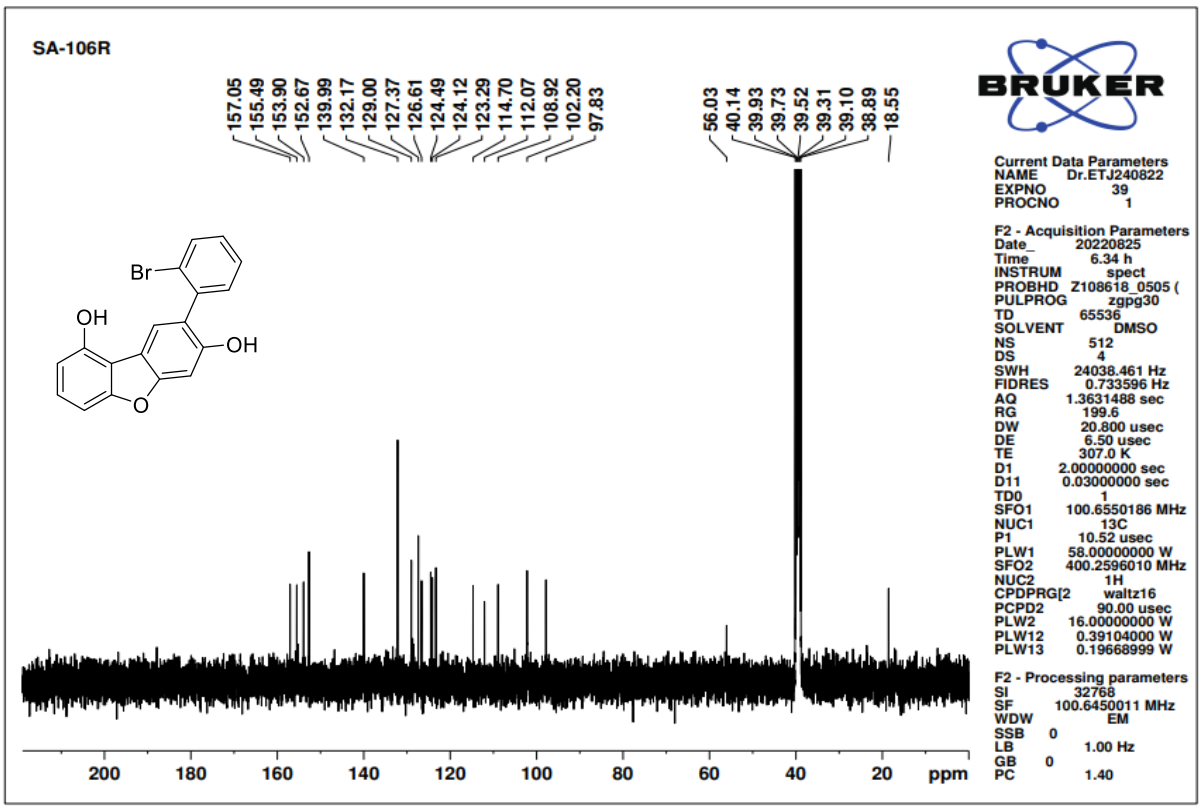


Figure 131: ^{13}C NMR spectrum of compound **7b**

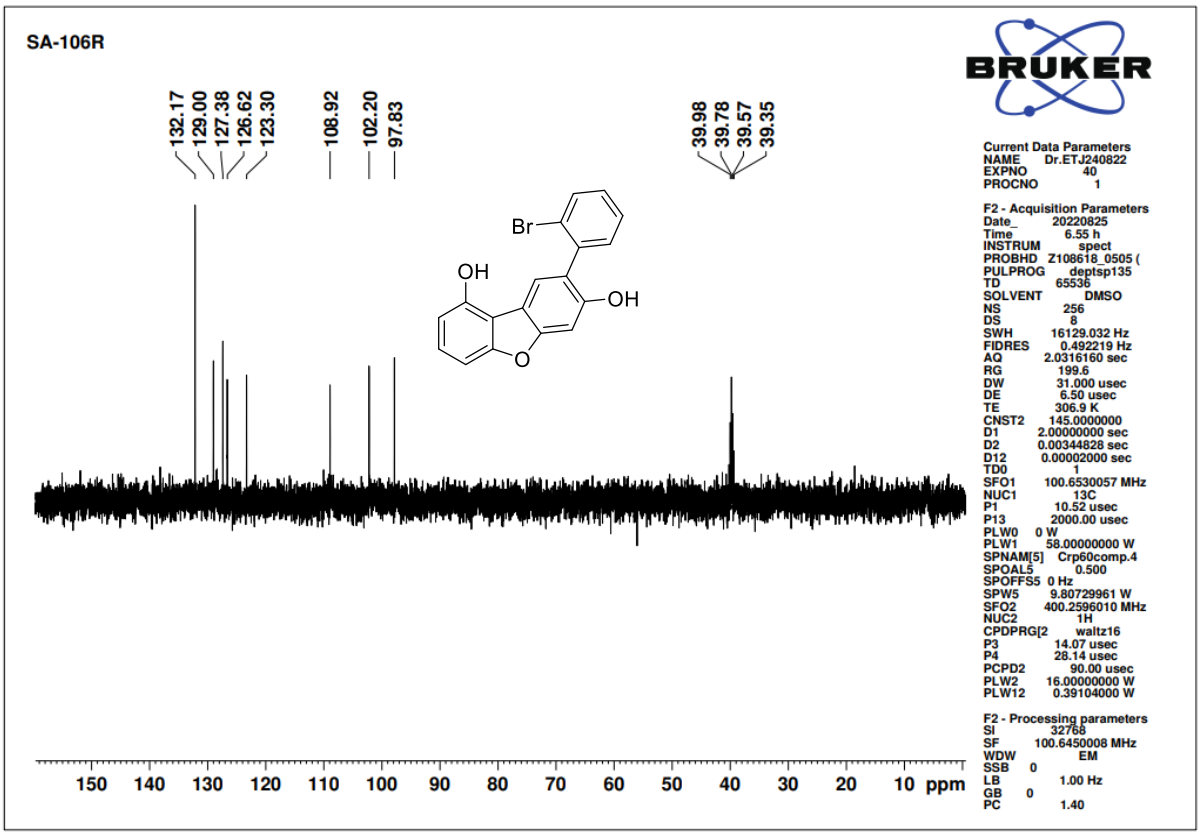


Figure 132: DEPT-135 NMR spectrum of compound **7b**

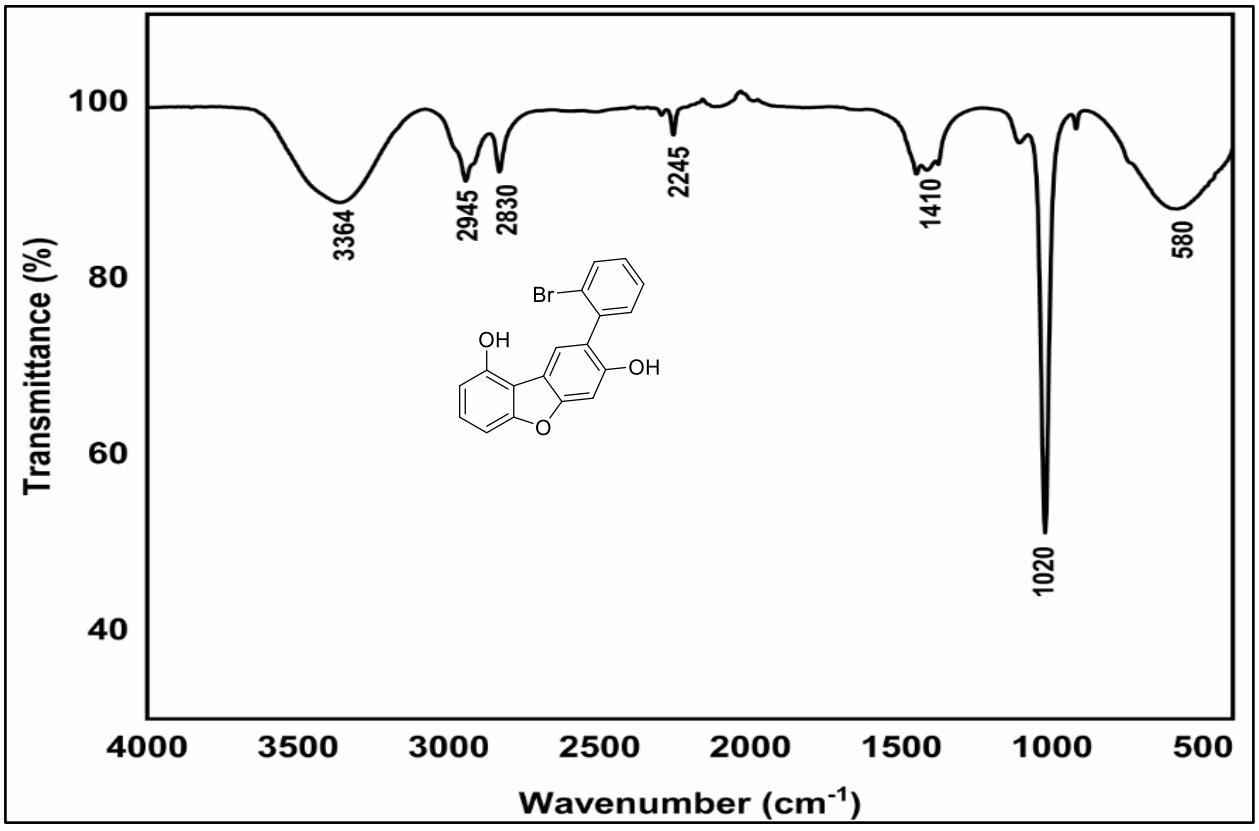


Figure 133: FT-IR spectrum of compound **7b**

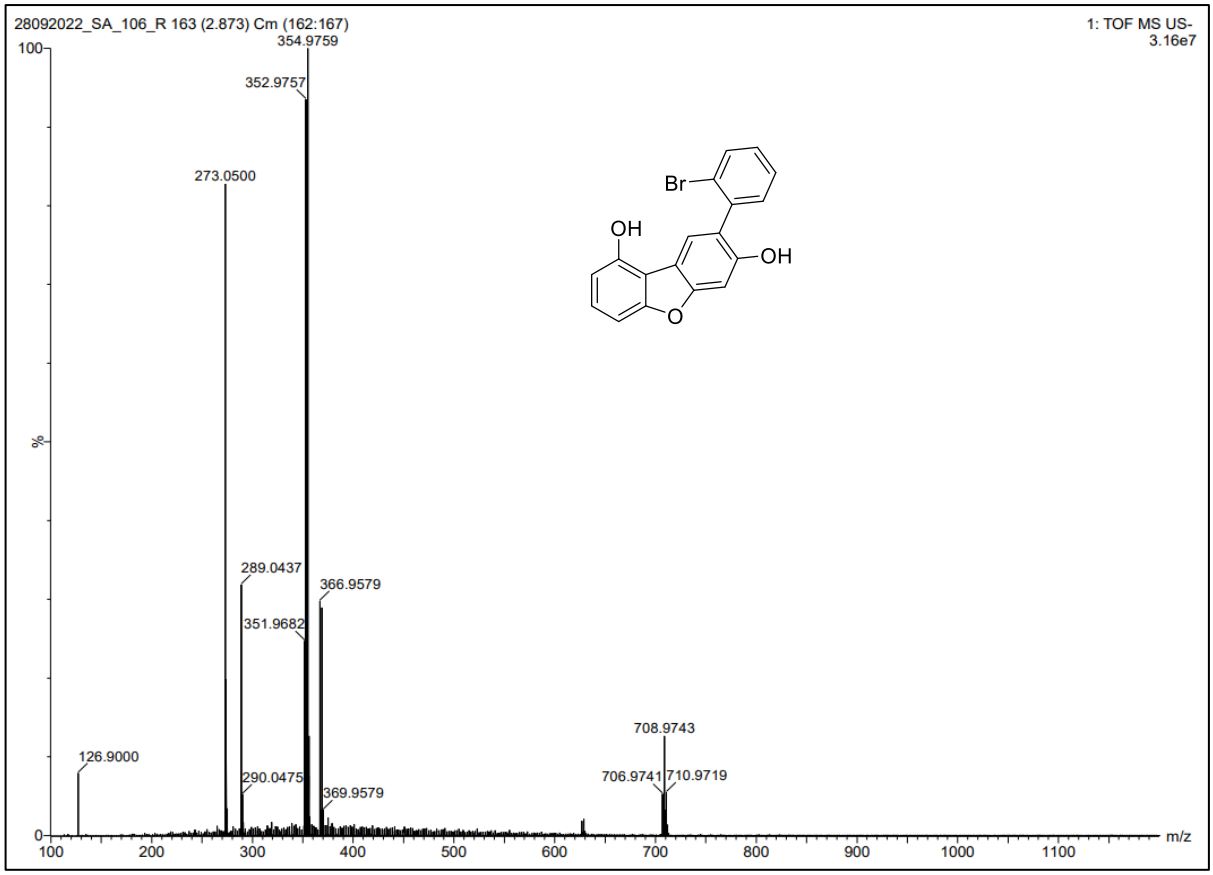


Figure 134: HRMS spectrum of compound **7b**

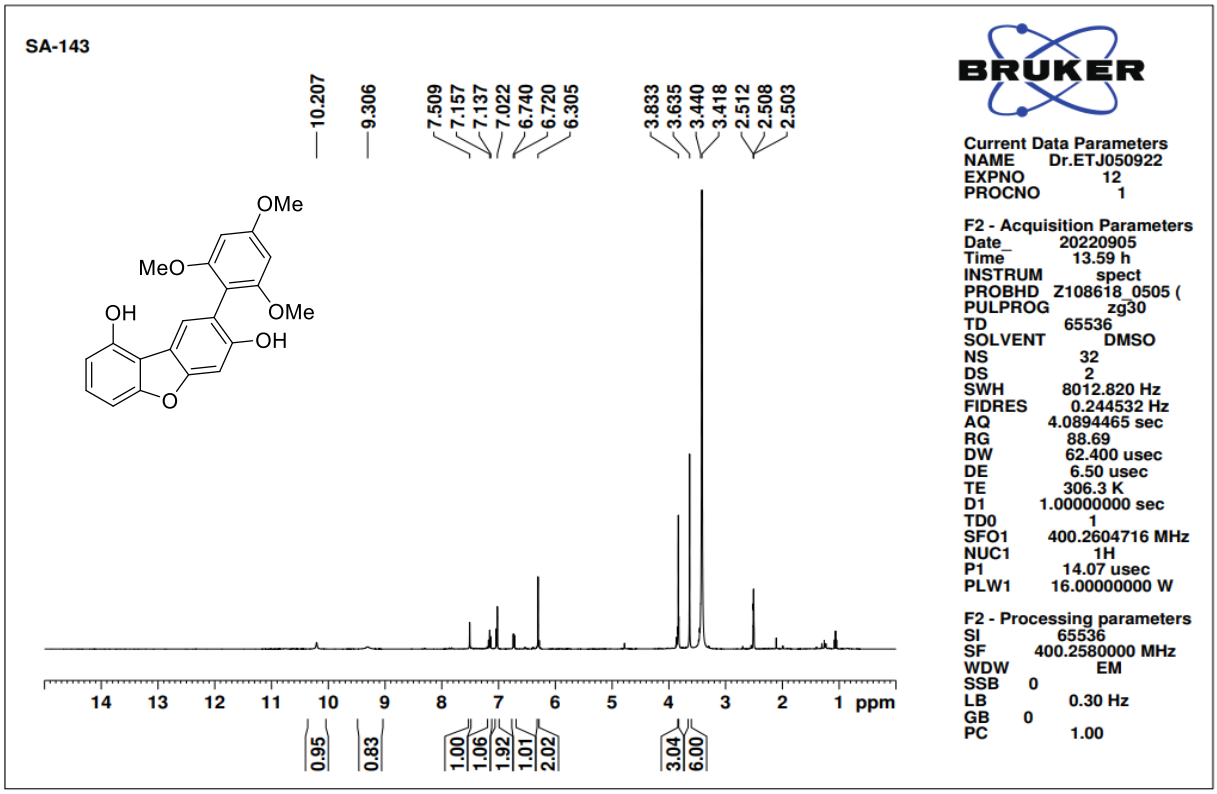


Figure 135: ^{1}H NMR spectrum of compound **7c**

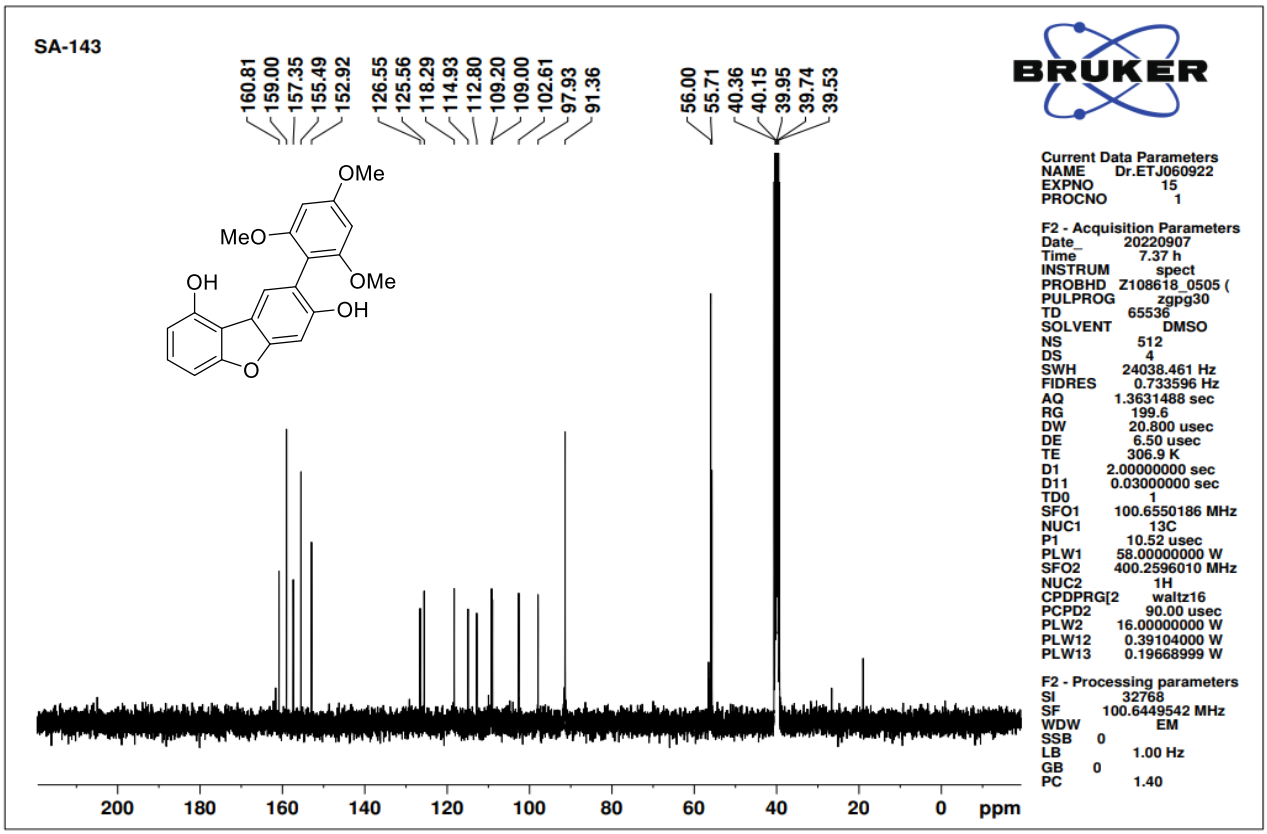


Figure 136: ^{13}C NMR spectrum of compound **7c**

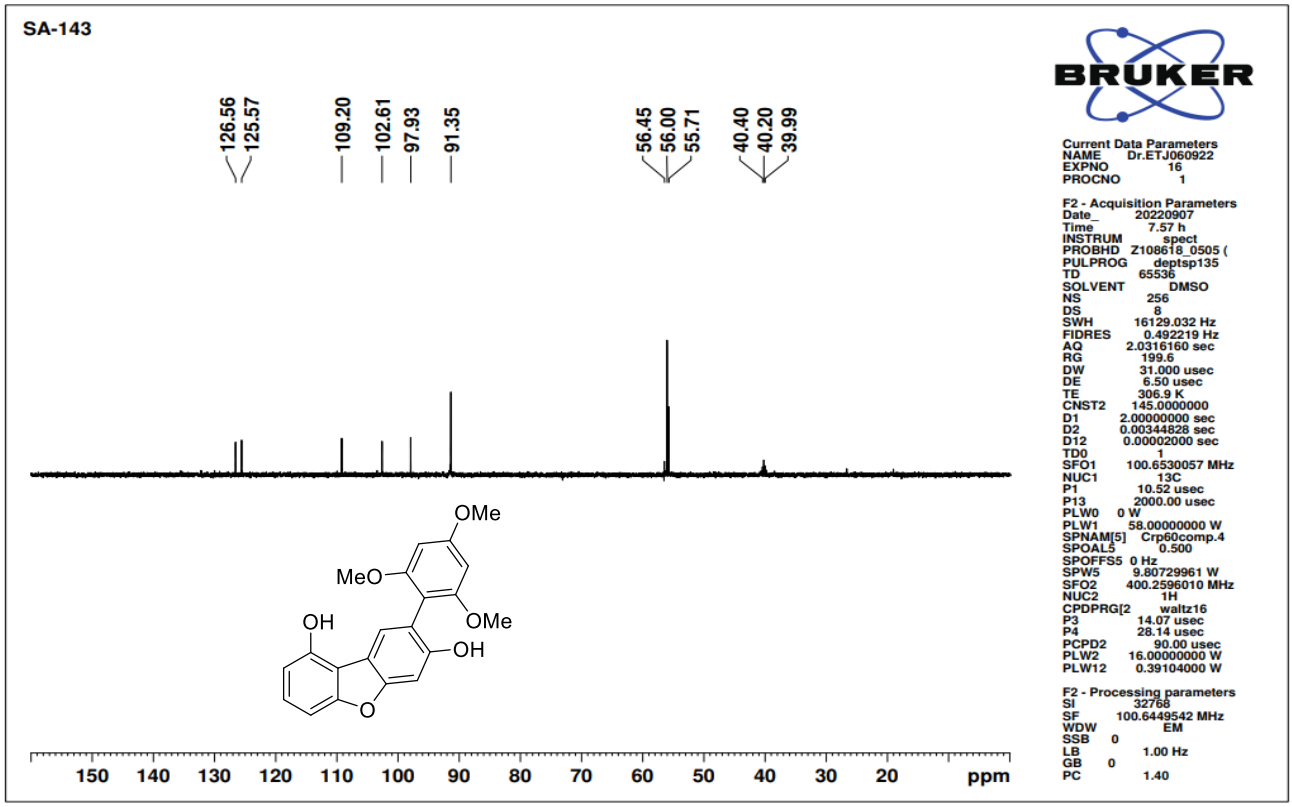


Figure 137: DEPT-135 NMR spectrum of compound **7c**

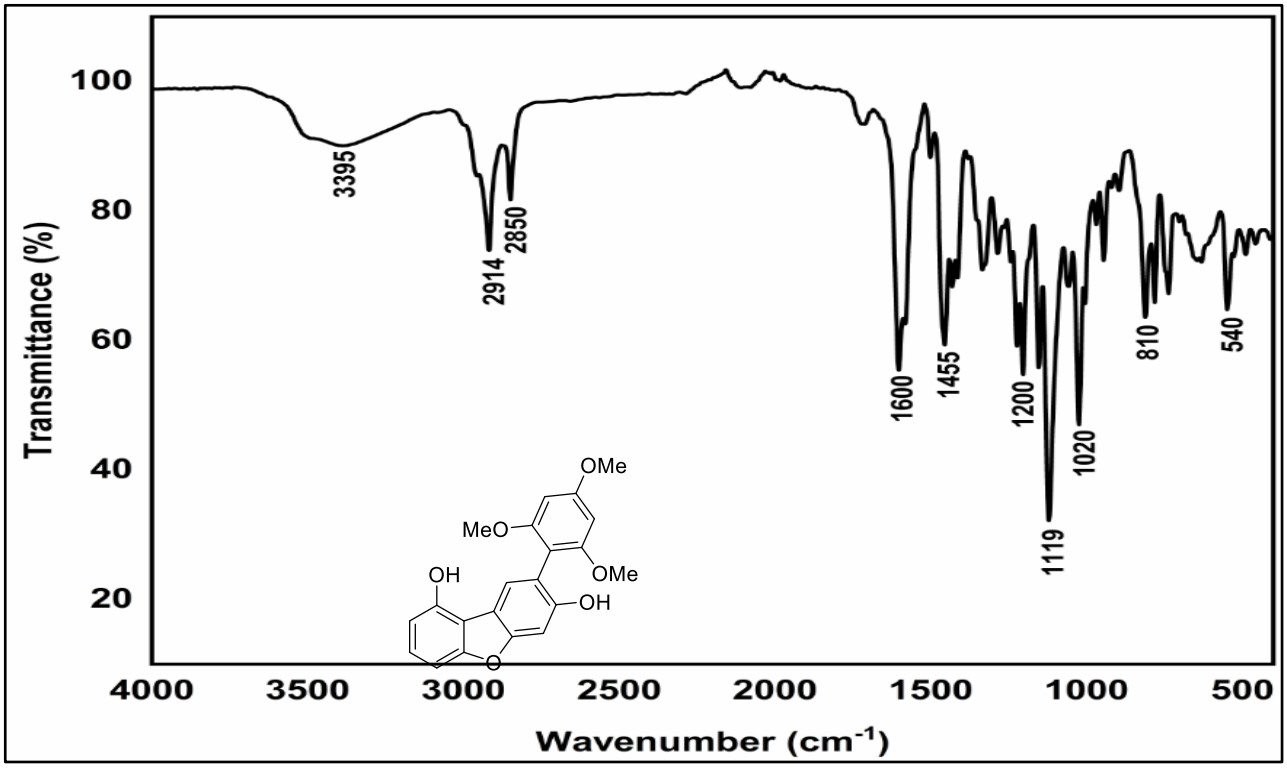


Figure 138: FT-IR spectrum of compound **7c**

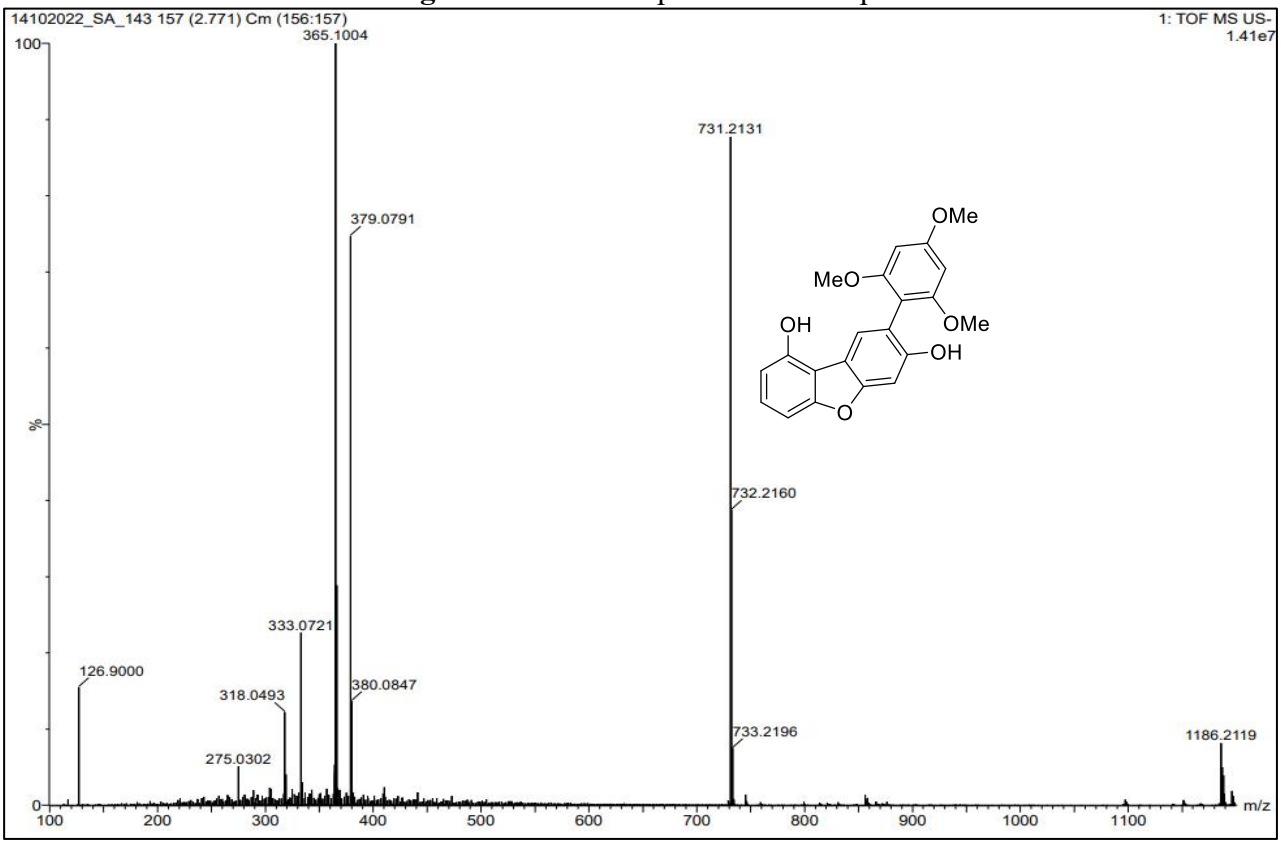


Figure 139: HRMS spectrum of compound **7c**

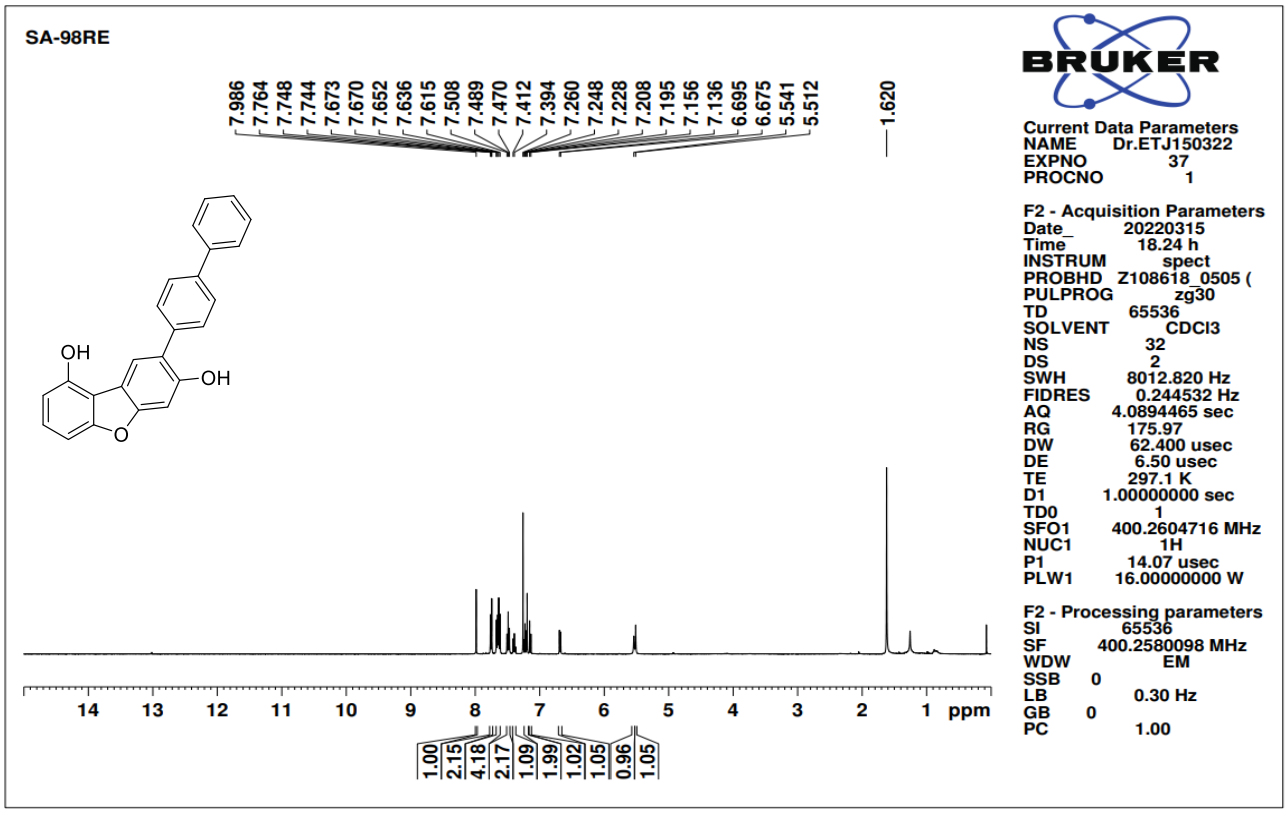


Figure 140: ^{1}H NMR spectrum of compound **7d**

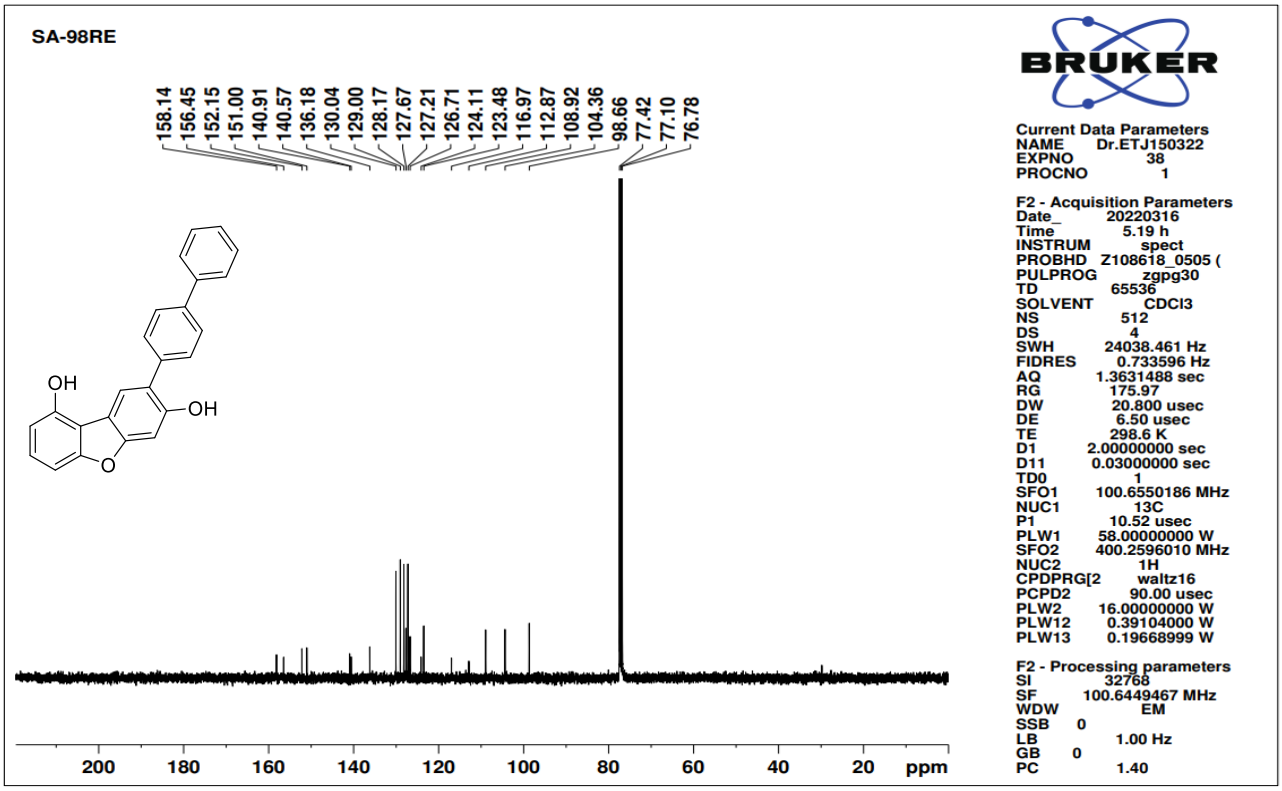


Figure 141: ^{13}C NMR spectrum of compound **7d**

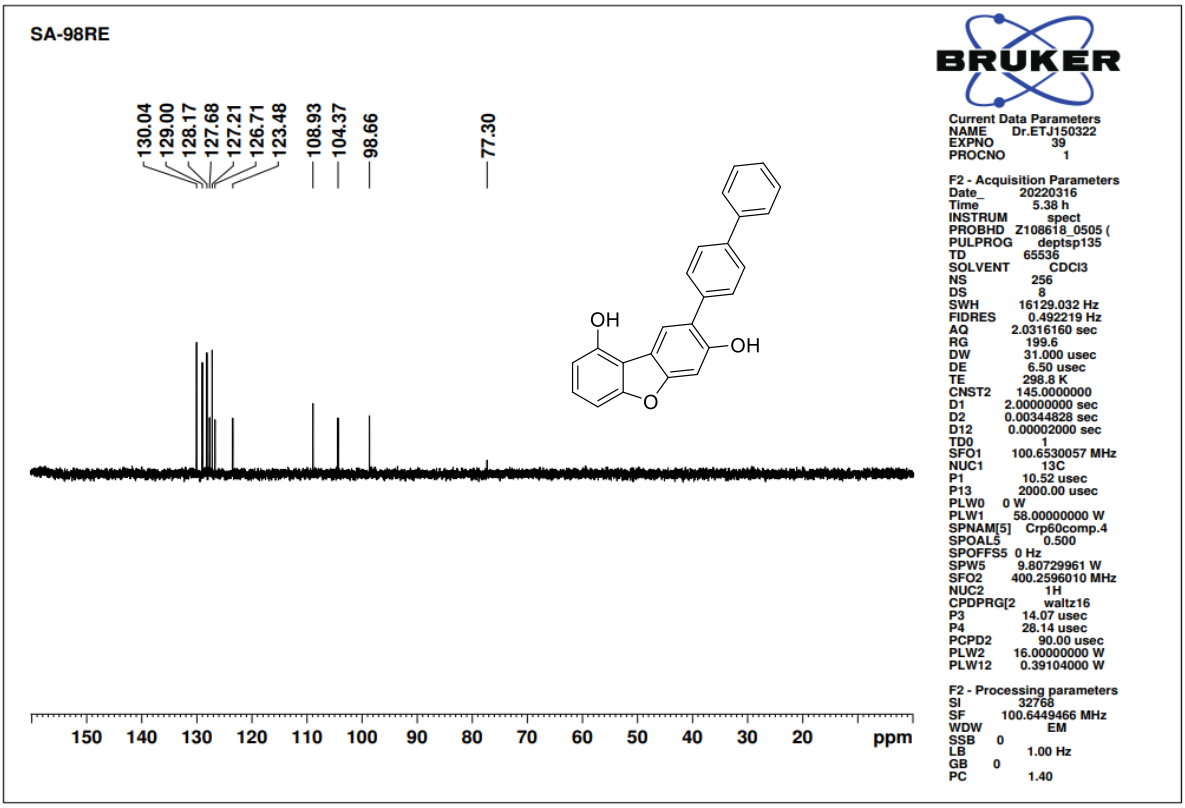


Figure 142: DEPT-135 NMR spectrum of compound **7d**

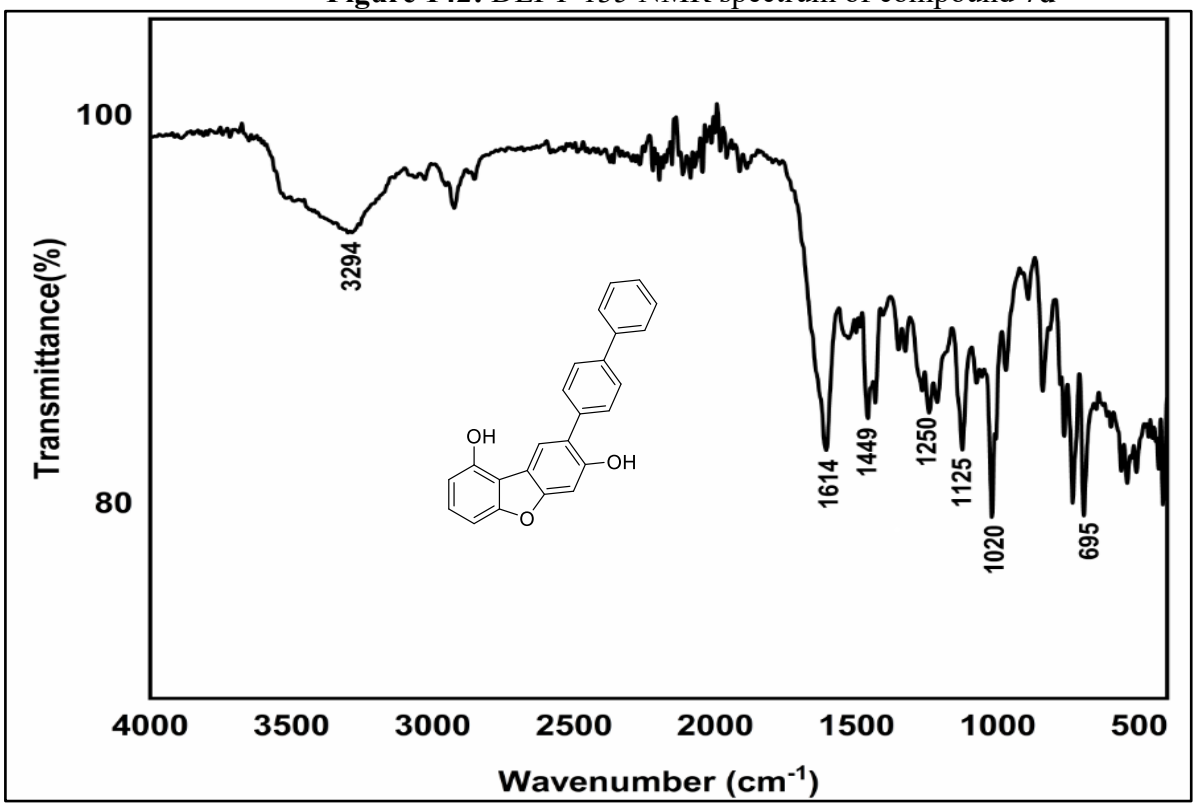


Figure 143: FT-IR spectrum of compound **7d**

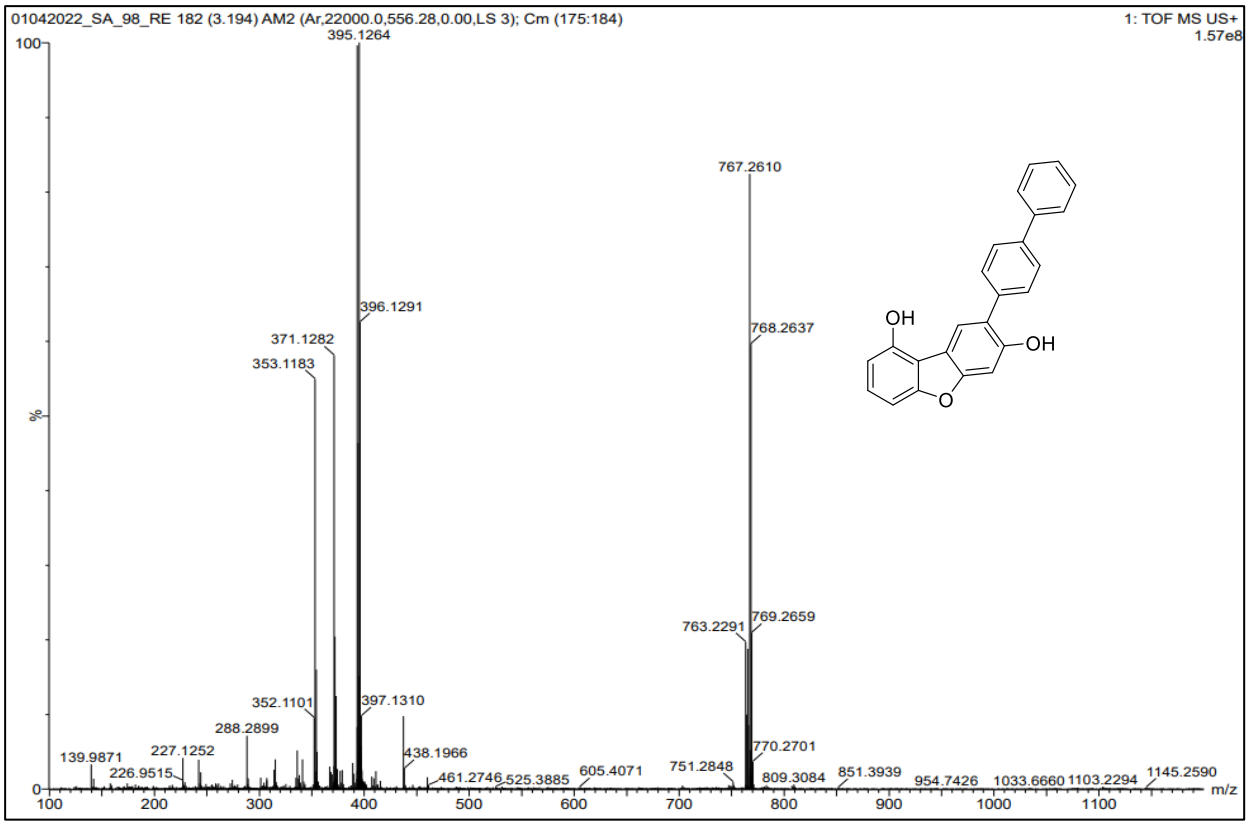


Figure 144: HRMS spectrum of compound **7d**

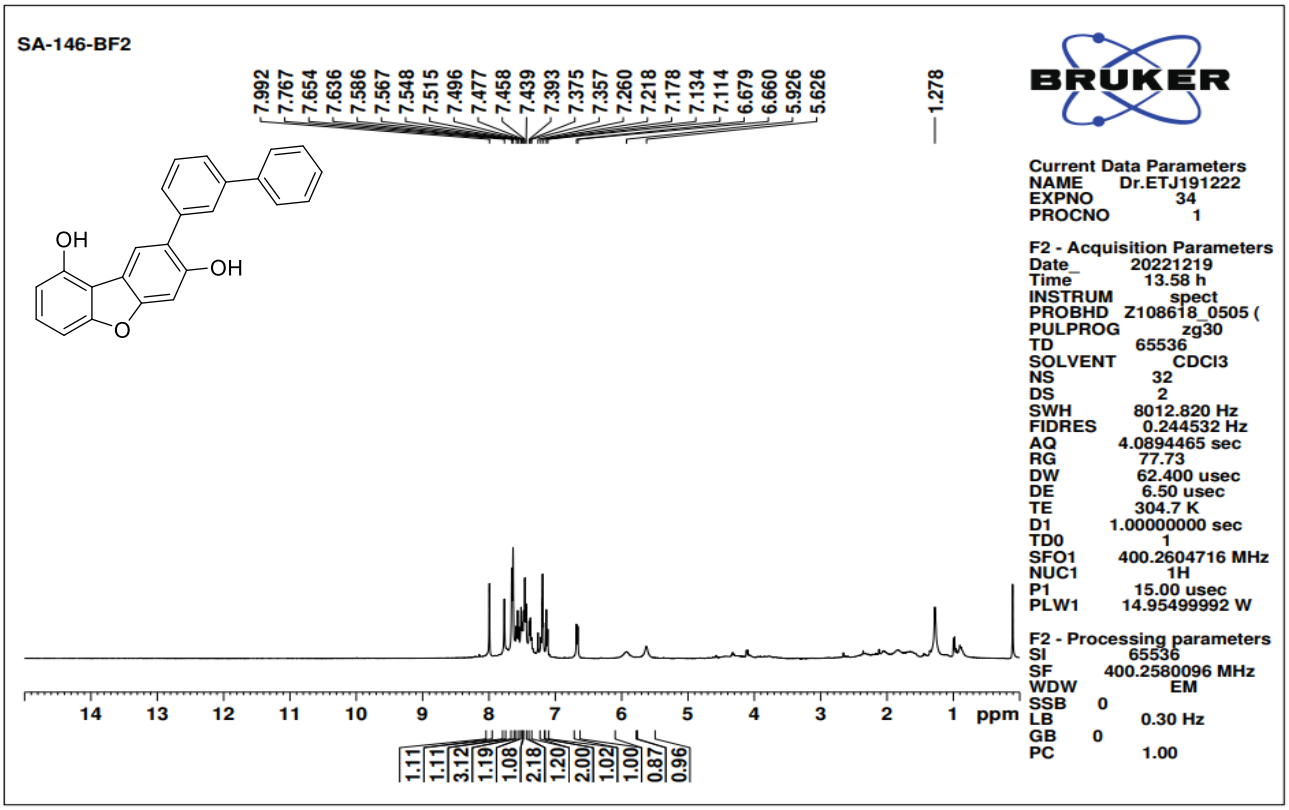


Figure 145: ^{1}H NMR spectrum of compound **7e**

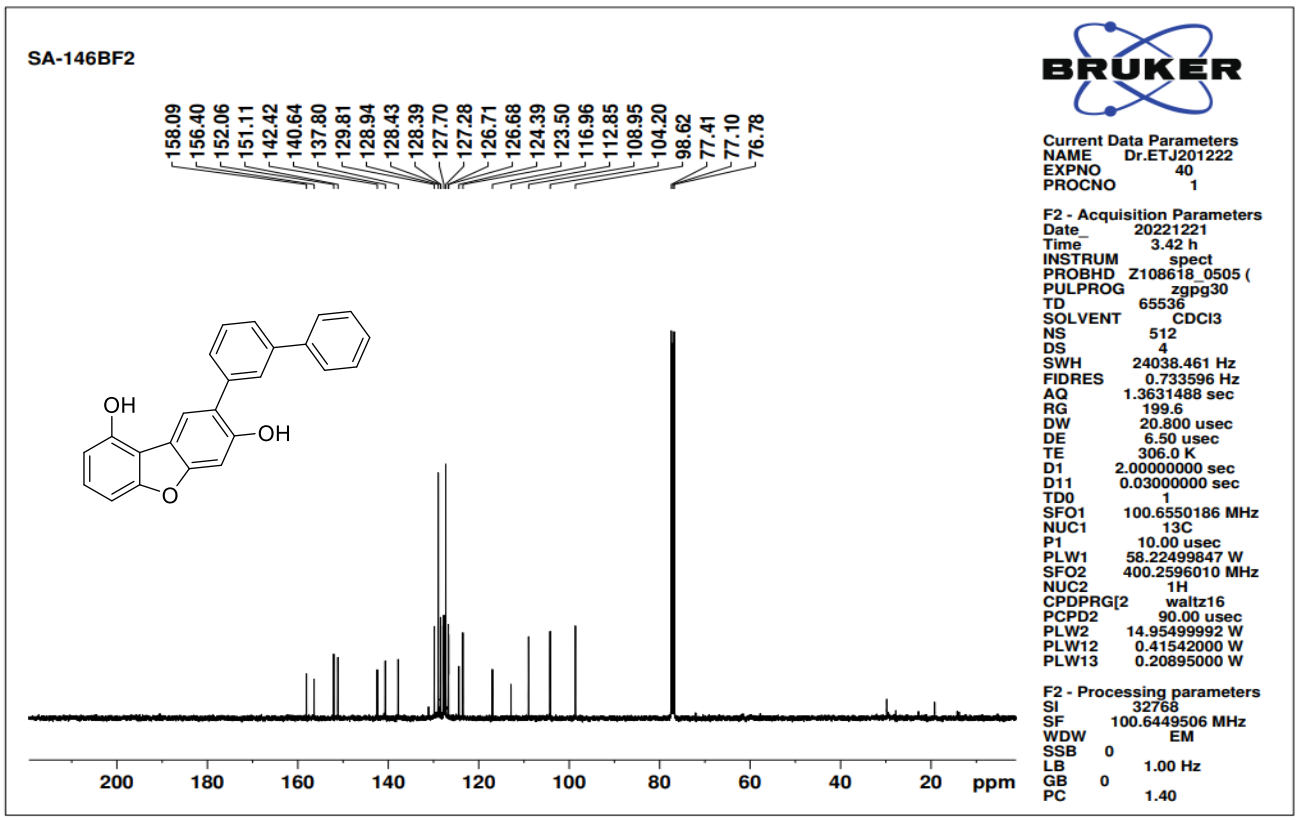


Figure 146: ^{13}C NMR spectrum of compound **7e**

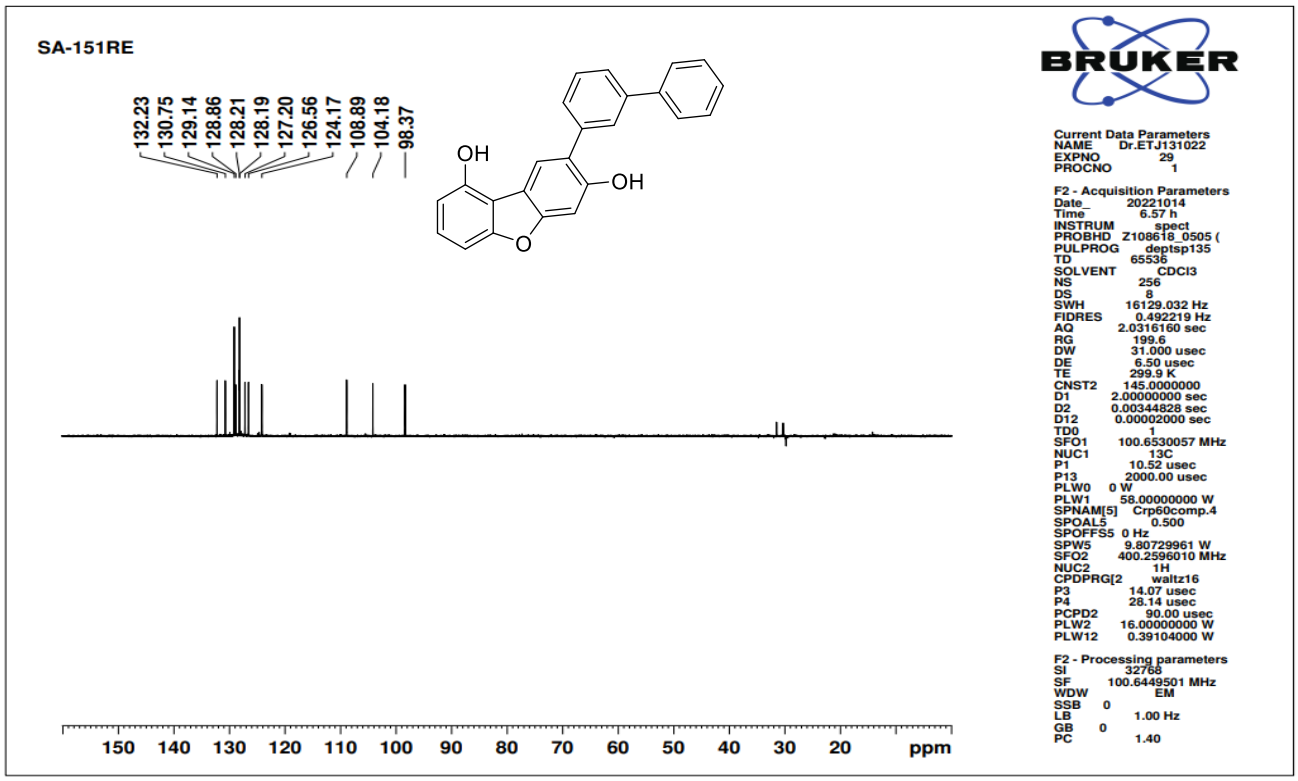


Figure 147: DEPT-135 NMR spectrum of compound **7e**

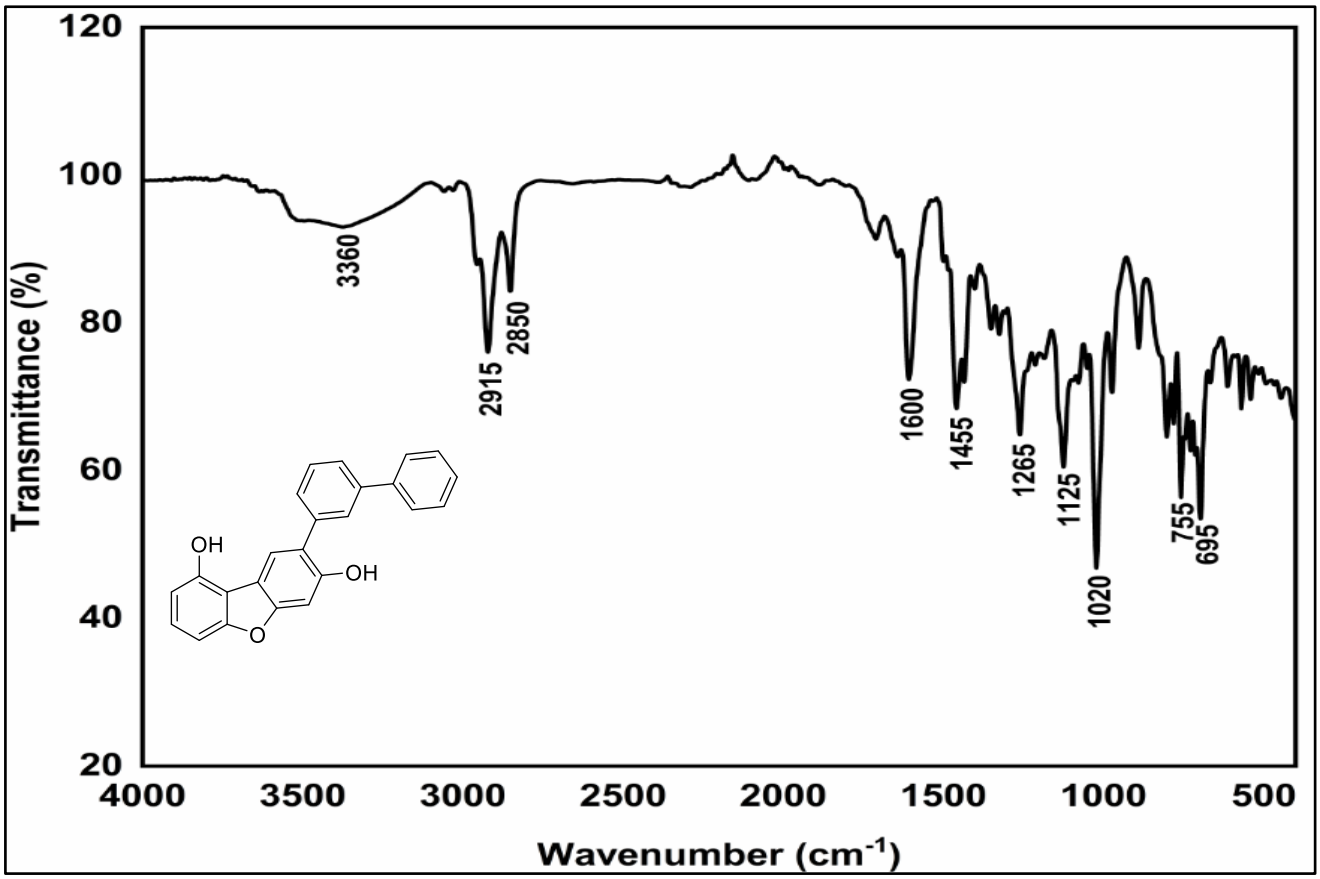


Figure 148: FT-IR spectrum of compound **7e**

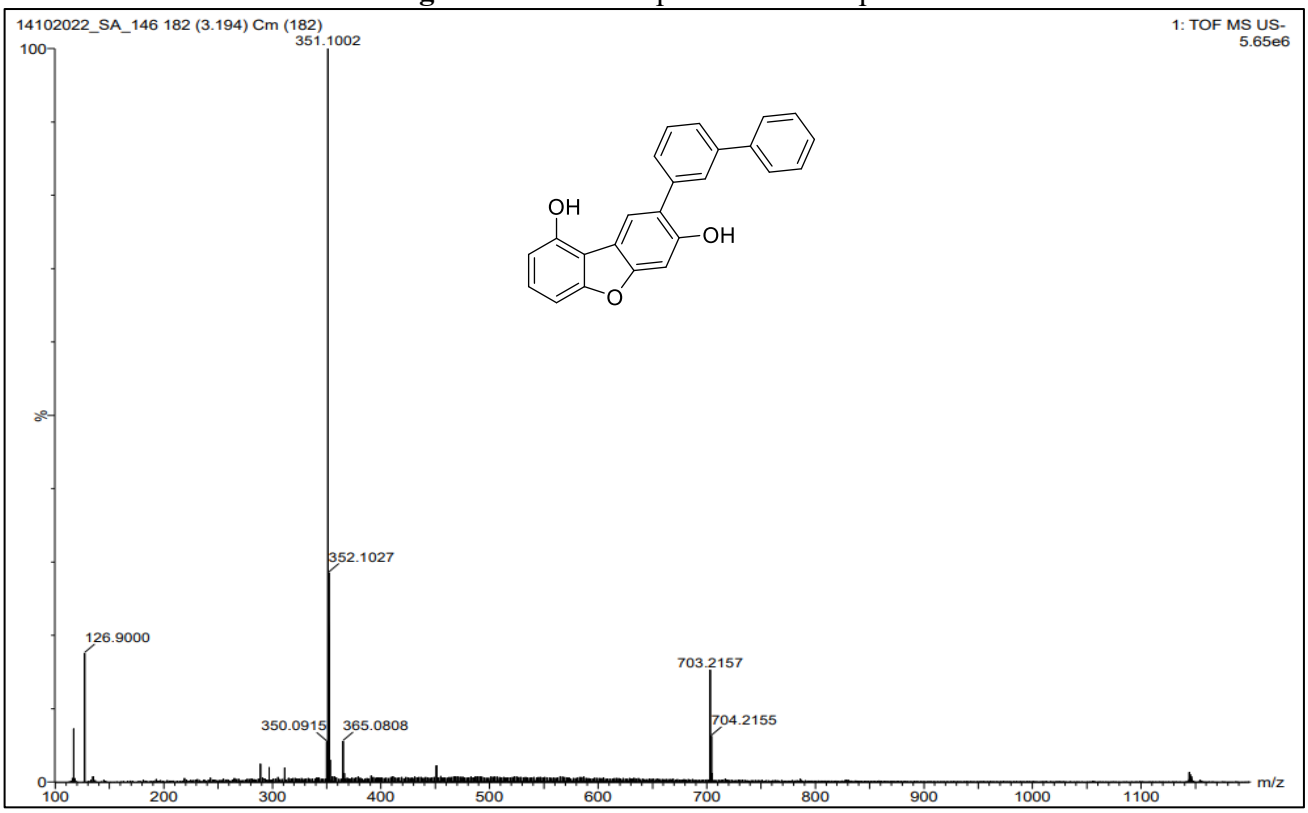


Figure 149: HRMS spectrum of compound **7e**

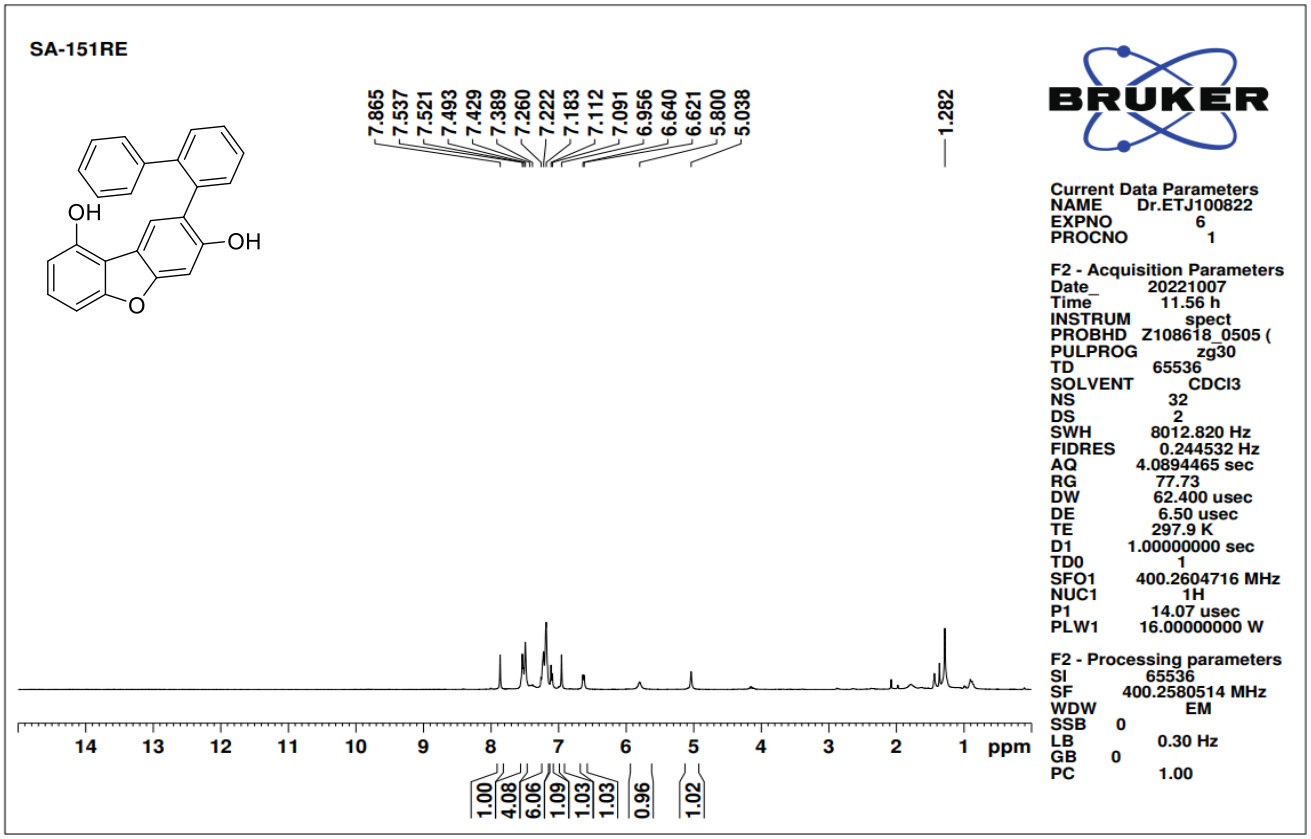


Figure 150: ^{1}H NMR spectrum of compound **7f**

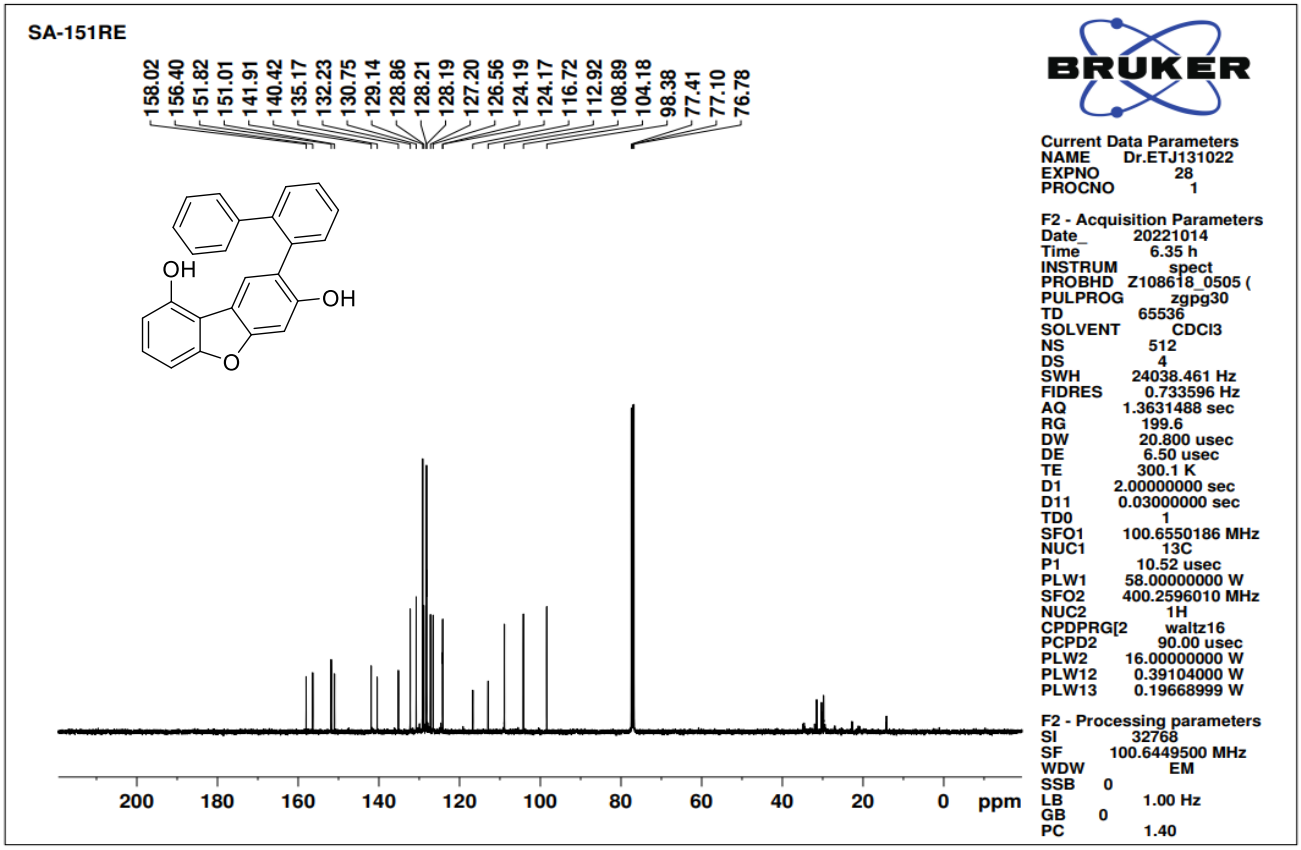


Figure 151: ^{13}C NMR spectrum of compound **7f**

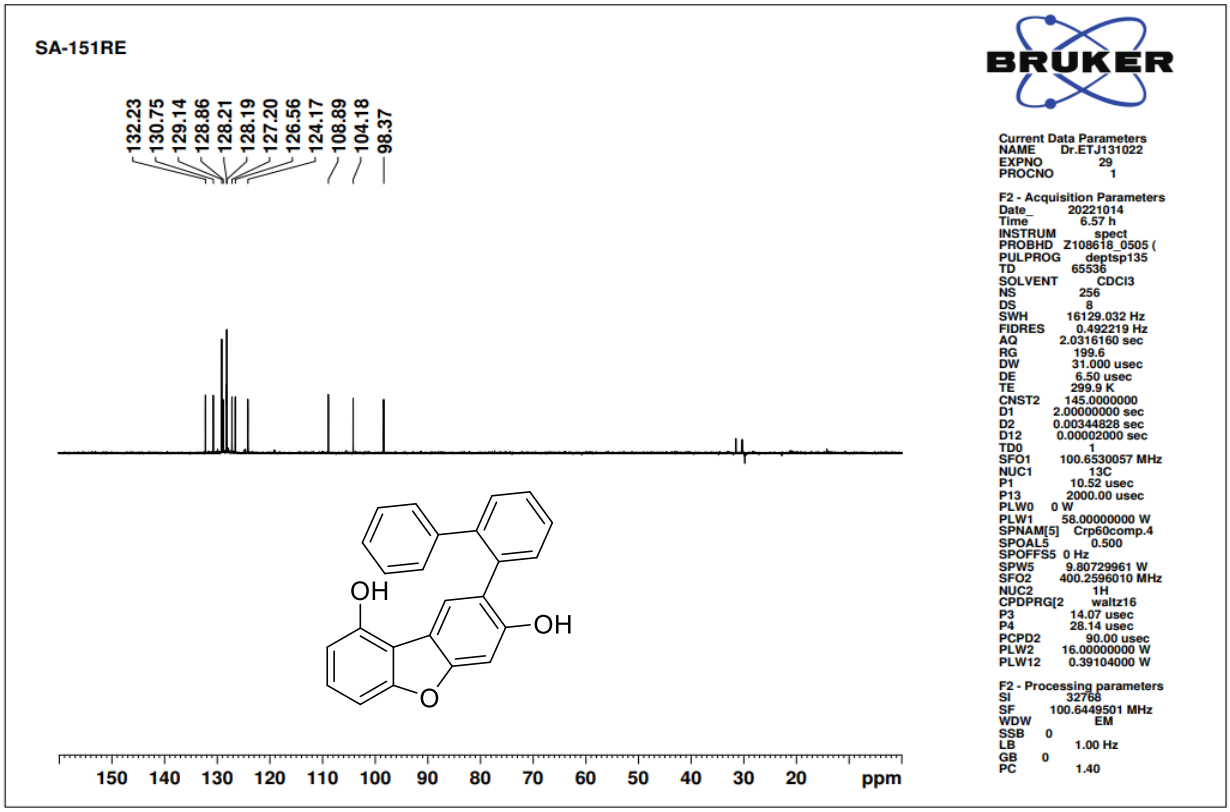


Figure 152: DEPT-135 NMR spectrum of compound **7f**

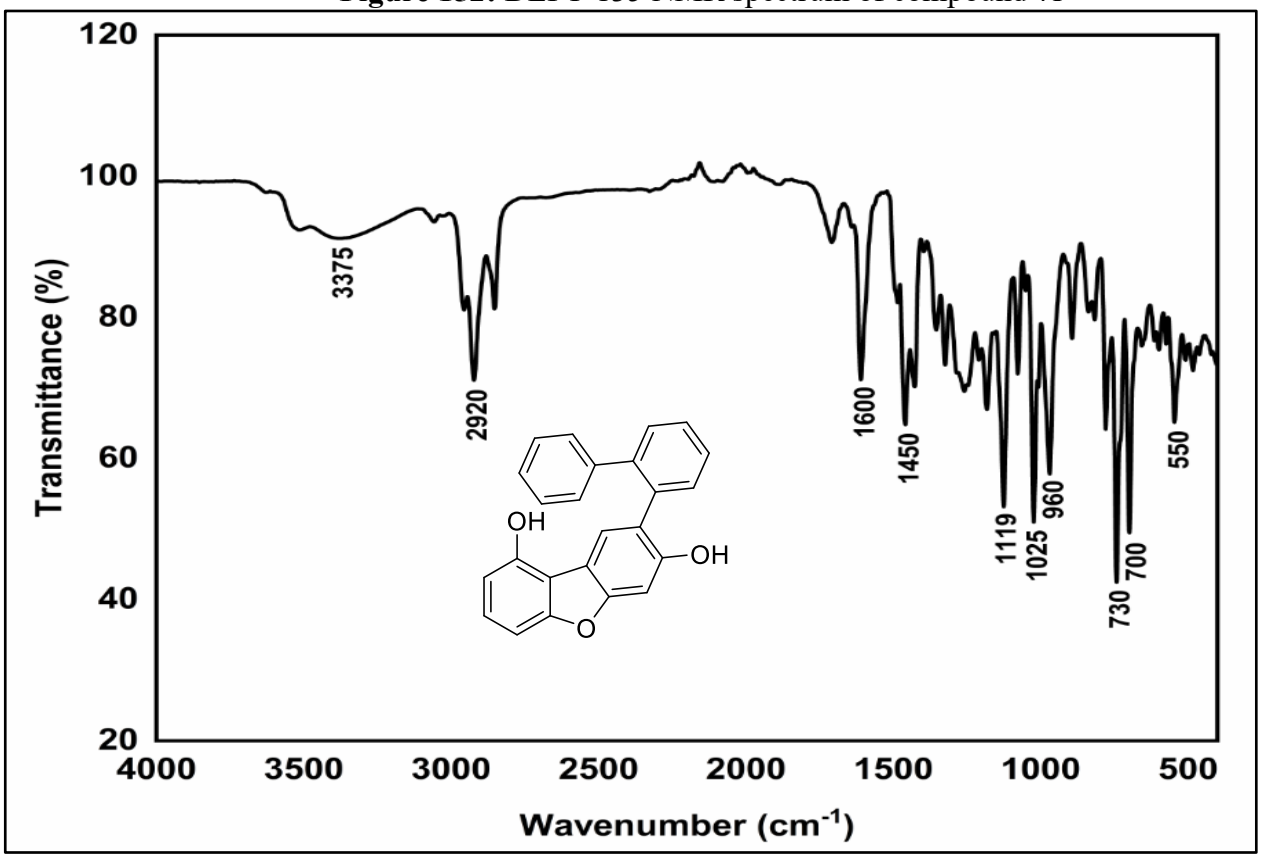


Figure 153: FT-IR spectrum of compound **7f**

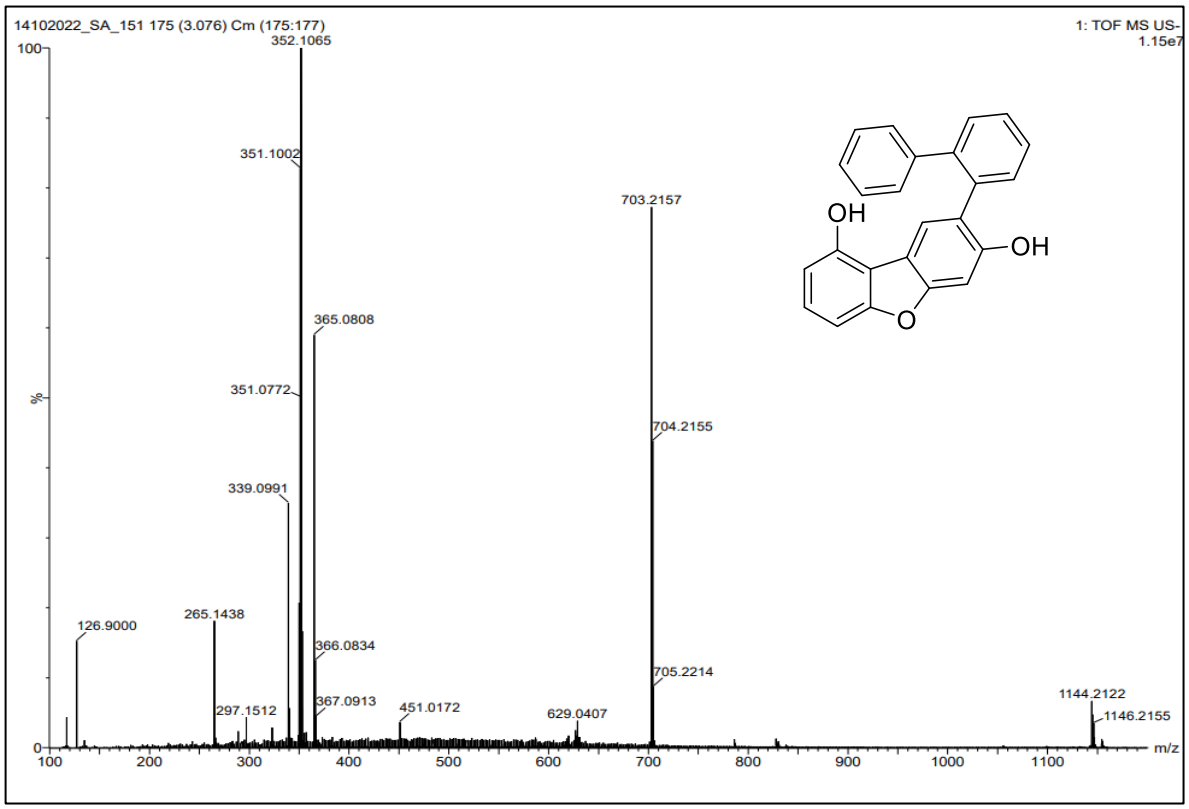


Figure 154: HRMS spectrum of compound **7f**

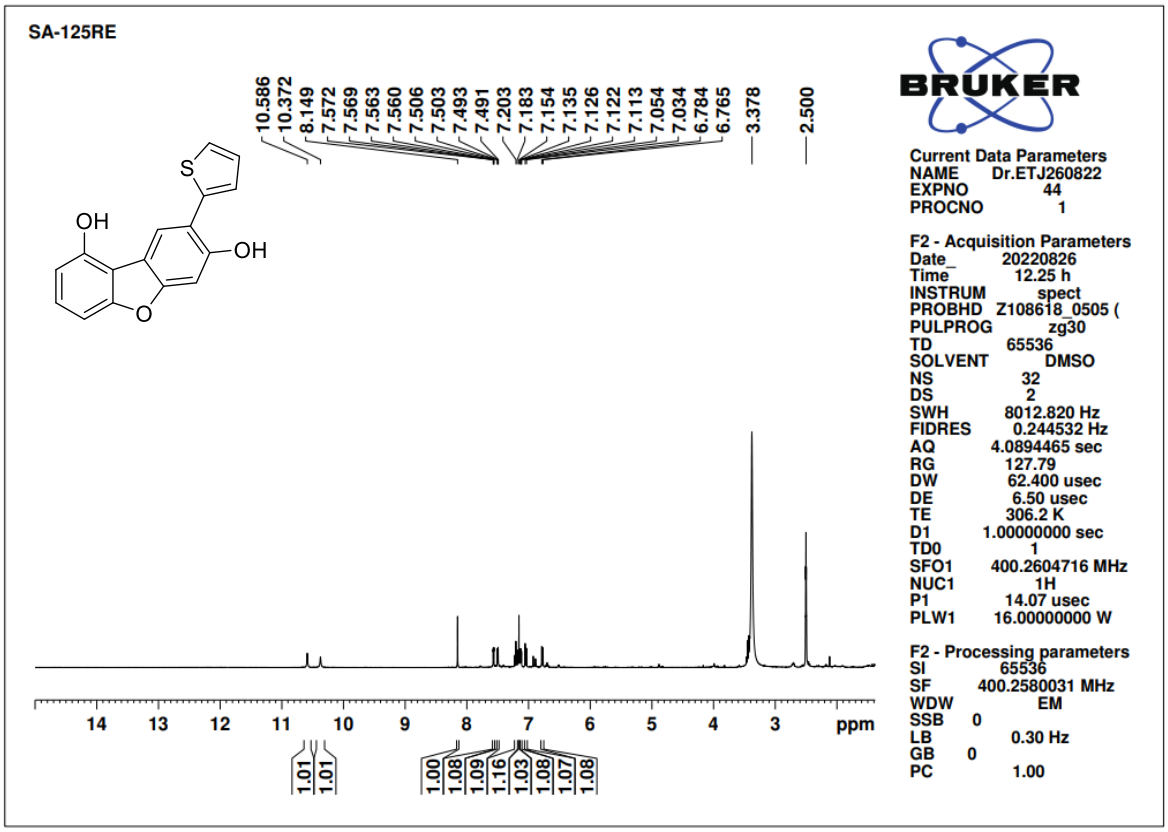


Figure 155: ^{1}H NMR spectrum of compound **7g**

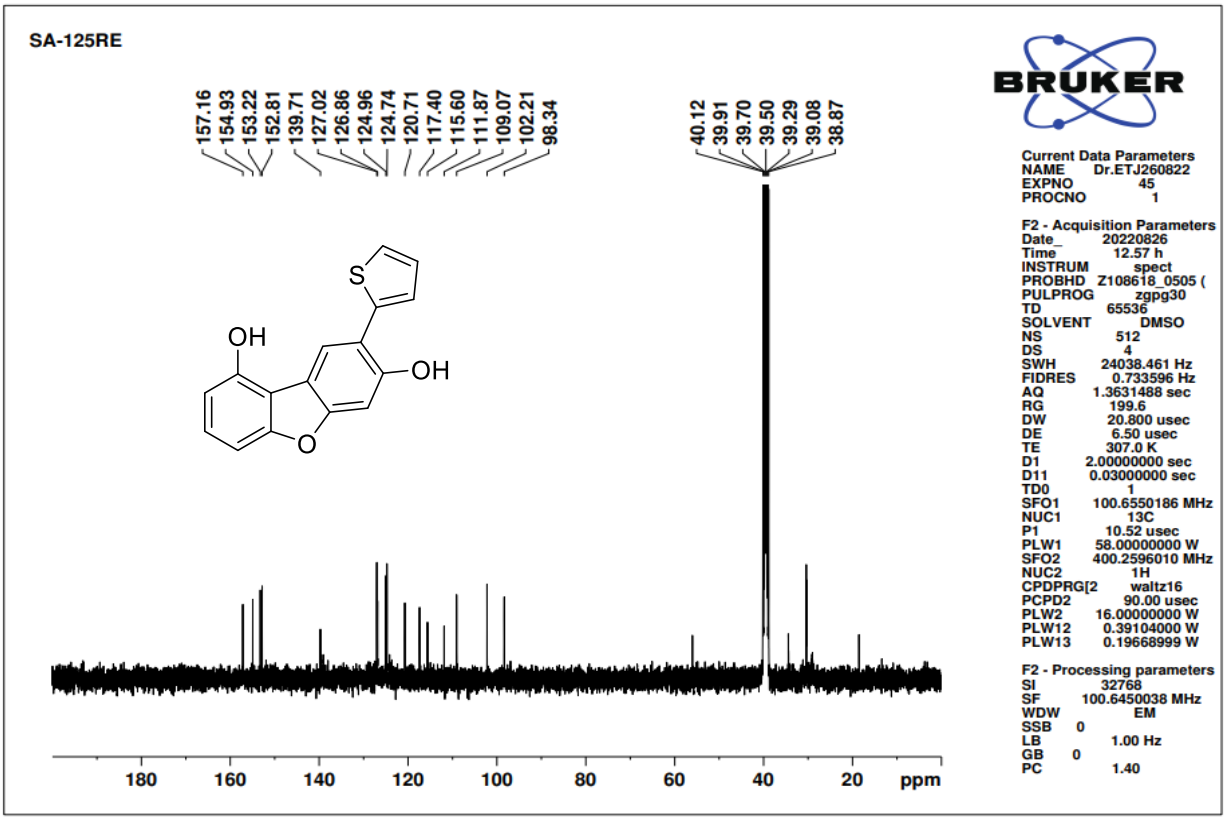


Figure 156: ^{13}C NMR spectrum of compound **7g**

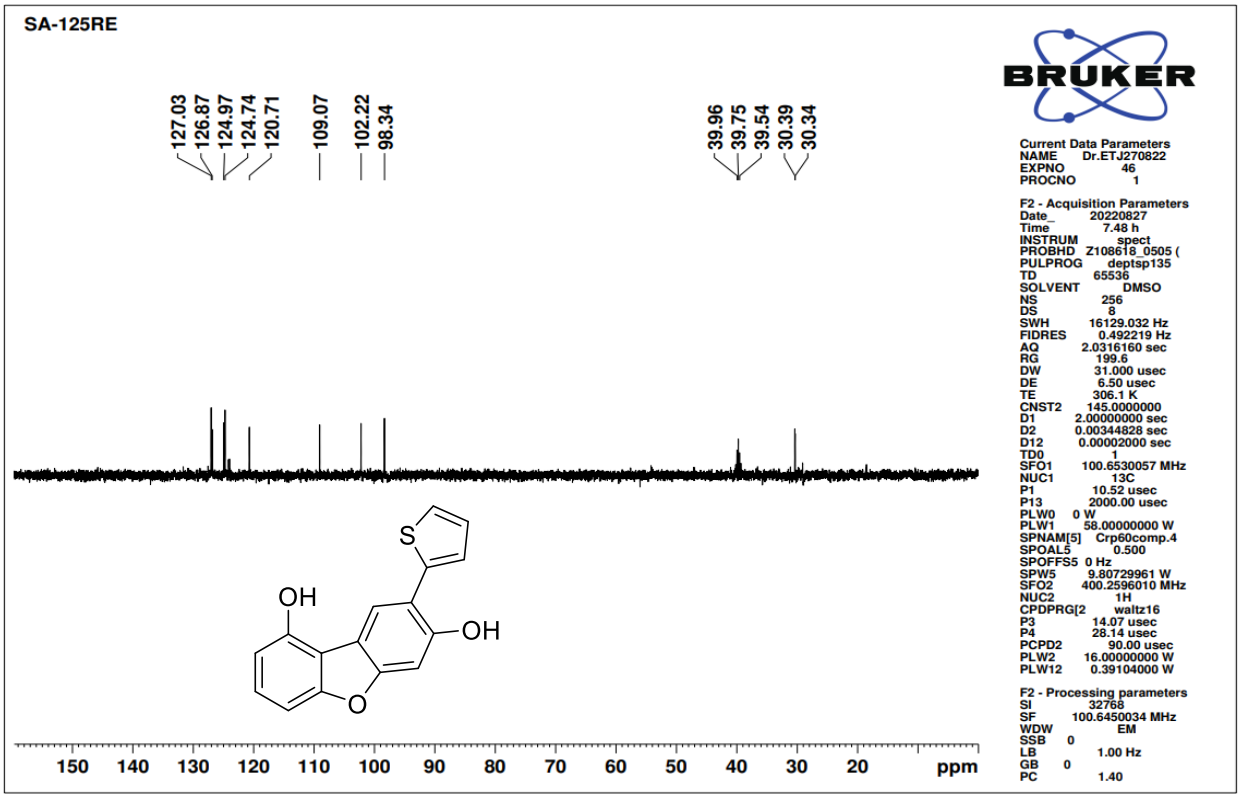


Figure 157: DEPT-135 NMR spectrum of compound **7g**

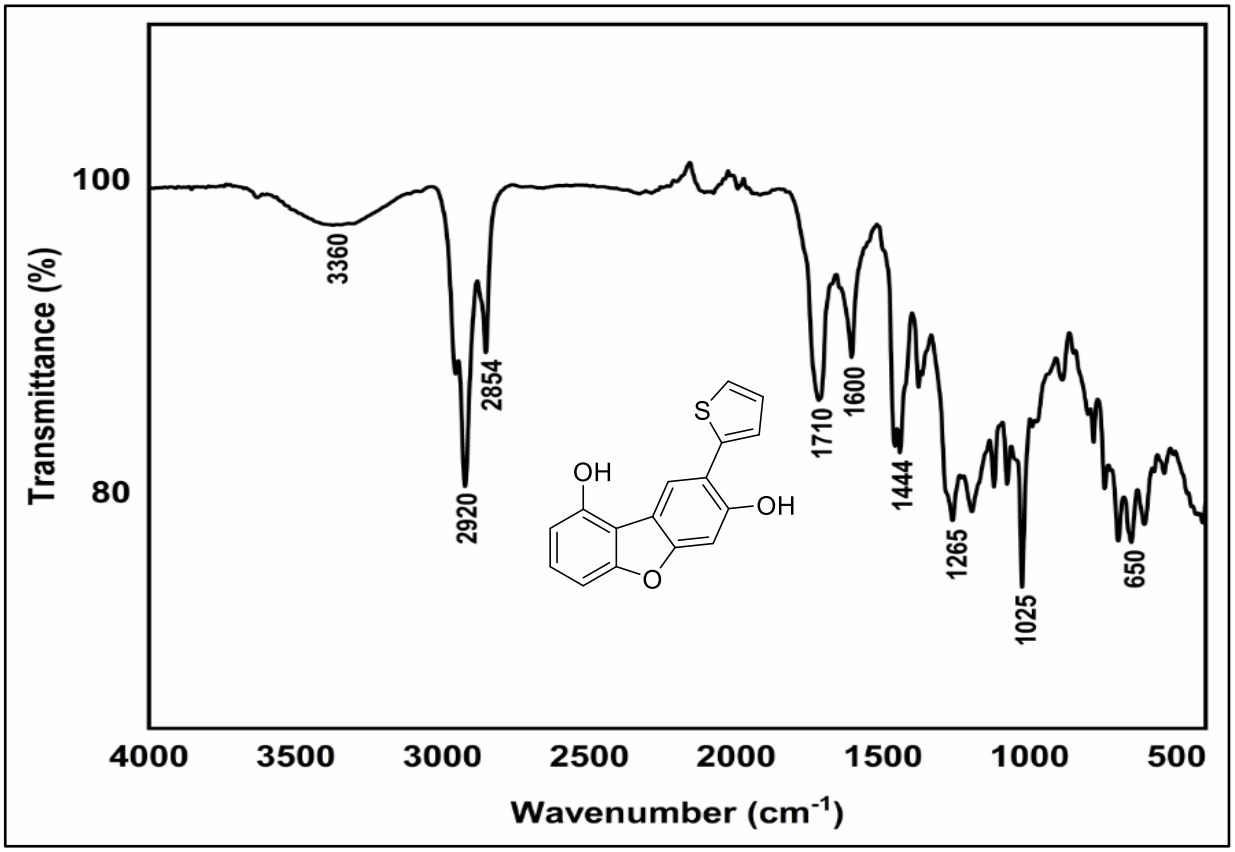


Figure 158: FT-IR spectrum of compound **7g**

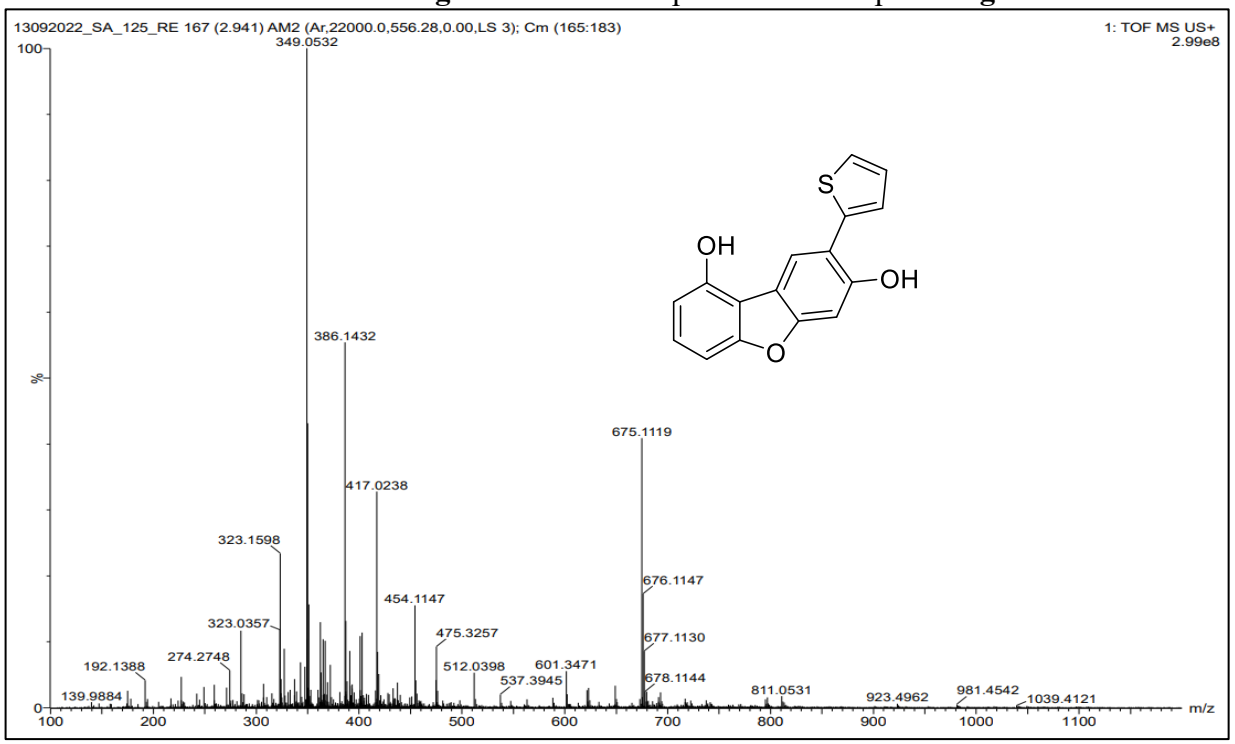


Figure 159: HRMS spectrum of compound **7g**

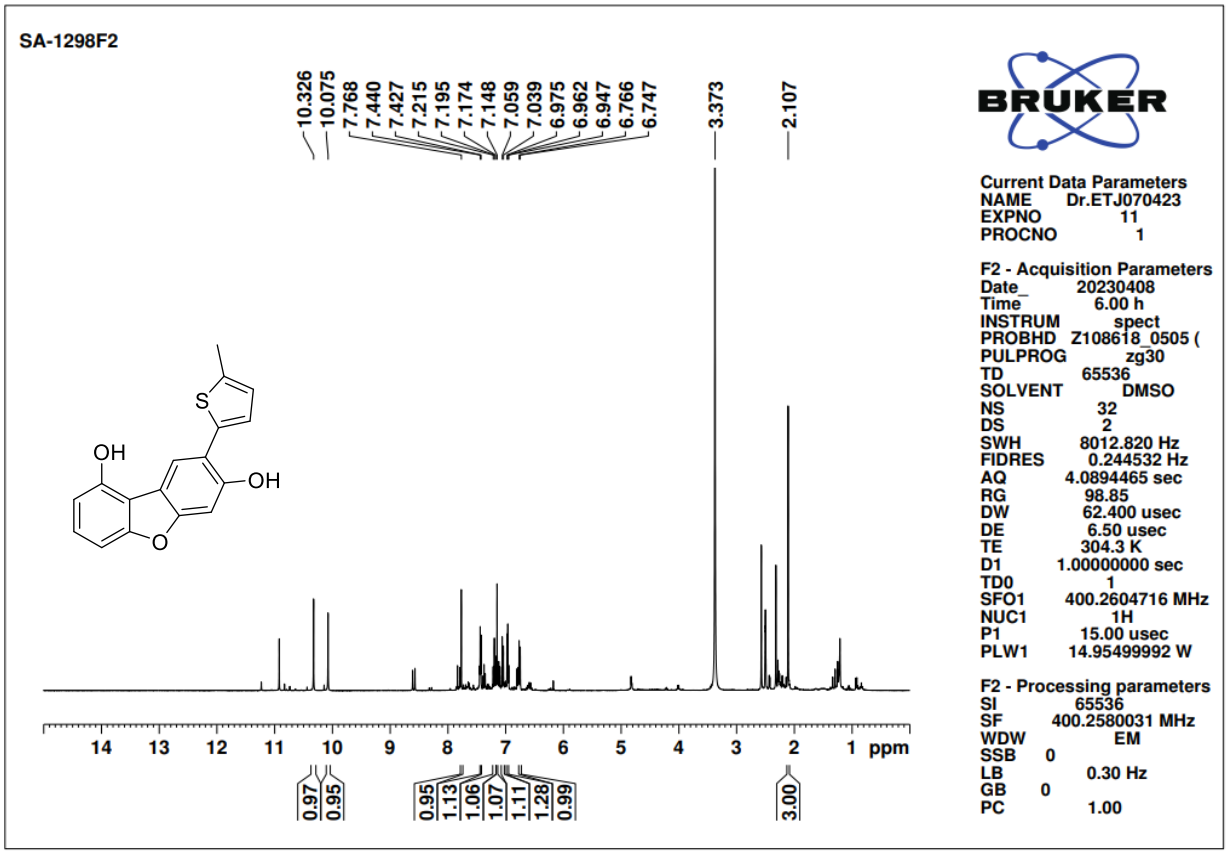


Figure 160: ^{1}H NMR spectrum of compound **7h**

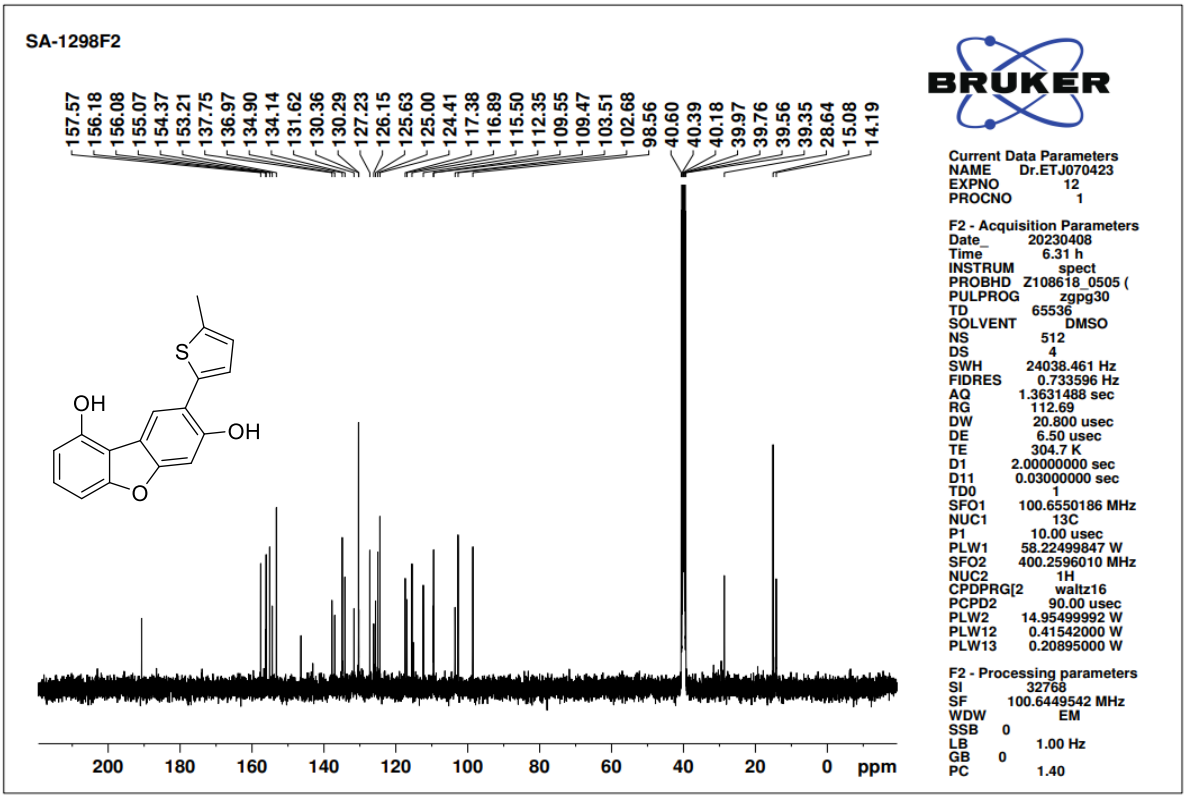


Figure 161: ^{13}C NMR spectrum of compound **7h**

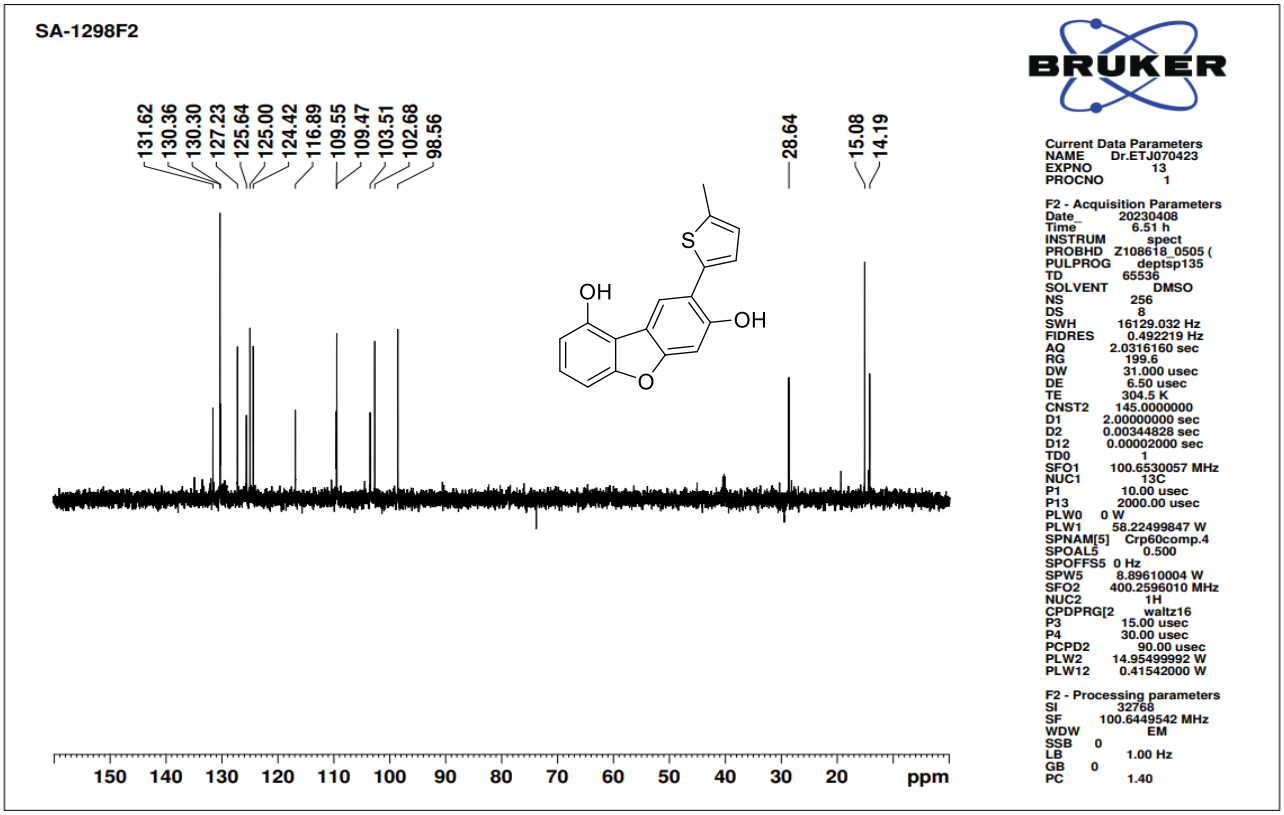


Figure 162: DEPT-135 NMR spectrum of compound **7h**

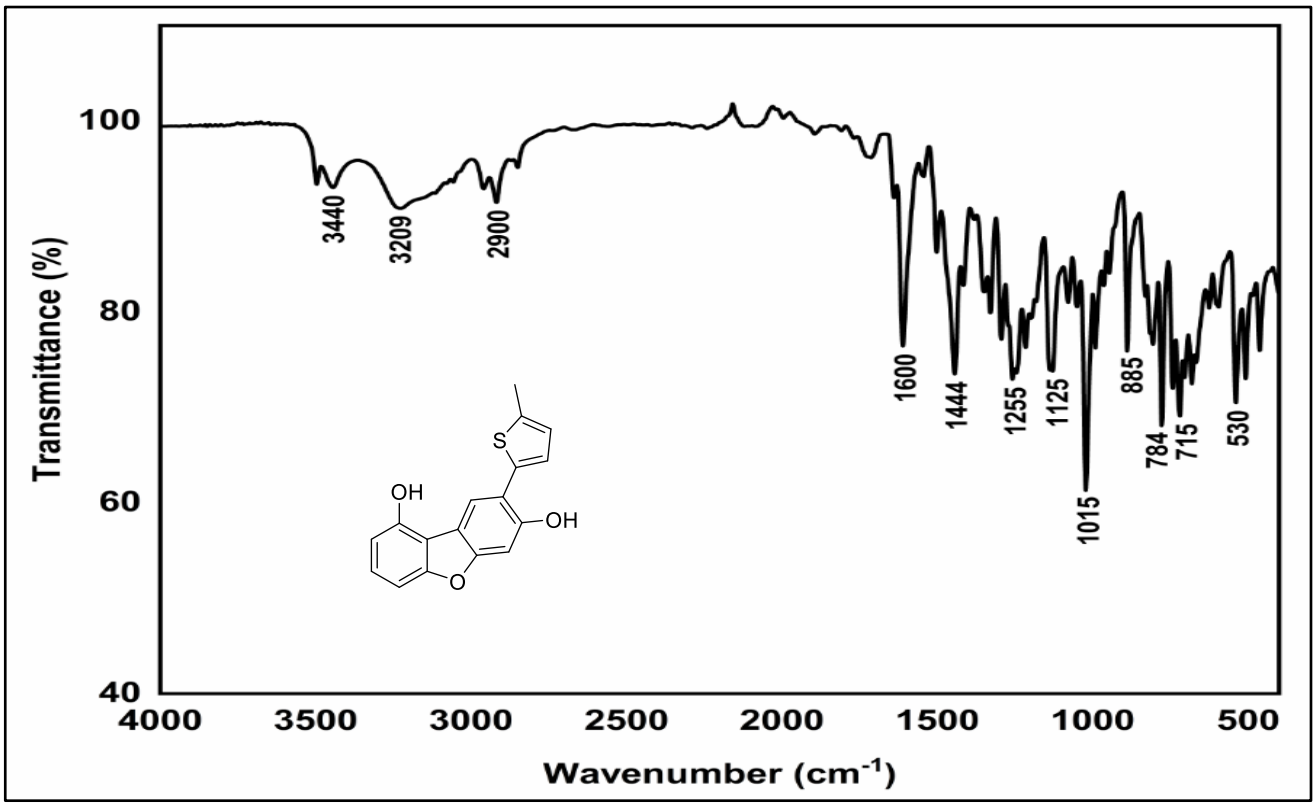


Figure 163: FT-IR spectrum of compound **7h**

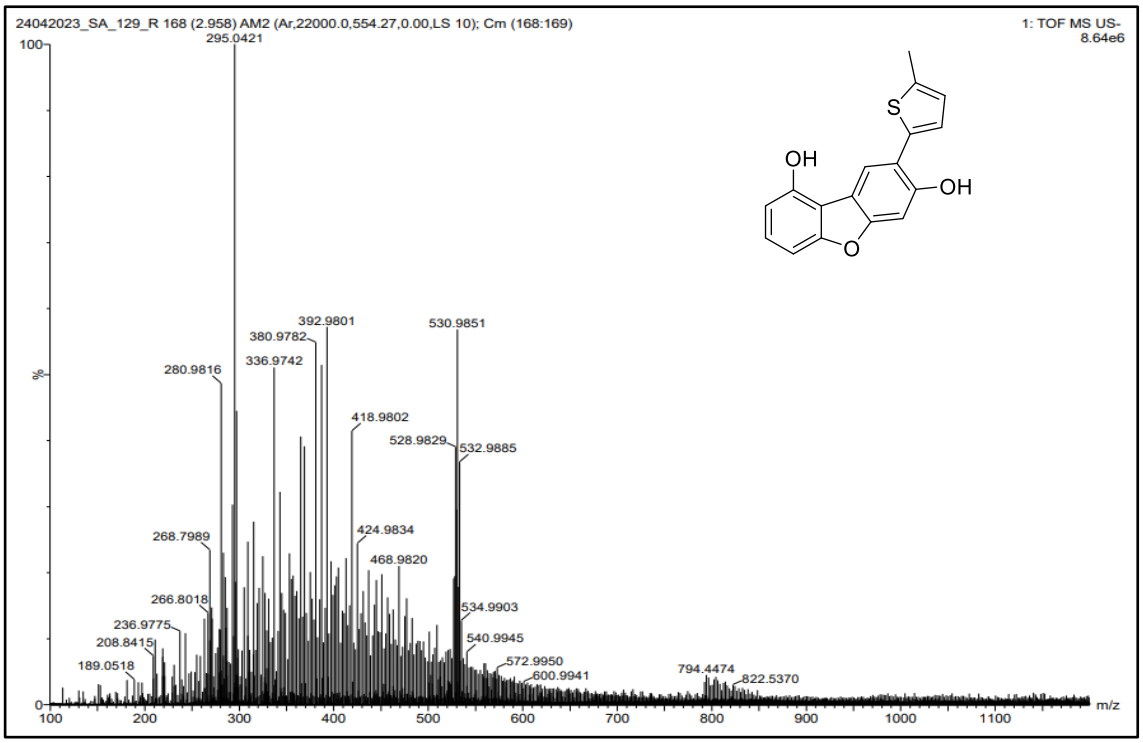


Figure 164: HRMS spectrum of compound **7h**

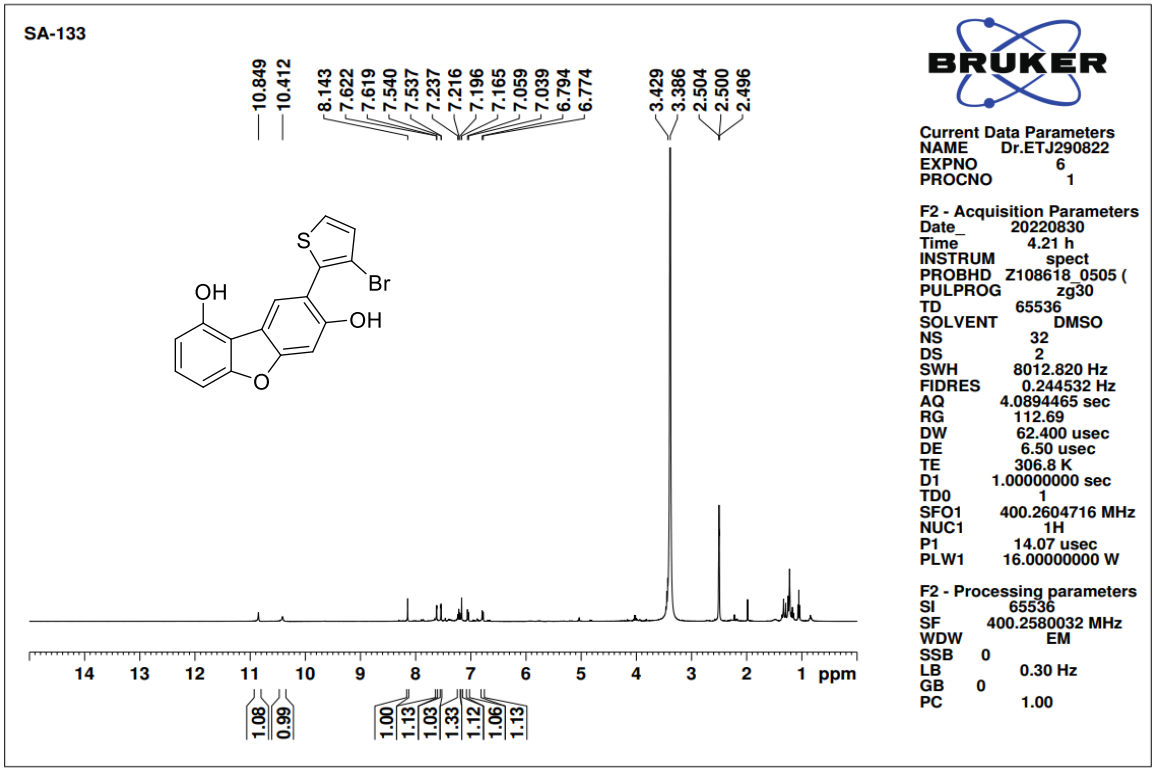


Figure 165: ^{1}H NMR spectrum of compound **7i**

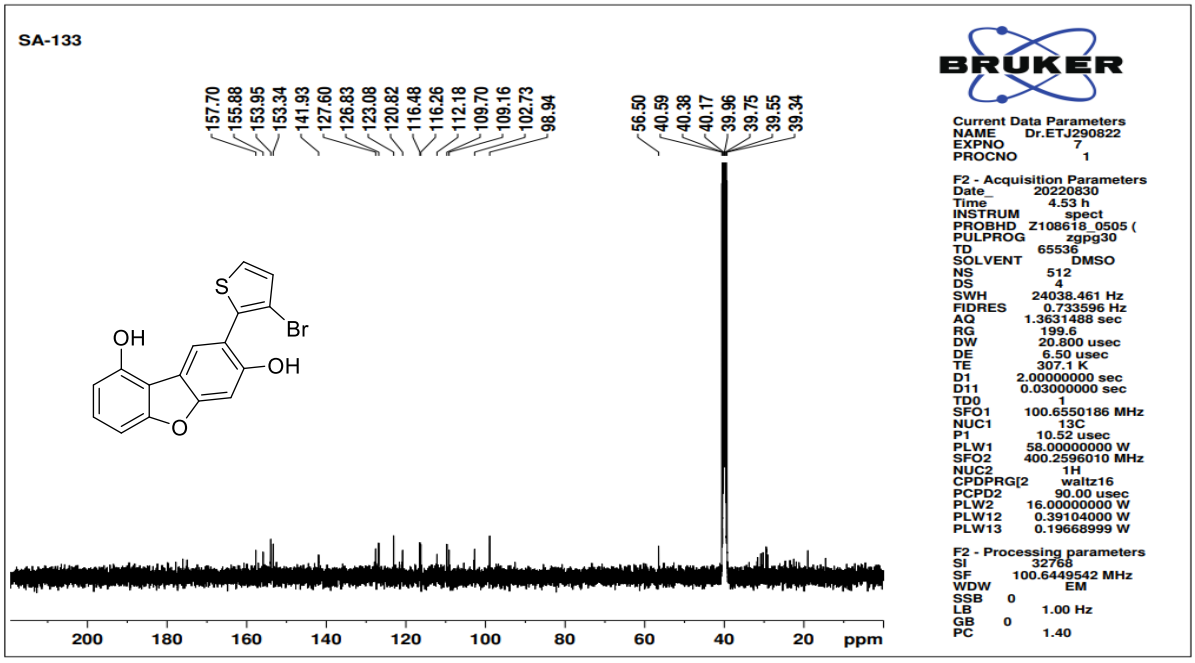


Figure 166: ^{13}C NMR spectrum of compound **7i**

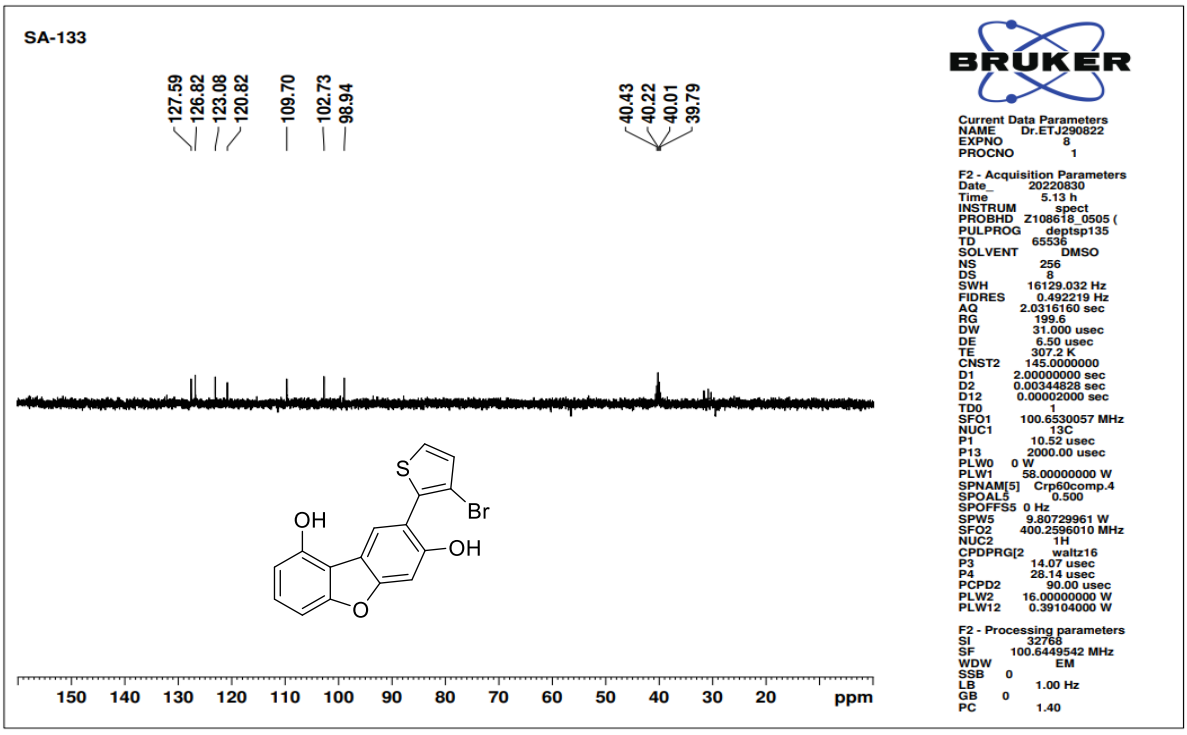


Figure 167: DEPT-135 NMR spectrum of compound **7i**

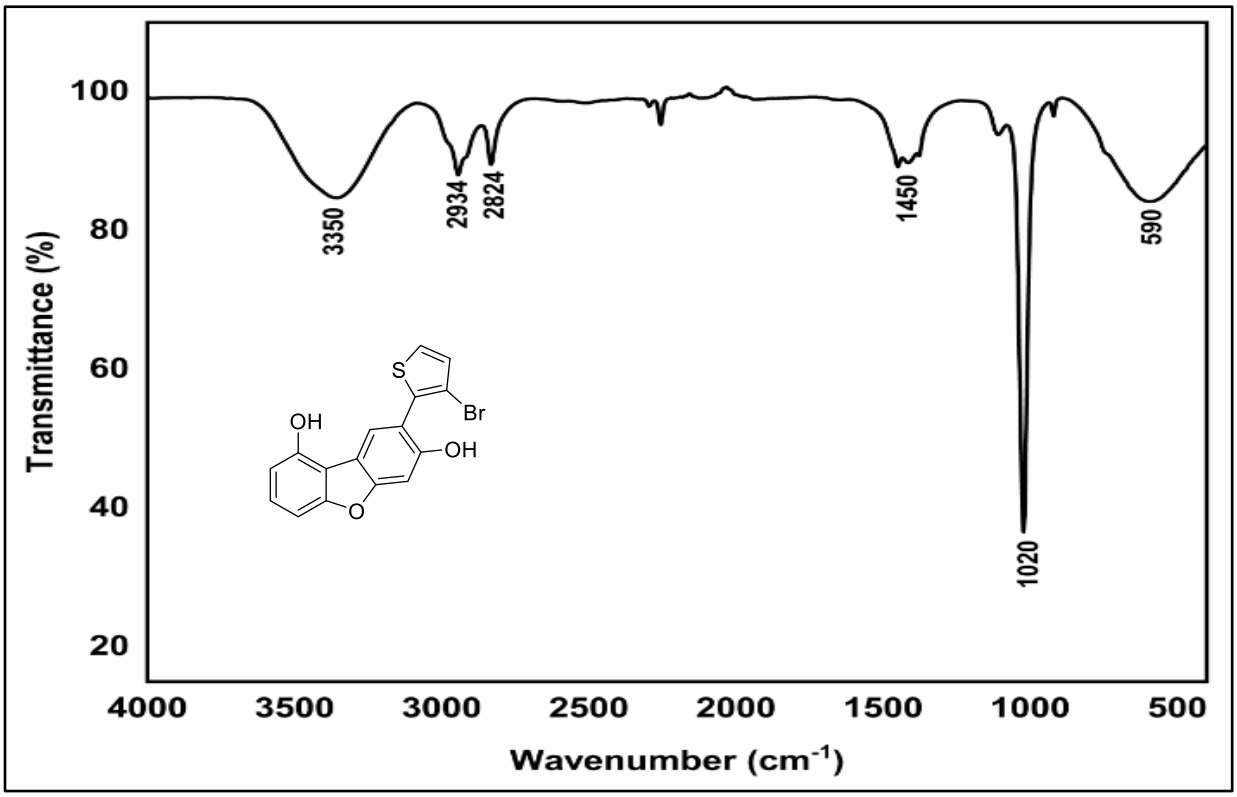


Figure 168: FT-IR spectrum of compound **7i**

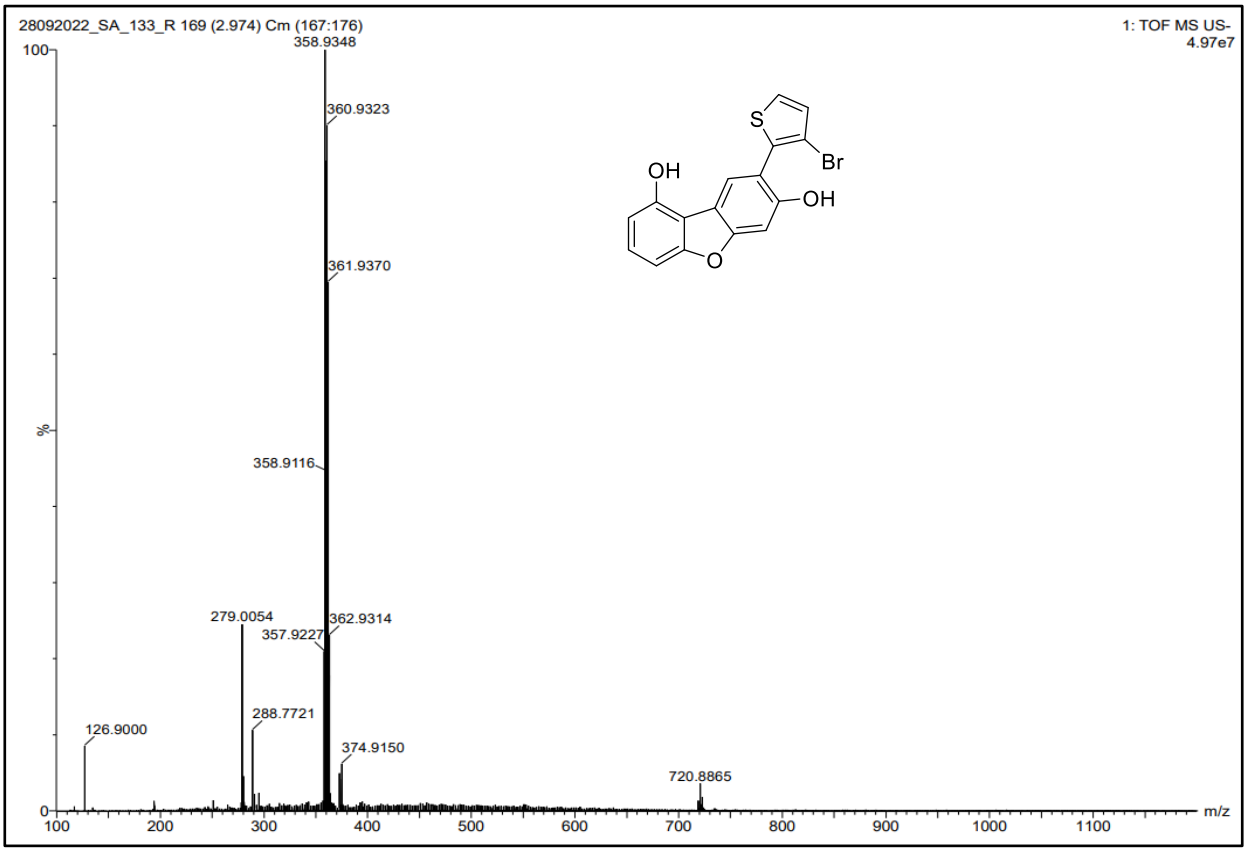


Figure 169: HRMS spectrum of compound **7i**

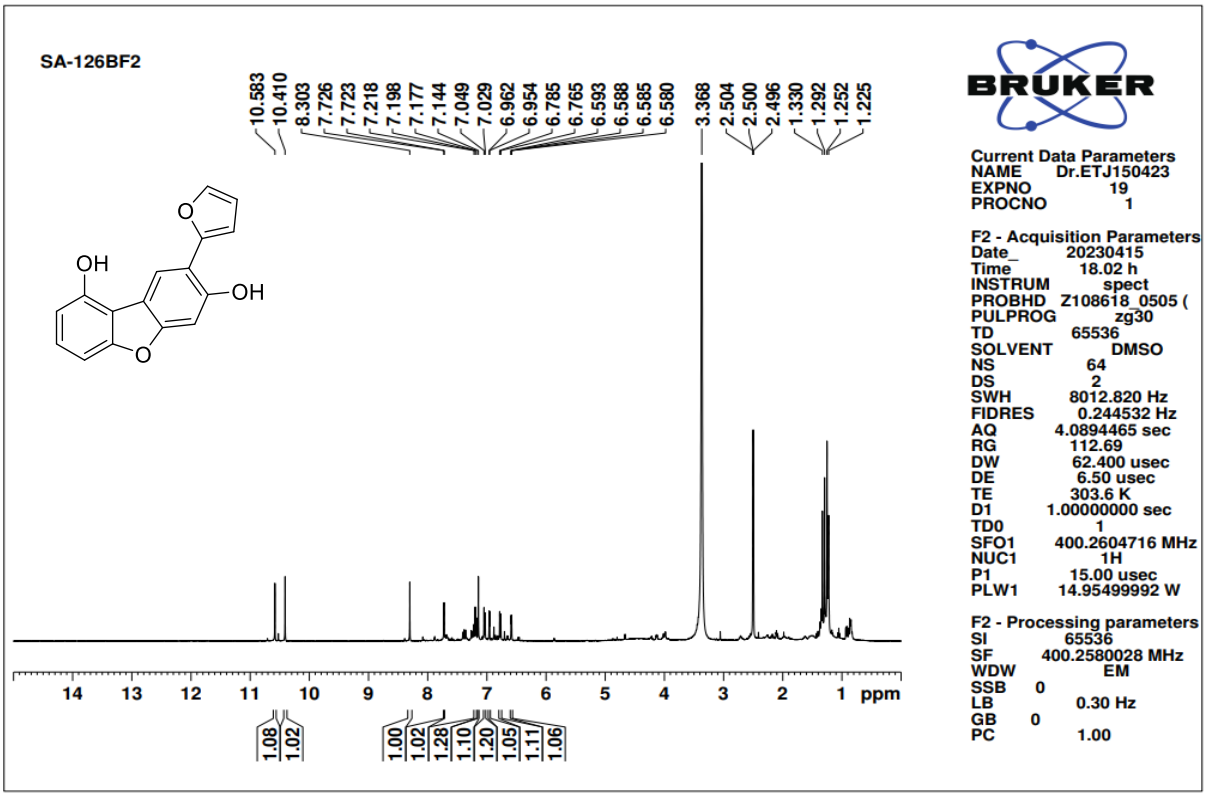


Figure 170: ^{1}H NMR spectrum of compound **7j**

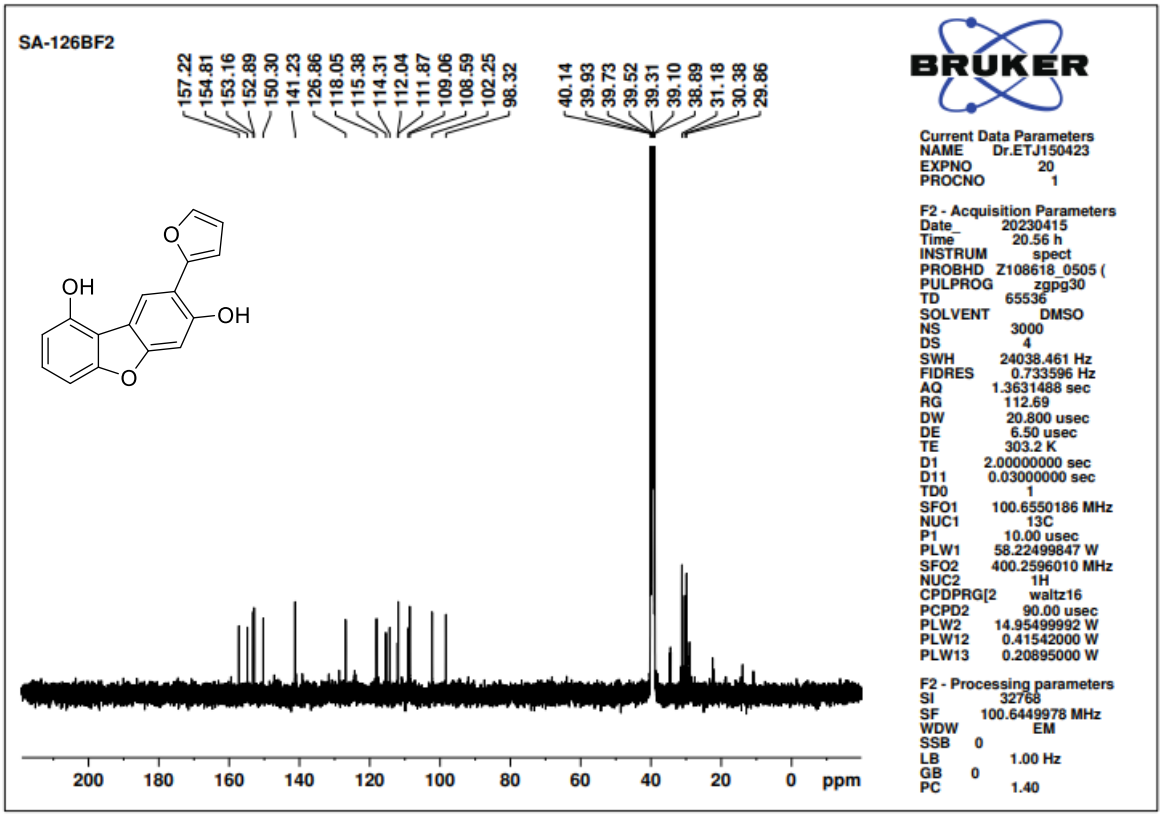


Figure 171: ^{13}C NMR spectrum of compound **7j**

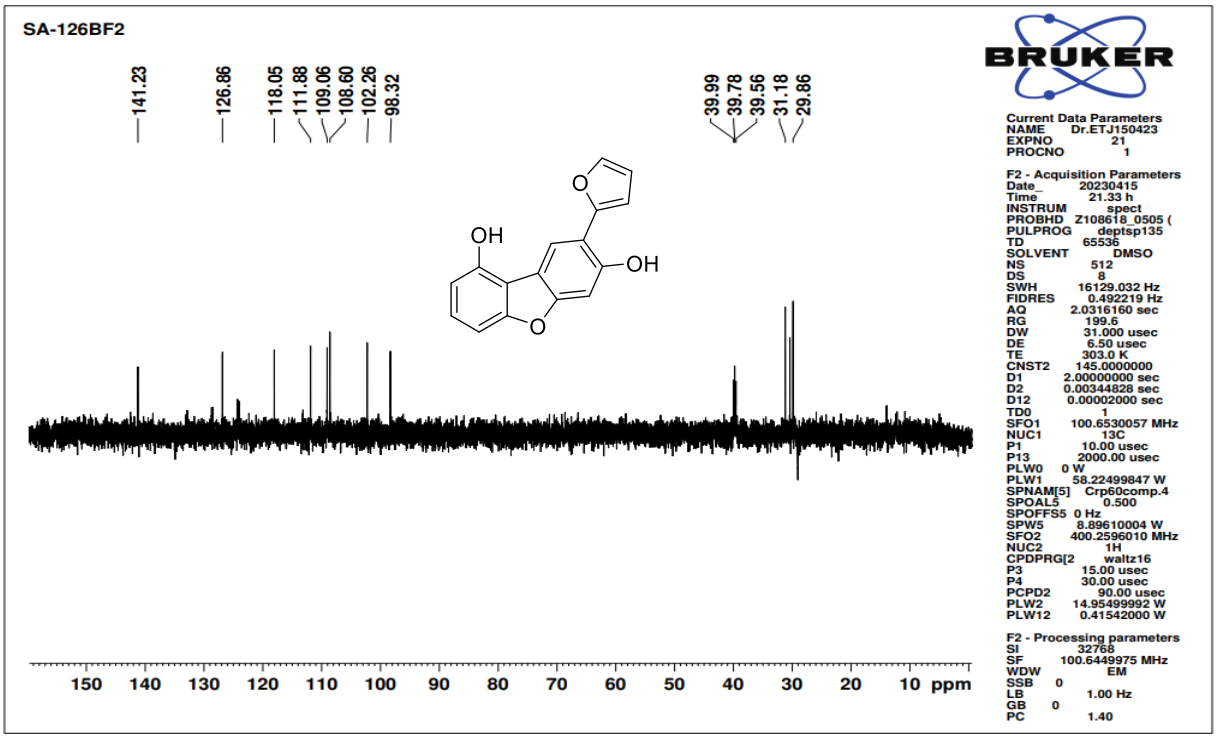


Figure 172: DEPT-135 NMR spectrum of compound **7j**

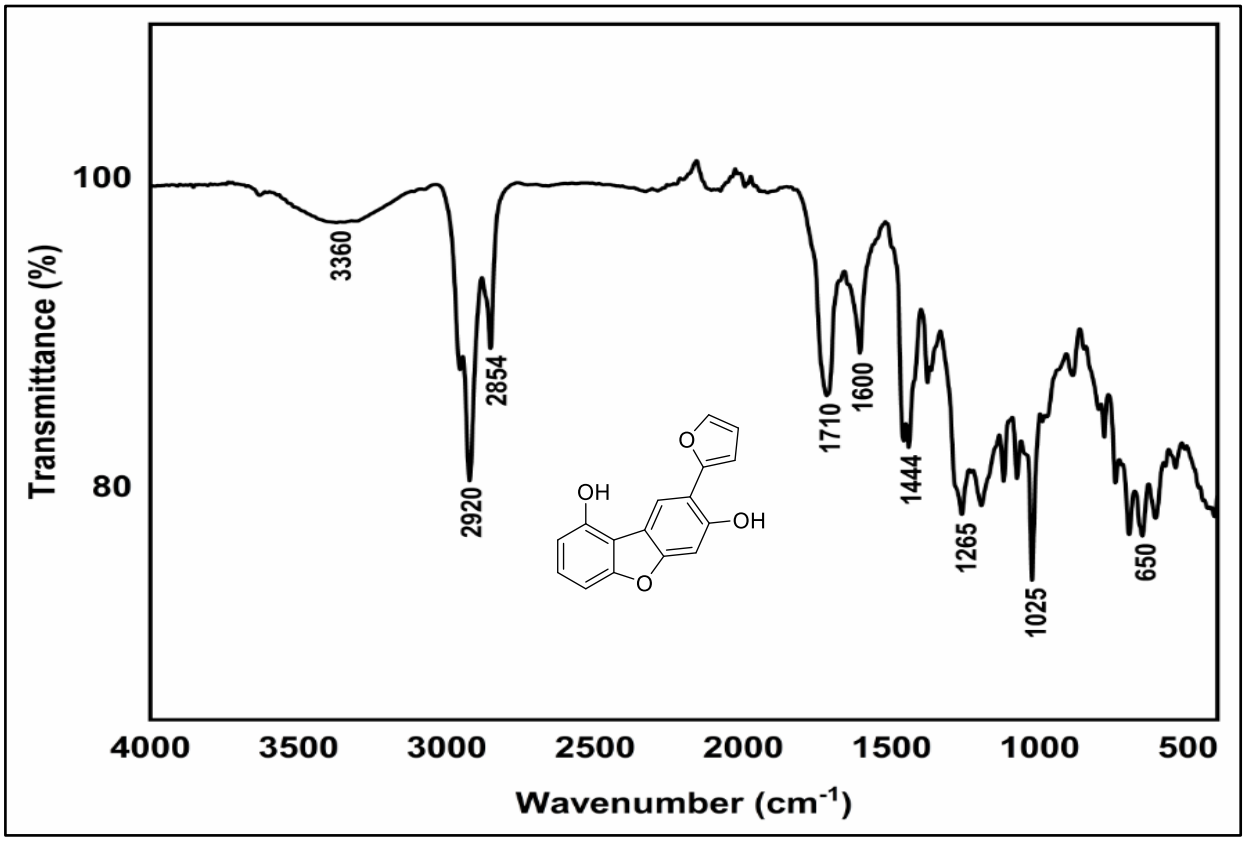


Figure 173: FT-IR spectrum of compound **7j**

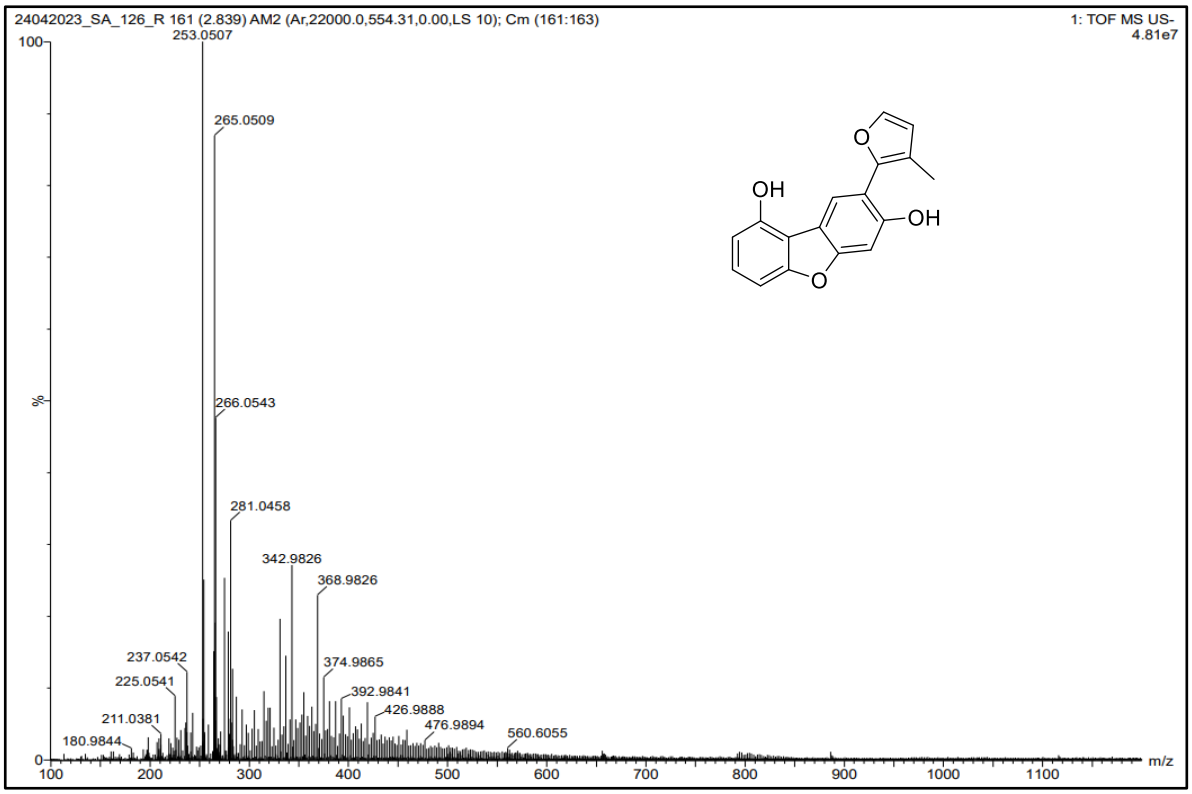


Figure 174: HRMS spectrum of compound **7j**

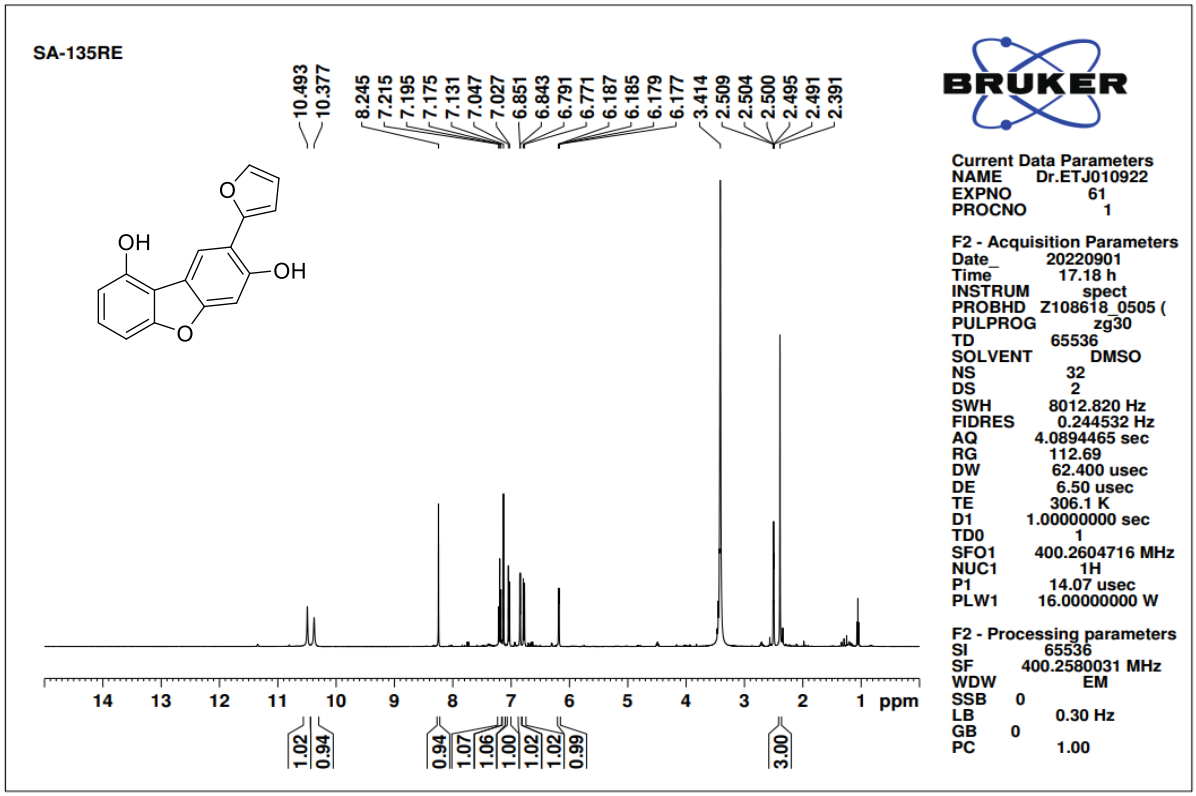


Figure 175: ^{1}H NMR spectrum of compound **7k**

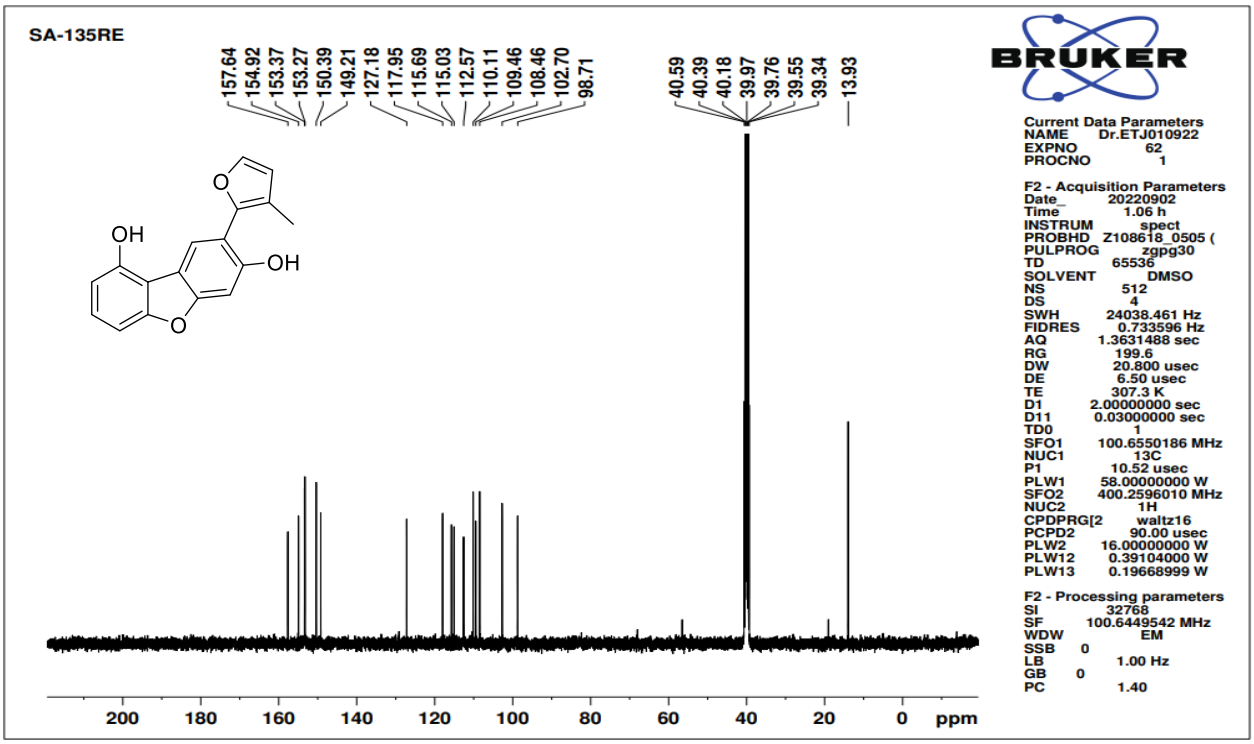


Figure 176: ^{13}C NMR spectrum of compound **7k**

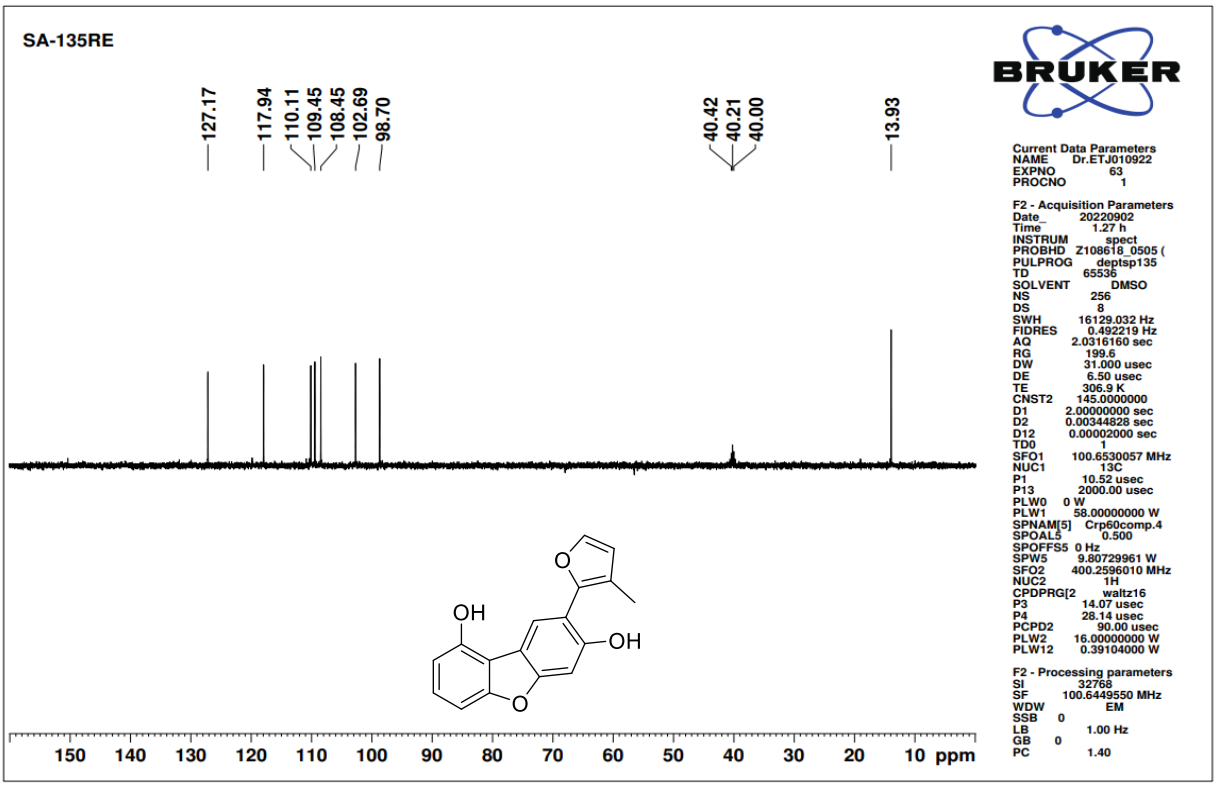


Figure 177: DEPT-135 NMR spectrum of compound **7k**

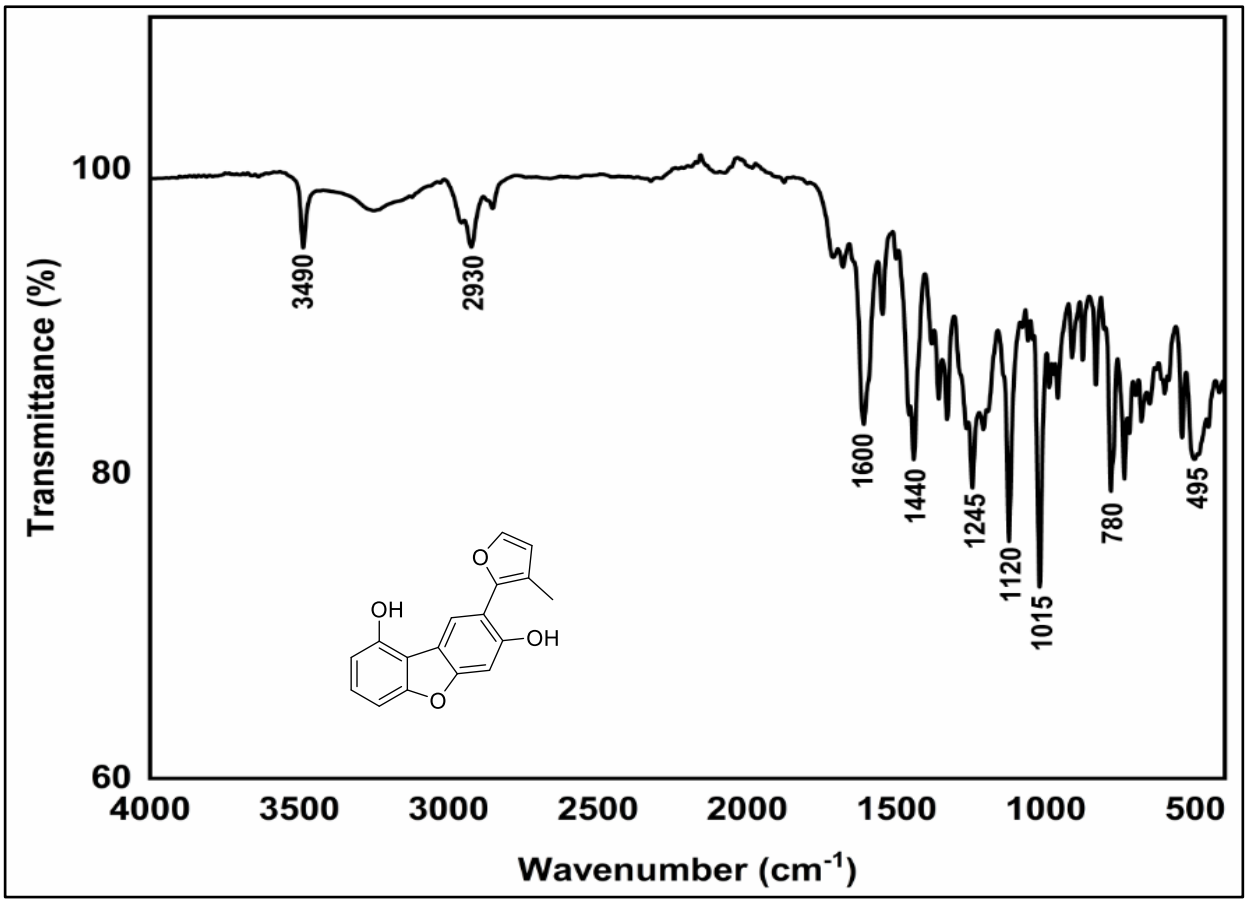


Figure 178: FT-IR spectrum of compound **7k**

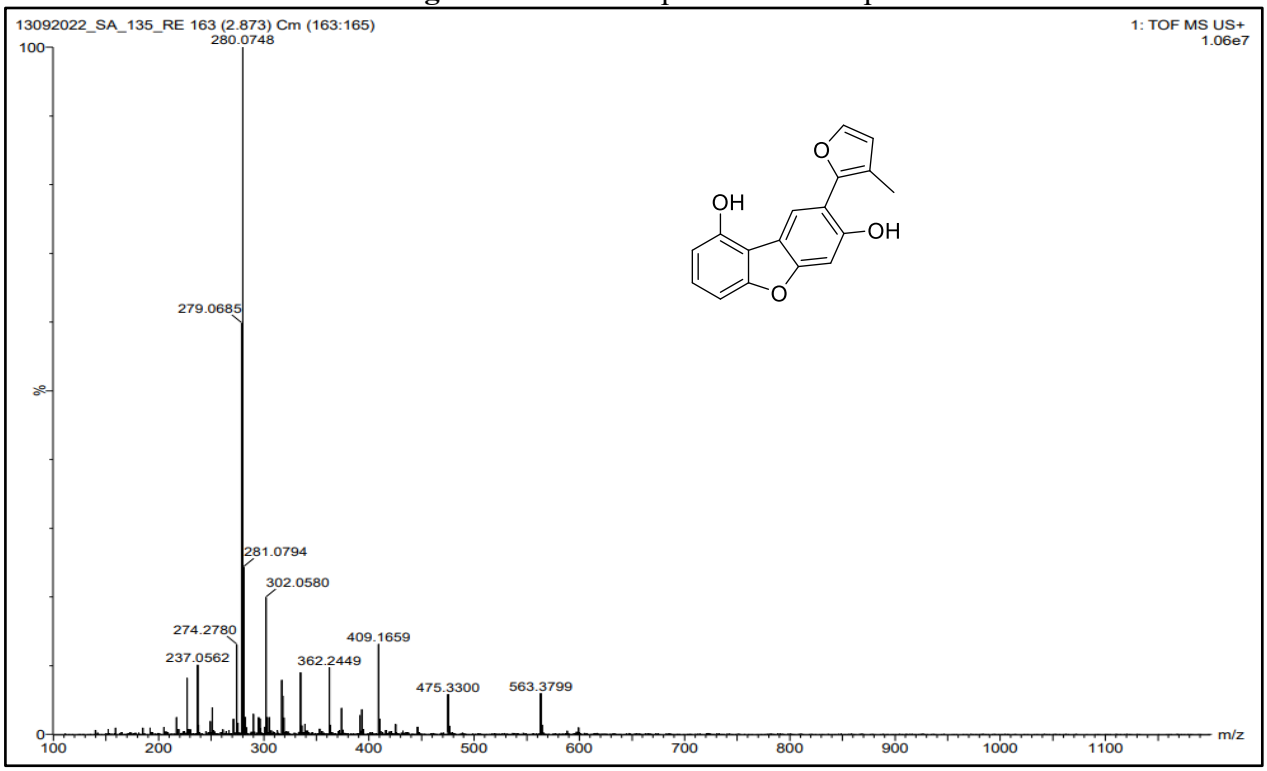


Figure 179: HRMS spectrum of compound **7k**

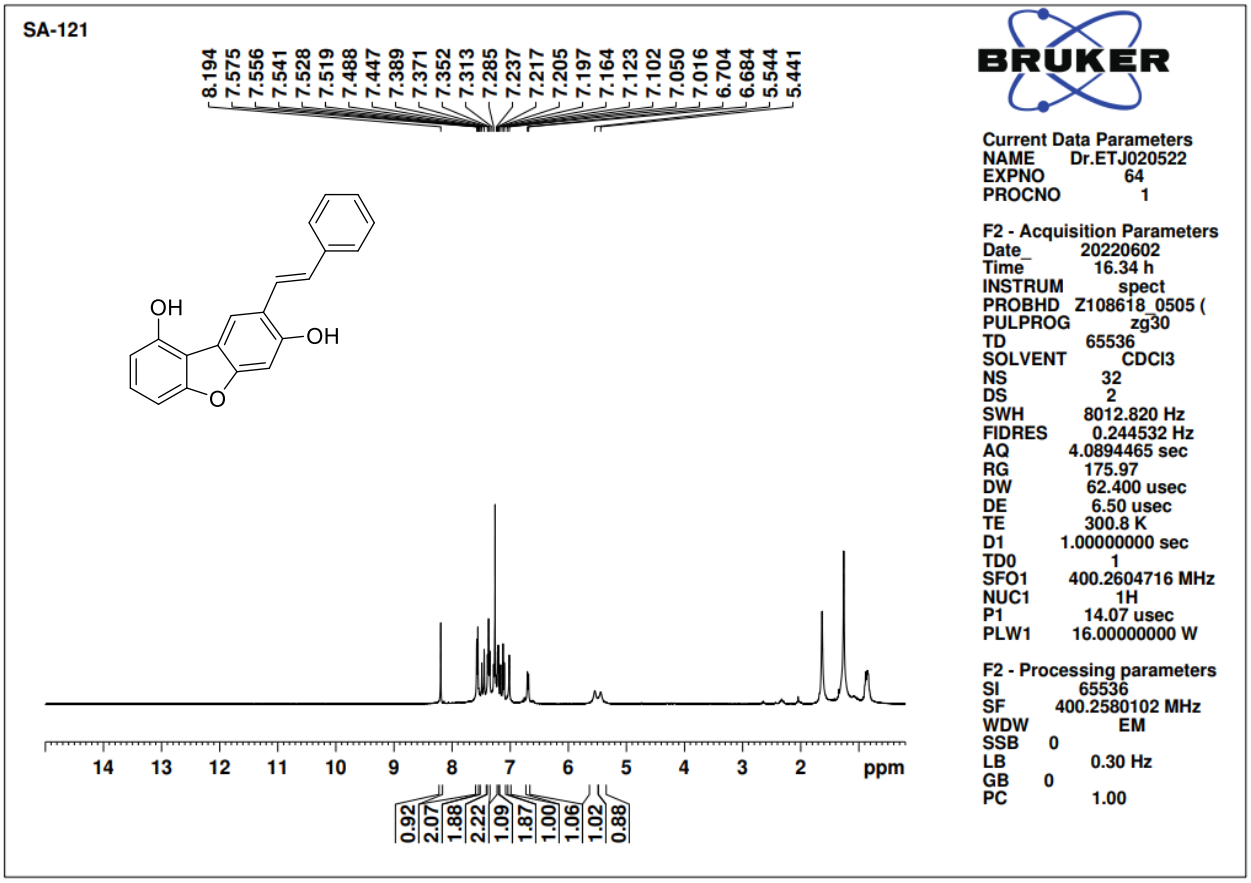


Figure 180: ^{1}H NMR spectrum of compound **7l**

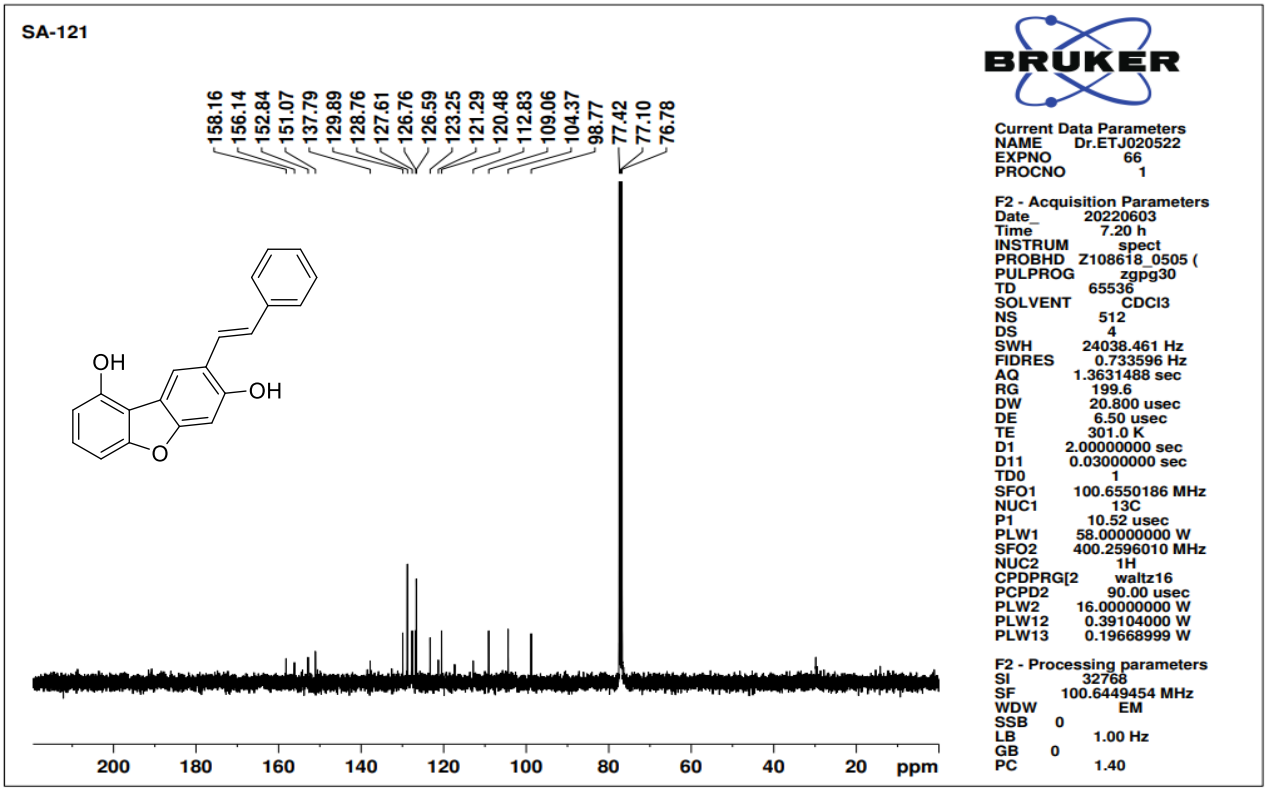


Figure 181: ^{13}C NMR spectrum of compound **7l**

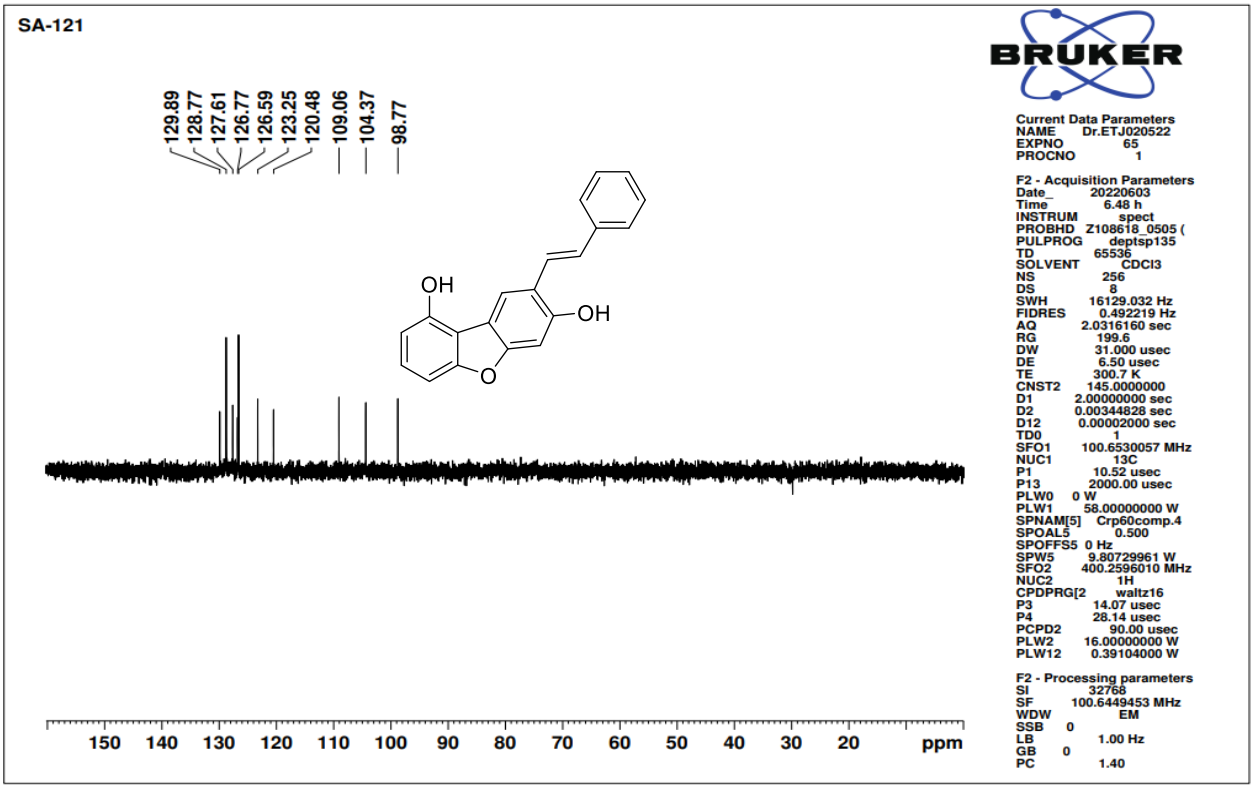


Figure 182: DEPT-135 NMR spectrum of compound **7l**

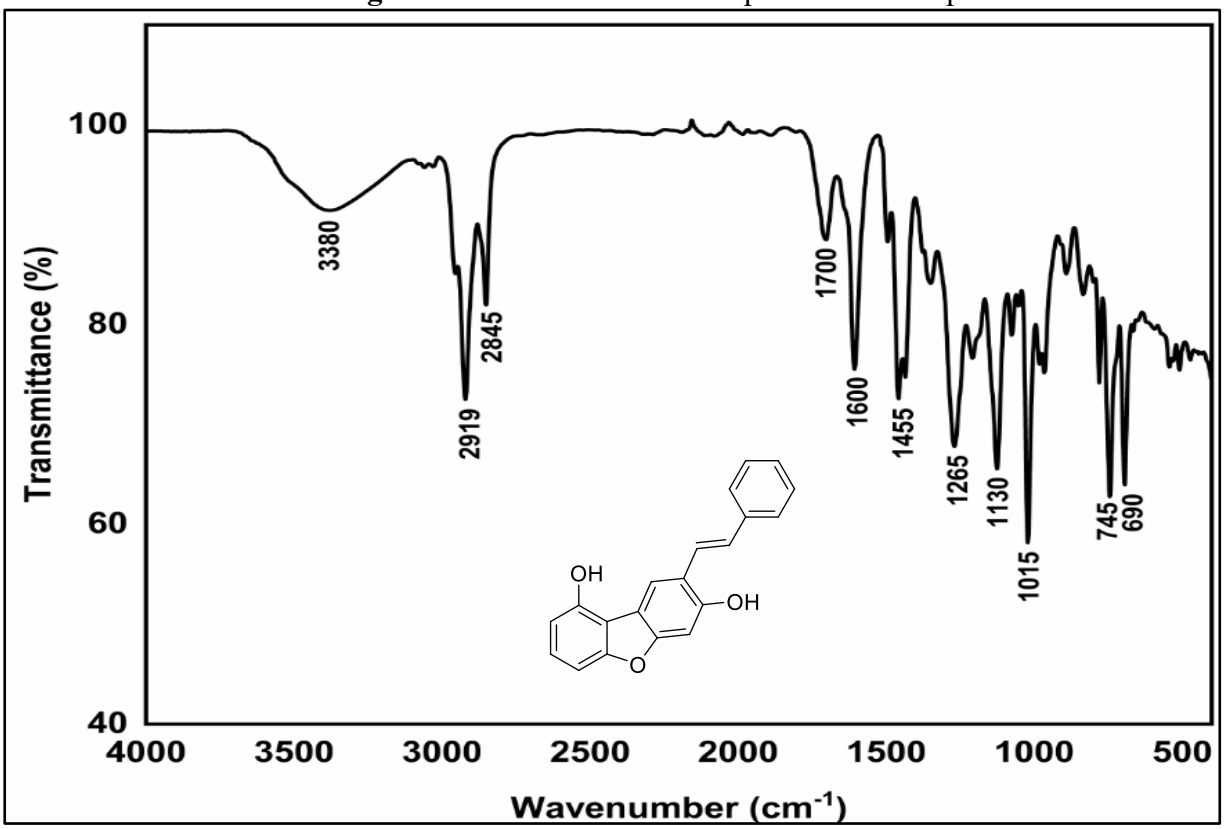


Figure 183: FT-IR spectrum of compound **7l**

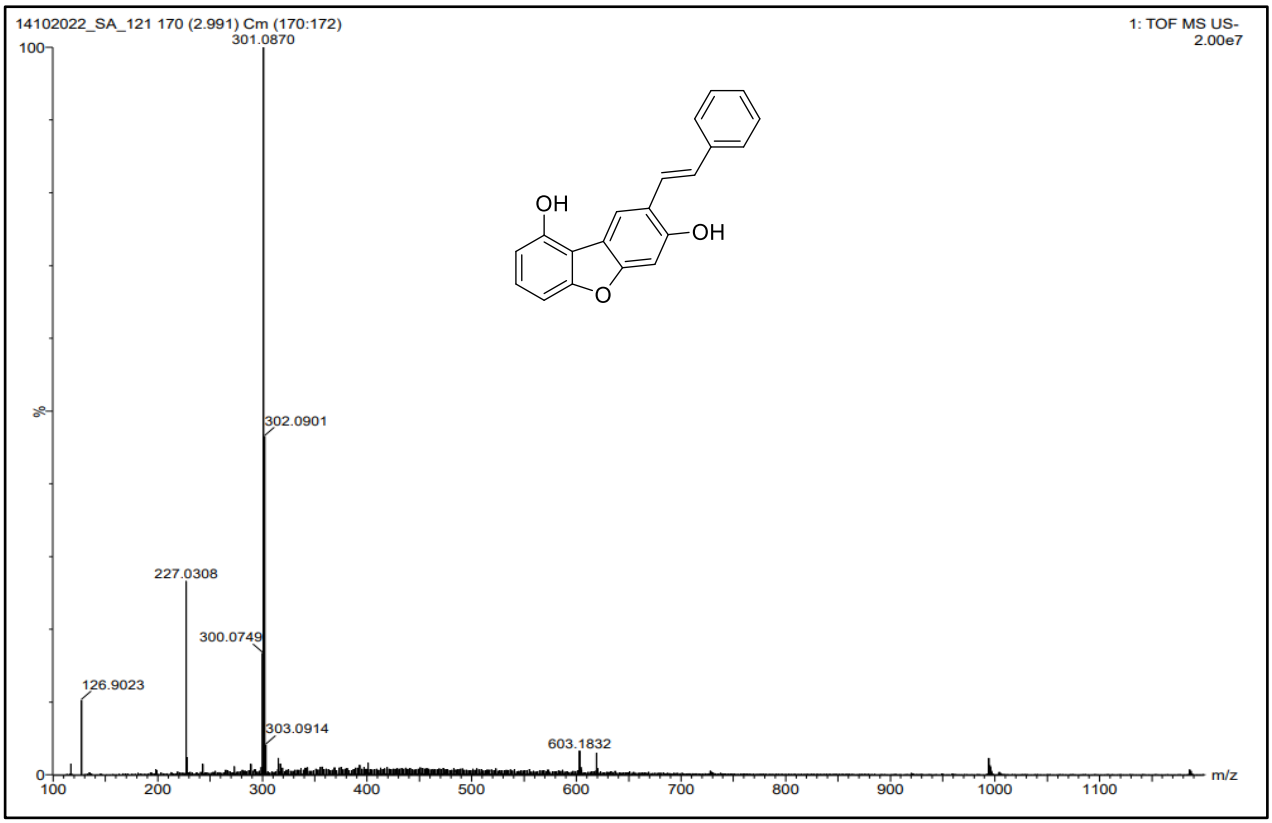


Figure 184: HRMS spectrum of compound **7l**

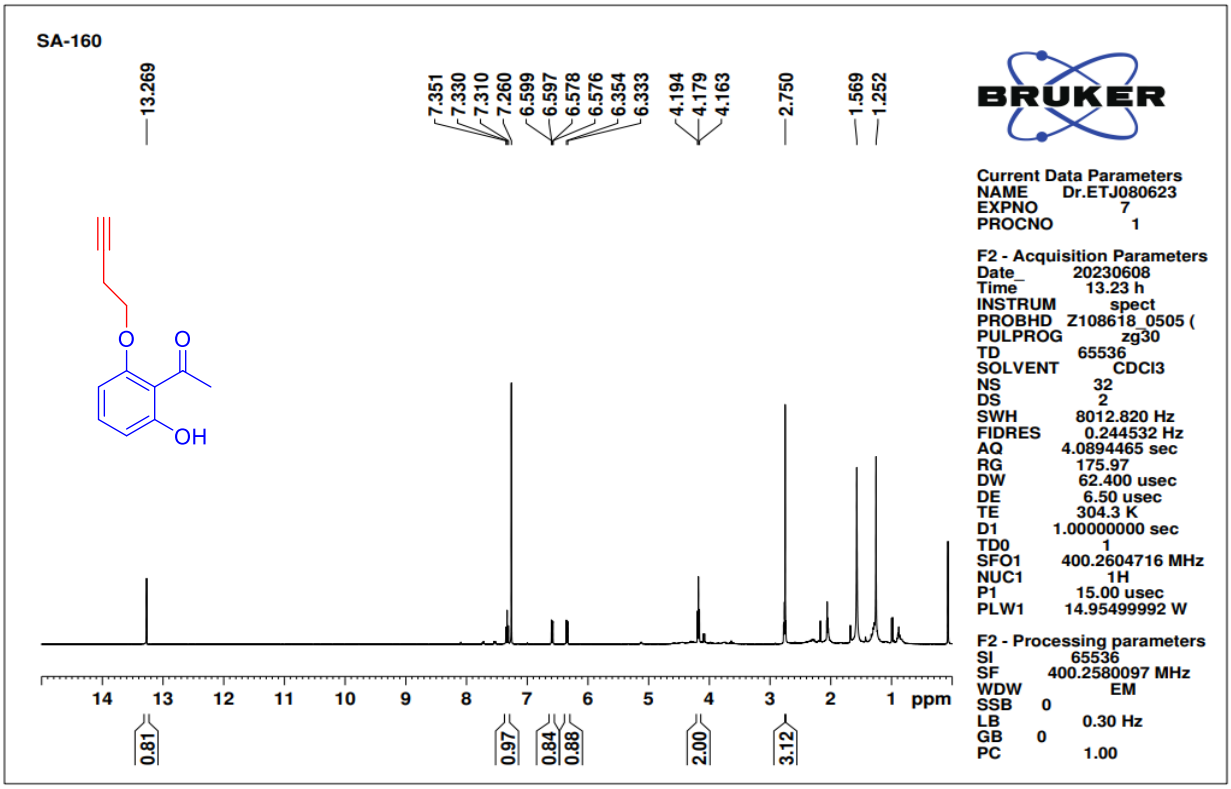


Figure 185: ^{1}H NMR spectrum of compound **14**

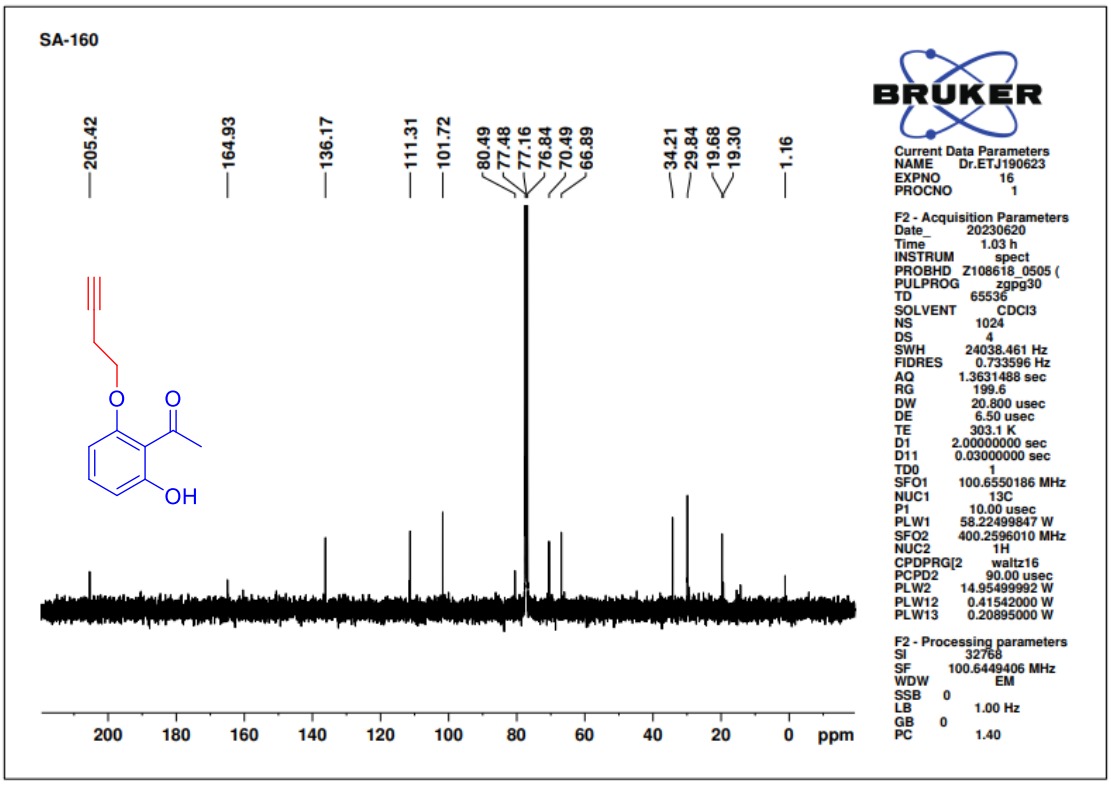


Figure 186: ^{13}C NMR spectrum of compound **14**

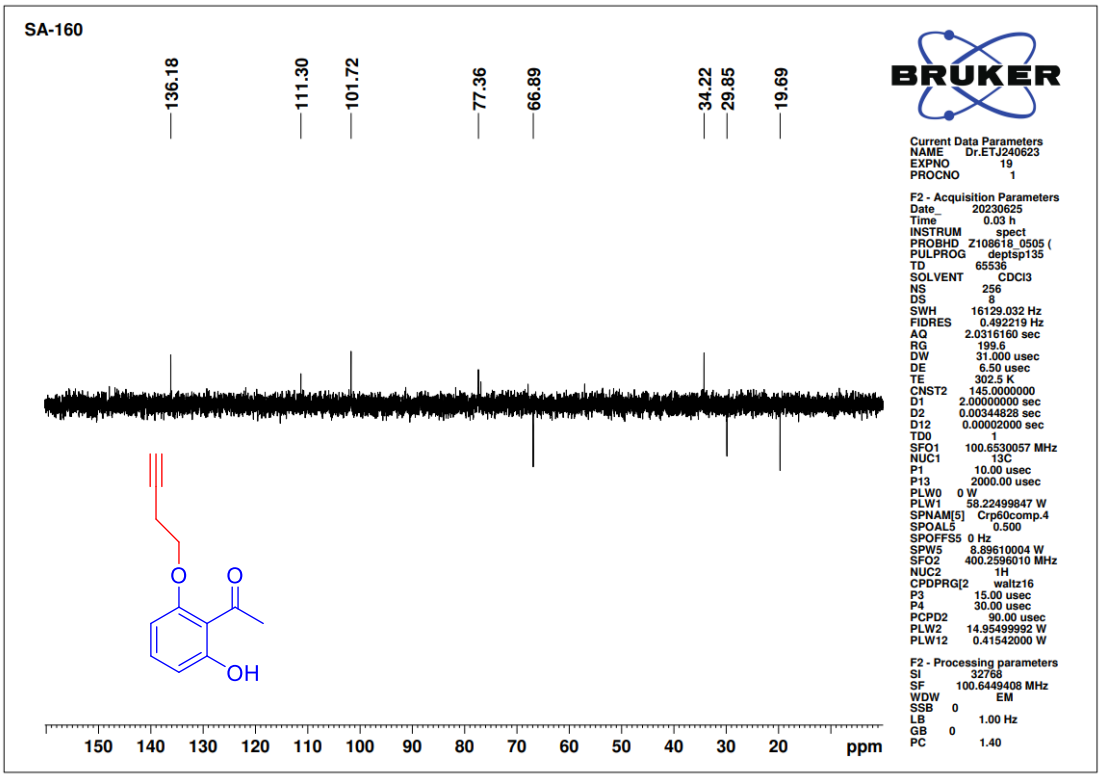


Figure 187: DEPT-135 NMR spectrum of compound **14**

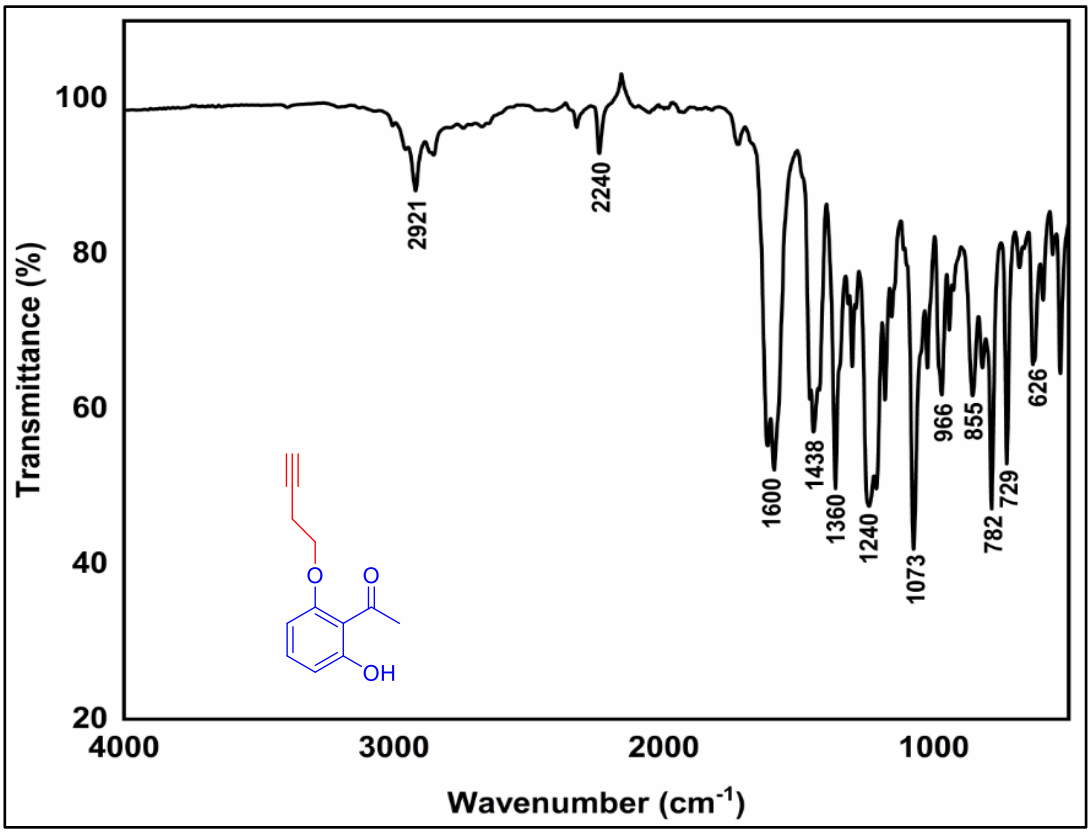


Figure 188: FT-IR spectrum of compound **14**

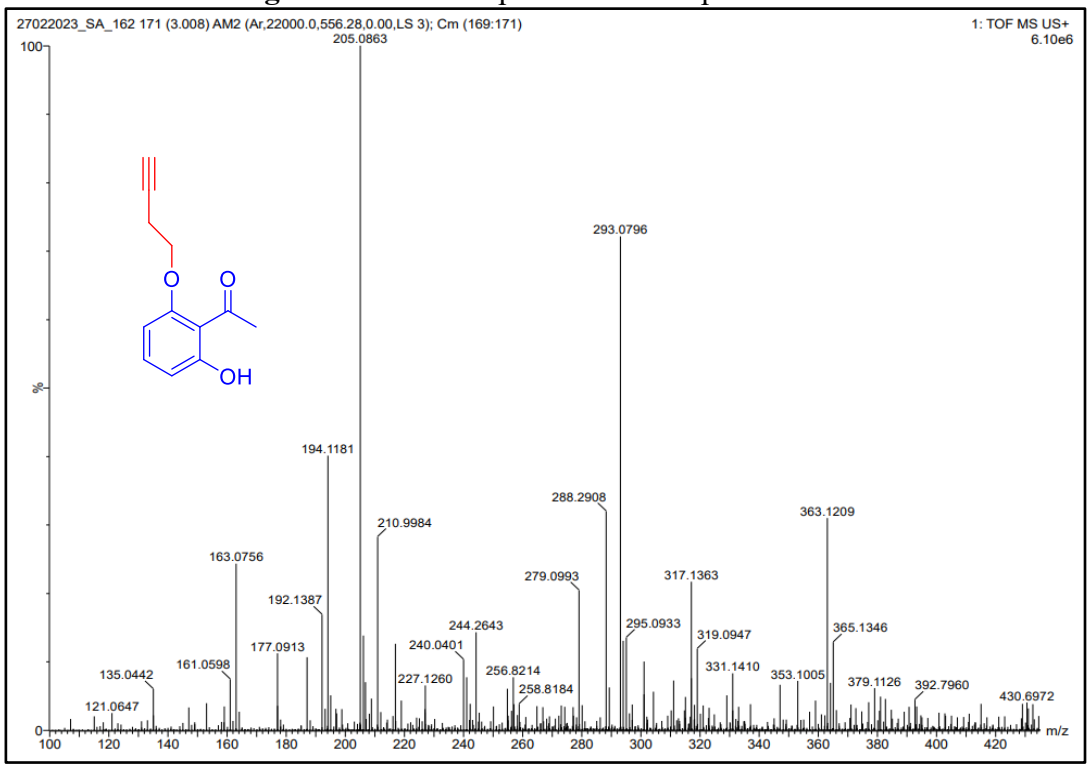


Figure 189: HRMS spectrum of compound **14**

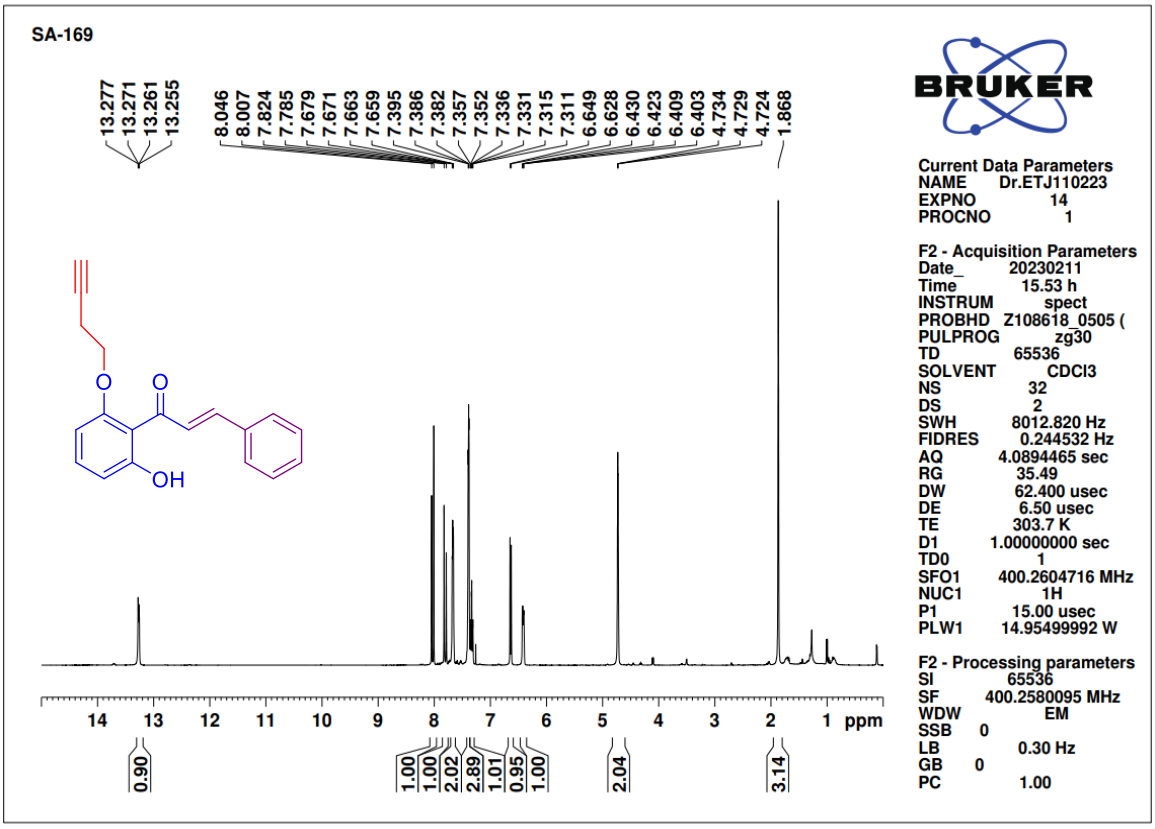


Figure 190: ^{1}H NMR spectrum of compound **14**

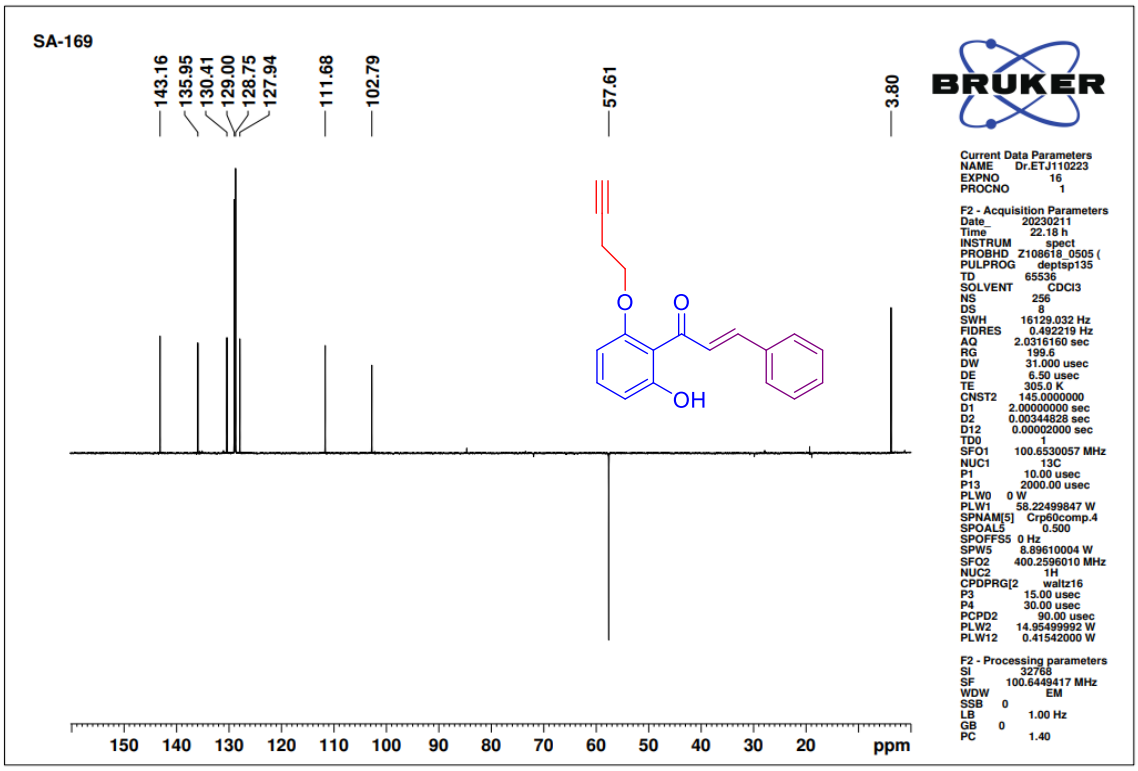


Figure 191: ^{13}C NMR spectrum of compound **14**

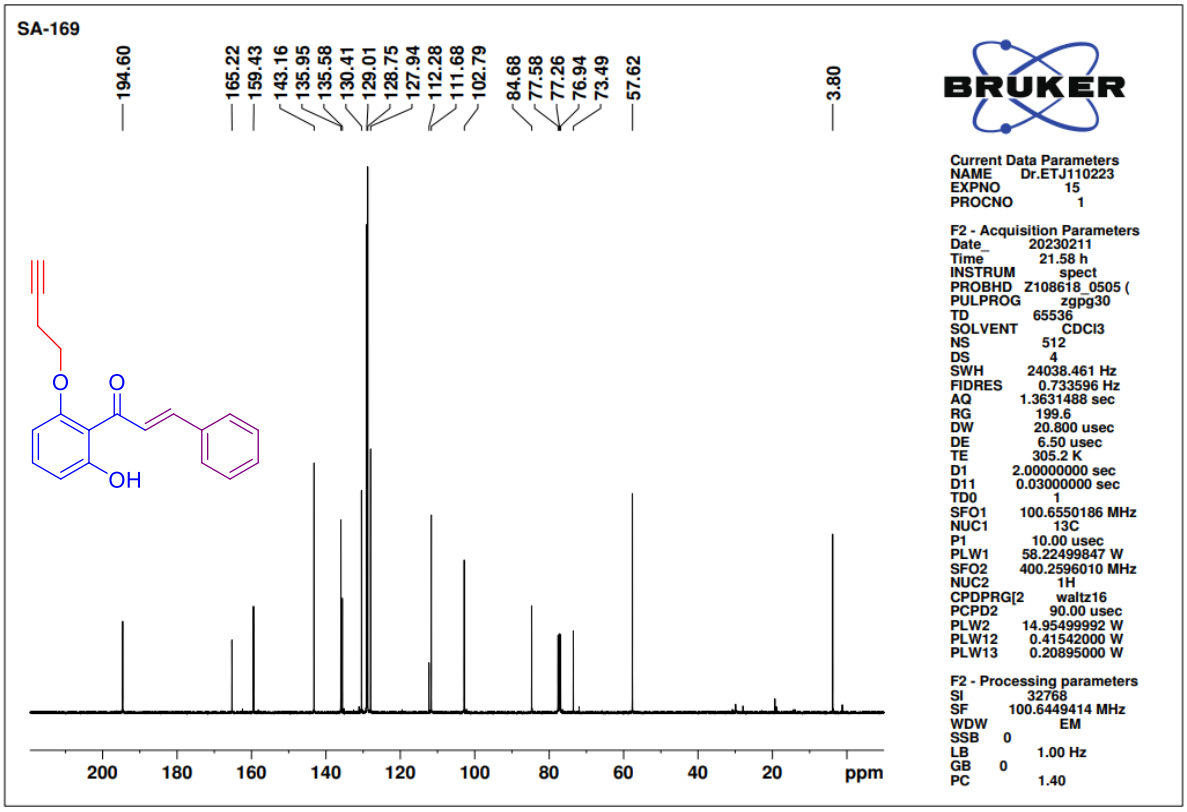


Figure 192: DEPT-135 NMR spectrum of compound **14**

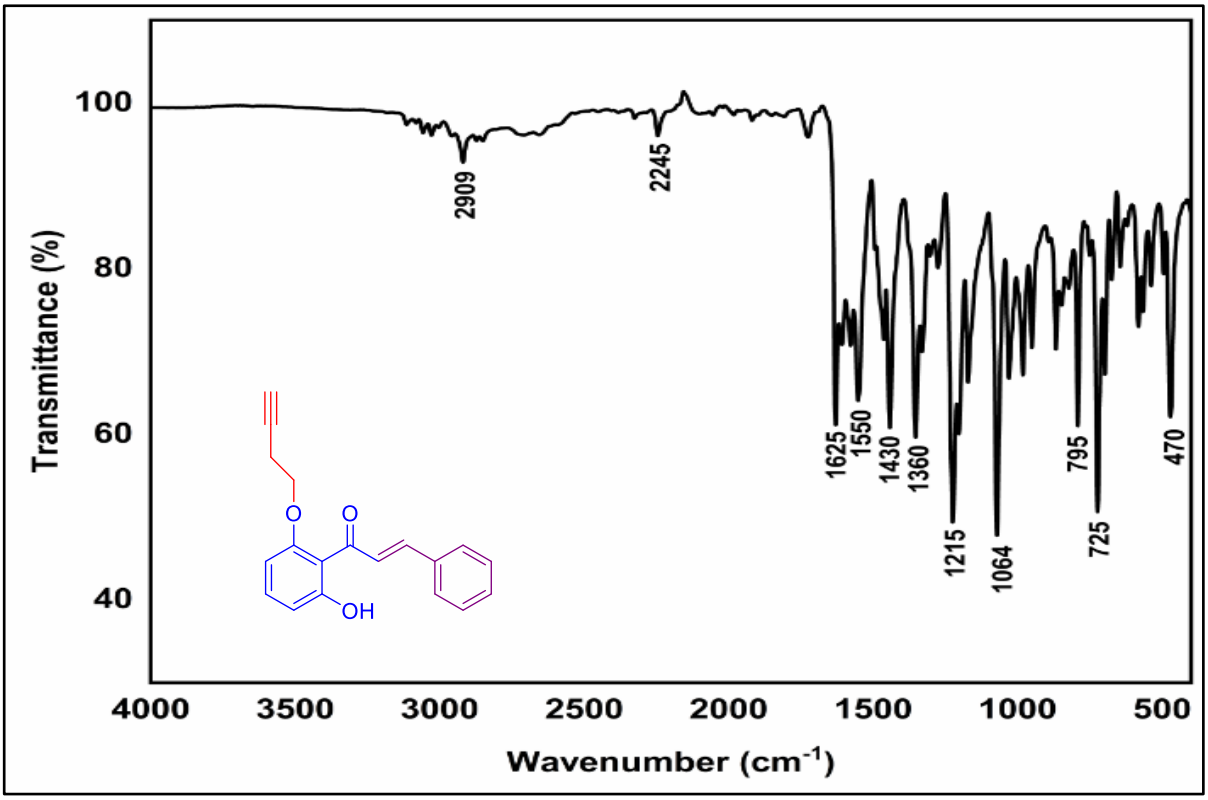


Figure 193: FT-IR spectrum of compound **14**

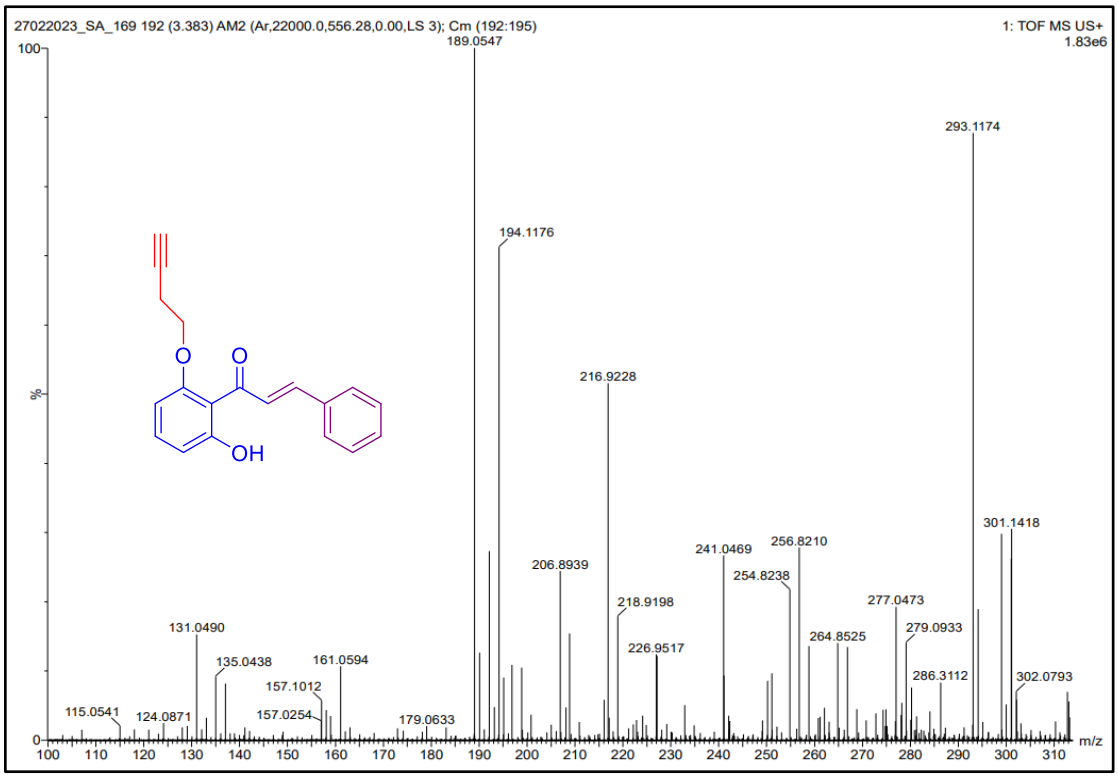


Figure 194: FT-IR spectrum of compound **14**

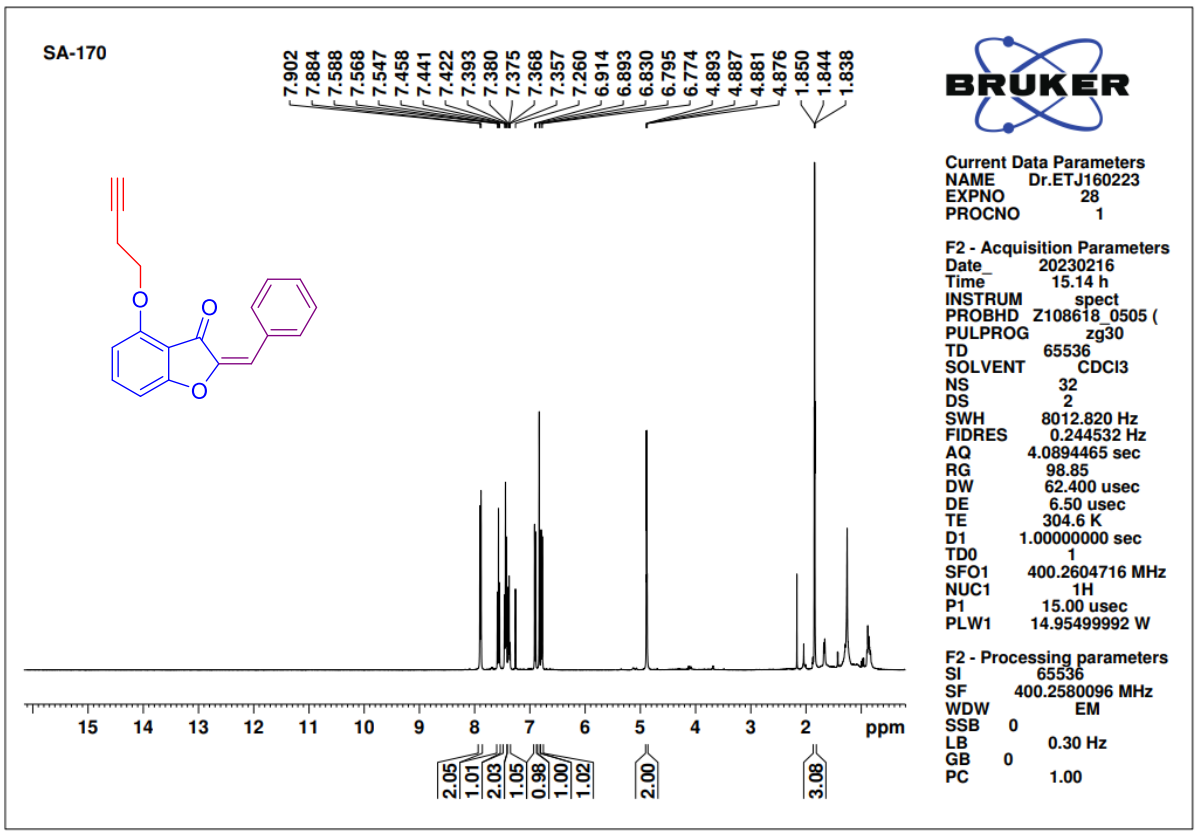


Figure 195: ^{1}H-NMR spectrum of compound **15**

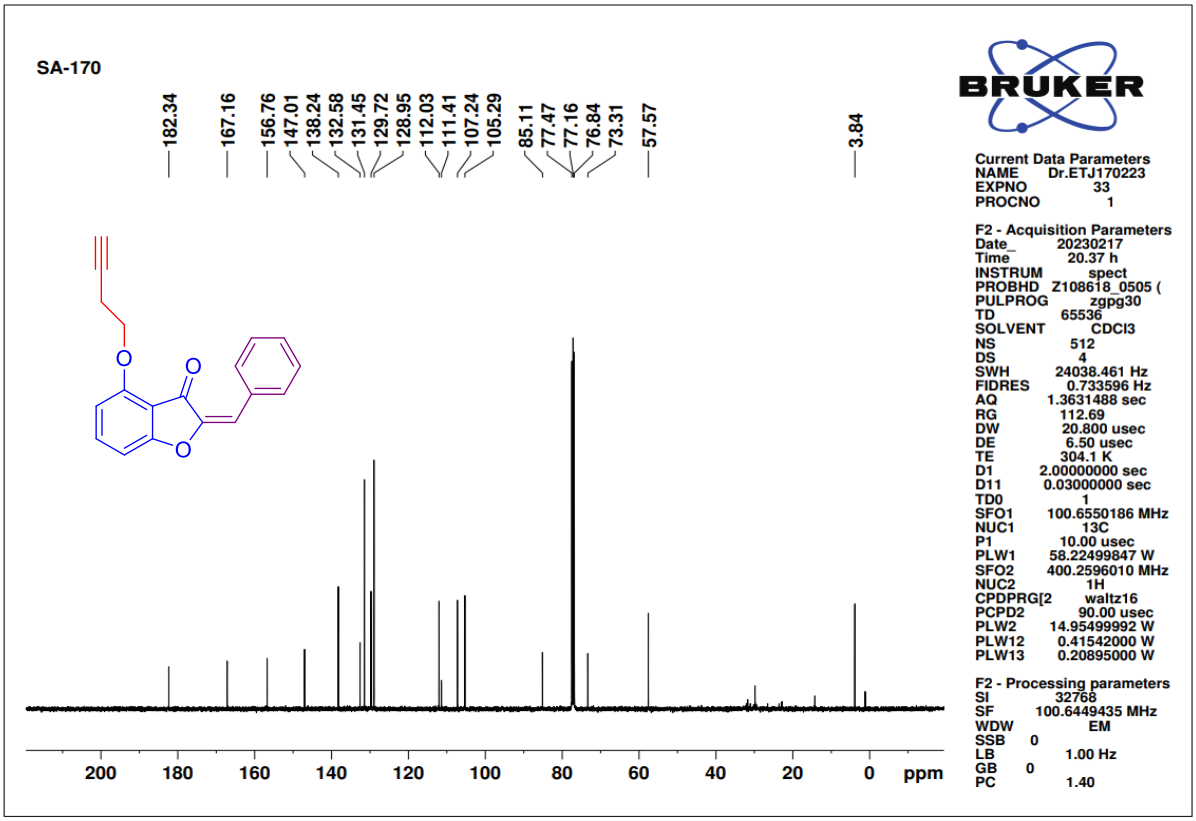


Figure 196: ^{13}C-NMR spectrum of compound **15**

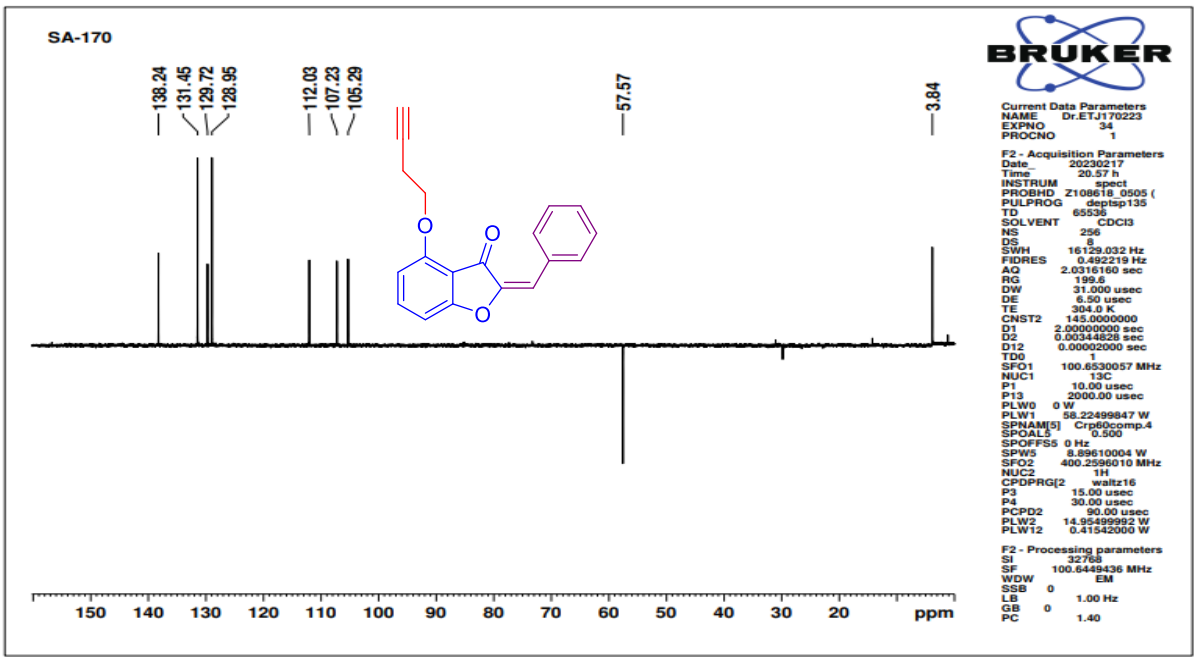


Figure 197: DEPT-135 NMR spectrum of compound **15**

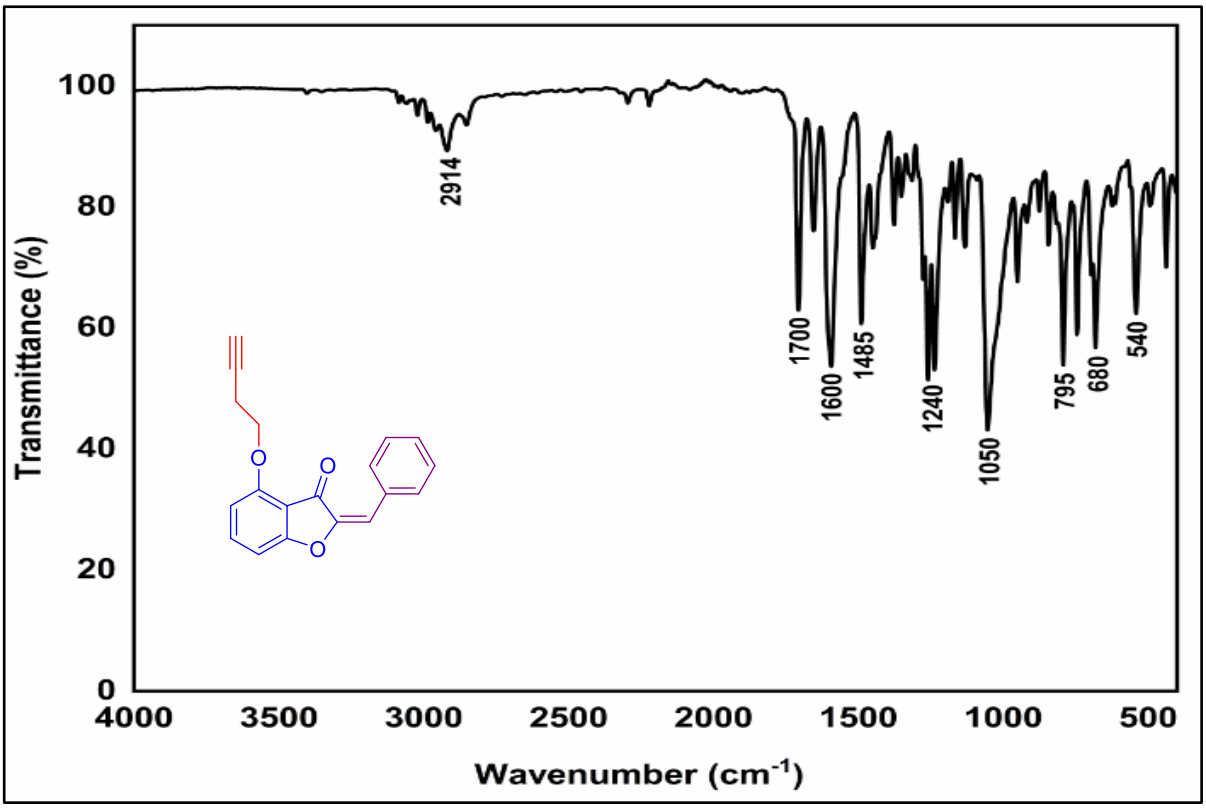


Figure 198: FT-IR spectrum of compound **15**

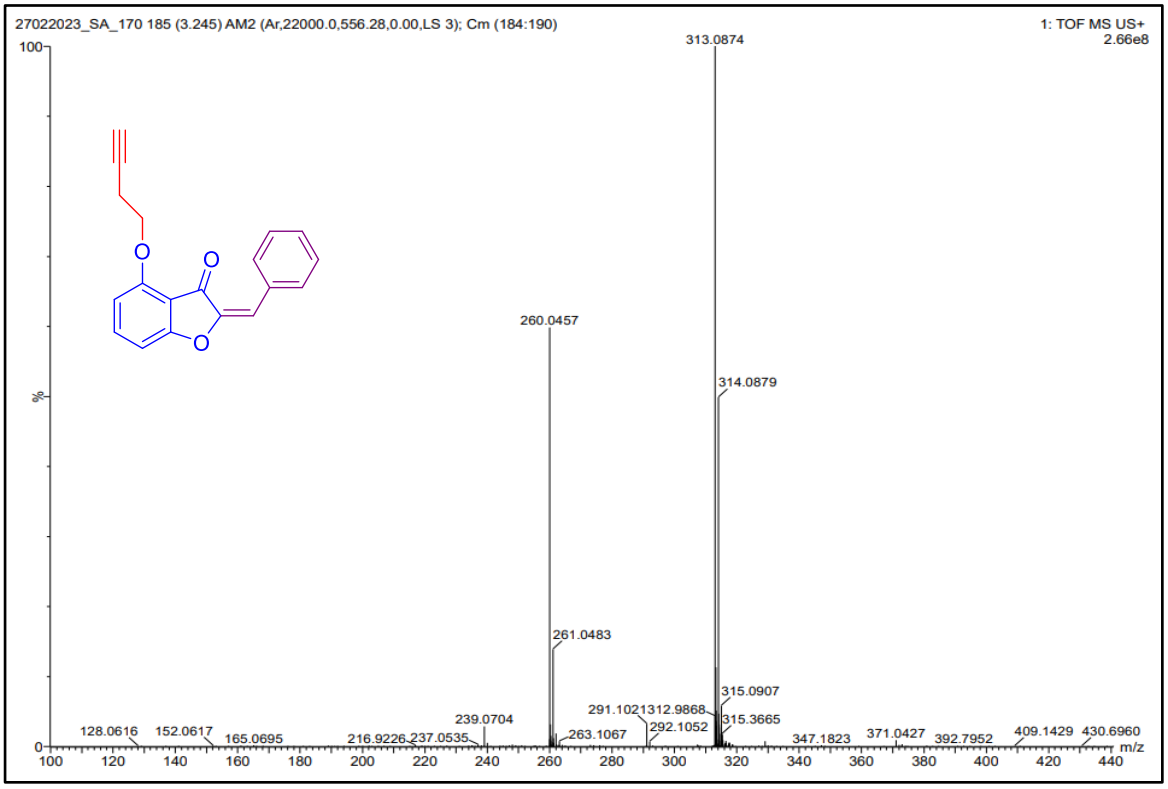


Figure 199: HRMS spectrum of compound **15**

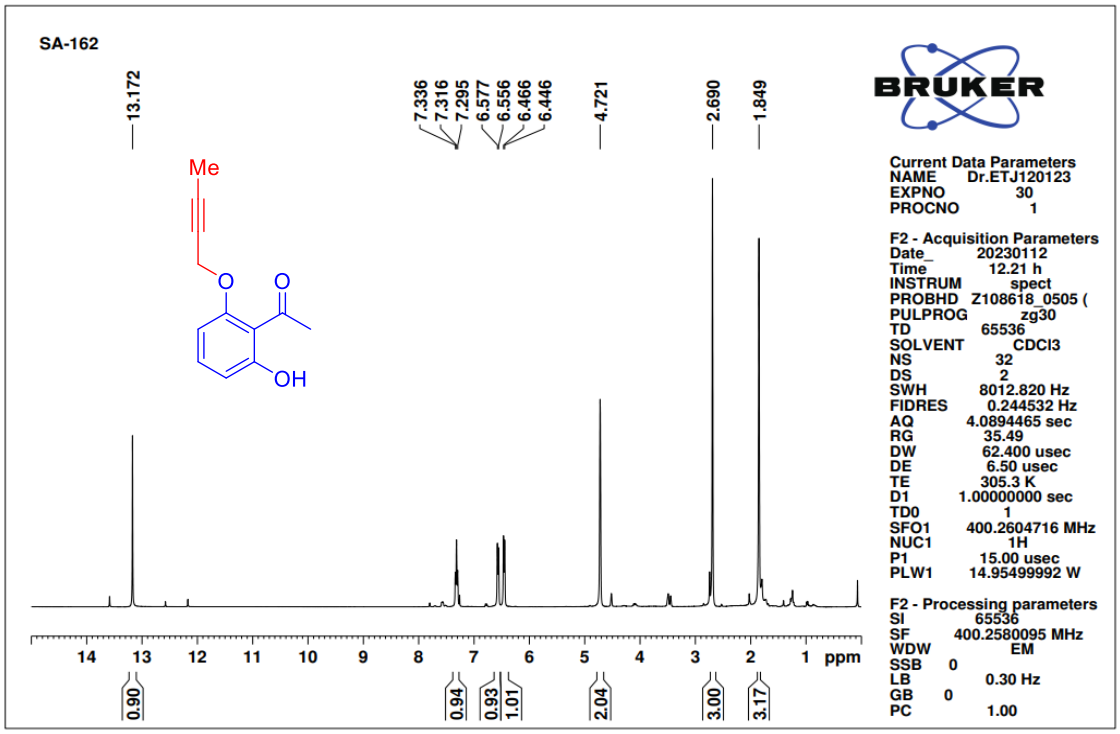


Figure 200: ^{1}H-NMR spectrum of compound **9**

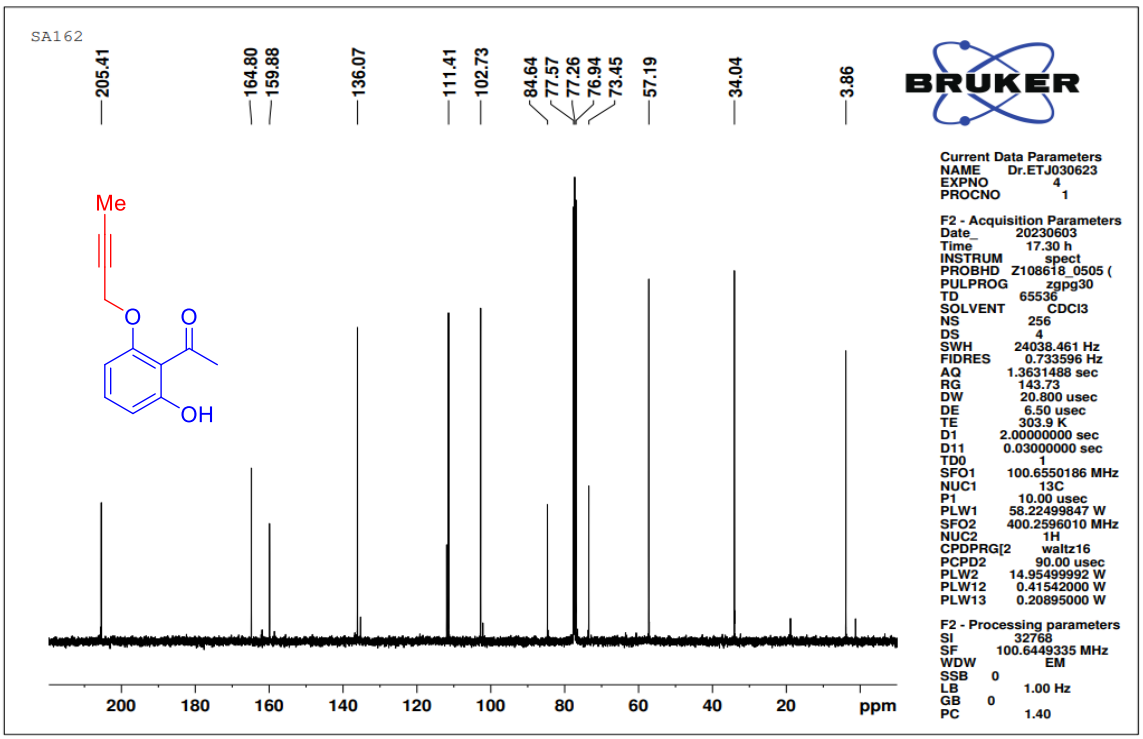


Figure 201: ^{13}C-NMR spectrum of compound **9**

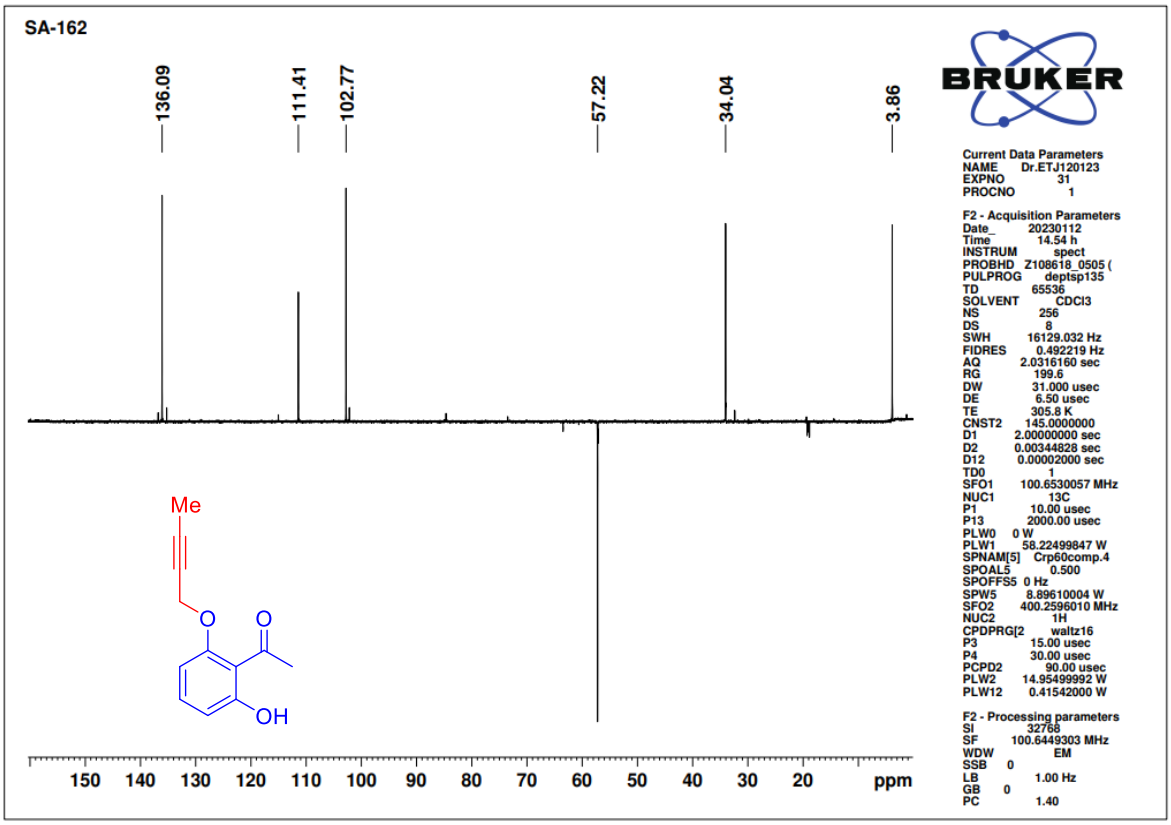


Figure 202: DEPT-135 NMR spectrum of compound **9**

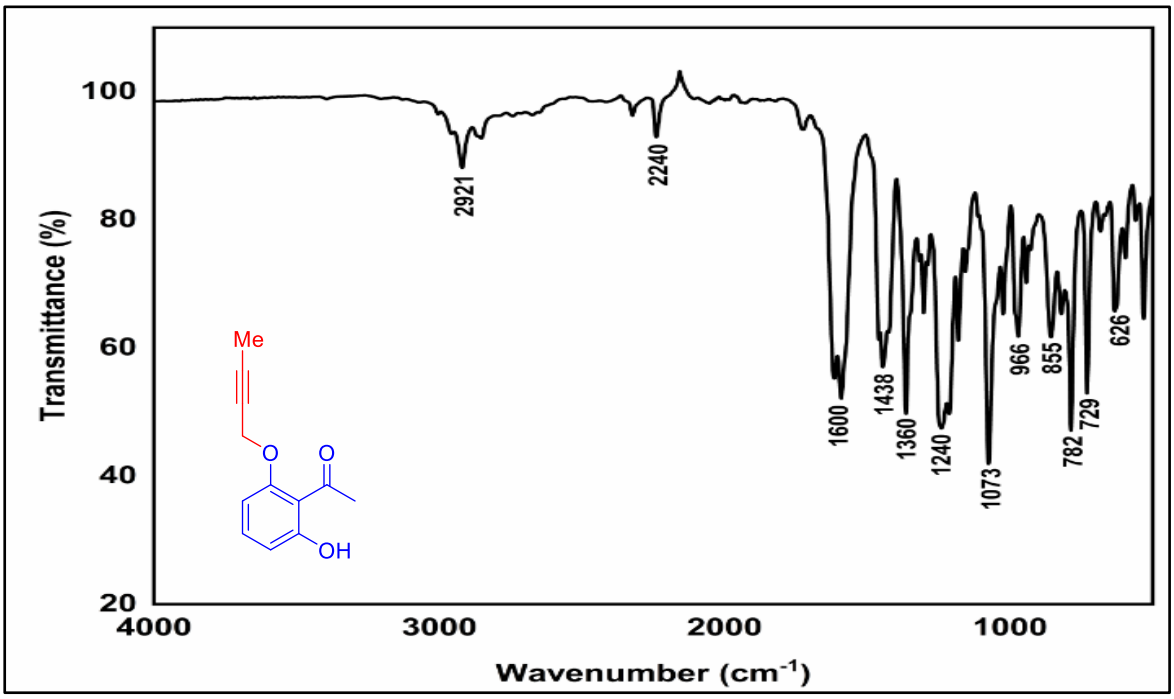


Figure 203: FT-IR spectrum of compound **9**

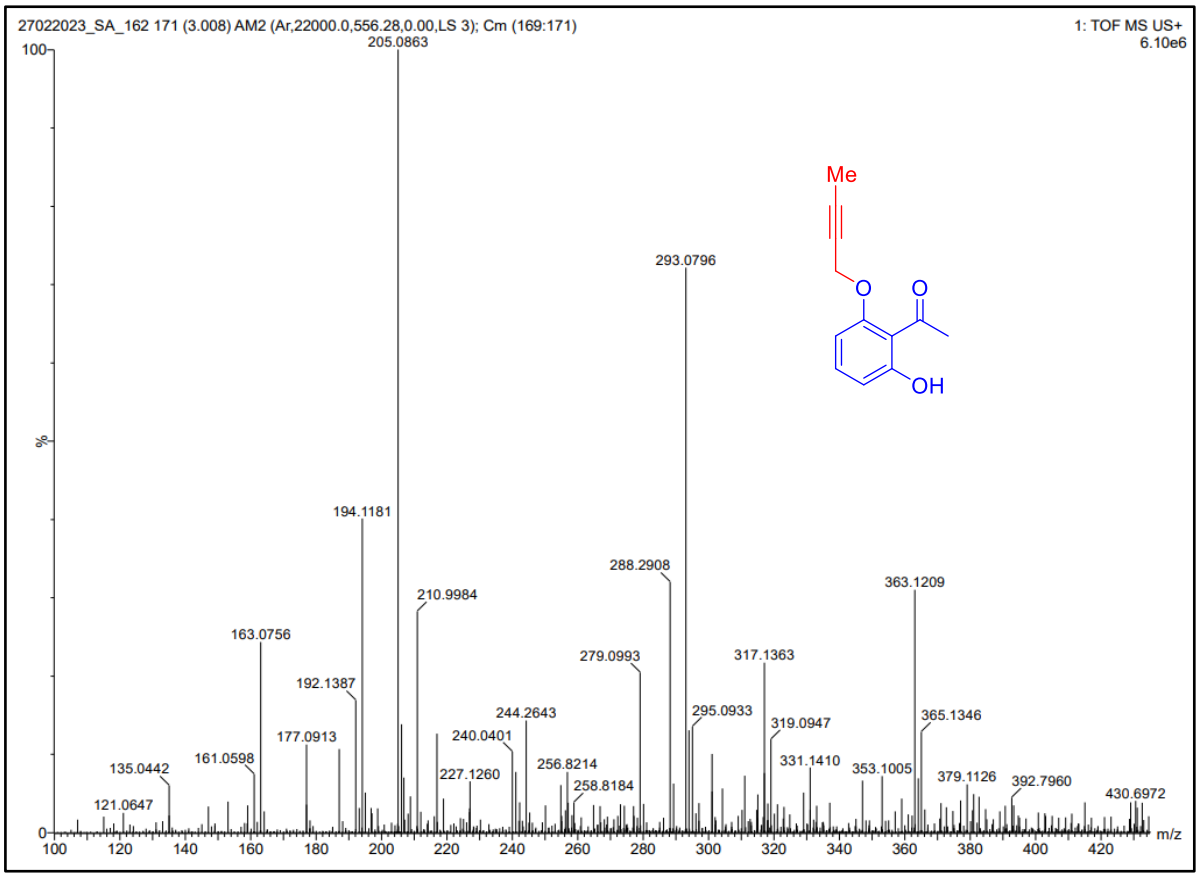


Figure 204: HRMS spectrum of compound **9**

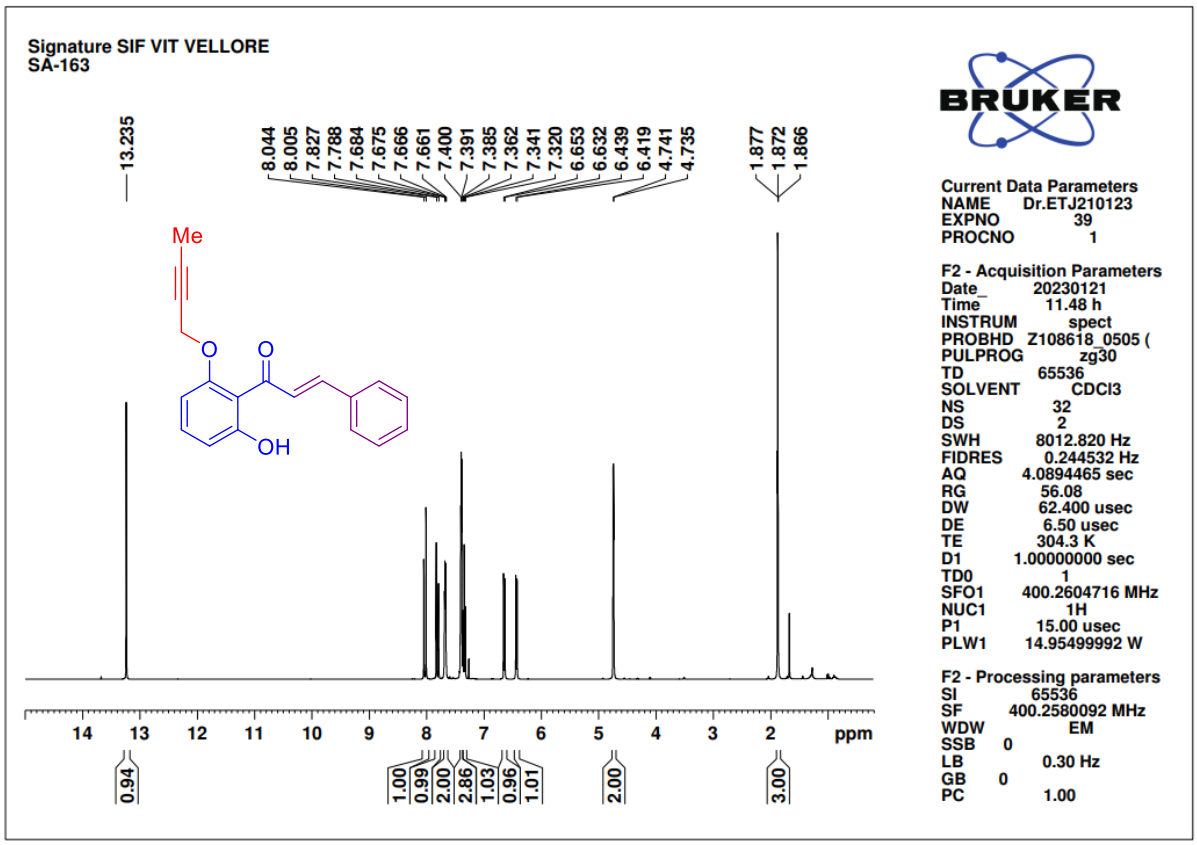


Figure 205: ^{1}H-NMR spectrum of compound **10**

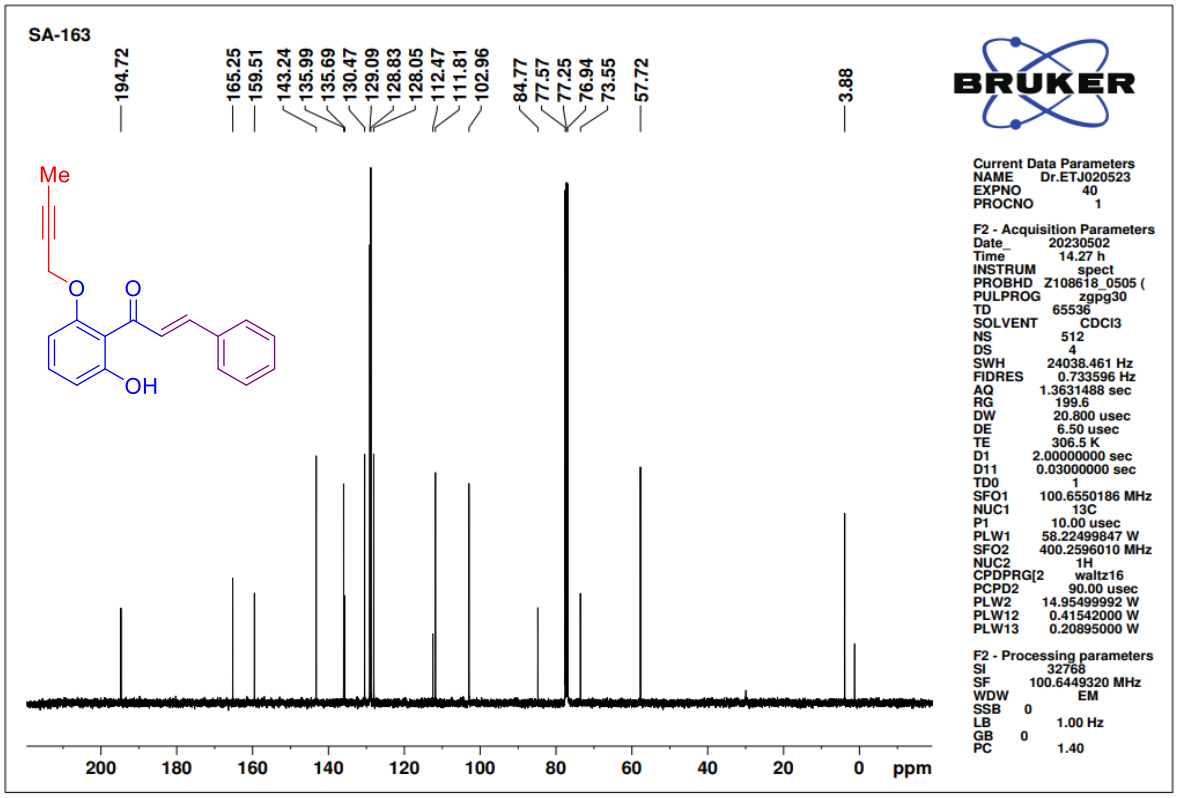


Figure 206: ^{13}C-NMR spectrum of compound **10**

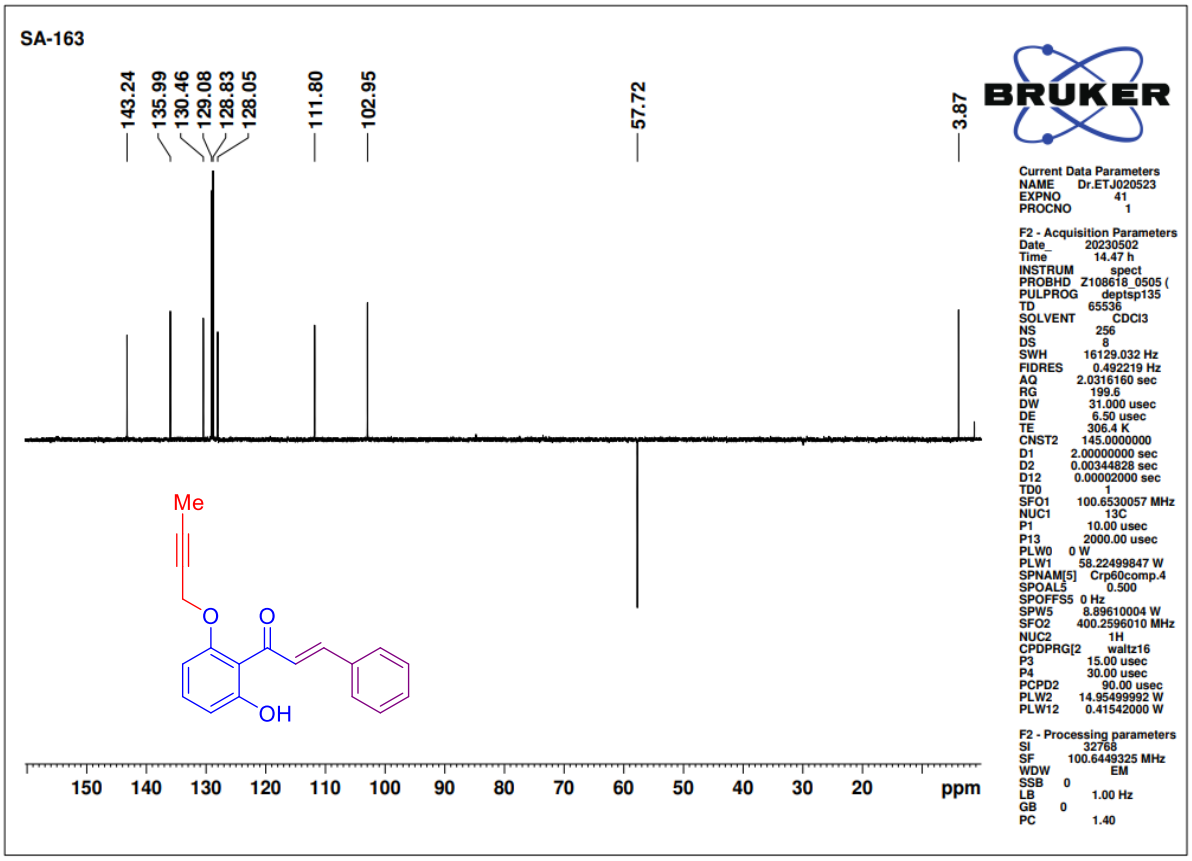


Figure 207: DEPT -135 NMR spectrum of compound **10**

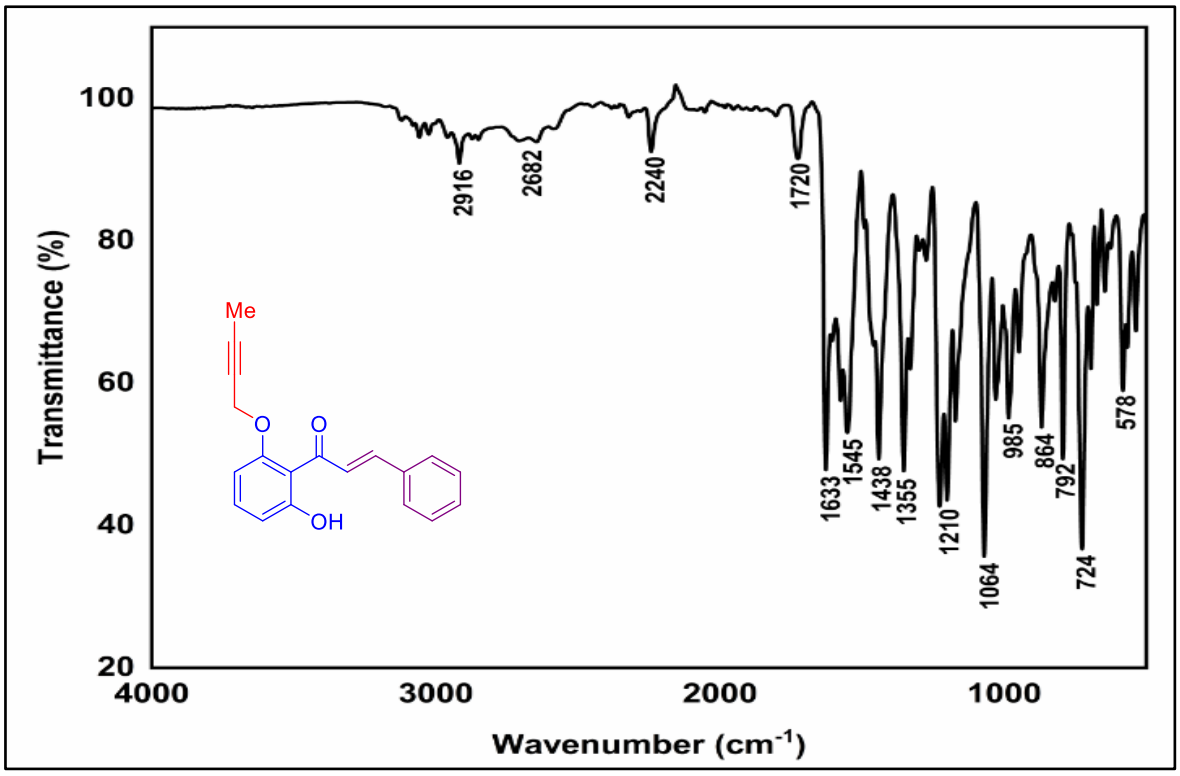


Figure 208: FT-IR spectrum of compound **10**

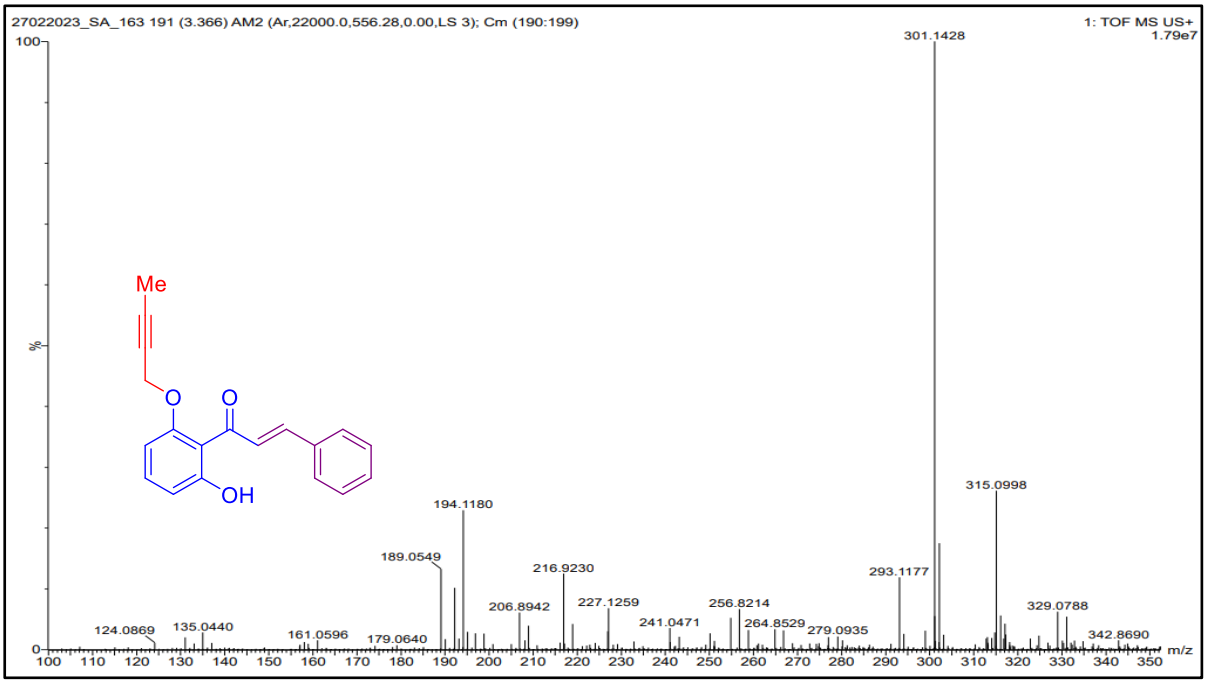


Figure 209: HRMS spectrum of compound **10**

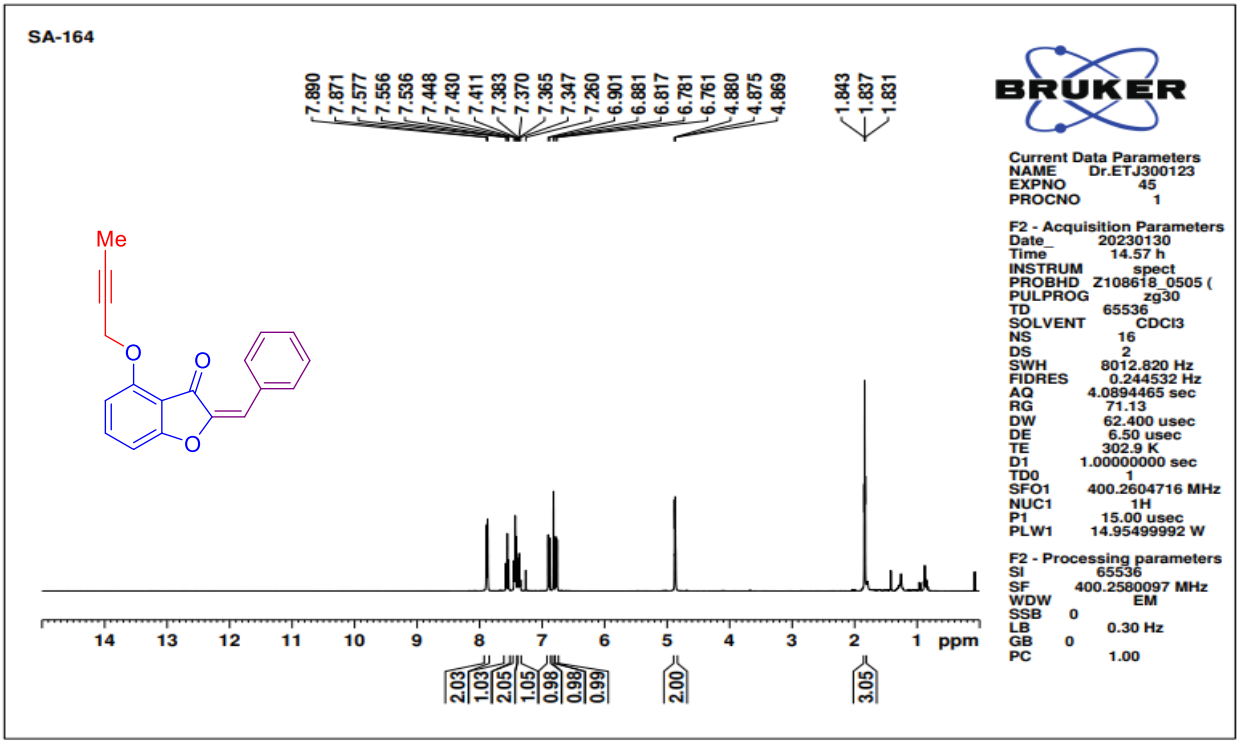


Figure 210: ^{1}H-NMR spectrum of compound **11**

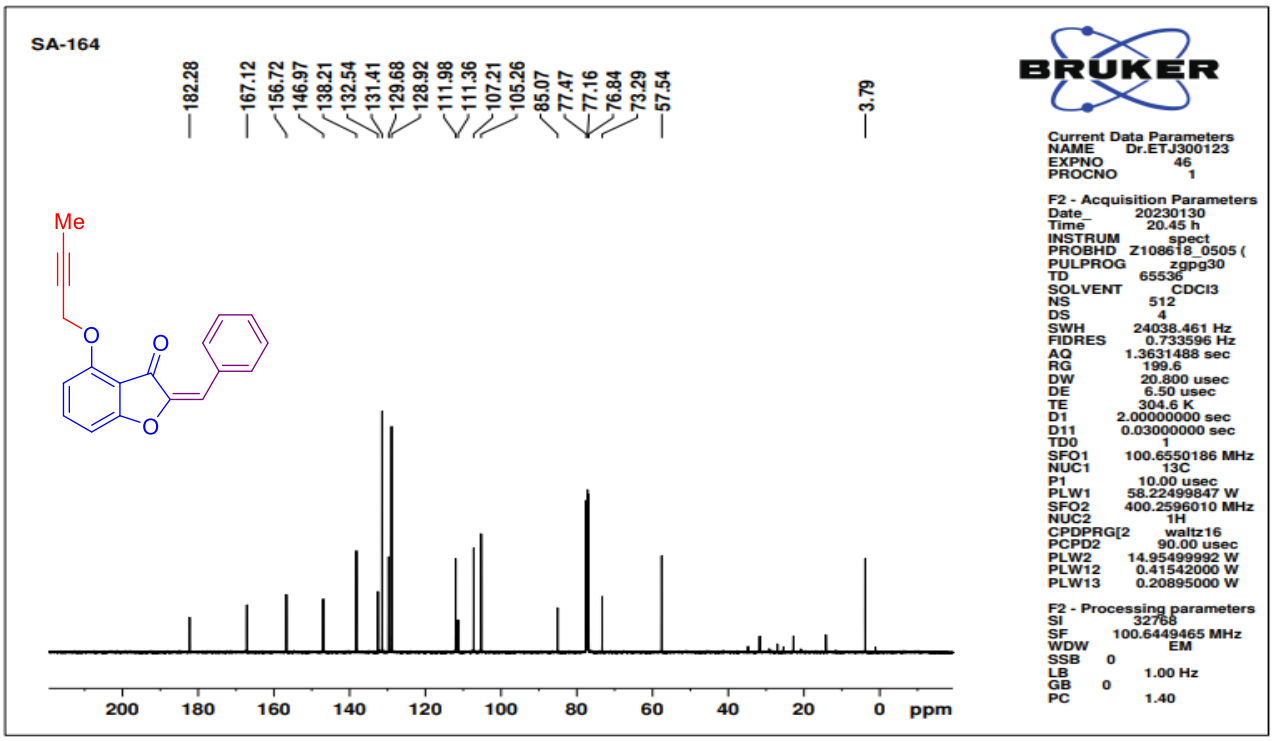


Figure 211: ^{13}C-NMR spectrum of compound **11**

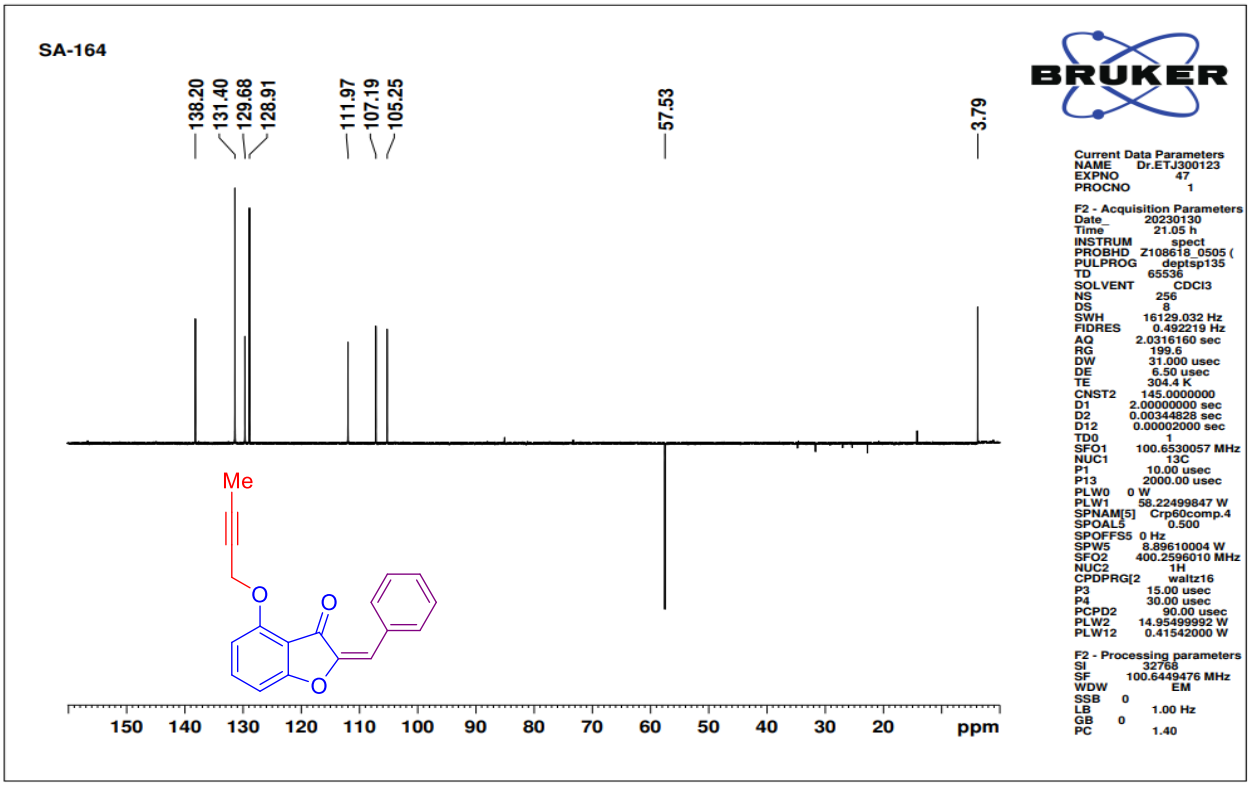


Figure 212: DEPT-135-NMR spectrum of compound **11**

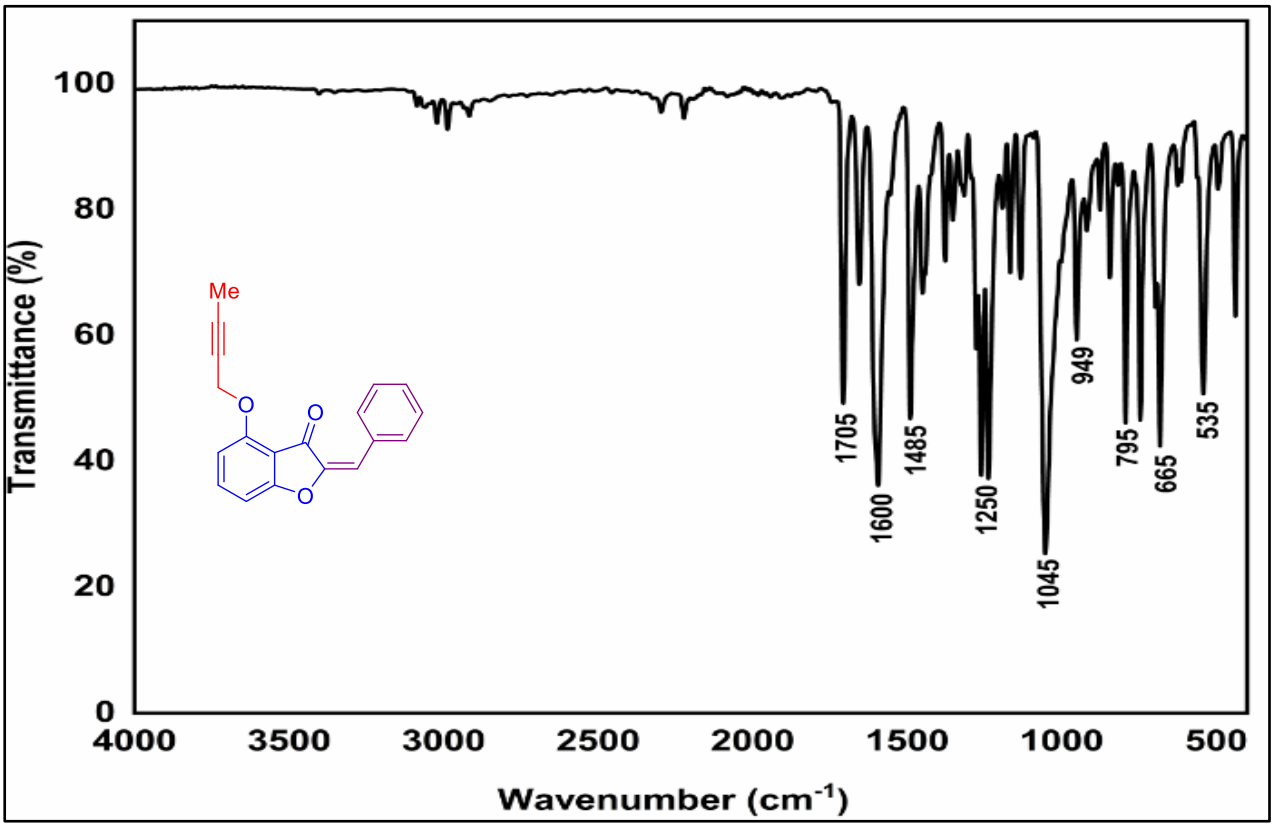


Figure 213: FT-IR spectrum of compound **11**

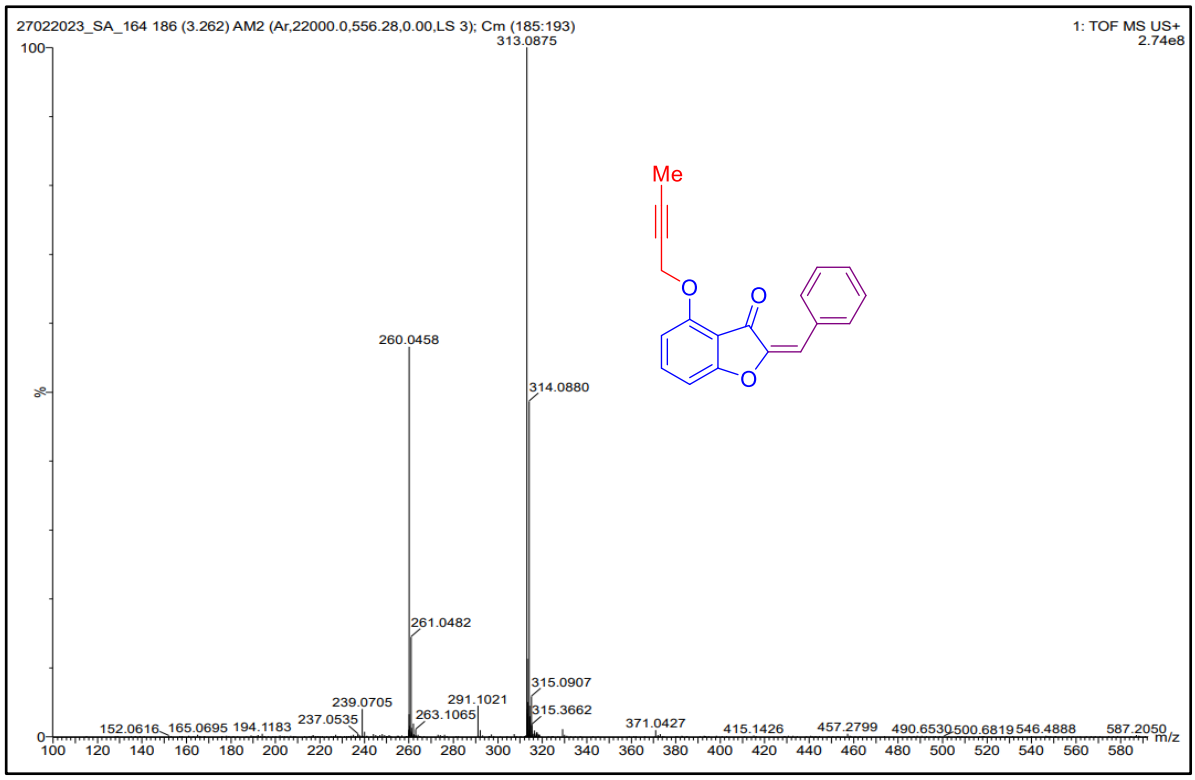


Figure 214: HRMS spectrum of compound **11**

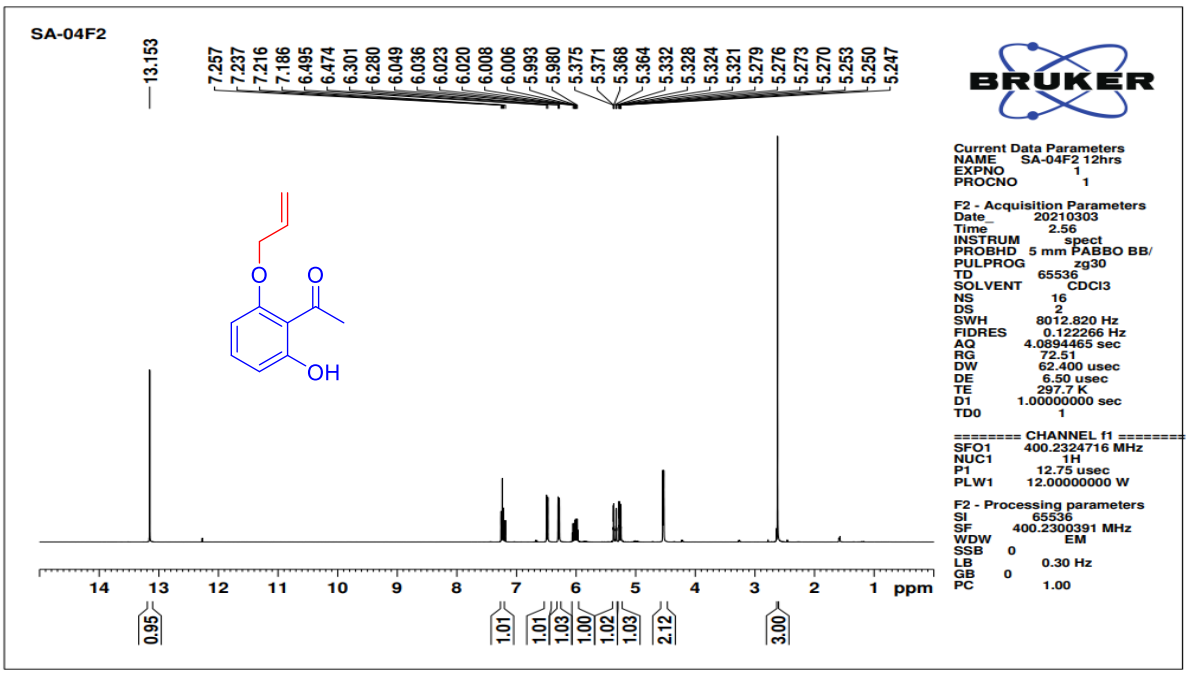


Figure 215: ^{13}H-NMR spectrum of compound **17**

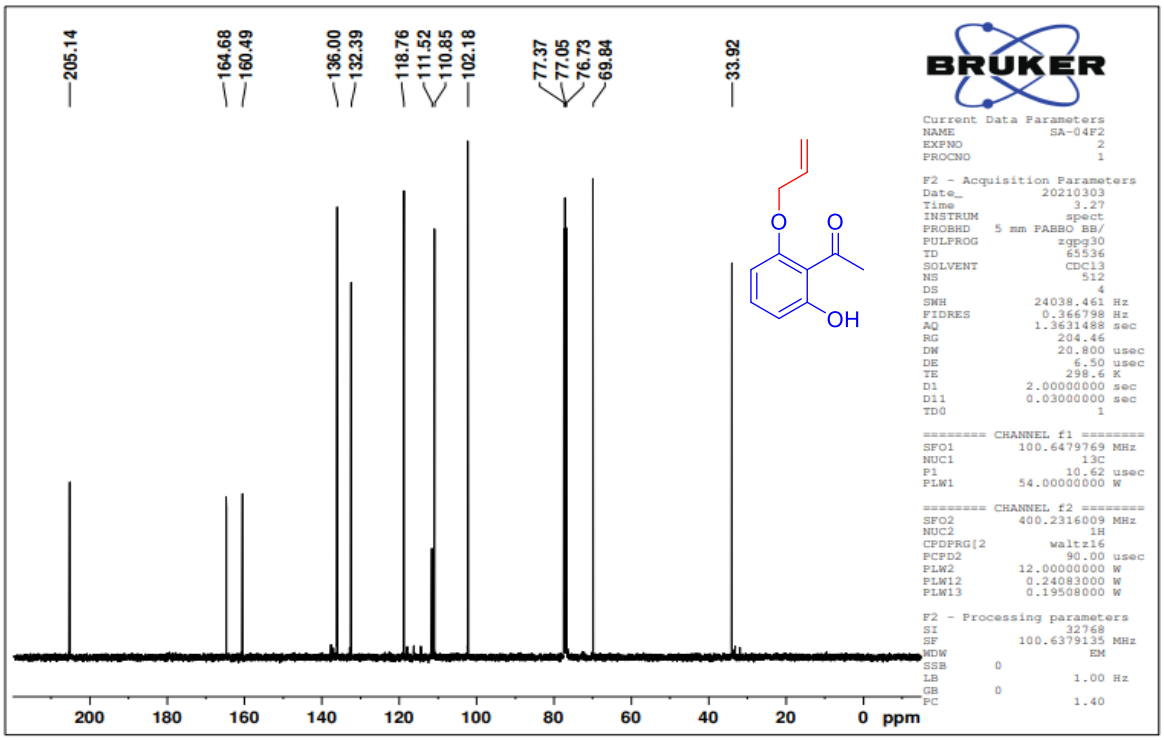


Figure 216: ^{13}C-NMR spectrum of compound **17**

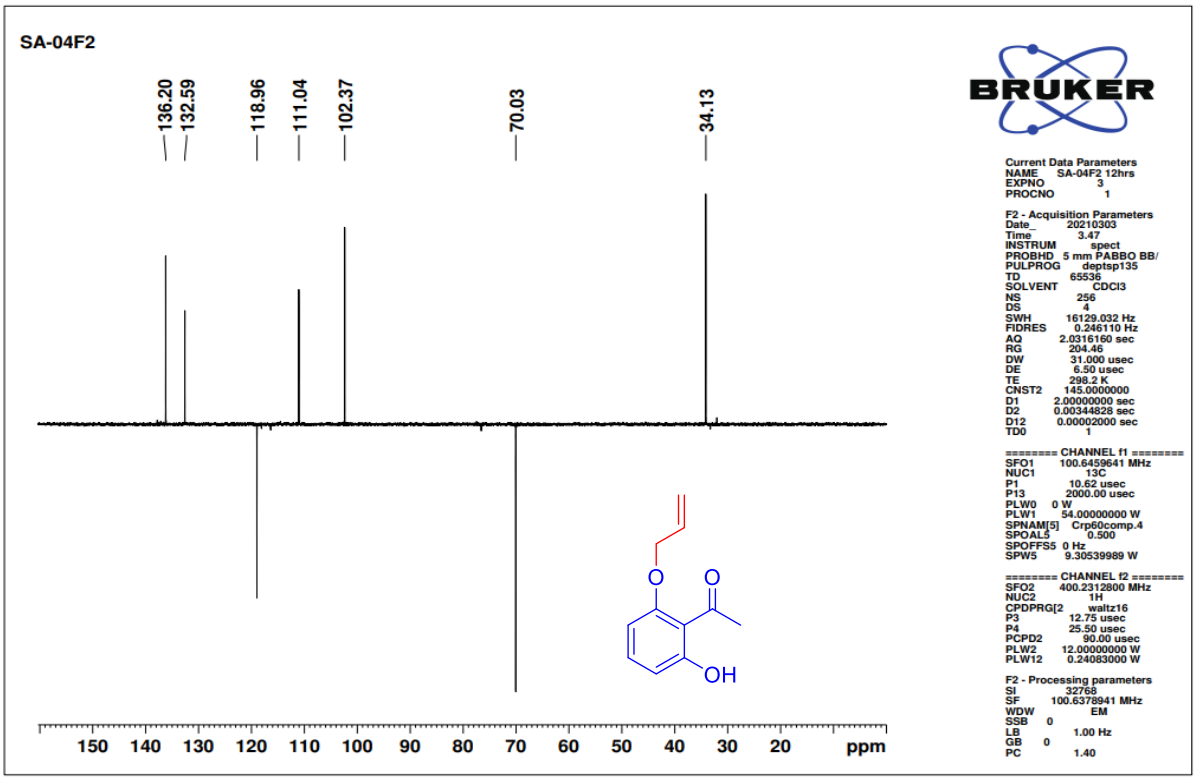


Figure 217: DEPT-135 NMR spectrum of compound **17**

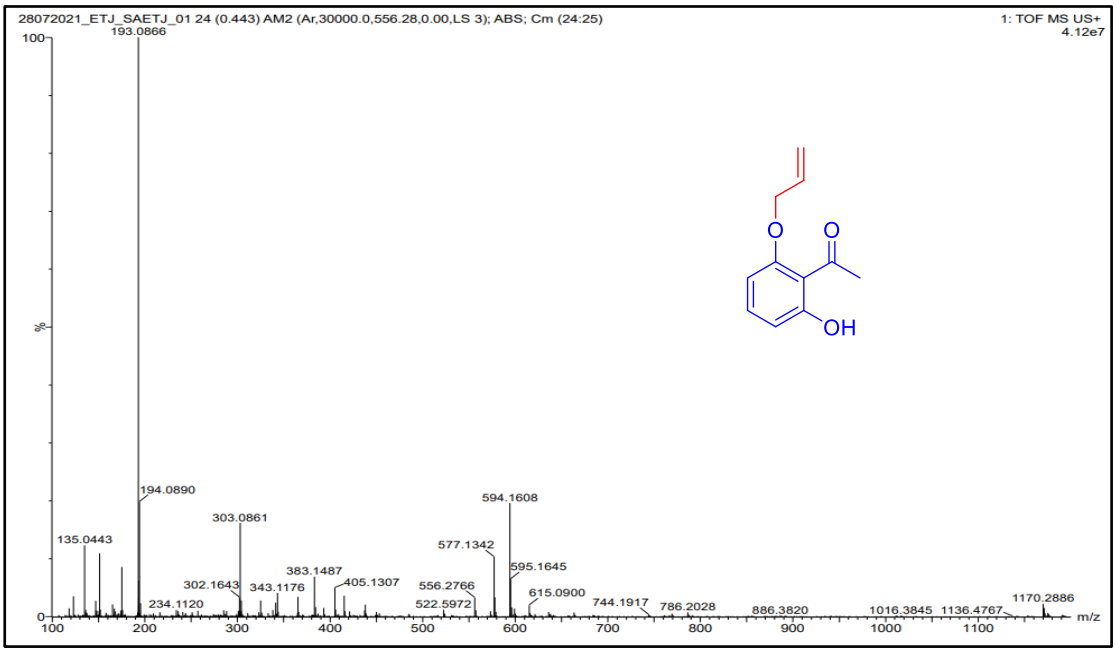


Figure 218: HRMS spectrum of compound **17**

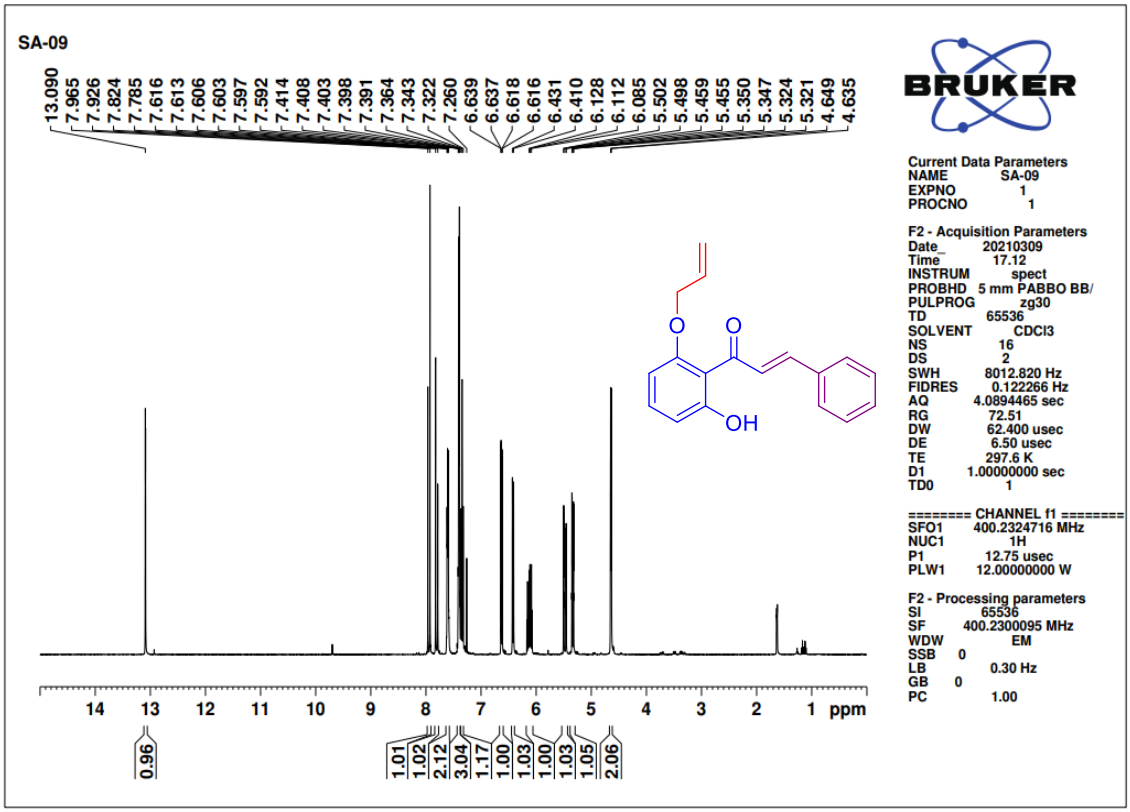


Figure 219: ^{1}H-NMR spectrum of compound **18**

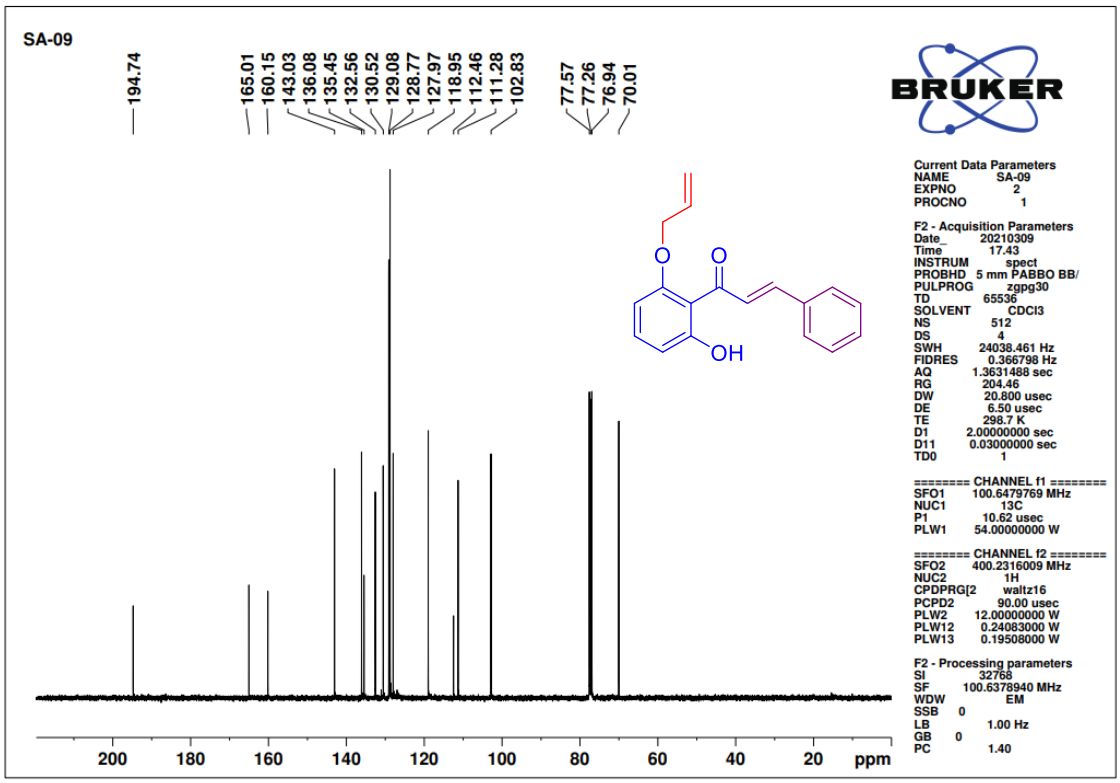


Figure 220: ^{13}C-NMR spectrum of compound **18**

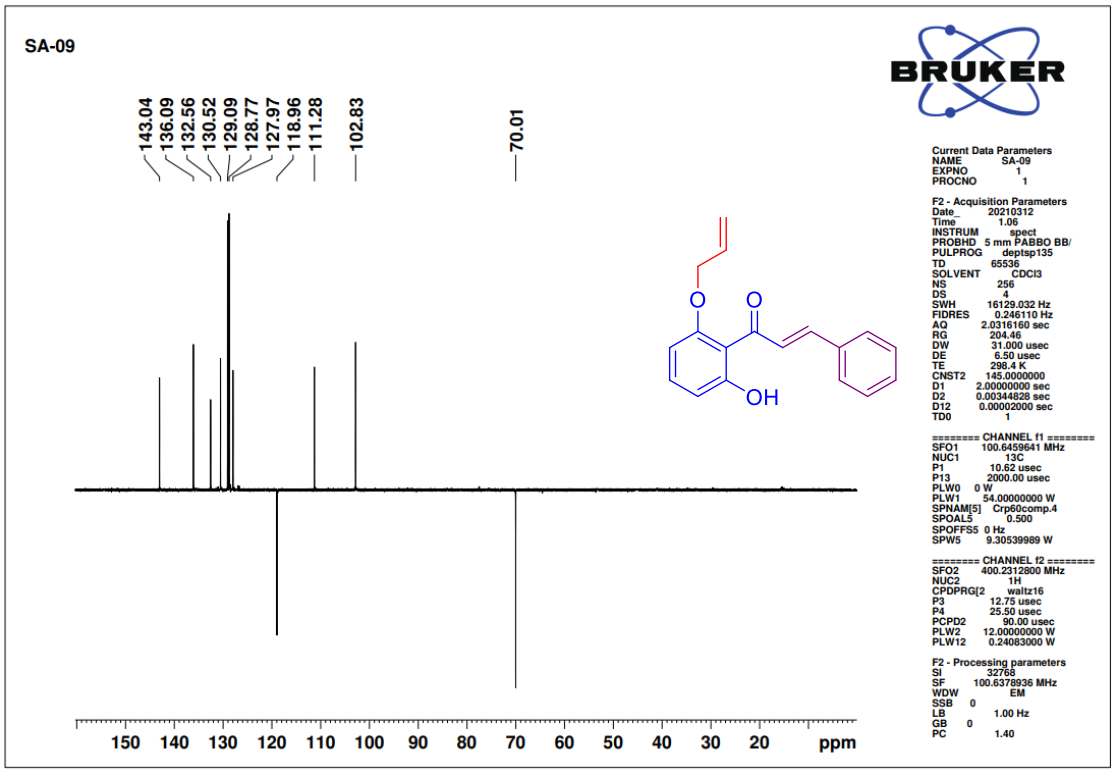


Figure 221: DEPT-135 NMR spectrum of compound **18**

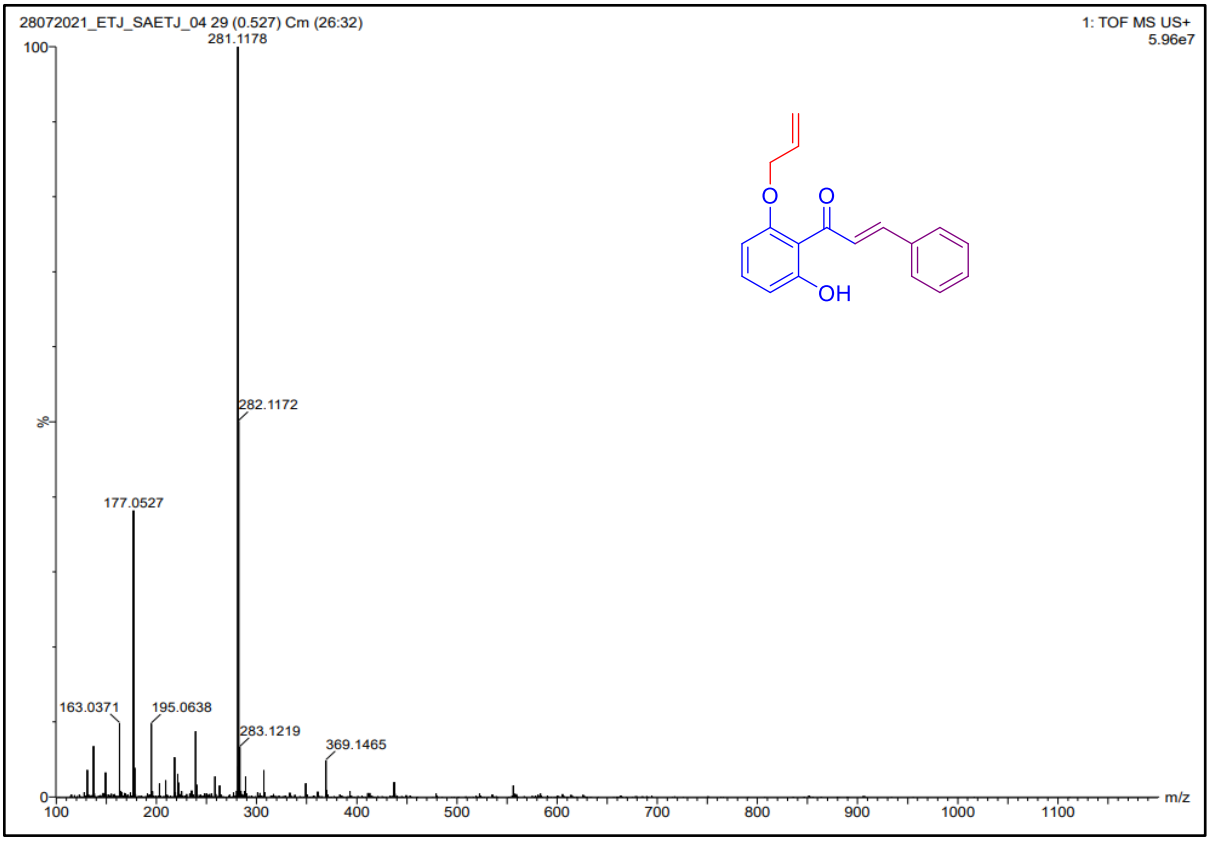


Figure 222: HRMS spectrum of compound **18**

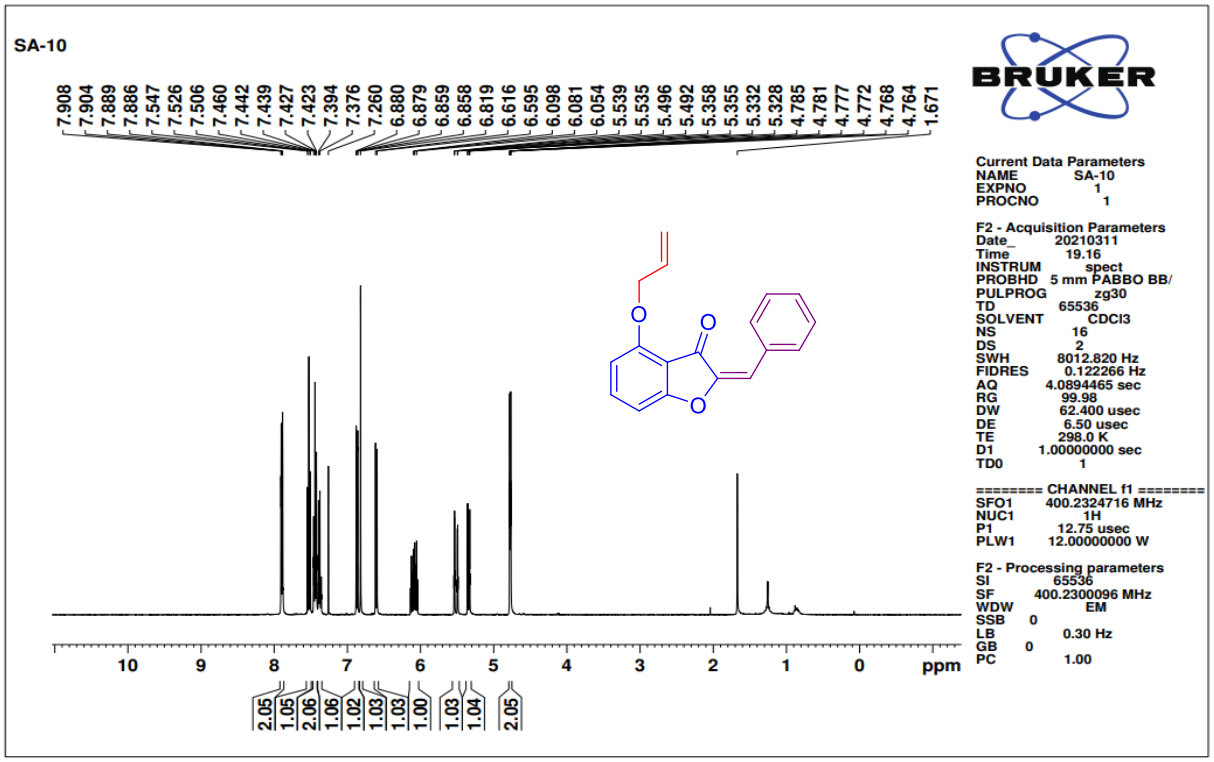


Figure 223: ^{1}H-NMR spectrum of compound **19**

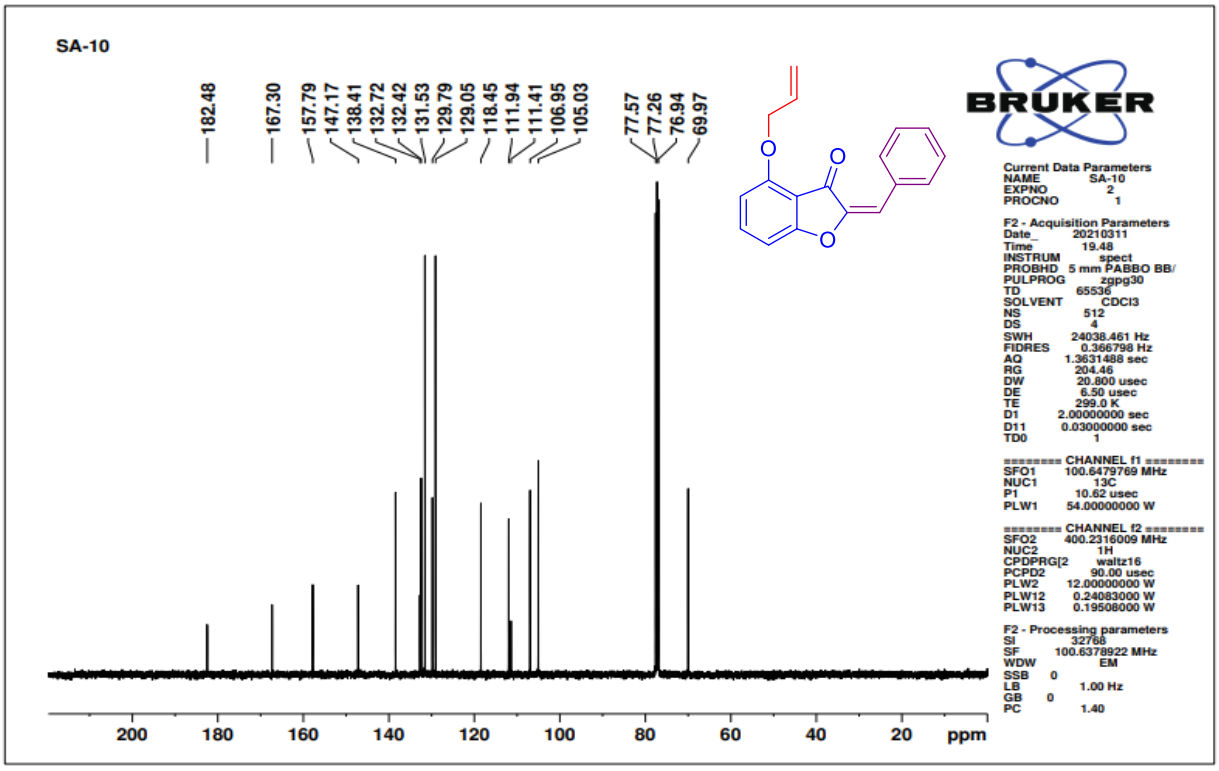


Figure 224: ^{13}C-NMR spectrum of compound **19**

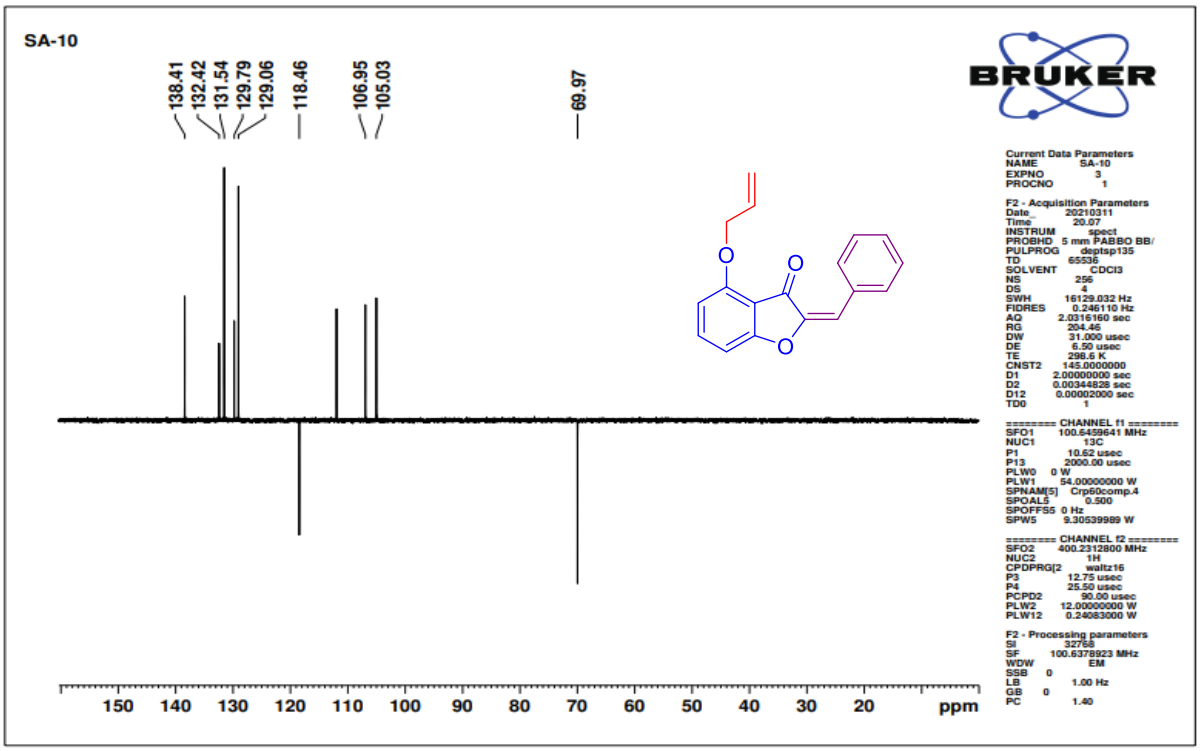


Figure 225: DEPT-135 NMR spectrum of compound **19**

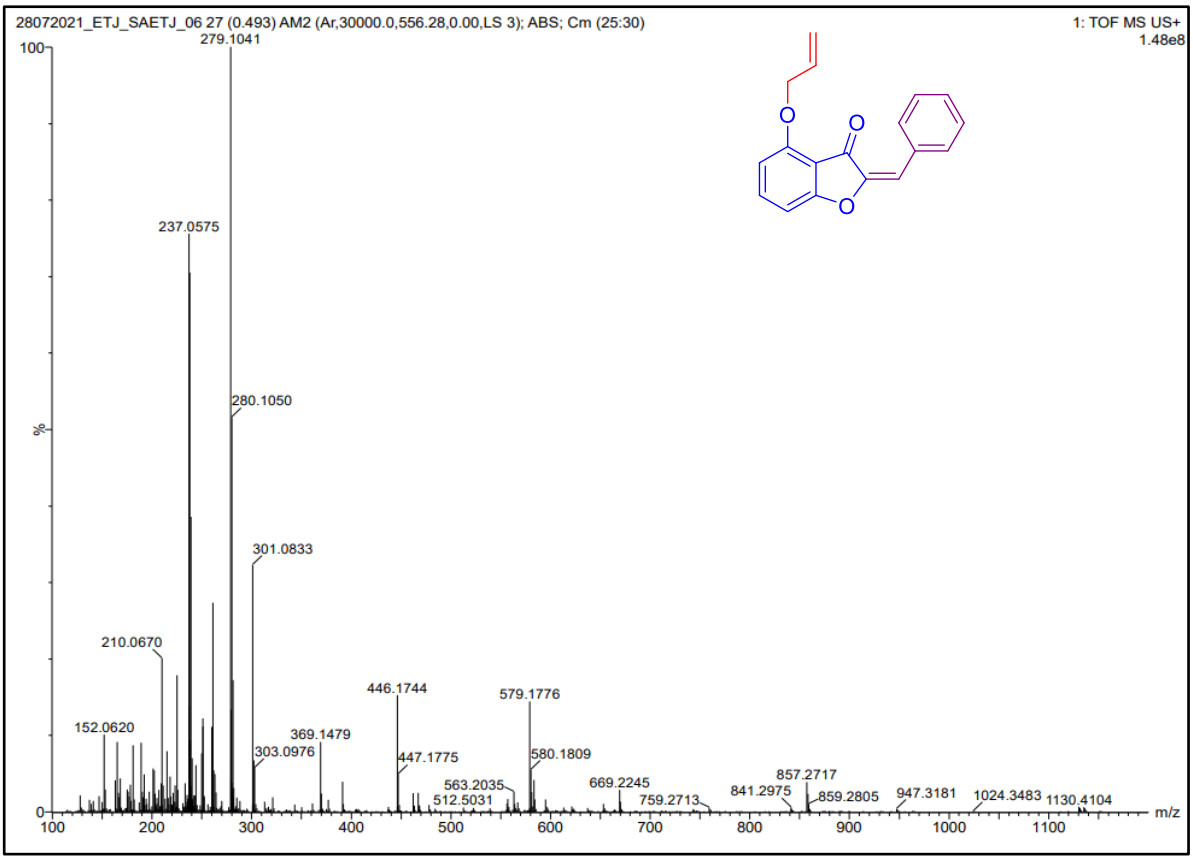


Figure 226: HRMS spectrum of compound **19**

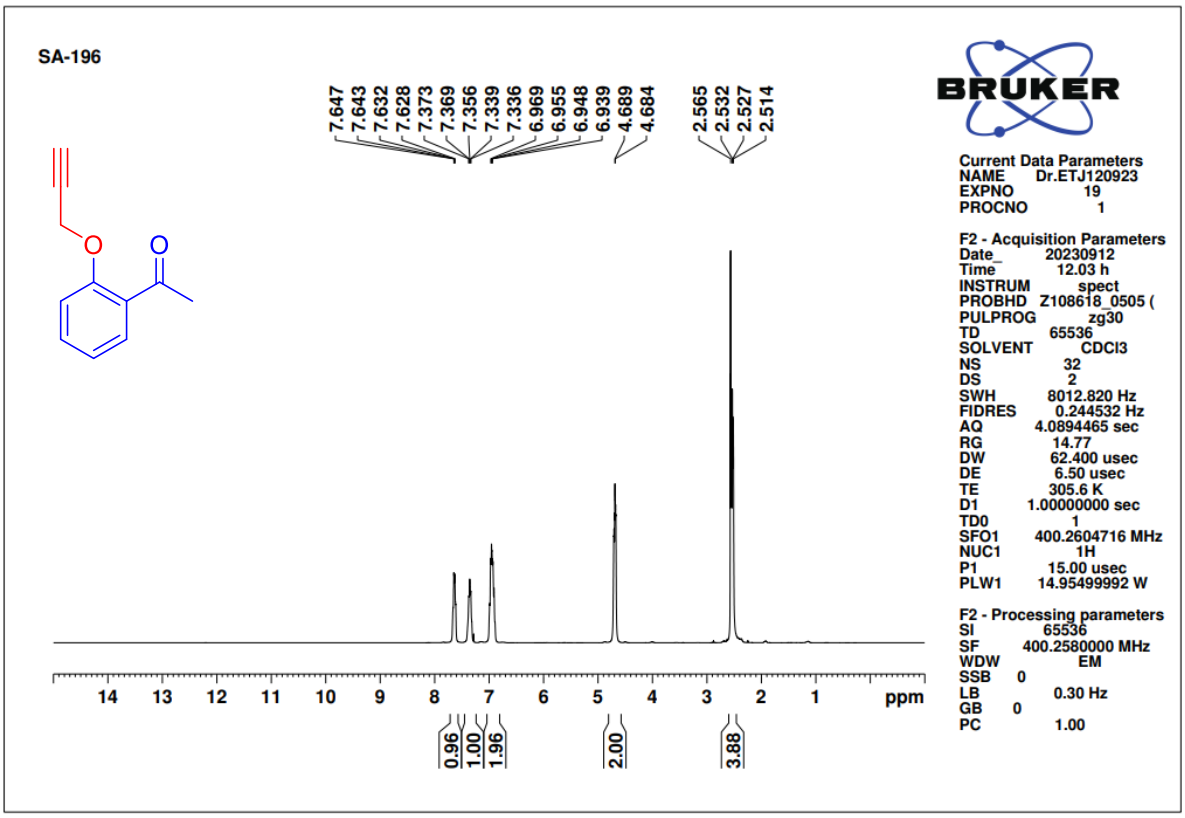


Figure 227: ^{1}H-NMR spectrum of compound **21**

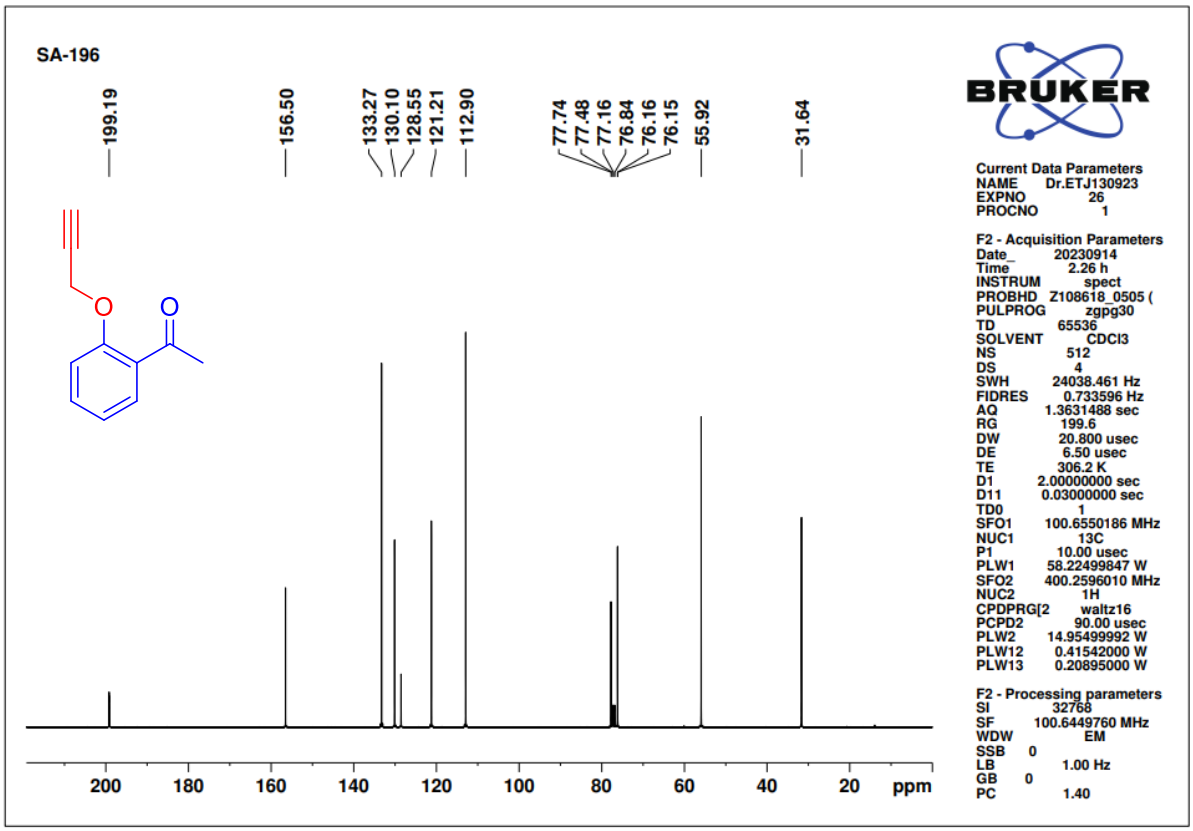


Figure 228: ^{13}C-NMR spectrum of compound **21**

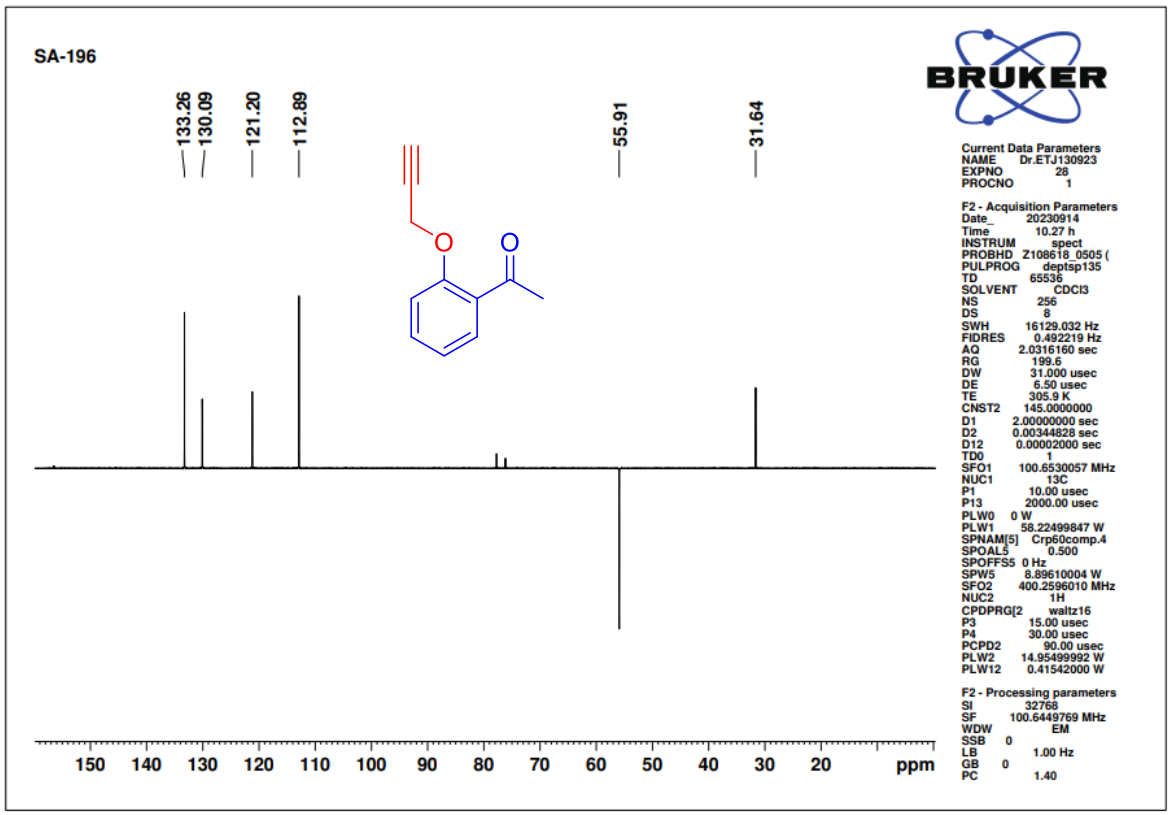


Figure 229: DEPT 135-NMR spectrum of compound **21**

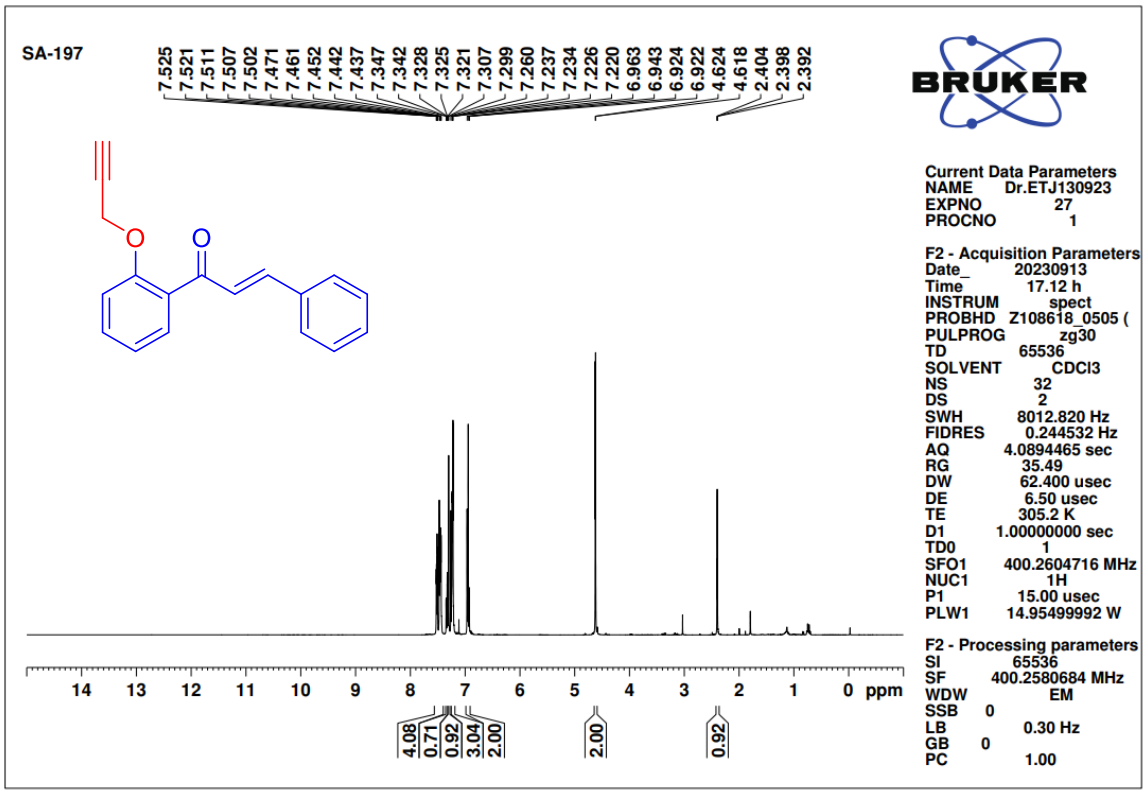


Figure 230: ^{1}H-NMR spectrum of compound **22**

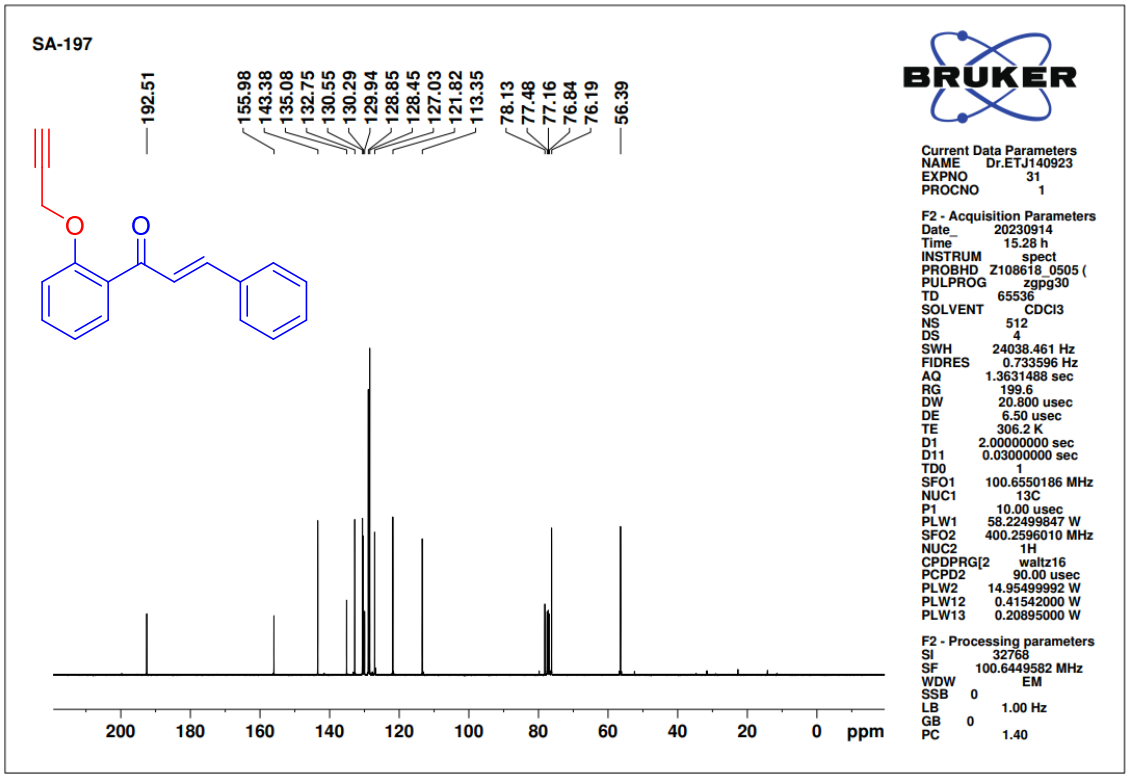


Figure 231: ^{13}C-NMR spectrum of compound **22**

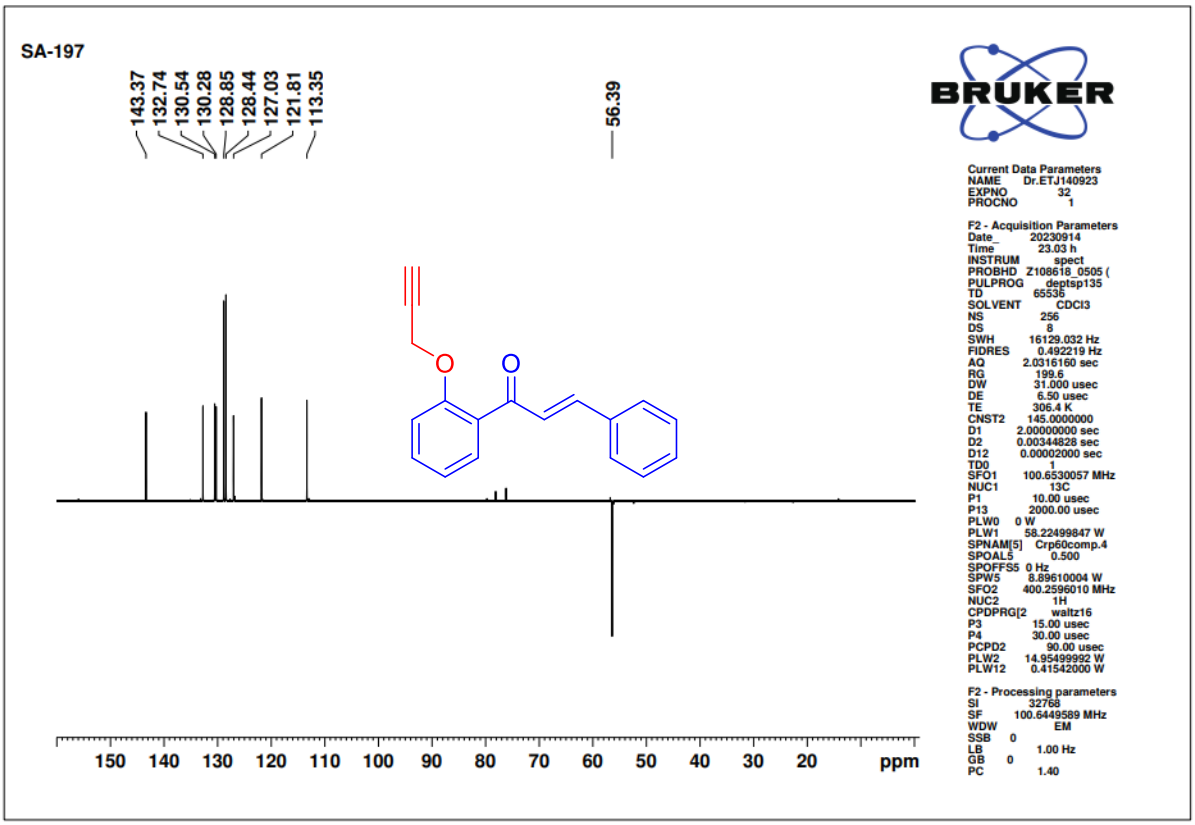


Figure 232: DEPT 135-NMR spectrum of compound **22**

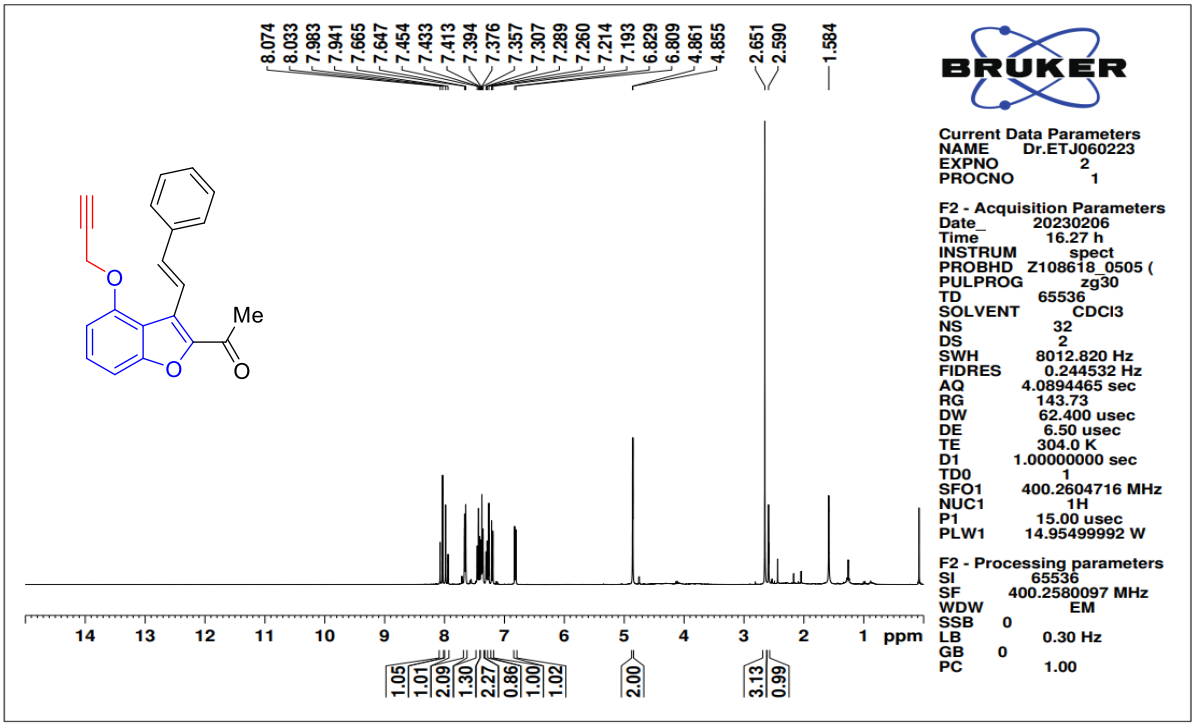


Figure 233: ^{1}H-NMR spectrum of compound **23**

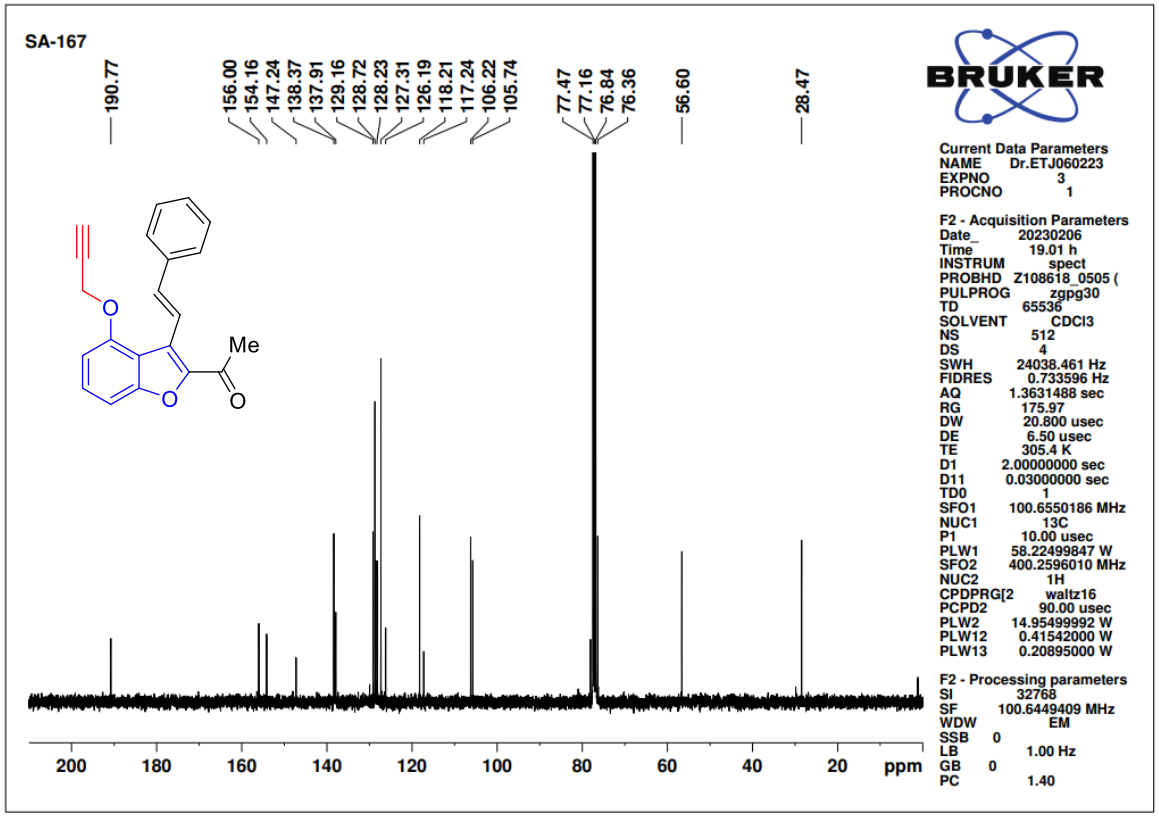


Figure 234: ^{13}C-NMR spectrum of compound **23**

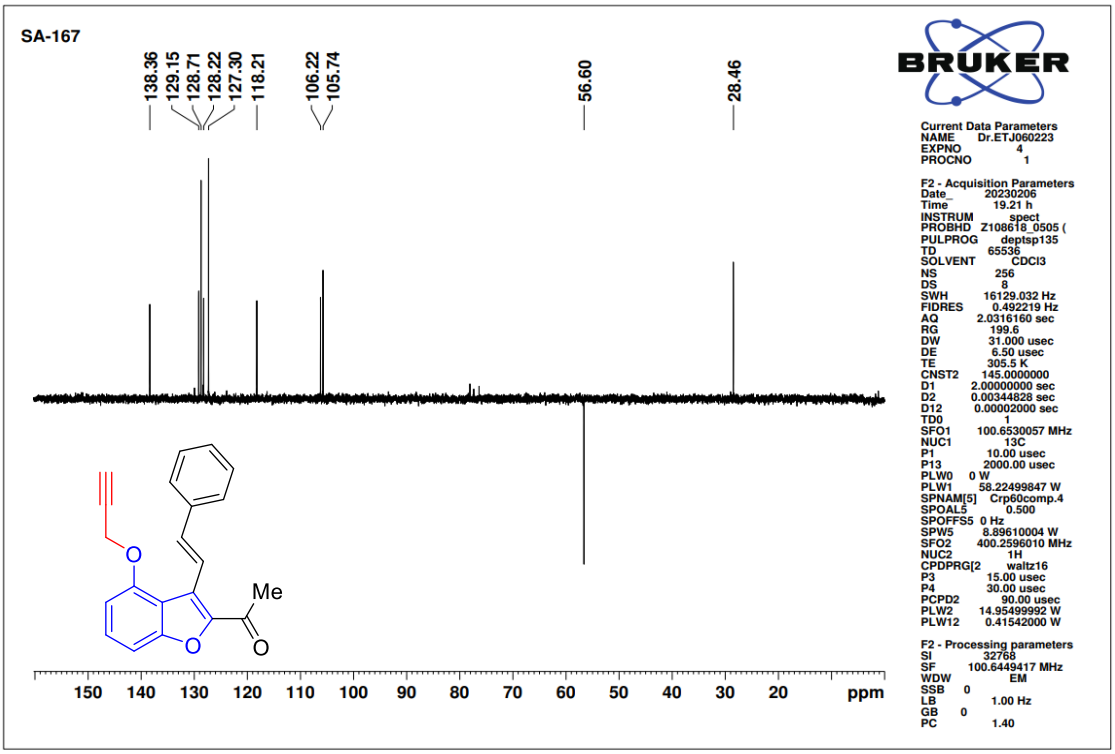


Figure 235: DEPT-135 NMR spectrum of compound **23**

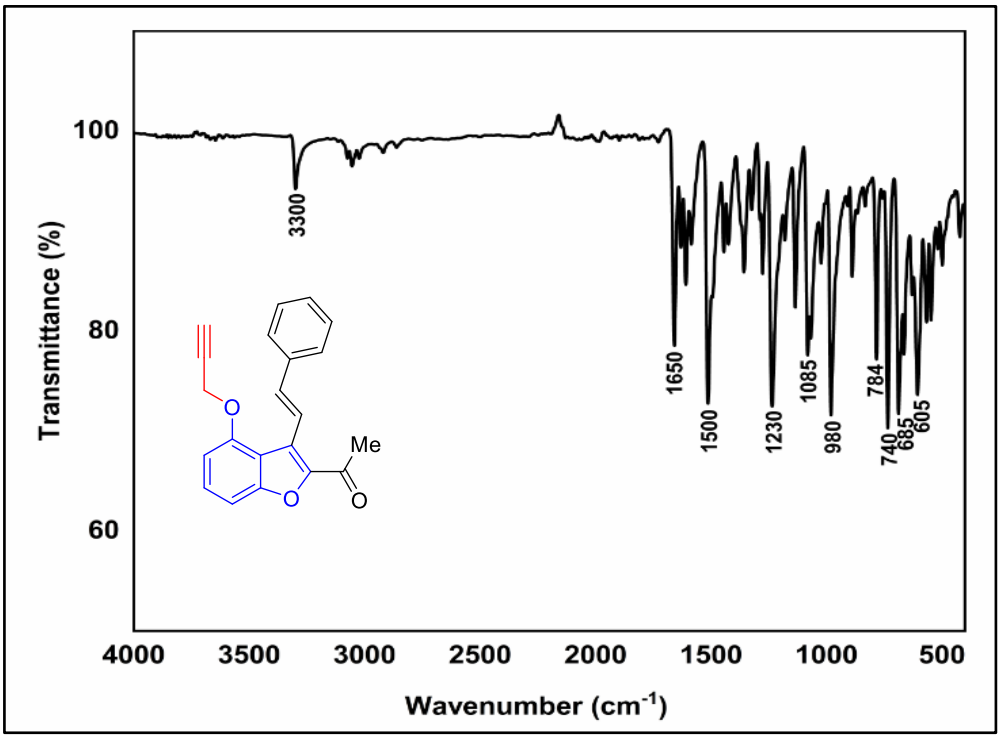


Figure 236: FT-IR spectrum of compound **23**

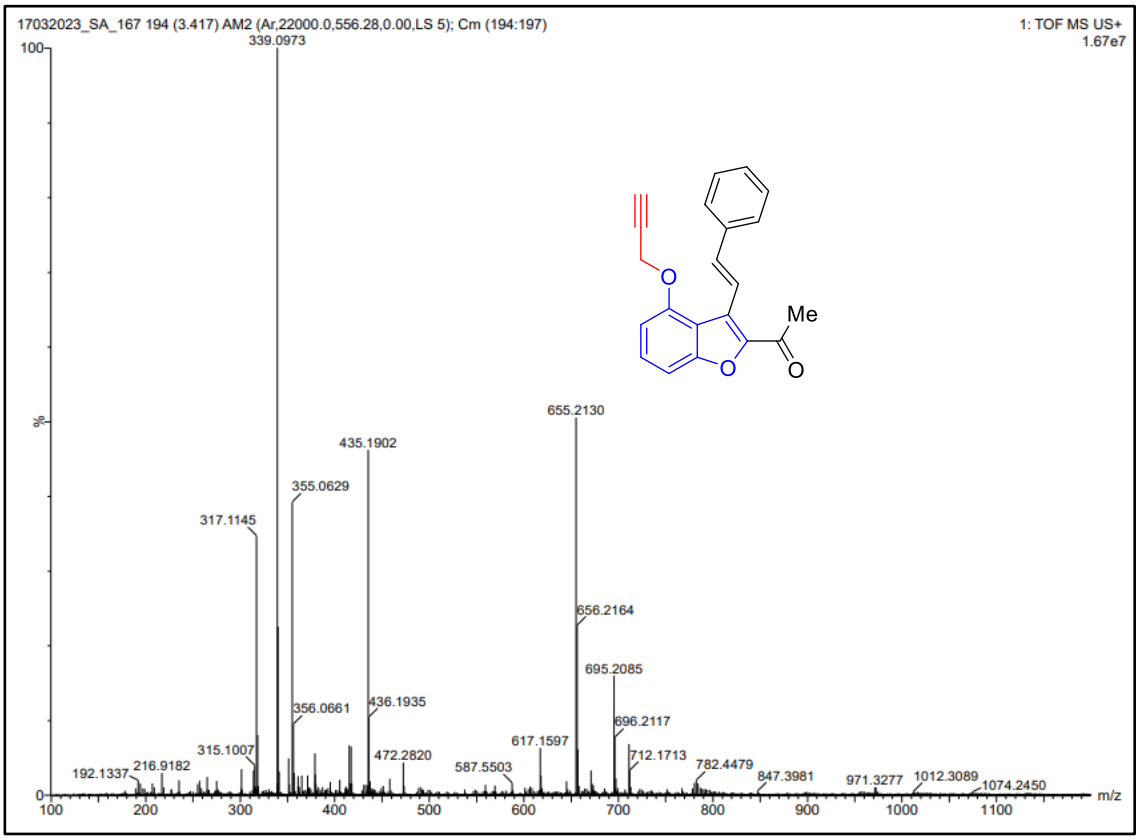


Figure 237: HRMS spectrum of compound **23**

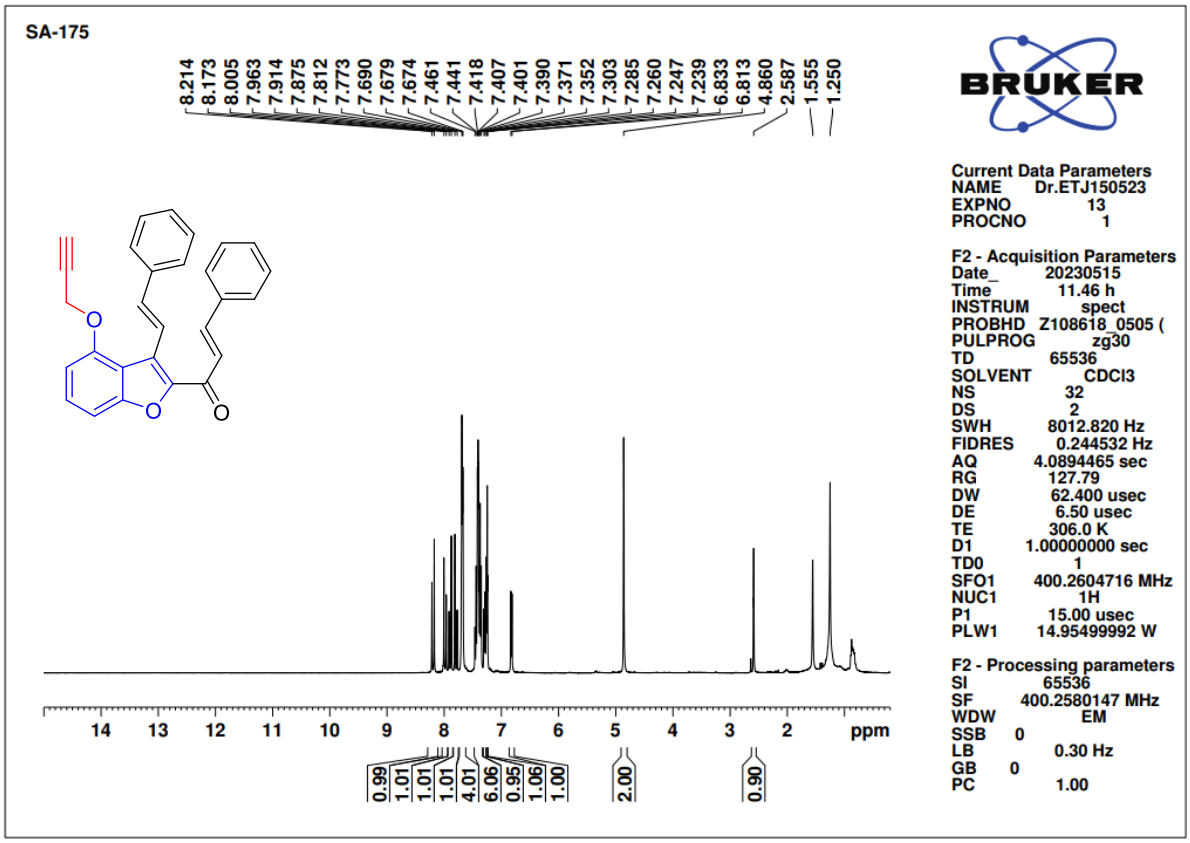


Figure 238: ^{1}H-NMR spectrum of compound **24**

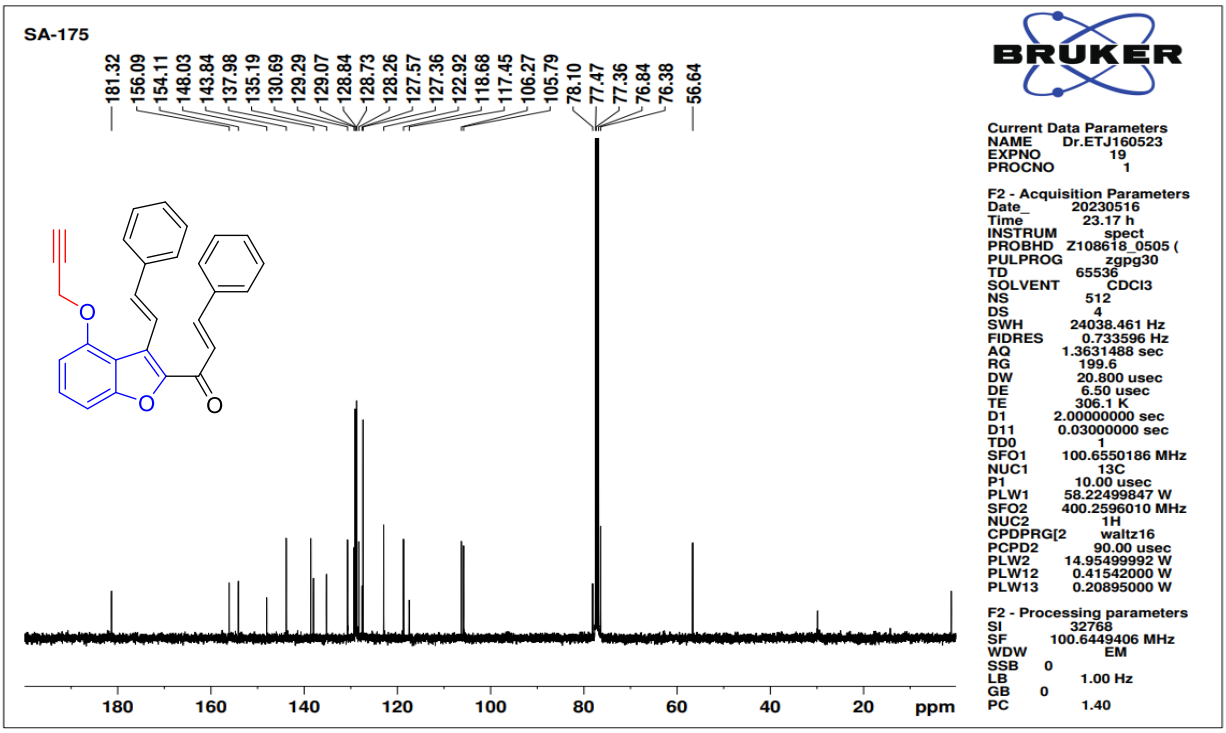


Figure 239: ^{13}C-NMR spectrum of compound **24**

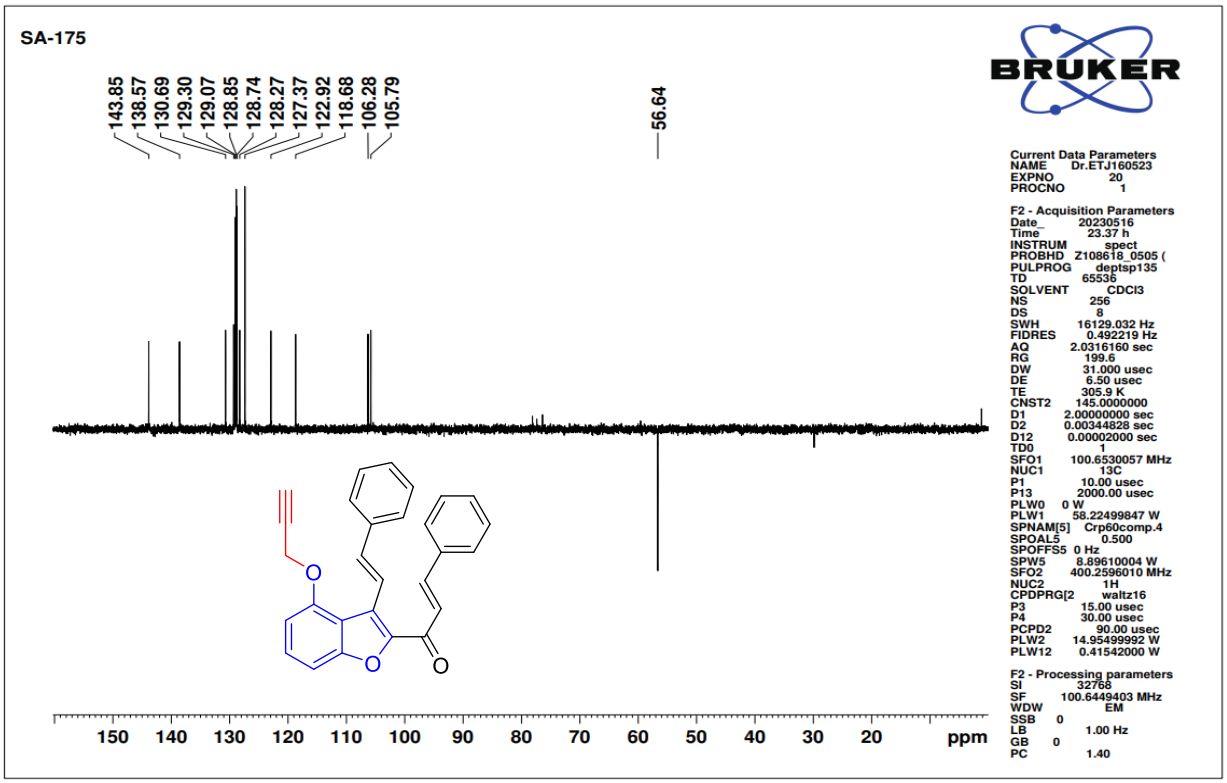


Figure 240: DEPT-135 NMR of compound **24**

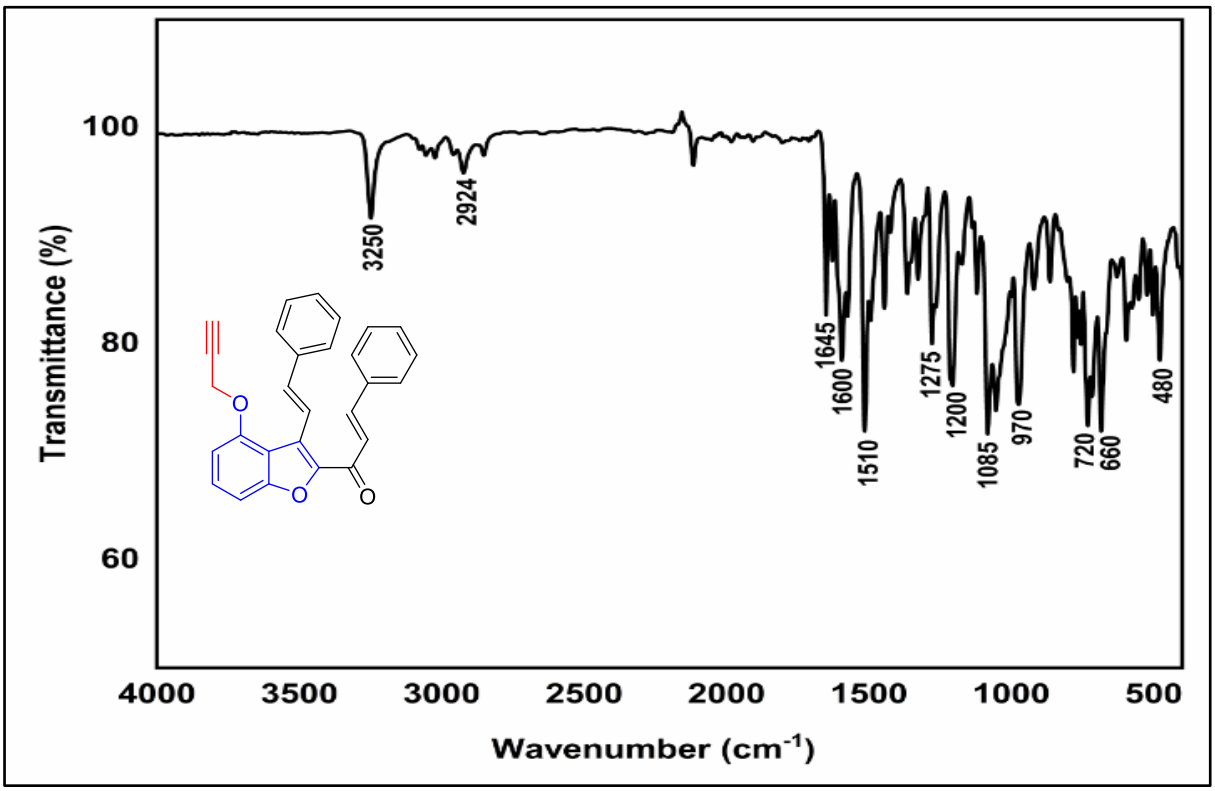


Figure 241: FT-IR spectrum of compound **24**

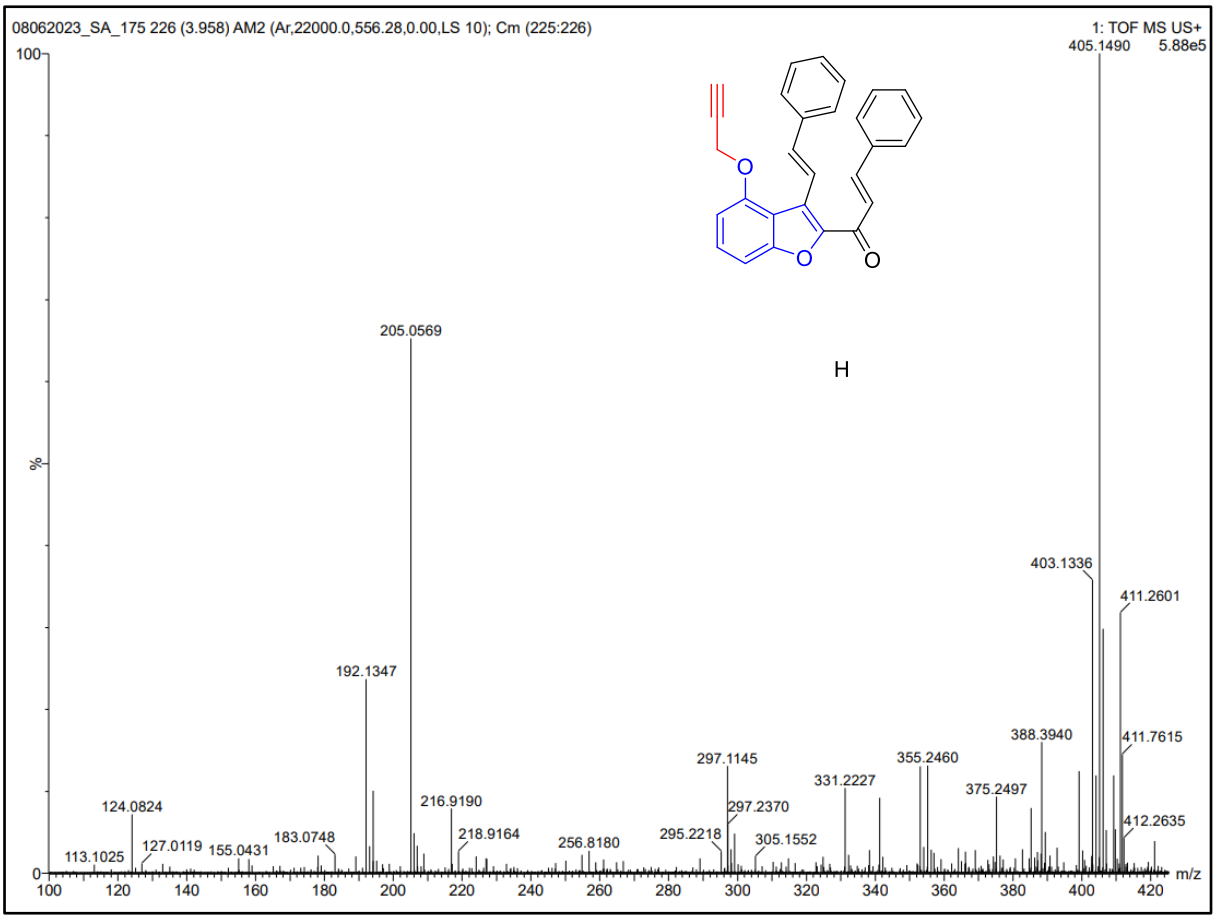


Figure 242: HRMS spectrum of compound **24**

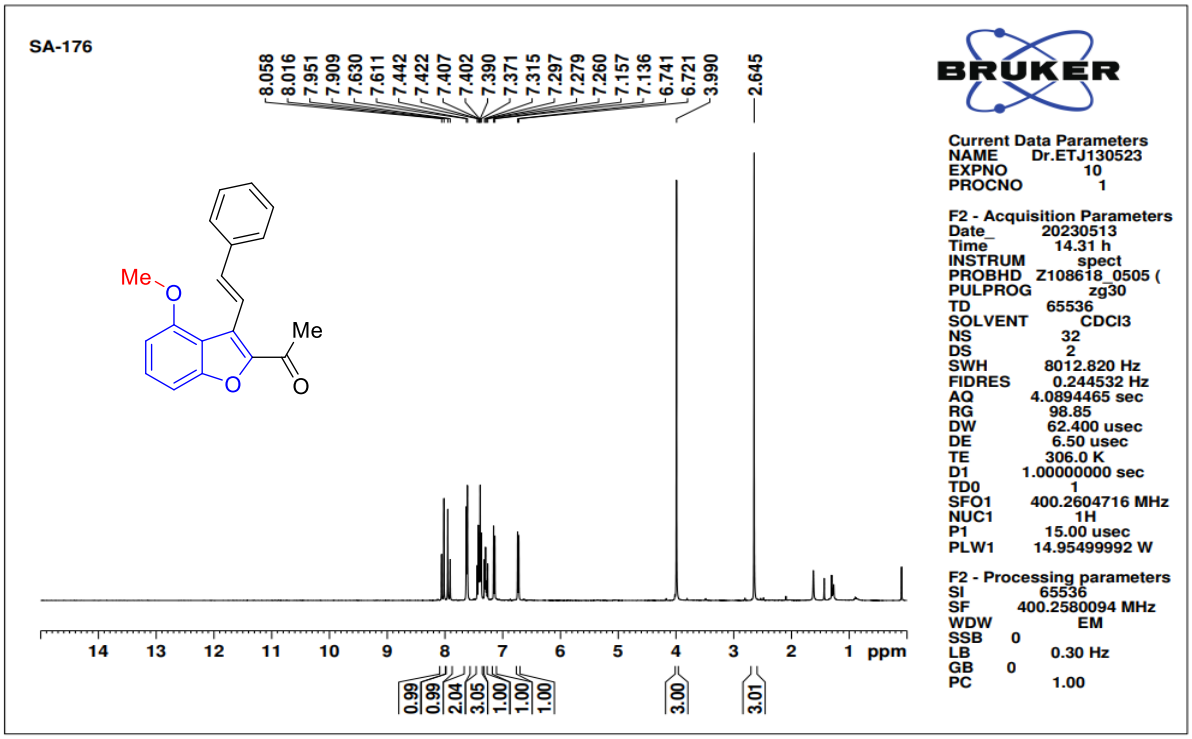


Figure 243: ^{1}H-NMR spectrum of compound **25**

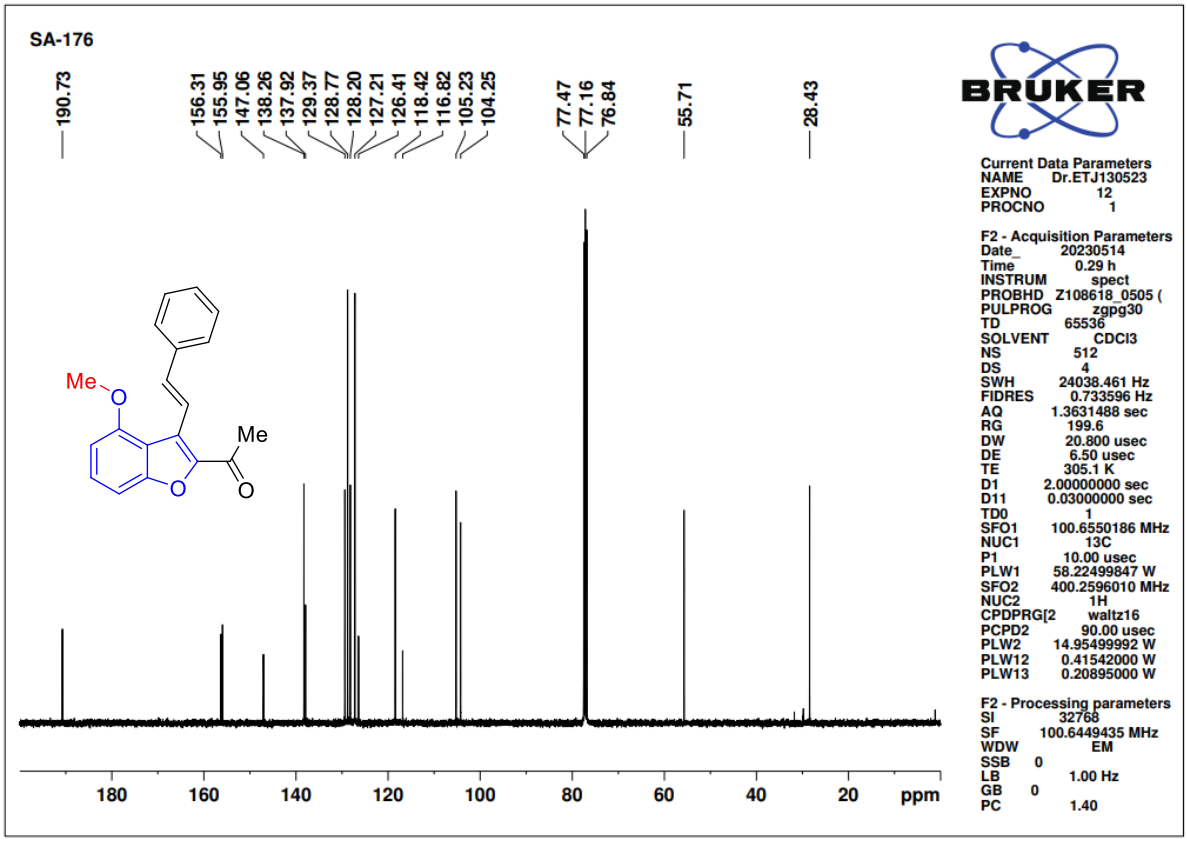


Figure 244: ^{13}C-NMR spectrum of compound **25**

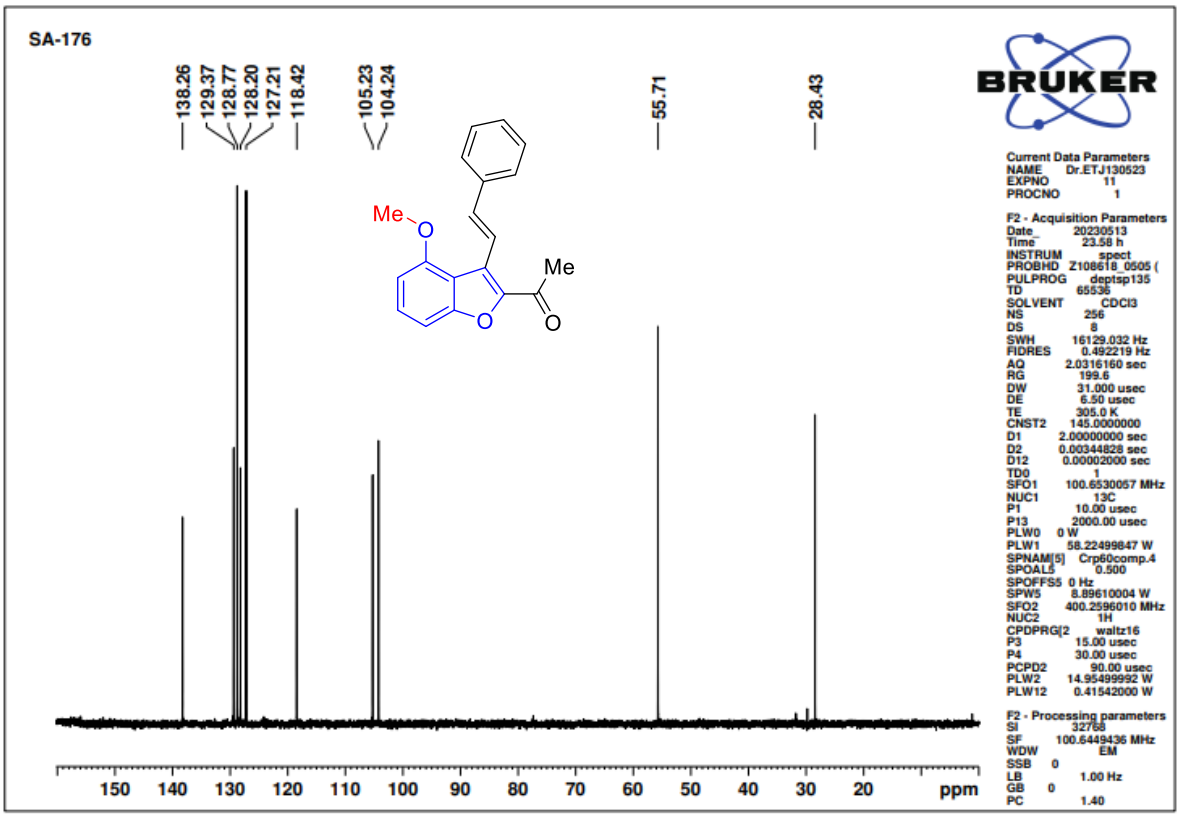


Figure 245: DEPT-135 NMR spectrum of compound **25**

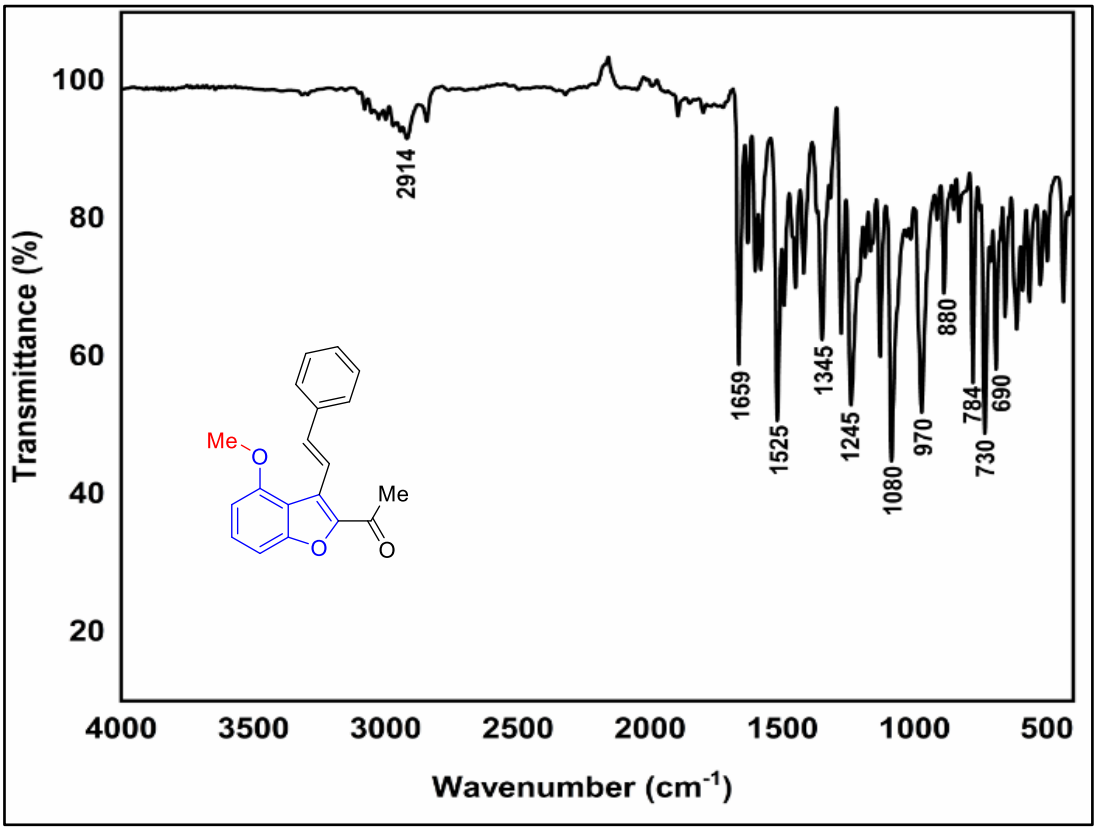


Figure 246: FT-IR spectrum of compound **25**

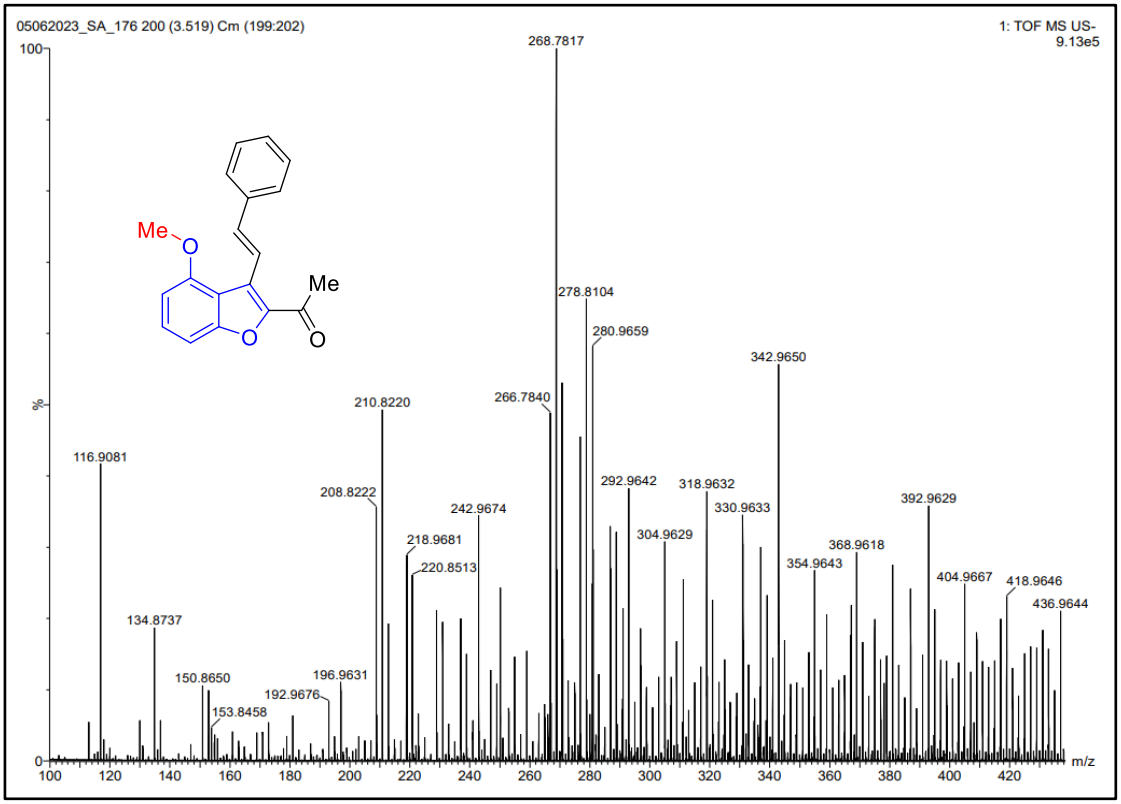


Figure 247: HRMS spectrum of compound **25**

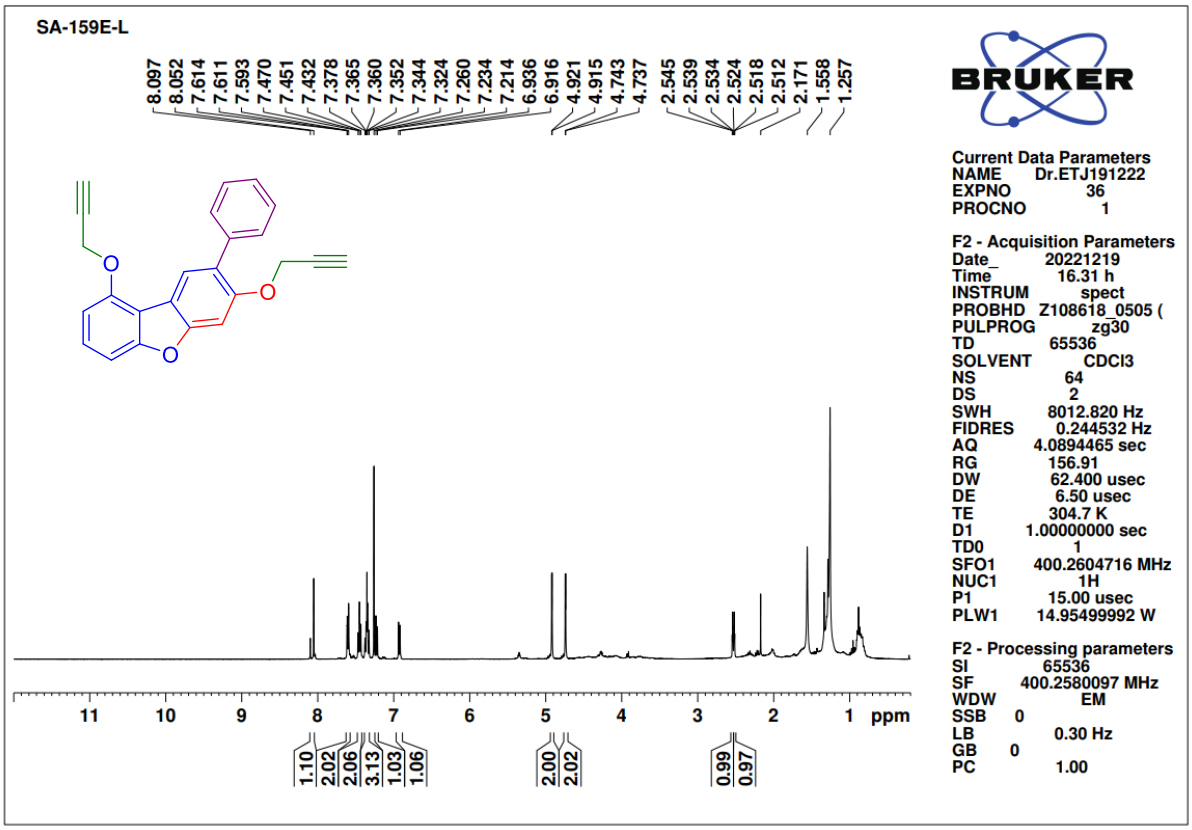


Figure 248: ^{1}H-NMR spectrum of compound **26**

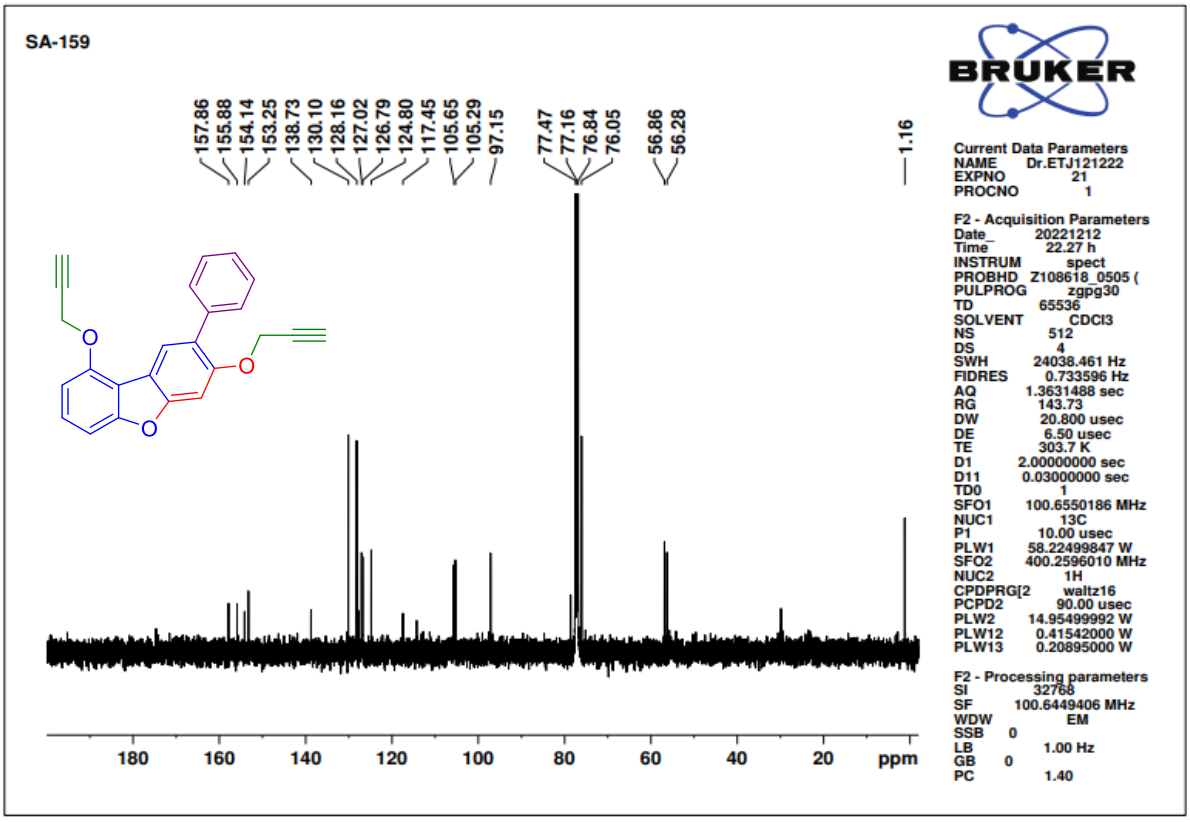


Figure 249: ^{13}C-NMR spectrum of compound **26**

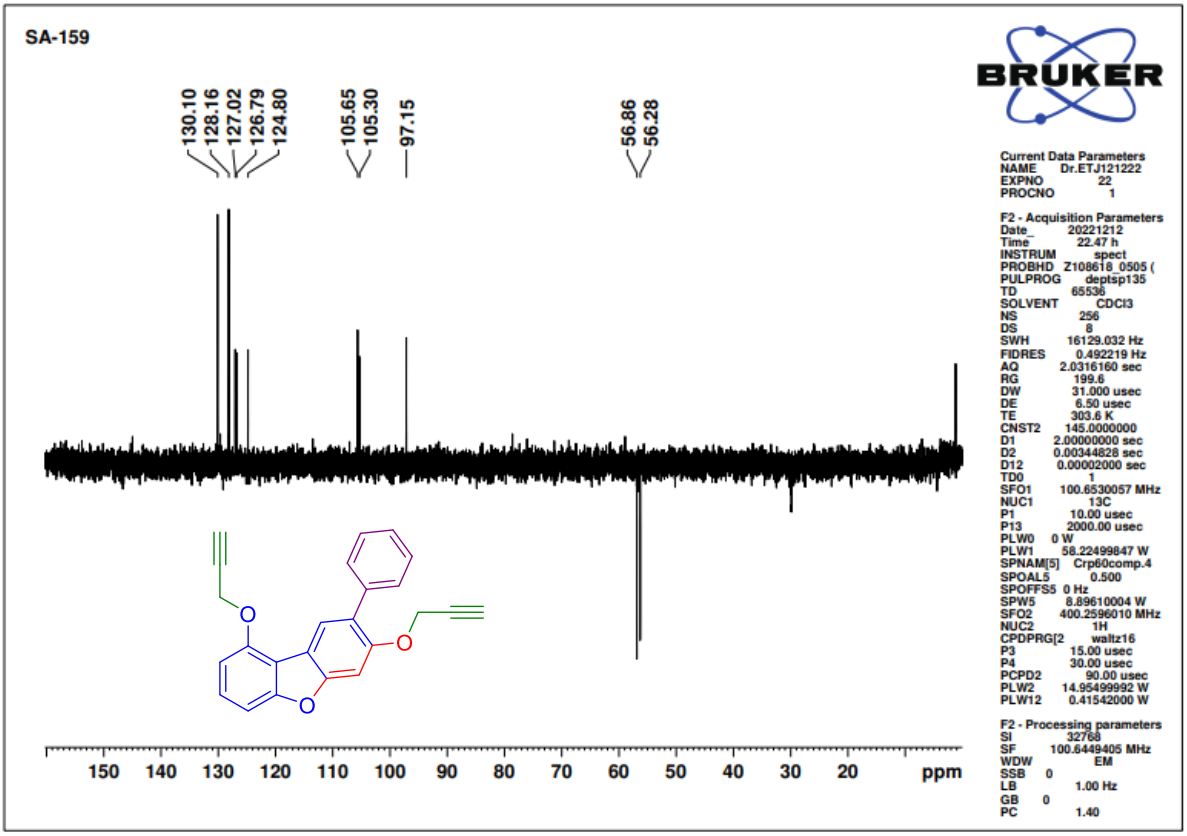


Figure 250: DEPT-135 NMR spectrum of compound **26**

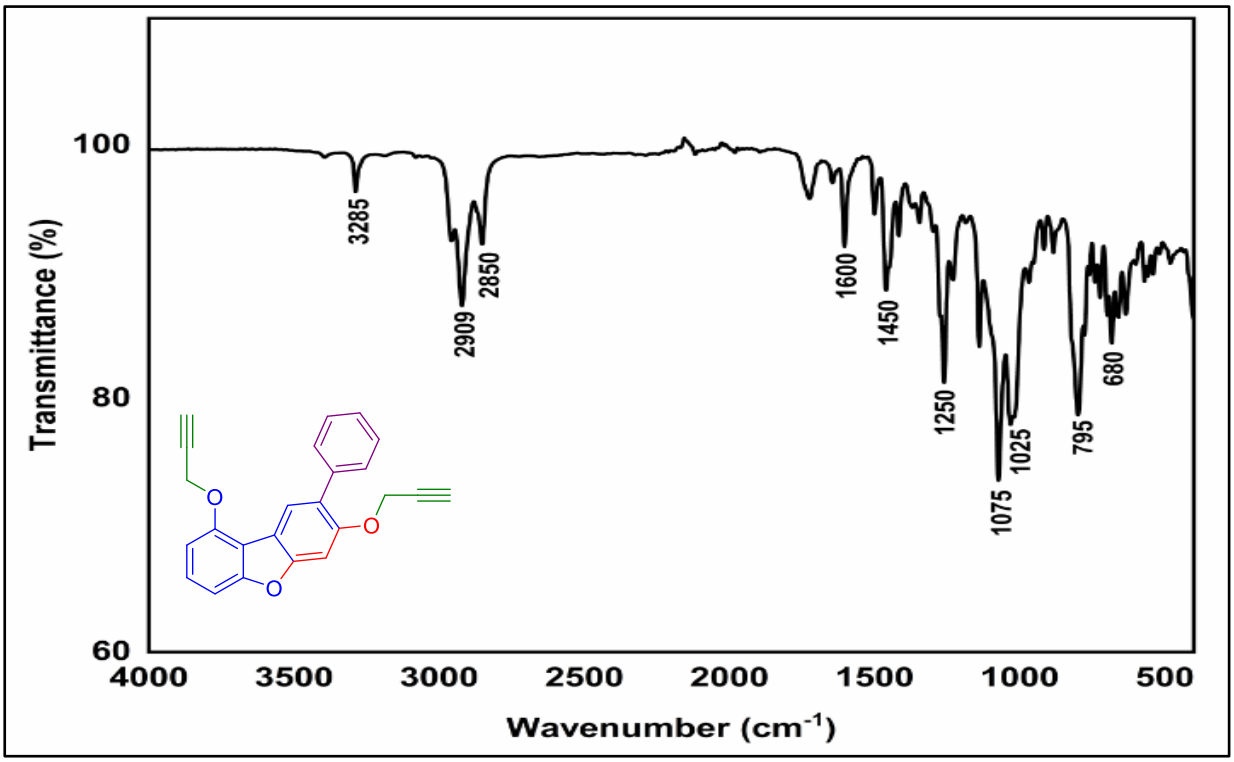


Figure 251: FT-IR spectrum of compound **26**

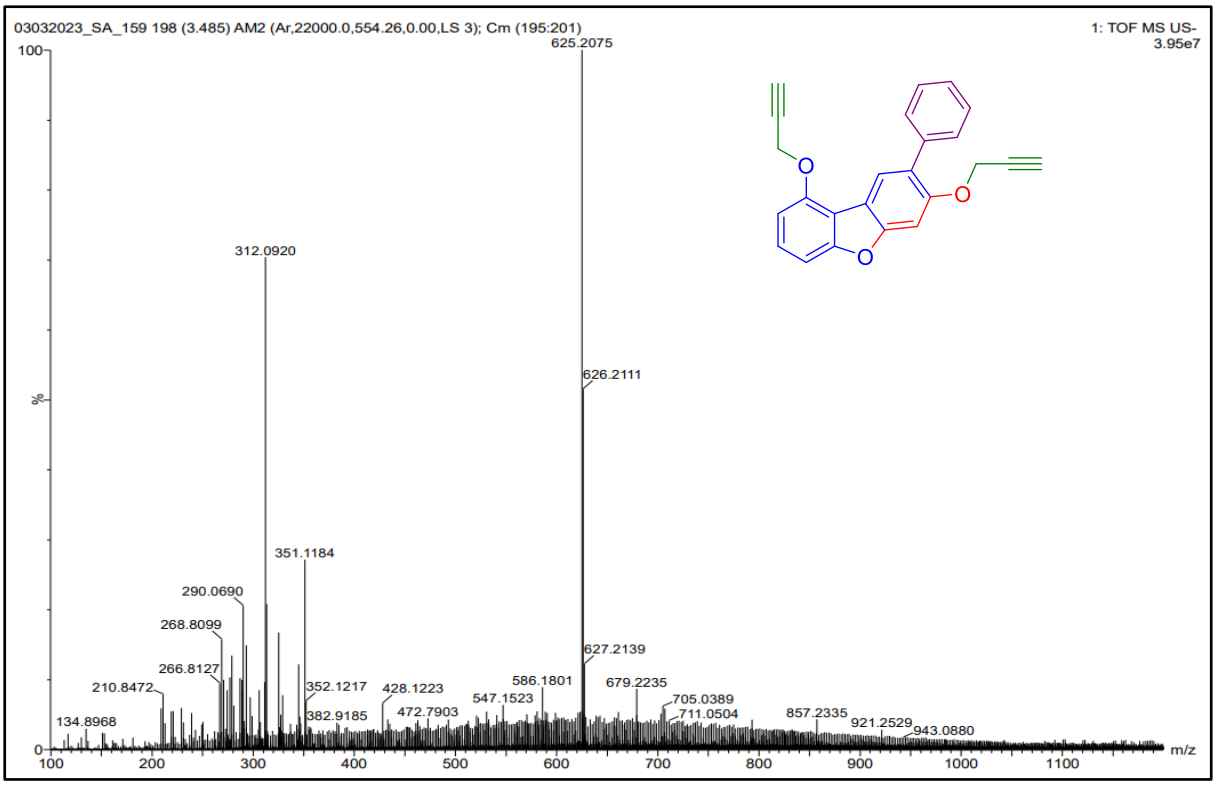


Figure 252: HRMS spectrum of compound **26**

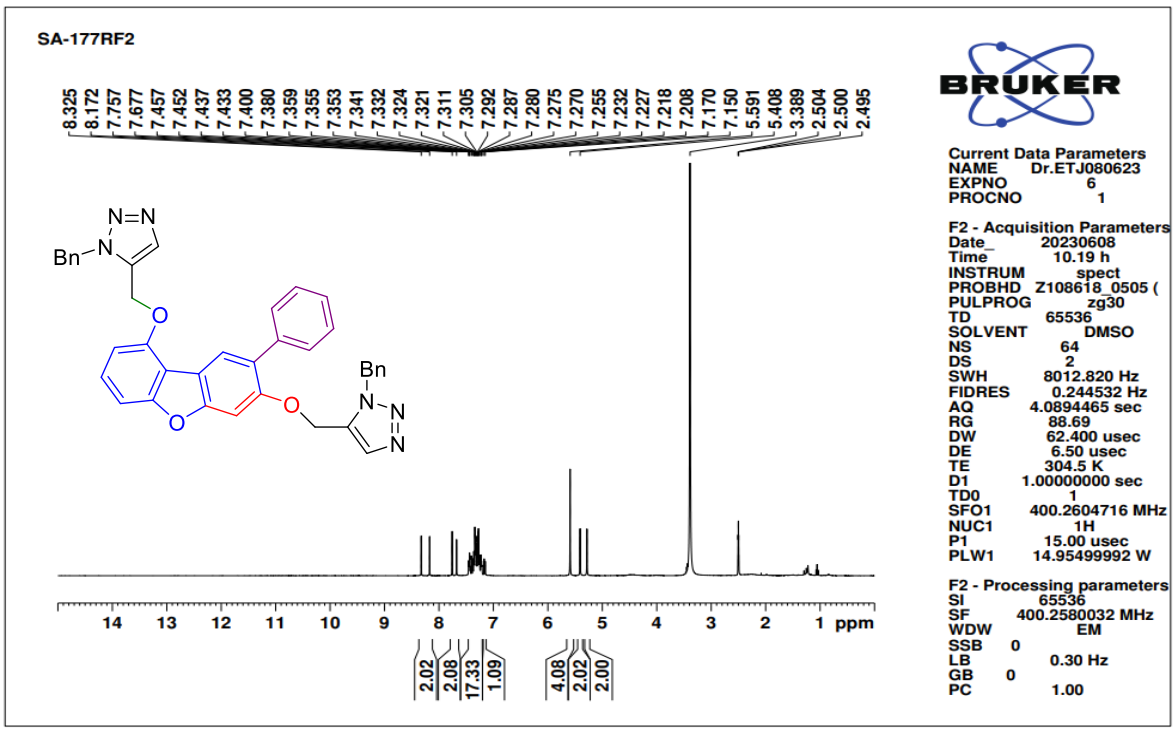


Figure 253: ^{1}H NMR spectrum of compound **27**

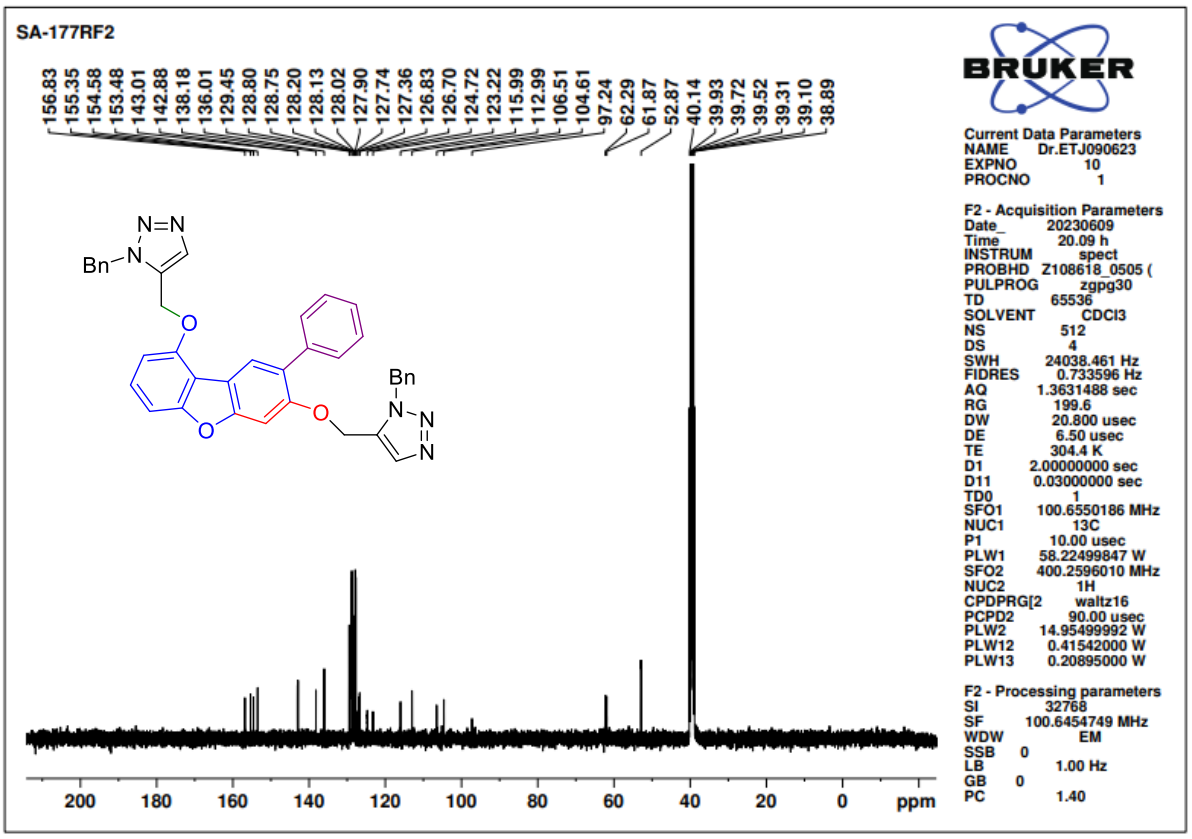


Figure 254: ^{13}C NMR spectrum of compound **27**

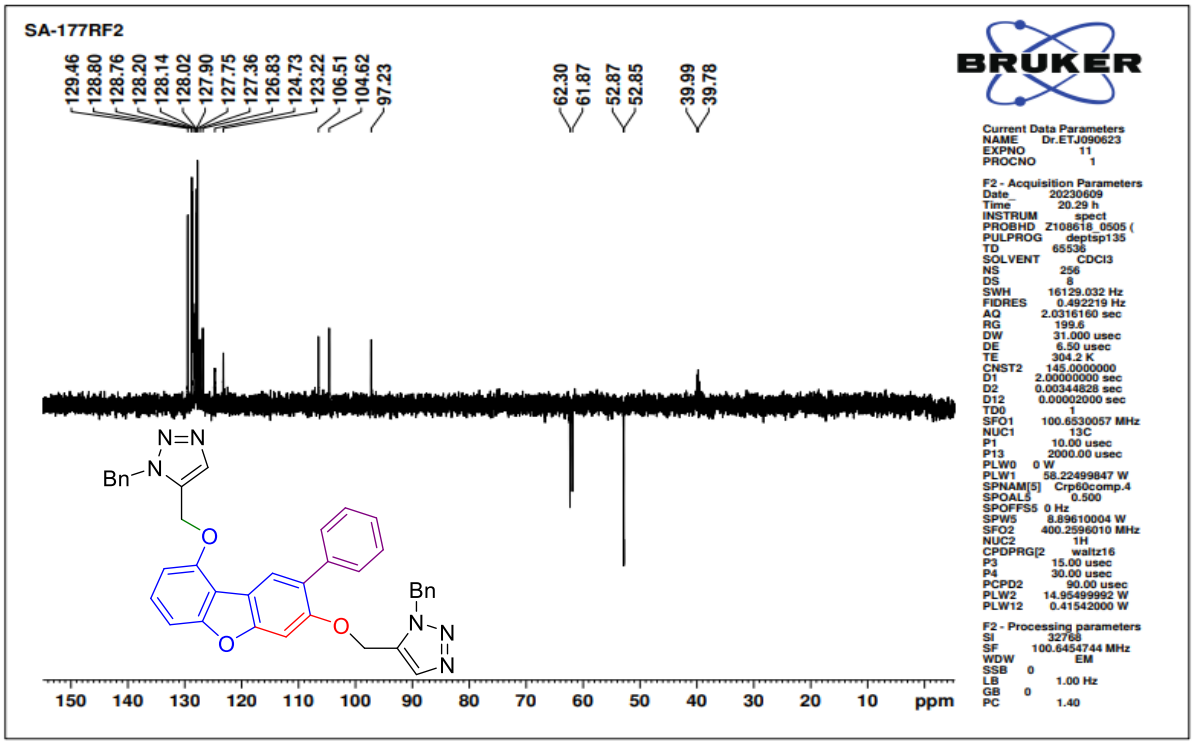


Figure 255: DEPT-135 NMR spectrum of compound **27**

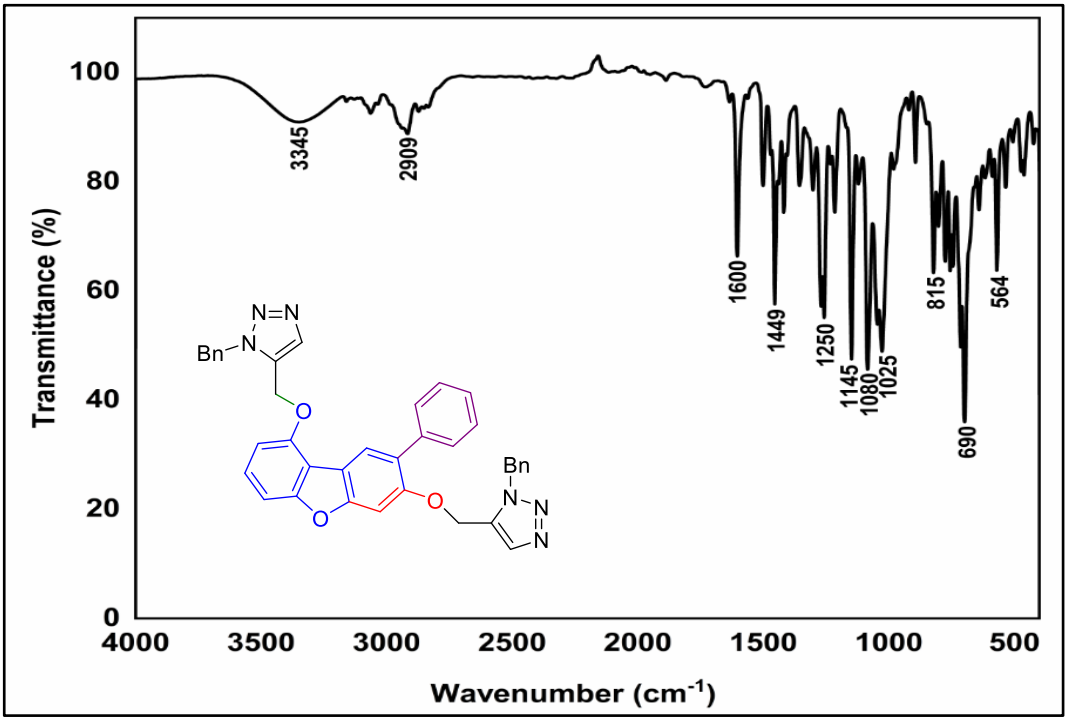


Figure 256: FT-IR spectrum of compound **27**

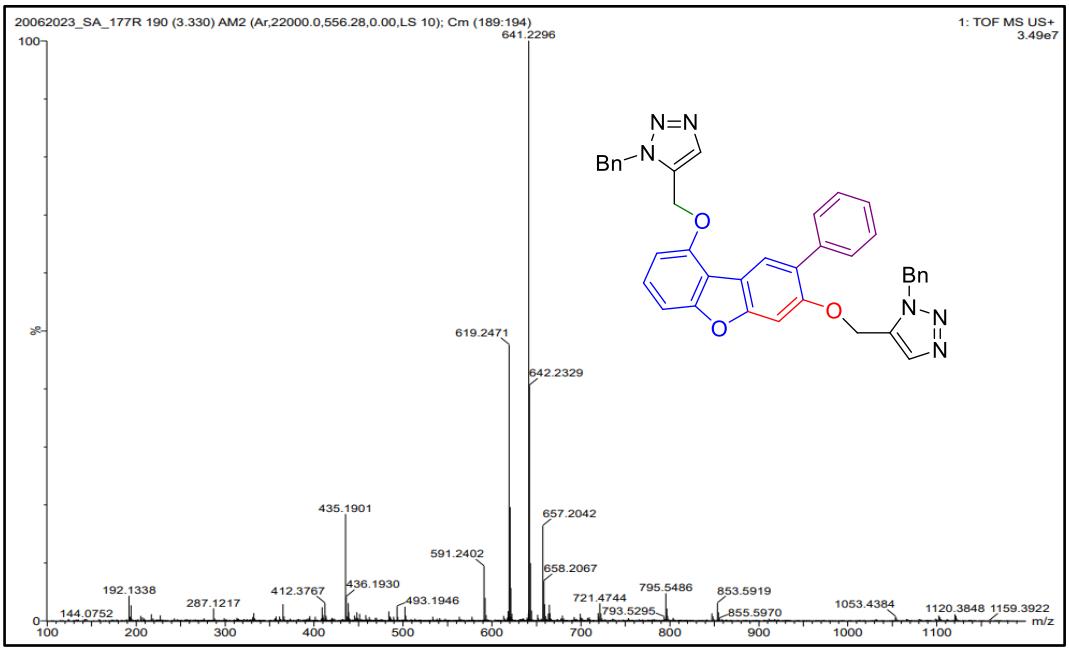


Figure 257: HRMS spectrum of compound **27**

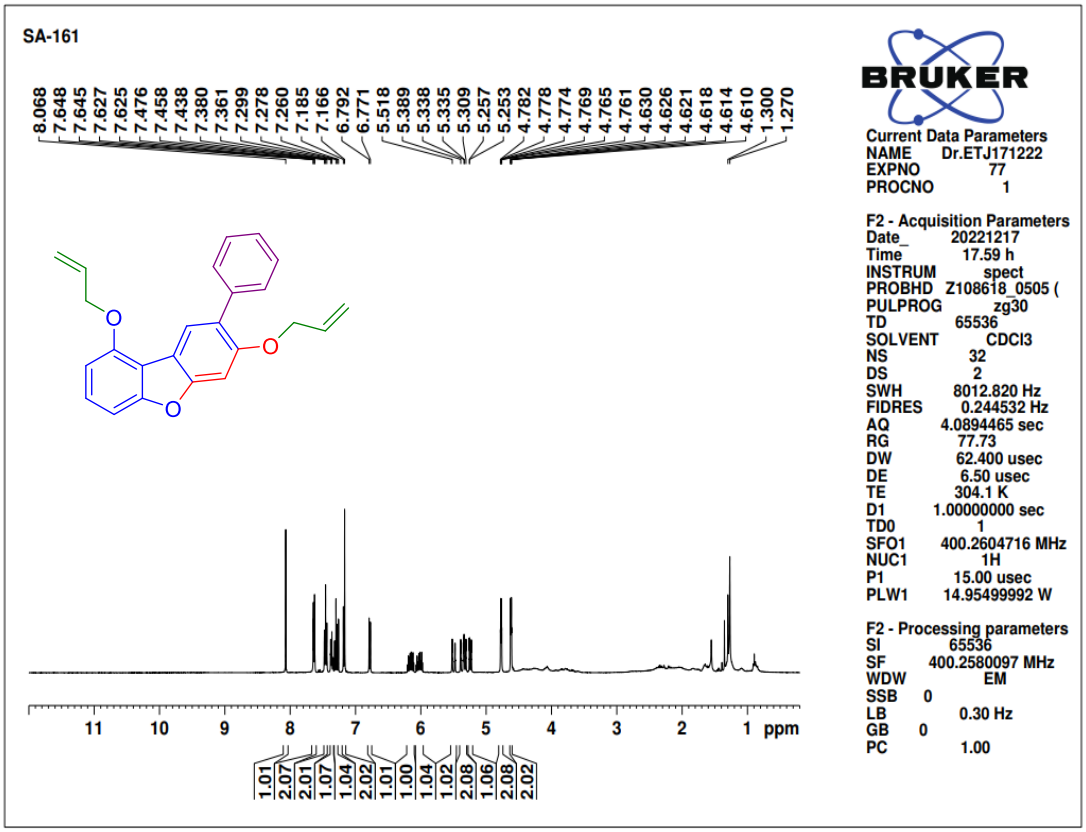


Figure 258: ^{1}H NMR spectrum of compound **28**

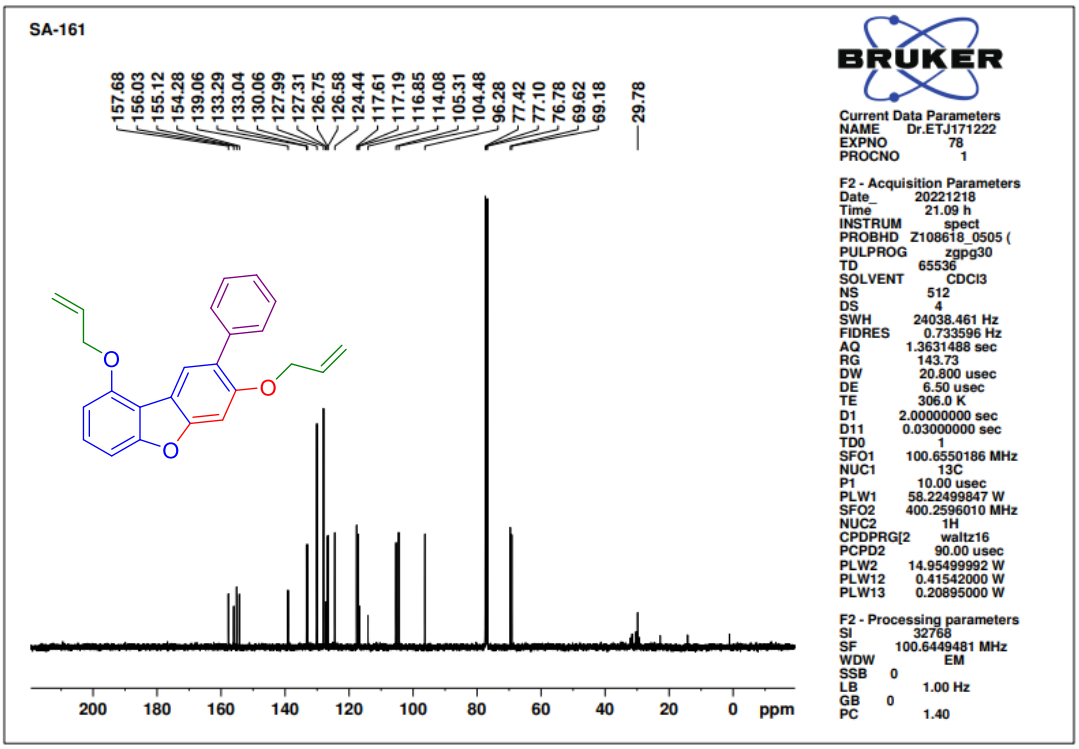


Figure 259: ^{13}C NMR spectrum of compound **28**

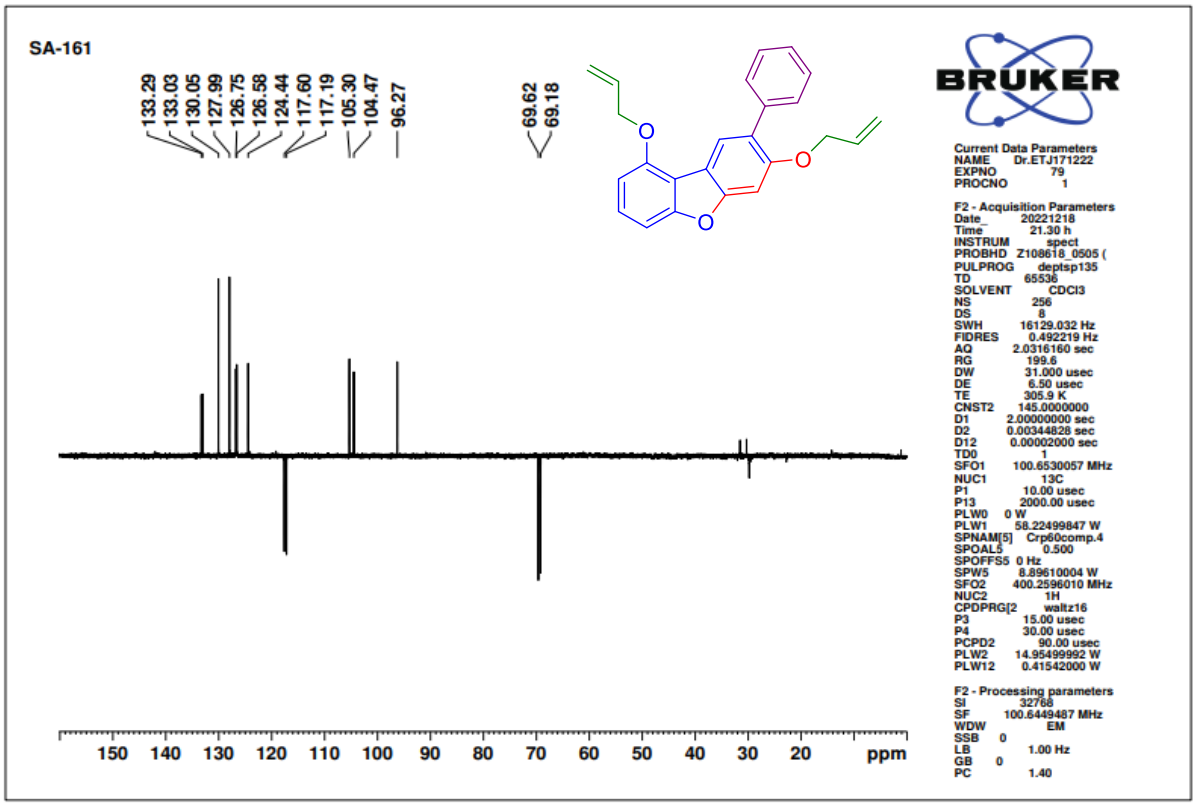


Figure 260: DEPT-135 NMR spectrum of compound **28**

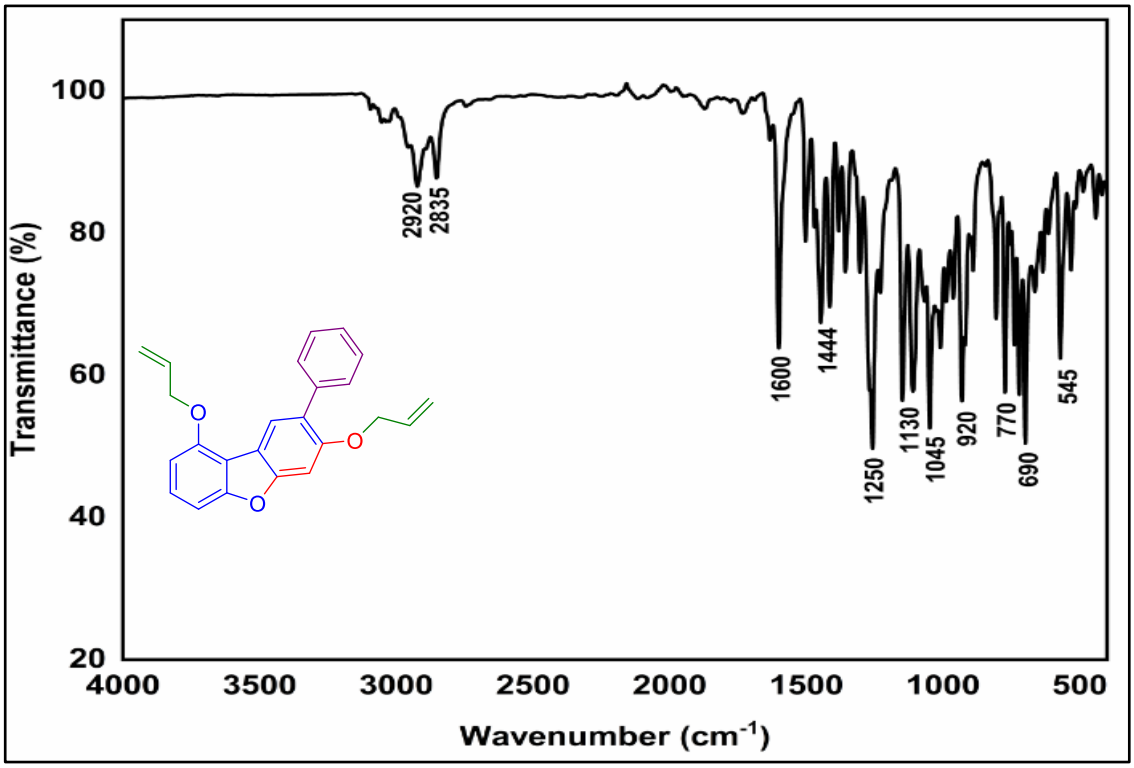


Figure 261: FT-IR spectrum of compound **28**

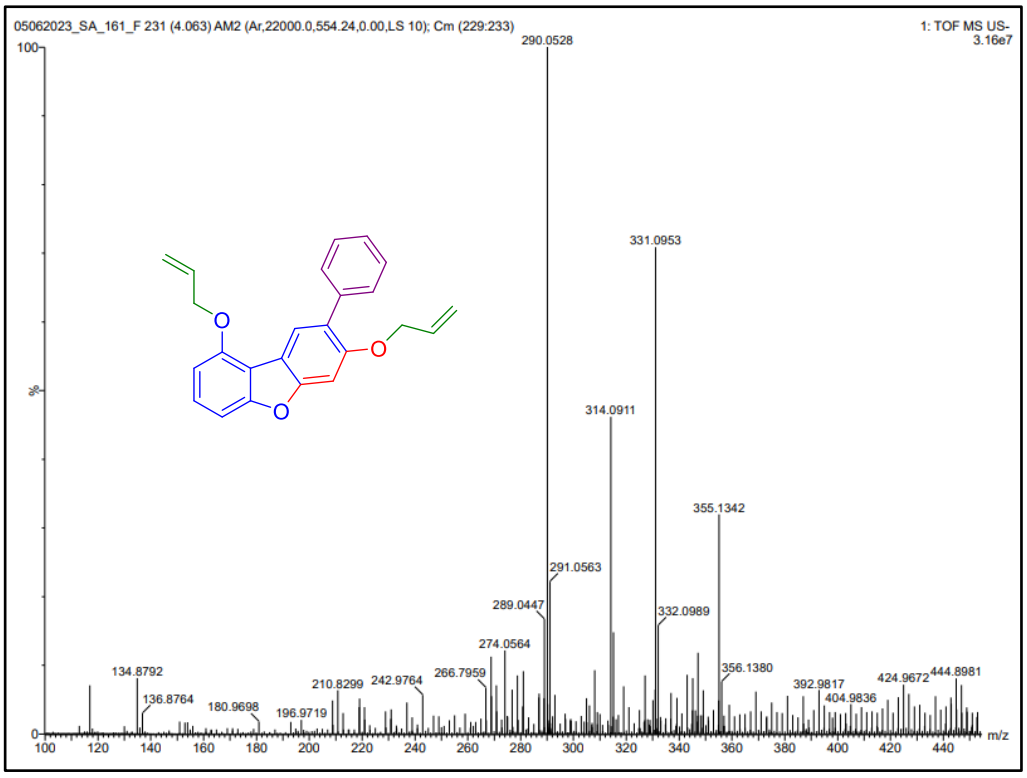


Figure 262: HRMS spectrum of compound **28**

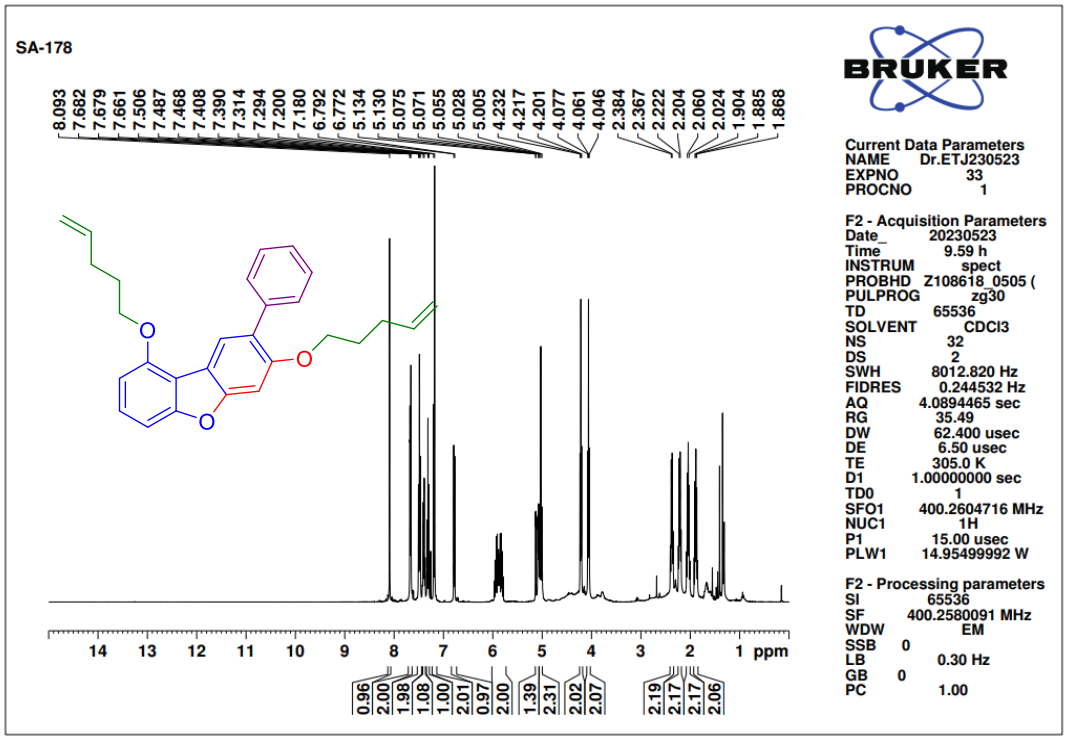


Figure 263: ^{1}H-NMR spectrum of compound **29**

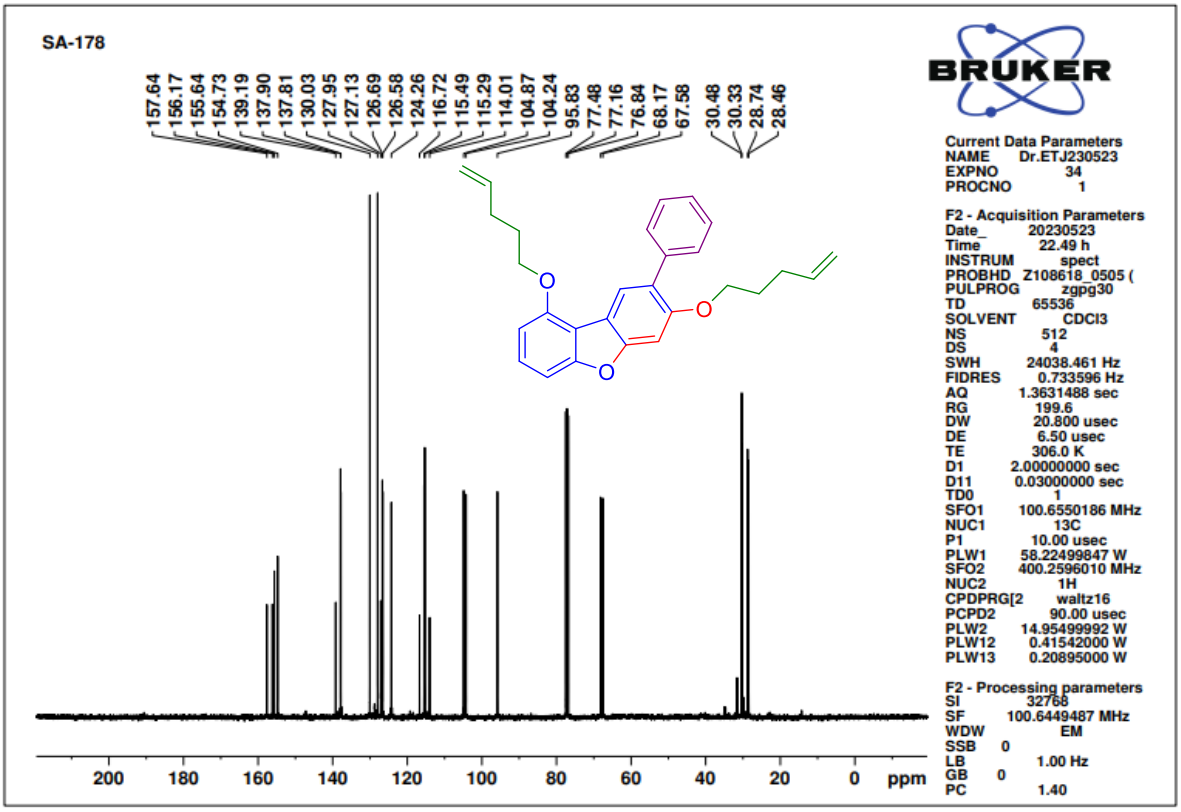


Figure 264: ^{13}C-NMR spectrum of compound **29**

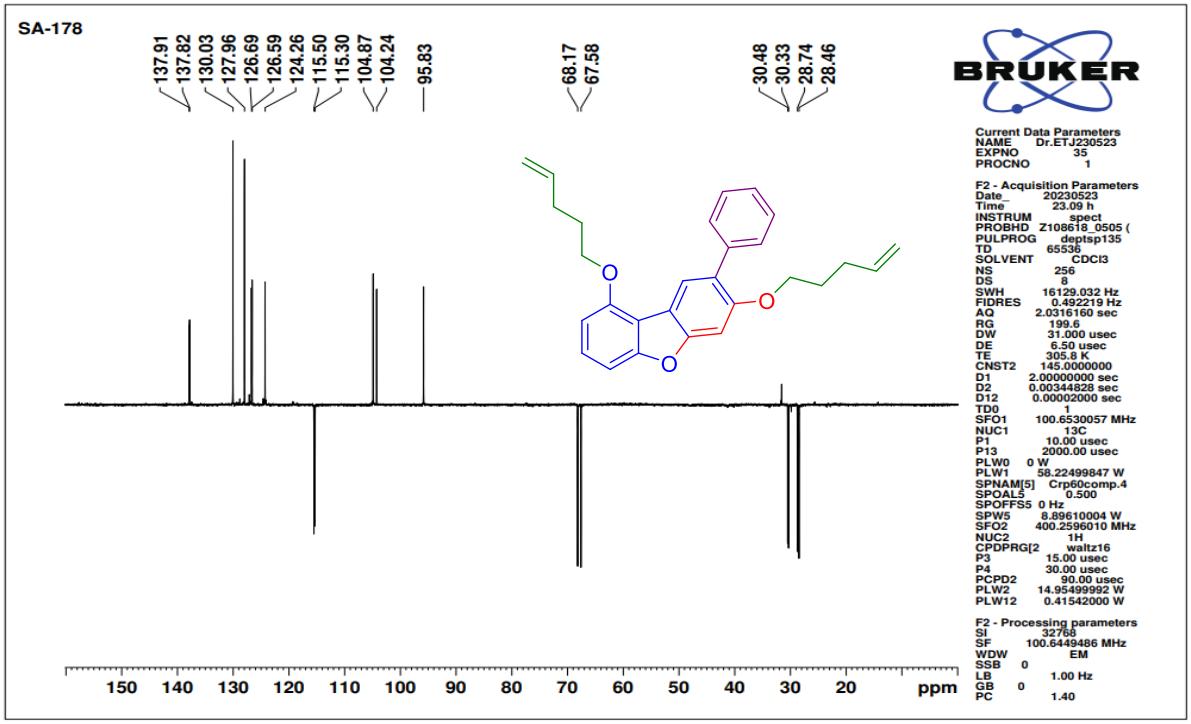


Figure 265: DEPT-135 NMR spectrum of compound **29**

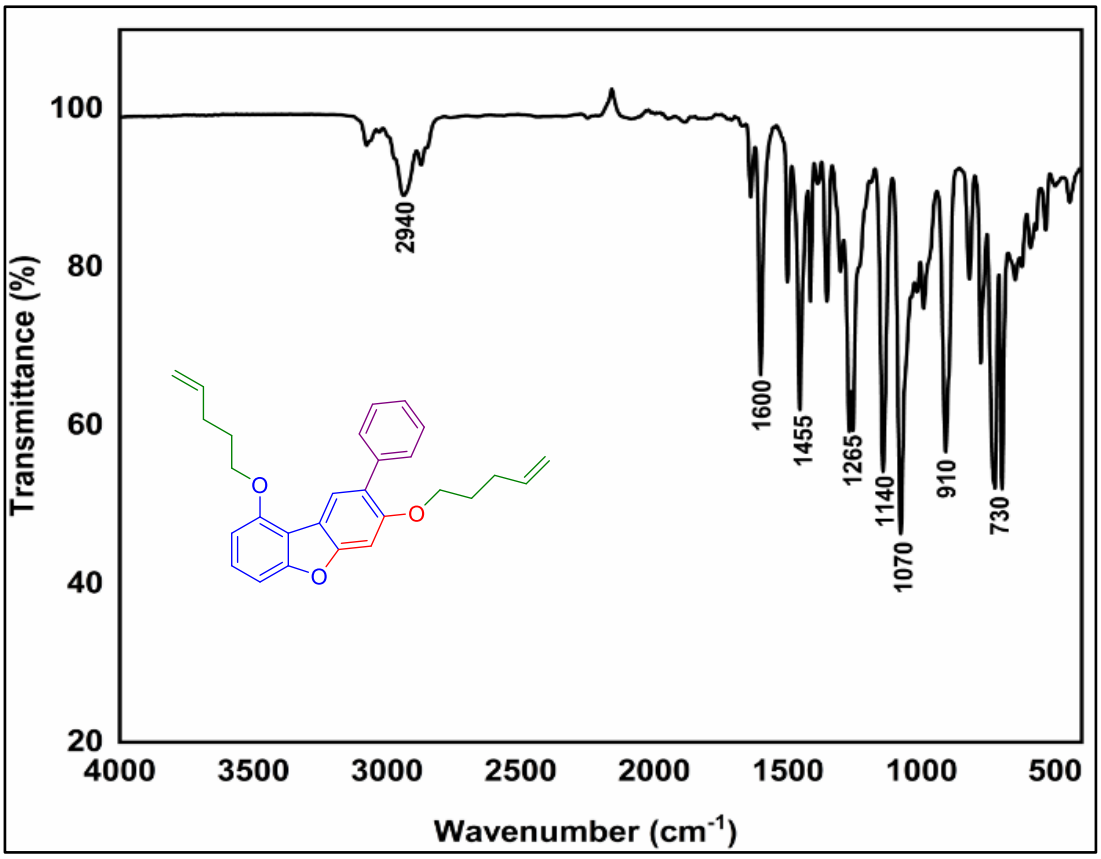


Figure 266: FT-IR spectrum of compound **29**

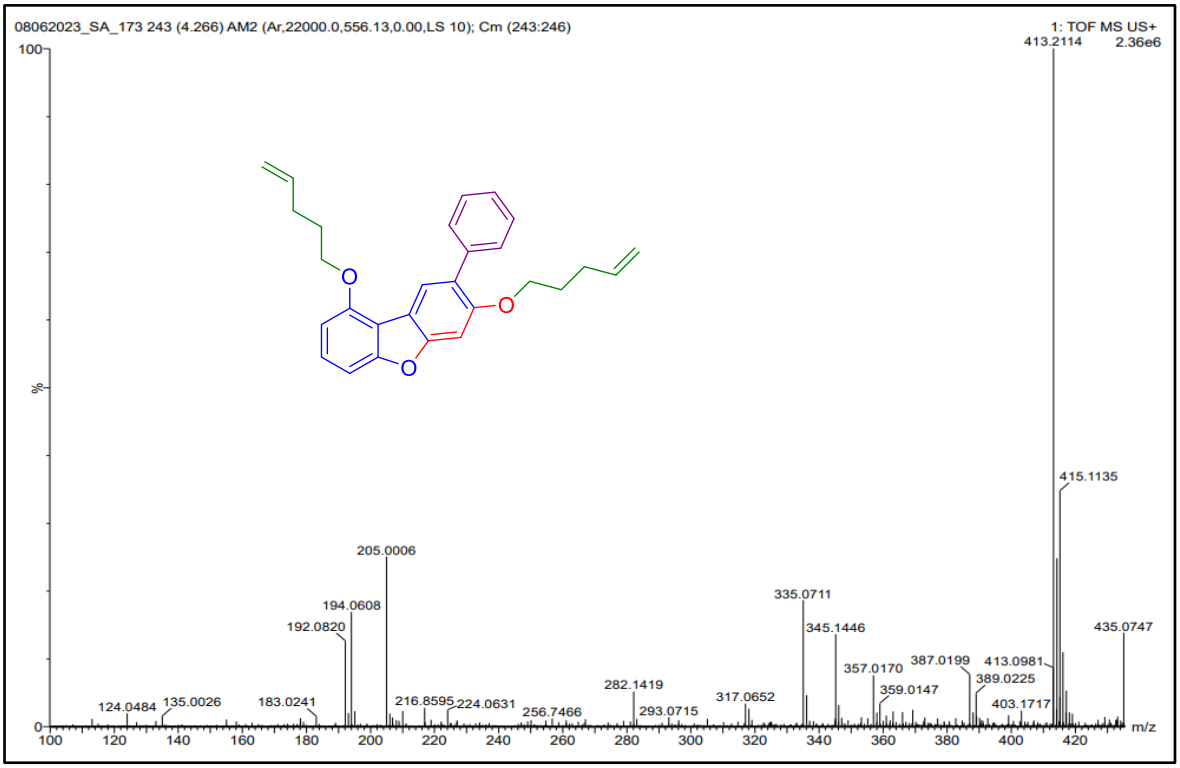
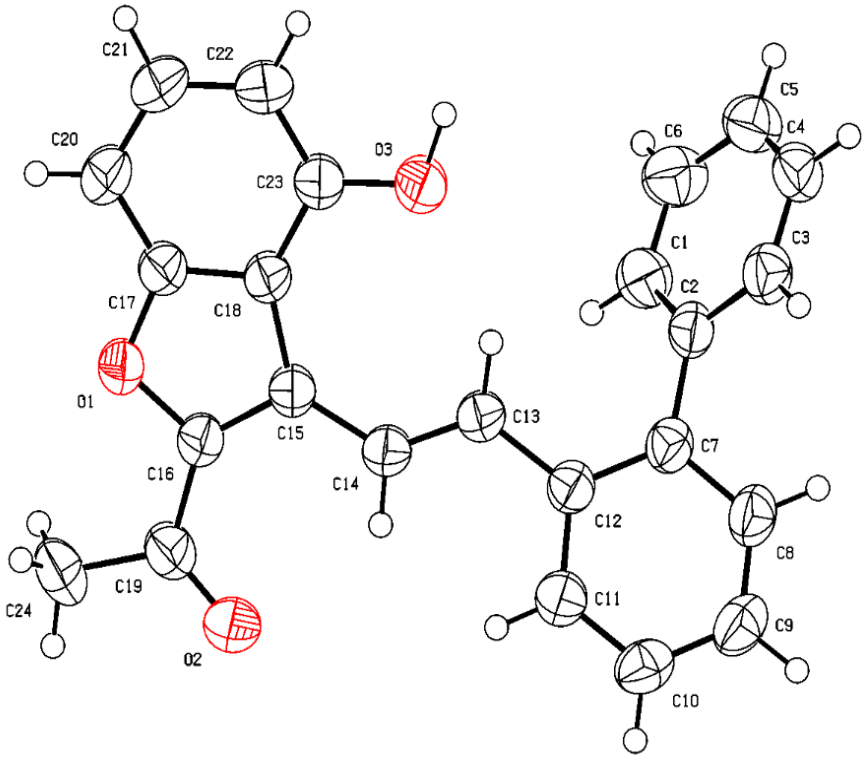


Figure 267: FT-IR spectrum of compound **29**

5. Basic crystallographic data for compounds **6f, 7d** and **23**

Crystal Structure Report for compound **6f**



CCDC NUMBER: 2266920

A specimen of $C_{24}H_{18}O_3$, approximate dimensions 0.117 mm x 0.134 mm x 0.245 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å).

The integration of the data using a monoclinic unit cell yielded a total of 26560 reflections to a maximum θ angle of 28.31° (0.75 Å resolution), of which 4550 were independent (average redundancy 5.837, completeness =99.6%, R_{int} = 4.63%, R_{sig} = 3.94%) and 2689 (59.10%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.3959(7) Å, b = 17.1806(10) Å, c = 10.1872(7) Å, β = 113.005(2)°, volume = 1835.9(2) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9800 and 0.9900.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{24}H_{18}O_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 248 variables converged at R1 = 4.90%, for the observed data and wR2 = 14.08% for all data. The goodness-of-fit was 1.024. The largest peak in the final difference electron density synthesis was 0.138 $e^-/Å^3$and the largest hole was -0.199 $e^-/Å^3$ with an RMS deviation of 0.036 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.282 g/cm^3 and F(000), 744 e^-.

Table 1. Sample and crystal data for compound **6f.**

Identification code	SA151BF1RE	
Chemical formula	$C_{24}H_{18}O_3$	
Formula weight	354.38 g/mol	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal size	0.117 x 0.134 x 0.245 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 11.3959(7) Å	α = 90°
	b = 17.1806(10) Å	β = 113.005(2) °
	c = 10.1872(7) Å	γ = 90°
Volume	1835.9(2) $Å^3$	
Z	4	
Density (calculated)	1.282 g/cm^3	
Absorption coefficient	0.084 mm^{-1}	
F (000)	744	

Table 2. Data collection and structure refinement for compound **6f.**

Theta range for data collection	2.27 to 28.31°

Index ranges	-15<=h<=13, -22<=k<=20, -13<=l<=13
Reflections collected	26560
Independent reflections	4550 [R(int) = 0.0463]
Max. and min. transmission	0.9900 and 0.9800
Structure solution technique	direct methods
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	Σ w $(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4550 / 0 / 248
Goodness-of-fit on F^2	1.024
Final R indices	2689 data; I>2σ(I) R1 = 0.0490, wR2 = 0.1070
	all data R1 = 0.1001, wR2 = 0.1408
Weighting scheme	$w=1/[\sigma^2(F_o^2) +(0.0508P)^2+0.5371P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.138 and -0.199 eÅ^{-3}
R.M.S. deviation from mean	0.036 eÅ^{-3}

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for compound **6f.**

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.69410(11)	0.47727(7)	0.02448(13)	0.0542(3)
O2	0.58927(15)	0.32554(8)	0.77378(16)	0.0793(5)
O3	0.42273(15)	0.66664(8)	0.73465(15)	0.0774(5)
C1	0.08381(19)	0.58691(11)	0.5324(2)	0.0591(5)
C2	0.09743(16)	0.58935(10)	0.40268(17)	0.0468(4)
C3	0.04860(17)	0.65399(11)	0.31615(19)	0.0547(5)
C4	0.98571(18)	0.71206(11)	0.3553(2)	0.0600(5)
C5	0.97018(19)	0.70742(12)	0.4817(2)	0.0644(5)
C6	0.0208(2)	0.64521(13)	0.5706(2)	0.0695(6)
C7	0.14954(17)	0.52239(10)	0.34976(17)	0.0461(4)
C8	0.07439(19)	0.49328(11)	0.21497(18)	0.0559(5)
C9	0.1104(2)	0.42890(11)	0.15928(19)	0.0591(5)
C10	0.22325(19)	0.39188(11)	0.23783(19)	0.0553(5)
C11	0.29945(18)	0.41996(10)	0.37068(19)	0.0523(5)
C12	0.26556(16)	0.48535(10)	0.43014(17)	0.0446(4)
C13	0.35151(16)	0.51548(10)	0.56966(18)	0.0480(4)
C14	0.44184(17)	0.47374(10)	0.66663(18)	0.0504(4)
C15	0.53316(16)	0.49601(9)	0.80636(18)	0.0453(4)
C16	0.61872(16)	0.44379(10)	0.89579(18)	0.0496(4)
C17	0.65652(16)	0.55296(10)	0.01675(19)	0.0493(4)
C18	0.55830(16)	0.56871(9)	0.88538(18)	0.0451(4)
C19	0.64560(19)	0.36197(11)	0.8837(2)	0.0610(5)
C20	0.71226(19)	0.60572(12)	0.1253(2)	0.0633(5)
C21	0.6658(2)	0.67976(12)	0.0982(2)	0.0745(6)
C22	0.5693(2)	0.69990(12)	0.9688(2)	0.0709(6)
C23	0.51522(18)	0.64612(10)	0.8618(2)	0.0563(5)
C24	0.7445(2)	0.32347(13)	0.0100(3)	0.0898(8)

Table 4. Bond lengths (Å) for compound **6f.**

O1-C17	1.362(2)	O1-C16	1.381(2)
O2-C19	1.223(2)	O3-C23	1.358(2)
O3-H1B	0.98(3)	C1-C6	1.375(3)
C1-C2	1.390(3)	C1-H1	0.930000
C2-C3	1.392(2)	C2-C7	1.489(2)
C3-C4	1.375(3)	C3-H3	0.930000
C4-C5	1.369(3)	C4-H4	0.930000
C5-C6	1.374(3)	C5-H5	0.930000
C6-H6	0.930000	C7-C8	1.396(2)
C7-C12	1.406(2)	C8-C9	1.377(3)
C8-H8	0.930000	C9-C10	1.377(3)
C9-H9	0.930000	C10-C11	1.378(2)
C10-H10	0.930000	C11-C12	1.400(2)
C11-H11	0.930000	C12-C13	1.469(2)
C13-C14	1.325(2)	C13-H13	0.930000
C14-C15	1.448(2)	C14-H14	0.930000
C15-C16	1.375(2)	C15-C18	1.453(2)
C16-C19	1.454(3)	C17-C20	1.378(3)
C17-C18	1.395(2)	C18-C23	1.405(2)
C19-C24	1.494(3)	C20-C21	1.364(3)
C20-H20	0.930000	C21-C22	1.391(3)
C21-H21	0.930000	C22-C23	1.377(3)
C22-H22	0.930000	C24-H24A	0.960000
C24-H24B	0.960000	C24-H24C	0.960000

Table 5. Bond angles (°) for compound **6f.**

C17-O1-C16	106.13(13)	C23-O3-H1B	110.5(15)
C6-C1-C2	120.80(18)	C6-C1-H1	119.600000
C2-C1-H1	119.600000	C1-C2-C3	117.44(17)
C1-C2-C7	121.96(16)	C3-C2-C7	120.30(16)
C4-C3-C2	121.33(18)	C4-C3-H3	119.300000
C2-C3-H3	119.300000	C5-C4-C3	120.27(18)
C5-C4-H4	119.900000	C3-C4-H4	119.900000
C4-C5-C6	119.4(2)	C4-C5-H5	120.300000
C6-C5-H5	120.300000	C5-C6-C1	120.7(2)
C5-C6-H6	119.600000	C1-C6-H6	119.600000
C8-C7-C12	119.10(17)	C8-C7-C2	117.04(15)
C12-C7-C2	123.79(15)	C9-C8-C7	121.73(18)
C9-C8-H8	119.100000	C7-C8-H8	119.100000
C10-C9-C8	119.53(17)	C10-C9-H9	120.200000
C8-C9-H9	120.200000	C9-C10-C11	119.73(18)
C9-C10-H10	120.100000	C11-C10-H10	120.100000
C10-C11-C12	122.09(17)	C10-C11-H11	119.000000
C12-C11-H11	119.000000	C11-C12-C7	117.81(15)
C11-C12-C13	120.58(16)	C7-C12-C13	121.57(16)
C14-C13-C12	124.09(16)	C14-C13-H13	118.000000
C12-C13-H13	118.000000	C13-C14-C15	129.82(17)
C13-C14-H14	115.100000	C15-C14-H14	115.100000
C16-C15-C14	122.00(16)	C16-C15-C18	104.99(14)

C14-C15-C18	133.01(15)	C15-C16-O1	111.97(15)
C15-C16-C19	133.84(16)	O1-C16-C19	114.19(15)
O1-C17-C20	123.08(16)	O1-C17-C18	110.92(14)
C20-C17-C18	125.99(17)	C17-C18-C23	116.32(15)
C17-C18-C15	105.98(14)	C23-C18-C15	137.63(16)
O2-C19-C16	121.32(17)	O2-C19-C24	120.78(18)
C16-C19-C24	117.89(18)	C21-C20-C17	115.48(18)
C21-C20-H20	122.300000	C17-C20-H20	122.300000
C20-C21-C22	121.64(18)	C20-C21-H21	119.200000
C22-C21-H21	119.200000	C23-C22-C21	121.80(19)
C23-C22-H22	119.100000	C21-C22-H22	119.100000
O3-C23-C22	121.39(17)	O3-C23-C18	119.85(16)
C22-C23-C18	118.75(17)	C19-C24-H24A	109.500000
C19-C24-H24B	109.500000	H24A-C24-H24B	109.500000
C19-C24-H24C	109.500000	H24A-C24-H24C	109.500000
H24B-C24-H24C	109.500000		

Table 6. Torsion angles (°) for **6f.**

C6-C1-C2-C3	2.0(3)	C6-C1-C2-C7	-171.66(18)
C1-C2-C3-C4	-2.0(3)	C7-C2-C3-C4	171.78(16)
C2-C3-C4-C5	0.2(3)	C3-C4-C5-C6	1.6(3)

C4-C5-C6-C1	-1.6(3)	C2-C1-C6-C5	-0.3(3)
C1-C2-C7-C8	124.68(19)	C3-C2-C7-C8	-48.8(2)
C1-C2-C7-C12	-52.2(2)	C3-C2-C7-C12	134.35(18)
C12-C7-C8-C9	0.6(3)	C2-C7-C8-C9	-176.40(17)
C7-C8-C9-C10	0.0(3)	C8-C9-C10-C11	-0.5(3)
C9-C10-C11-C12	0.5(3)	C10-C11-C12-C7	0.1(3)
C10-C11-C12-C13	-177.60(17)	C8-C7-C12-C11	-0.6(2)
C2-C7-C12-C11	176.13(16)	C8-C7-C12-C13	177.07(16)
C2-C7-C12-C13	-6.2(3)	C11-C12-C13-C14	-21.8(3)
C7-C12-C13-C14	160.60(18)	C12-C13-C14-C15	179.29(17)
C13-C14-C15-C16	177.94(19)	C13-C14-C15-C18	-1.0(3)
C14-C15-C16-O1	-178.45(15)	C18-C15-C16-O1	0.7(2)
C14-C15-C16-C19	1.2(3)	C18-C15-C16-C19	-179.6(2)
C17-O1-C16-C15	-0.5(2)	C17-O1-C16-C19	179.77(17)
C16-O1-C17-C20	-178.71(18)	C16-O1-C17-C18	0.01(19)
O1-C17-C18-C23	-177.08(16)	C20-C17-C18-C23	1.6(3)
O1-C17-C18-C15	0.4(2)	C20-C17-C18-C15	179.09(19)
C16-C15-C18-C17	-0.7(2)	C14-C15-C18-C17	178.36(19)
C16-C15-C18-C23	176.0(2)	C14-C15-C18-C23	-5.0(4)
C15-C16-C19-O2	2.9(4)	O1-C16-C19-O2	-177.41(19)

C15-C16-C19-C24	-177.1(2)	O1-C16-C19-C24	2.6(3)
O1-C17-C20-C21	177.93(19)	C18-C17-C20-C21	-0.6(3)
C17-C20-C21-C22	-0.4(3)	C20-C21-C22-C23	0.4(4)
C21-C22-C23-O3	-178.7(2)	C21-C22-C23-C18	0.7(3)
C17-C18-C23-O3	177.83(17)	C15-C18-C23-O3	1.4(4)
C17-C18-C23-C22	-1.6(3)	C15-C18-C23-C22	-178.0(2)

Table 7. Anisotropic atomic displacement parameters ($Å^2$) for compound **6f.**

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	0.0466(7)	0.0458(7)	0.0533(7)	-0.0015(6)	0.0013(6)	0.0019(5)
O2	0.0915(11)	0.0421(8)	0.0748(10)	-0.0075(7)	0.0005(8)	0.0088(7)
O3	0.0885(11)	0.0381(7)	0.0690(9)	-0.0006(6)	-0.0087(8)	0.0066(7)
C1	0.0712(13)	0.0503(11)	0.0526(11)	0.0077(9)	0.0208(10)	0.0037(10)
C2	0.0425(9)	0.0439(10)	0.0444(9)	0.0031(7)	0.0065(7)	-0.0030(7)
C3	0.0559(11)	0.0513(11)	0.0478(10)	0.0068(8)	0.0102(9)	-0.0008(9)
C4	0.0566(12)	0.0435(10)	0.0637(12)	0.0053(9)	0.0062(10)	0.0026(9)
C5	0.0595(12)	0.0511(12)	0.0773(14)	-0.0054(10)	0.0209(11)	0.0028(9)
C6	0.0860(15)	0.0614(14)	0.0658(13)	-0.0018(11)	0.0349(12)	0.0003(12)
C7	0.0506(10)	0.0413(9)	0.0399(9)	0.0049(7)	0.0108(8)	-0.0041(8)
C8	0.0585(11)	0.0563(12)	0.0408(9)	0.0047(8)	0.0063(9)	-0.0014(9)
C9	0.0717(13)	0.0589(12)	0.0385(9)	-0.0023(9)	0.0127(9)	-0.0116(10)
C10	0.0692(13)	0.0461(10)	0.0510(10)	-0.0052(8)	0.0241(10)	-0.0095(9)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	0.0553(11)	0.0450(10)	0.0507(10)	0.0009(8)	0.0143(9)	-0.0010(8)
C12	0.0480(10)	0.0391(9)	0.0416(9)	0.0028(7)	0.0118(8)	-0.0031(7)
C13	0.0481(10)	0.0392(9)	0.0480(10)	-0.0024(7)	0.0094(8)	-0.0013(8)
C14	0.0550(11)	0.0369(9)	0.0484(10)	-0.0014(7)	0.0086(8)	-0.0004(8)
C15	0.0438(9)	0.0384(9)	0.0461(9)	0.0016(7)	0.0092(8)	-0.0016(7)
C16	0.0463(10)	0.0432(10)	0.0479(10)	-0.0018(8)	0.0060(8)	0.0001(8)
C17	0.0431(9)	0.0427(10)	0.0539(10)	-0.0020(8)	0.0101(8)	-0.0017(8)
C18	0.0423(9)	0.0378(9)	0.0475(9)	-0.0012(7)	0.0093(7)	-0.0028(7)
C19	0.0540(11)	0.0441(11)	0.0690(13)	0.0007(10)	0.0067(10)	0.0046(9)
C20	0.0563(12)	0.0558(12)	0.0584(12)	-0.0093(9)	0.0015(9)	-0.0063(9)
C21	0.0741(14)	0.0540(13)	0.0709(14)	-0.0202(11)	0.0017(11)	-0.0075(11)
C22	0.0730(14)	0.0411(11)	0.0780(14)	-0.0121(10)	0.0072(11)	-0.0004(10)
C23	0.0556(11)	0.0408(10)	0.0574(11)	-0.0005(8)	0.0057(9)	-0.0006(8)
C24	0.0742(15)	0.0621(14)	0.0963(17)	0.0039(12)	-0.0066(13)	0.0251(12)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for compound **6f.**

	x/a	**y/b**	**z/c**	**U(eq)**
H1B	0.410(3)	0.7229(18)	0.730(3)	0.116000
H1	0.1178	0.5453	0.5941	0.071000
H3	0.0587	0.6580	0.2301	0.066000
H4	-0.0464	0.7547	0.2957	0.072000
H5	-0.0742	0.7460	0.5071	0.077000
H6	0.0123	0.6425	0.6577	0.083000
H8	-0.0020	0.5180	0.1614	0.067000
H9	0.0588	0.4105	0.0692	0.071000

	x/a	y/b	z/c	U(eq)
H10	0.2480	0.3481	0.2014	0.066000
H11	0.3758	0.3947	0.4225	0.063000
H13	0.3419	0.5671	0.5912	0.058000
H14	0.4475	0.4223	0.6411	0.060000
H20	0.7771	0.5918	1.2113	0.076000
H21	0.6995	0.7177	1.1680	0.089000
H22	0.5405	0.7511	0.9541	0.085000
H24A	0.7256	0.3324	1.0927	0.135000
H24B	0.8268	0.3448	1.0256	0.135000
H24C	0.7447	0.2685	0.9929	0.135000

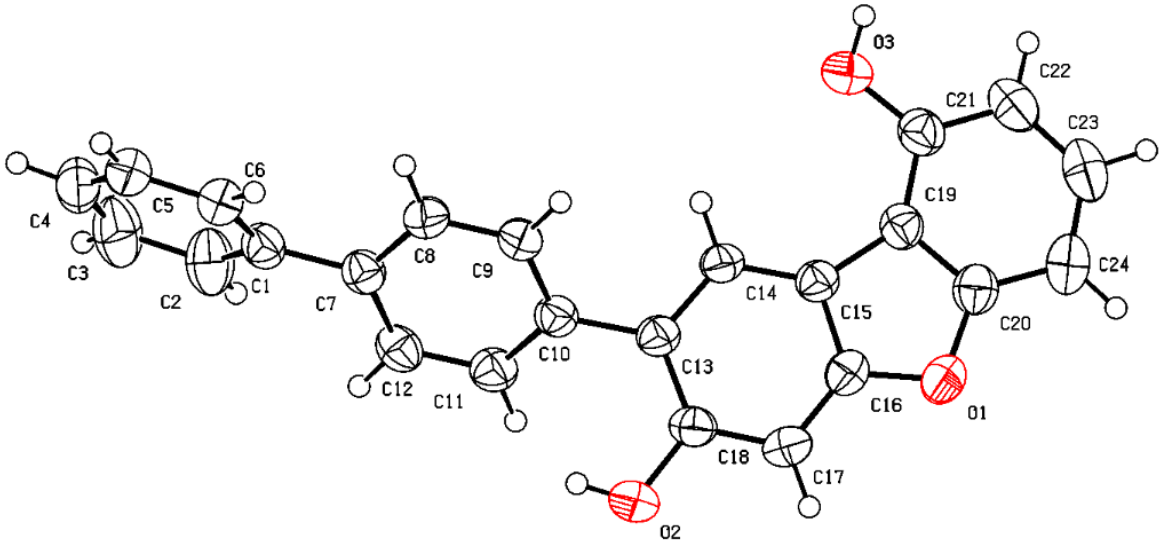
Table 9. Hydrogen bond distances (Å) and angles (°) for compound **6f.**

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O3-H1B···O2#1	0.98(3)	1.76(3)	2.7331(19)	172.(2)
C22-H22···O2#1	0.930000	2.560000	3.247(3)	131.500000

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, y+1/2, -z+3/2

Crystal Structure Report for compound **7d**



CCDC NUMBER: 2181857

A specimen of $C_{24}H_{16}O_3$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å).

The integration of the data using a triclinic unit cell yielded a total of 38013 reflections to a maximum θ angle of 28.29° (0.75 Å resolution), of which 4227 were independent (average redundancy 8.993, completeness = 99.2%, R_{int} = 3.90%, R_{sig} = 2.55%) and 3088 (73.05%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.1787(5) Å, b = 9.1920(5) Å, c = 11.2622(6) Å, α = 105.164(2)°, β = 92.910(2)°, γ = 109.138(2)°, volume = 856.66(8) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I).

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{24}H_{16}O_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 250 variables converged at R1 = 4.65%, for the observed data and wR2 = 13.66% for all data. The goodness-of-fit was 0.954. The largest peak in the final difference electron density synthesis was 0.200 $e^-/Å^3$ and the largest hole was -0.164 $e^-/Å^3$ with an RMS deviation of 0.032 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.366 g/cm^3 and F (000), 368 e^-.

Table 1. Sample and crystal data for compound **7d.**

Identification code	work_3	
Chemical formula	$C_{24}H_{16}O_3$	
Formula weight	352.37 g/mol	
Temperature	302(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.1787(5) Å	α = 105.164(2) °
	b = 9.1920(5) Å	β = 92.910(2) °
	c = 11.2622(6) Å	γ = 109.138(2) °
Volume	856.66(8) $Å^3$	
Z	2	
Density (calculated)	1.366 g/cm^3	
Absorption coefficient	0.090 mm^{-1}	
F (000)	368	

Table 2. Data collection and structure refinement for compound **7d.**

Theta range for data collection	2.38 to 28.29°
Index ranges	-12<=h<=12, -12<=k<=12, -15<=l<=14
Reflections collected	38013
Independent reflections	4227 [R(int) = 0.0390]
Structure solution technique	direct methods
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)

Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	Σ w $(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4227 / 0 / 250	
Goodness-of-fit on F^2	0.954	
Final R indices	3088 data; I>2σ(I)	R1 = 0.0465, wR2 = 0.1138
	all data	R1 = 0.0713, wR2 = 0.1366
Weighting scheme	$w=1/[\sigma^2(F_o^2) +(0.0605P)^2+0.3197P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.200 and -0.164 eÅ^{-3}	
R.M.S. deviation from mean	0.032 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for compound **7d.**

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
O1	0.93069(13)	0.31243(14)	0.27708(10)	0.0515(3)
O2	0.81086(16)	0.01954(14)	0.57457(12)	0.0588(3)
O3	0.69277(17)	0.67468(16)	0.45184(12)	0.0645(4)
C1	0.40847(18)	0.18307(19)	0.01344(14)	0.0443(3)
C2	0.2608(2)	0.0697(3)	0.00242(18)	0.0657(5)
C3	0.1830(2)	0.0688(3)	0.1055(2)	0.0767(6)
C4	0.2509(2)	0.1792(3)	0.21932(19)	0.0648(5)
C5	0.3987(2)	0.2875(2)	0.23254(17)	0.0576(4)

	x/a	y/b	z/c	U(eq)
C6	0.4764(2)	0.2898(2)	0.13057(15)	0.0491(4)
C7	0.48993(17)	0.19430(18)	0.90376(13)	0.0410(3)
C8	0.58789(18)	0.34361(18)	0.89676(14)	0.0441(3)
C9	0.66221(18)	0.35717(17)	0.79465(14)	0.0430(3)
C10	0.64191(17)	0.22282(17)	0.69378(13)	0.0401(3)
C11	0.54265(18)	0.07392(18)	0.70035(14)	0.0458(4)
C12	0.46949(18)	0.06017(18)	0.80347(15)	0.0460(4)
C13	0.72158(17)	0.24327(17)	0.58436(13)	0.0398(3)
C14	0.72101(17)	0.36770(17)	0.53553(13)	0.0406(3)
C15	0.79482(17)	0.38730(17)	0.43332(13)	0.0396(3)
C16	0.86867(17)	0.28085(18)	0.38110(13)	0.0428(3)
C17	0.87666(18)	0.15912(18)	0.42745(14)	0.0466(4)
C18	0.80221(18)	0.14243(17)	0.52934(14)	0.0434(3)
C19	0.81457(17)	0.49504(17)	0.35706(13)	0.0422(3)
C20	0.89531(18)	0.4431(2)	0.26337(15)	0.0475(4)
C21	0.7716(2)	0.62749(19)	0.35875(15)	0.0488(4)
C22	0.8079(2)	0.6996(2)	0.26531(17)	0.0583(4)
C23	0.8869(2)	0.6428(2)	0.17307(17)	0.0639(5)
C24	0.9327(2)	0.5129(2)	0.16951(16)	0.0599(5)

Table 4. Bond lengths (Å) for compound **7d.**

O1-C16	1.3850(18)	O1-C20	1.386(2)
O2-C18	1.3775(18)	O3-C21	1.363(2)
C1-C2	1.389(2)	C1-C6	1.389(2)
C1-C7	1.485(2)	C2-C3	1.394(3)
C3-C4	1.373(3)	C4-C5	1.367(3)

C5-C6	1.384(2)	C7-C12	1.389(2)
C7-C8	1.397(2)	C8-C9	1.379(2)
C9-C10	1.394(2)	C10-C11	1.397(2)
C10-C13	1.487(2)	C11-C12	1.384(2)
C13-C14	1.394(2)	C13-C18	1.409(2)
C14-C15	1.387(2)	C15-C16	1.392(2)
C15-C19	1.447(2)	C16-C17	1.373(2)
C17-C18	1.382(2)	C19-C20	1.392(2)
C19-C21	1.393(2)	C20-C24	1.376(2)
C21-C22	1.383(2)	C22-C23	1.385(3)
C23-C24	1.383(3)		

Table 5. Bond angles (°) for compound **7d.**

C16-O1-C20	105.61(11)	C2-C1-C6	117.69(15)
C2-C1-C7	121.59(15)	C6-C1-C7	120.69(14)
C1-C2-C3	120.29(19)	C4-C3-C2	120.75(18)
C5-C4-C3	119.54(17)	C4-C5-C6	120.05(18)
C5-C6-C1	121.60(16)	C12-C7-C8	117.39(14)
C12-C7-C1	122.21(14)	C8-C7-C1	120.38(13)
C9-C8-C7	121.33(14)	C8-C9-C10	121.44(14)
C9-C10-C11	117.15(13)	C9-C10-C13	119.70(13)
C11-C10-C13	123.12(13)	C12-C11-C10	121.36(14)
C11-C12-C7	121.32(14)	C14-C13-C18	118.24(13)
C14-C13-C10	119.82(13)	C18-C13-C10	121.92(13)
C15-C14-C13	120.13(13)	C14-C15-C16	118.80(13)

C14-C15-C19	135.75(14)	C16-C15-C19	105.42(13)
C17-C16-O1	124.82(13)	C17-C16-C15	123.53(14)
O1-C16-C15	111.65(13)	C16-C17-C18	116.41(13)
O2-C18-C17	115.75(13)	O2-C18-C13	121.42(14)
C17-C18-C13	122.84(14)	C20-C19-C21	118.78(14)
C20-C19-C15	106.26(13)	C21-C19-C15	134.96(14)
C24-C20-O1	125.16(16)	C24-C20-C19	123.79(17)
O1-C20-C19	111.05(13)	O3-C21-C22	124.41(16)
O3-C21-C19	117.08(14)	C22-C21-C19	118.49(16)
C21-C22-C23	120.78(17)	C24-C23-C22	122.18(17)
C20-C24-C23	115.96(17)		

Table 6. Anisotropic atomic displacement parameters ($Å^2$) for compound **7d.**

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	0.0554(7)	0.0589(7)	0.0463(6)	0.0158(5)	0.0179(5)	0.0262(5)
O2	0.0807(9)	0.0507(7)	0.0633(8)	0.0250(6)	0.0223(7)	0.0387(6)
O3	0.0964(10)	0.0494(7)	0.0627(8)	0.0213(6)	0.0263(7)	0.0392(7)
C1	0.0435(8)	0.0481(8)	0.0479(8)	0.0214(7)	0.0088(6)	0.0188(7)
C2	0.0505(10)	0.0807(13)	0.0583(11)	0.0283(10)	0.0064(8)	0.0076(9)
C3	0.0501(10)	0.1005(17)	0.0845(15)	0.0502(13)	0.0193(10)	0.0140(11)
C4	0.0701(12)	0.0864(14)	0.0662(12)	0.0451(11)	0.0313(10)	0.0433(11)
C5	0.0736(12)	0.0605(10)	0.0529(10)	0.0235(8)	0.0222(9)	0.0349(9)
C6	0.0539(9)	0.0483(9)	0.0487(9)	0.0162(7)	0.0134(7)	0.0203(7)
C7	0.0402(7)	0.0433(8)	0.0414(8)	0.0150(6)	0.0041(6)	0.0158(6)

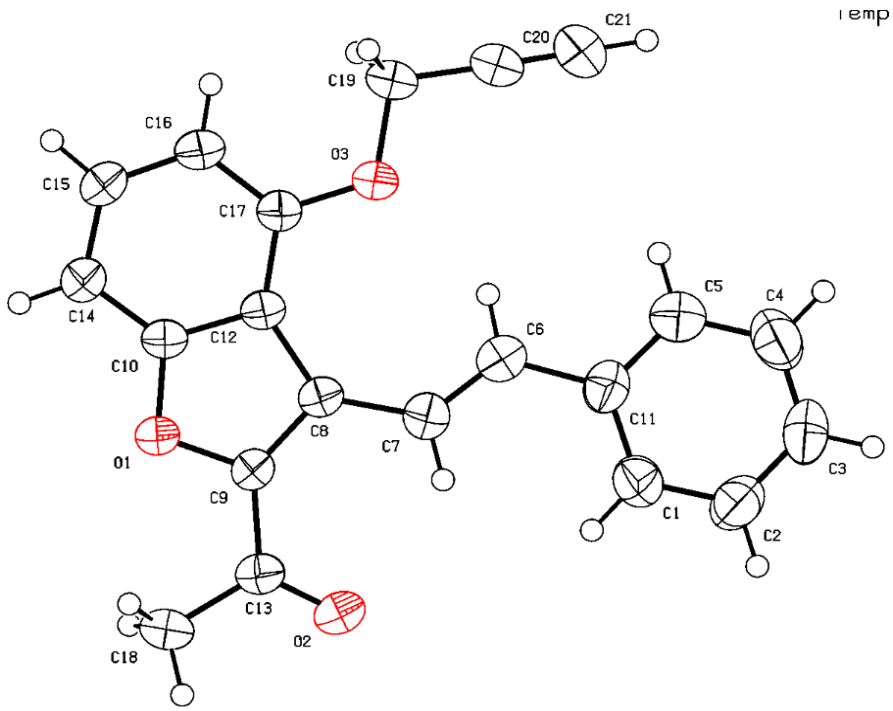
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C8	0.0501(8)	0.0374(7)	0.0434(8)	0.0083(6)	0.0095(6)	0.0161(6)
C9	0.0488(8)	0.0343(7)	0.0454(8)	0.0121(6)	0.0098(6)	0.0133(6)
C10	0.0442(8)	0.0394(7)	0.0389(7)	0.0121(6)	0.0048(6)	0.0174(6)
C11	0.0545(9)	0.0361(7)	0.0413(8)	0.0060(6)	0.0032(7)	0.0137(6)
C12	0.0474(8)	0.0369(7)	0.0492(9)	0.0144(6)	0.0029(7)	0.0082(6)
C13	0.0458(8)	0.0355(7)	0.0366(7)	0.0071(6)	0.0054(6)	0.0152(6)
C14	0.0488(8)	0.0374(7)	0.0380(7)	0.0084(6)	0.0080(6)	0.0203(6)
C15	0.0434(8)	0.0368(7)	0.0371(7)	0.0082(6)	0.0051(6)	0.0146(6)
C16	0.0427(8)	0.0448(8)	0.0383(7)	0.0084(6)	0.0072(6)	0.0150(6)
C17	0.0506(9)	0.0434(8)	0.0485(9)	0.0079(7)	0.0098(7)	0.0241(7)
C18	0.0500(8)	0.0365(7)	0.0450(8)	0.0100(6)	0.0049(6)	0.0188(6)
C19	0.0455(8)	0.0404(7)	0.0372(7)	0.0107(6)	0.0037(6)	0.0117(6)
C20	0.0461(8)	0.0507(9)	0.0426(8)	0.0133(7)	0.0057(6)	0.0138(7)
C21	0.0566(9)	0.0415(8)	0.0452(8)	0.0127(6)	0.0052(7)	0.0141(7)
C22	0.0696(11)	0.0483(9)	0.0551(10)	0.0225(8)	0.0016(9)	0.0141(8)
C23	0.0692(12)	0.0662(12)	0.0536(10)	0.0311(9)	0.0083(9)	0.0101(9)
C24	0.0586(10)	0.0743(12)	0.0476(9)	0.0241(9)	0.0159(8)	0.0185(9)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for compound **7d.**

	x/a	**y/b**	**z/c**	**U(eq)**
H1	0.775(3)	0.024(3)	0.644(2)	0.088000
H1B	0.704(3)	0.776(3)	0.465(2)	0.097000
H2	0.2135	-0.0060	0.9259	0.079000
H3	0.0840	-0.0075	1.0971	0.092000
H4	0.1968	0.1803	1.2869	0.078000
H5	0.4470	0.3596	1.3101	0.069000

	x/a	y/b	z/c	U(eq)
H6	0.5766	0.3645	1.1407	0.059000
H8	0.6033	0.4357	0.9623	0.053000
H9	0.7273	0.4581	0.7930	0.052000
H11	0.5254	-0.0179	0.6341	0.055000
H12	0.4054	-0.0409	0.8056	0.055000
H14	0.6710	0.4377	0.5716	0.049000
H17	0.9293	0.0915	0.3922	0.056000
H22	0.7789	0.7873	0.2644	0.070000
H23	0.9098	0.6938	0.1115	0.077000
H24	0.9857	0.4749	0.1074	0.072000

Crystal Structure Report for compound **23**



CCDC NUMBER: 2247453

A specimen of $C_{21}H_{16}O_3$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å).

The integration of the data using a monoclinic unit cell yielded a total of 28657 reflections to a maximum θ angle of 28.34° (0.75 Å resolution), of which 3966 were independent (average redundancy 7.226, completeness = 99.2%, R_{int} = 4.84%, R_{sig} = 3.81%) and 2476 (62.43%) were greater than $2\sigma(F^2)$. The final cell constants of a = 10.4864(11) Å, b = 10.0490(9) Å, c = 15.2051(13) Å, β = 89.824(3) °, volume = 1602.3(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6532 and 0.7457.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/n 1, with Z = 4 for the formula unit, $C_{21}H_{16}O_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 218 variables converged at R1 = 5.51%, for the observed data and wR2 = 15.20% for all data. The goodness-of-fit was 1.026. The largest peak in the final difference electron density synthesis was 0.352 $e^-/Å^3$ and the largest hole was -0.245 $e^-/Å^3$ with an RMS deviation of 0.037 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.311 g/cm^3 and F (000), 664 e^-.

Table 1. Sample and crystal data for compound **23.**

Identification code	workSA_167
Chemical formula	$C_{21}H_{16}O_3$
Formula weight	316.34 g/mol
Temperature	300(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic

Space group	P 1 21/n 1	
Unit cell dimensions	a = 10.4864(11) Å	α = 90°
	b = 10.0490(9) Å	β = 89.824(3) °
	c = 15.2051(13) Å	γ = 90°
Volume	1602.3(3) $Å^3$	
Z	4	
Density (calculated)	1.311 g/cm^3	
Absorption coefficient	0.087 mm^{-1}	
F (000)	664	

Table 2. Data collection and structure refinement for compound **23.**

Theta range for data collection	2.43 to 28.34°	
Index ranges	-13<=h<=13, -13<=k<=11, -20<=l<=20	
Reflections collected	28657	
Independent reflections	3966 [R(int) = 0.0484]	
Max. and min. transmission	0.7457 and 0.6532	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma w (F_o^2 - F_c^2)^2$	
Data / restraints / parameters	3966 / 0 / 218	
Goodness-of-fit on F^2	1.026	
Final R indices	2476 data; I>2σ(I)	R1 = 0.0551, wR2 = 0.1238

	all data	R1 = 0.1002, wR2 = 0.1520
Weighting scheme	$w=1/[\sigma^2(F_o^2) +(0.0557P)^2+0.6585P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.352 and -0.245 eÅ^{-3}	
R.M.S. deviation from mean	0.037 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for compound **23.**

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
O1	0.54921(13)	0.41774(12)	0.86596(8)	0.0483(4)
O2	0.59766(17)	0.13335(13)	0.73541(10)	0.0667(5)
O3	0.61266(14)	0.72382(12)	0.64072(8)	0.0511(4)
C1	0.7087(2)	0.2540(2)	0.46295(14)	0.0576(5)
C2	0.7445(2)	0.2038(2)	0.38214(15)	0.0642(6)
C3	0.7585(2)	0.2863(3)	0.31159(14)	0.0668(6)
C4	0.7379(2)	0.4188(3)	0.32103(15)	0.0729(7)
C5	0.7015(2)	0.4705(2)	0.40126(15)	0.0632(6)
C6	0.64507(19)	0.4501(2)	0.55805(13)	0.0517(5)
C7	0.63714(19)	0.3884(2)	0.63337(12)	0.0489(5)
C8	0.59973(17)	0.43682(17)	0.72008(11)	0.0398(4)
C9	0.58096(18)	0.35099(17)	0.78961(11)	0.0428(4)
C10	0.54565(19)	0.54943(17)	0.84438(12)	0.0451(4)
C11	0.68609(18)	0.3899(2)	0.47381(12)	0.0490(5)
C12	0.57737(17)	0.56882(16)	0.75594(11)	0.0390(4)
C13	0.58656(19)	0.20557(18)	0.79945(12)	0.0467(5)

	x/a	y/b	z/c	U(eq)
C14	0.5130(2)	0.6475(2)	0.90390(14)	0.0620(6)
C15	0.5152(2)	0.7752(2)	0.87138(14)	0.0640(6)
C16	0.5489(2)	0.80259(19)	0.78472(13)	0.0539(5)
C17	0.57943(18)	0.70199(17)	0.72679(11)	0.0420(4)
C18	0.5771(2)	0.15078(19)	0.89081(13)	0.0552(5)
C19	0.6030(2)	0.85757(18)	0.60893(13)	0.0512(5)
C20	0.6204(3)	0.8541(2)	0.51437(15)	0.0655(6)
C21	0.6270(4)	0.8533(3)	0.43821(18)	0.1097(12)

Table 4. Bond lengths (Å) for compound **23.**

O1-C10	1.364(2)	O1-C9	1.381(2)
O2-C13	1.220(2)	O3-C17	1.371(2)
O3-C19	1.432(2)	C1-C2	1.379(3)
C1-C11	1.396(3)	C2-C3	1.363(3)
C3-C4	1.357(4)	C4-C5	1.378(3)
C5-C11	1.378(3)	C6-C7	1.305(3)
C6-C11	1.479(3)	C7-C8	1.458(2)
C8-C9	1.378(2)	C8-C12	1.453(2)
C9-C13	1.470(3)	C10-C14	1.380(3)
C10-C12	1.398(2)	C12-C17	1.410(2)
C13-C18	1.497(3)	C14-C15	1.375(3)
C15-C16	1.391(3)	C16-C17	1.378(3)
C19-C20	1.449(3)	C20-C21	1.160(3)

Table 5. Bond angles (°) for **23.**

C10-O1-C9	106.01(13)	C17-O3-C19	117.03(14)
C2-C1-C11	120.6(2)	C3-C2-C1	120.5(2)

C4-C3-C2	119.8(2)	C3-C4-C5	120.5(2)
C11-C5-C4	121.2(2)	C7-C6-C11	125.67(19)
C6-C7-C8	130.65(19)	C9-C8-C12	105.13(15)
C9-C8-C7	121.49(16)	C12-C8-C7	133.36(16)
C8-C9-O1	111.99(15)	C8-C9-C13	133.99(16)
O1-C9-C13	114.01(15)	O1-C10-C14	122.83(17)
O1-C10-C12	111.10(15)	C14-C10-C12	126.07(17)
C5-C11-C1	117.47(19)	C5-C11-C6	119.1(2)
C1-C11-C6	123.47(19)	C10-C12-C17	115.98(15)
C10-C12-C8	105.75(15)	C17-C12-C8	138.27(16)
O2-C13-C9	120.93(17)	O2-C13-C18	121.86(17)
C9-C13-C18	117.21(16)	C15-C14-C10	115.27(18)
C14-C15-C16	121.95(19)	C17-C16-C15	121.22(18)
O3-C17-C16	123.41(16)	O3-C17-C12	117.10(15)
C16-C17-C12	119.48(16)	O3-C19-C20	107.68(16)
C21-C20-C19	176.1(3)		

Table 6. Anisotropic atomic displacement parameters ($Å^2$) for compound **23.**

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	0.0746(9)	0.0298(7)	0.0404(7)	0.0001(5)	0.0093(6)	-0.0021(6)
O2	0.1106(13)	0.0347(8)	0.0548(9)	-0.0059(6)	0.0114(8)	0.0001(8)
O3	0.0794(10)	0.0312(7)	0.0427(7)	0.0043(5)	0.0101(6)	0.0033(6)
C1	0.0676(14)	0.0556(13)	0.0496(11)	0.0030(10)	0.0074(10)	0.0069(10)
C2	0.0708(15)	0.0549(13)	0.0668(15)	0.0151(11)	0.0108(11)	0.0022(11)
C3	0.0716(15)	0.0842(18)	0.0445(12)	0.0124(11)	0.0106(10)	0.0030(13)
C4	0.0862(17)	0.0832(19)	0.0493(13)	0.0124(12)	0.0064(12)	0.0031(14)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C5	0.0748(15)	0.0540(13)	0.0609(13)	0.0031(11)	0.0011(11)	0.0063(11)
C6	0.0615(13)	0.0431(11)	0.0503(11)	-0.0033(9)	0.0025(9)	0.0021(9)
C7	0.0584(12)	0.0449(11)	0.0434(10)	-0.0017(8)	0.0040(9)	-0.0011(9)
C8	0.0461(10)	0.0327(9)	0.0405(9)	-0.0018(7)	0.0014(7)	-0.0009(7)
C9	0.0561(11)	0.0341(9)	0.0380(9)	-0.0027(7)	0.0051(8)	0.0002(8)
C10	0.0621(12)	0.0305(9)	0.0427(10)	0.0006(7)	0.0053(8)	-0.0041(8)
C11	0.0482(11)	0.0539(12)	0.0449(10)	-0.0095(9)	0.0021(8)	-0.0035(9)
C12	0.0464(10)	0.0310(9)	0.0396(9)	-0.0008(7)	0.0011(7)	-0.0026(7)
C13	0.0575(12)	0.0334(9)	0.0491(11)	0.0000(8)	0.0045(9)	-0.0004(8)
C14	0.1024(18)	0.0387(11)	0.0447(11)	-0.0039(9)	0.0161(11)	0.0035(11)
C15	0.1067(18)	0.0367(11)	0.0487(12)	-0.0083(9)	0.0143(11)	0.0003(11)
C16	0.0798(14)	0.0312(10)	0.0506(11)	-0.0008(8)	0.0046(10)	-0.0031(9)
C17	0.0527(11)	0.0342(9)	0.0392(9)	0.0004(7)	0.0021(8)	-0.0022(8)
C18	0.0735(14)	0.0362(10)	0.0558(12)	0.0084(9)	0.0036(10)	0.0026(9)
C19	0.0691(13)	0.0339(10)	0.0506(11)	0.0085(8)	0.0029(9)	0.0011(9)
C20	0.1013(18)	0.0404(11)	0.0546(13)	0.0103(10)	0.0102(12)	0.0043(11)
C21	0.212(4)	0.0624(17)	0.0546(16)	0.0123(13)	0.0290(19)	0.014(2)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for compound **23.**

	x/a	**y/b**	**z/c**	**U(eq)**
H1	0.6994	0.1967	0.5106	0.069000
H2	0.7593	0.1131	0.3757	0.077000
H3	0.7821	0.2518	0.2572	0.080000
H4	0.7484	0.4752	0.2730	0.087000
H5	0.6871	0.5615	0.4065	0.076000

	x/a	y/b	z/c	U(eq)
H6	0.6230	0.5397	0.5573	0.062000
H7	0.6590	0.2988	0.6314	0.059000
H14	0.4912	0.6286	0.9619	0.074000
H15	0.4934	0.8453	0.9084	0.077000
H16	0.5510	0.8904	0.7655	0.065000
H18A	0.6306	0.2016	0.9293	0.083000
H18B	0.6043	0.0596	0.8909	0.083000
H18C	0.4903	0.1560	0.9108	0.083000
H19A	0.6679	0.9129	0.6358	0.061000
H19B	0.5200	0.8943	0.6234	0.061000
H21	0.6324	0.8527	0.3772	0.132000