Supplementary Information

One-pot metal-free protocol for the synthesis of chalcogenated furans from 1, 4-enediones and thiols

Venkatachalam Rajeshkumar*, Chinnaraj Neelamegam, and Sambandam Anandan

Department of Chemistry, National Institute of Technology, Tiruchirappalli-620015, India.

E-mail: orgrajeshkumar@gmail.com; vrajesh@nitt.edu

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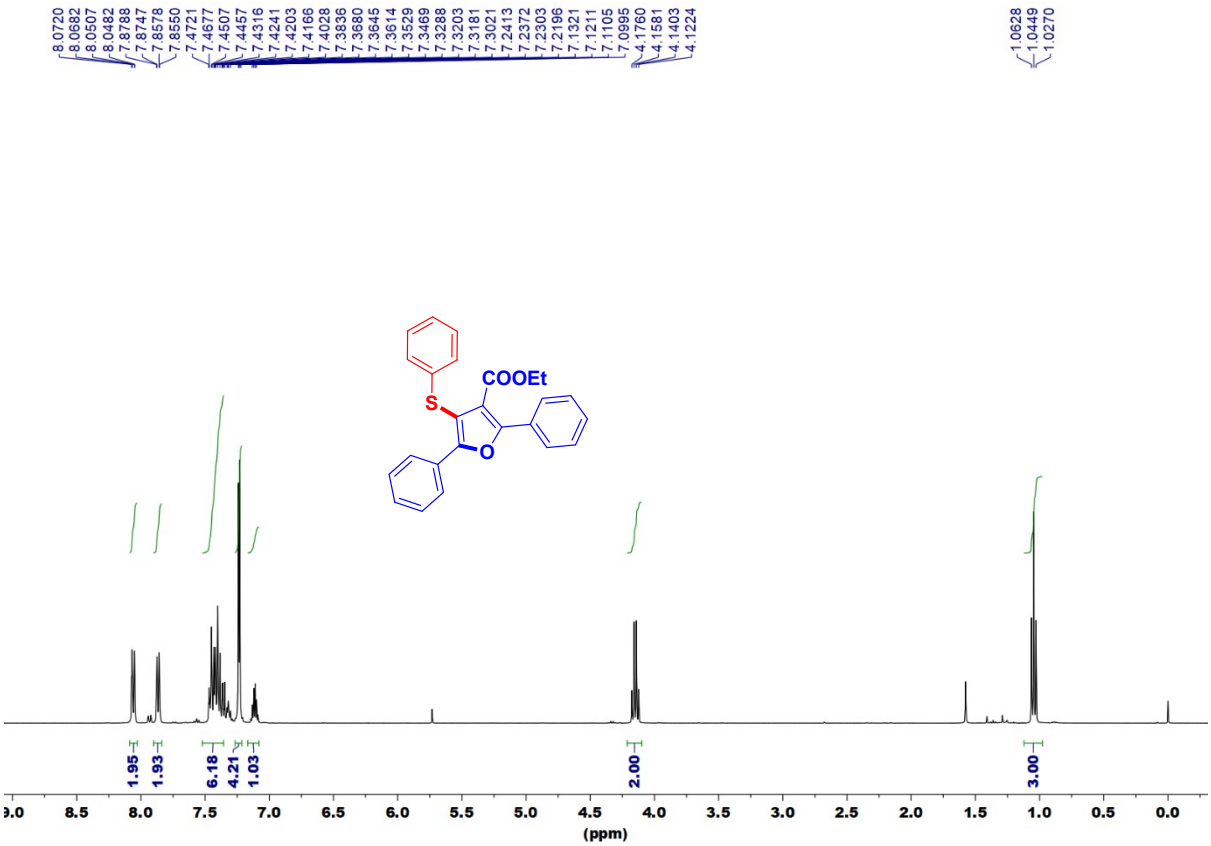

Figure S1. ^{1}H NMR spectrum of compound **3a** (400 MHz, $CDCl_3$)

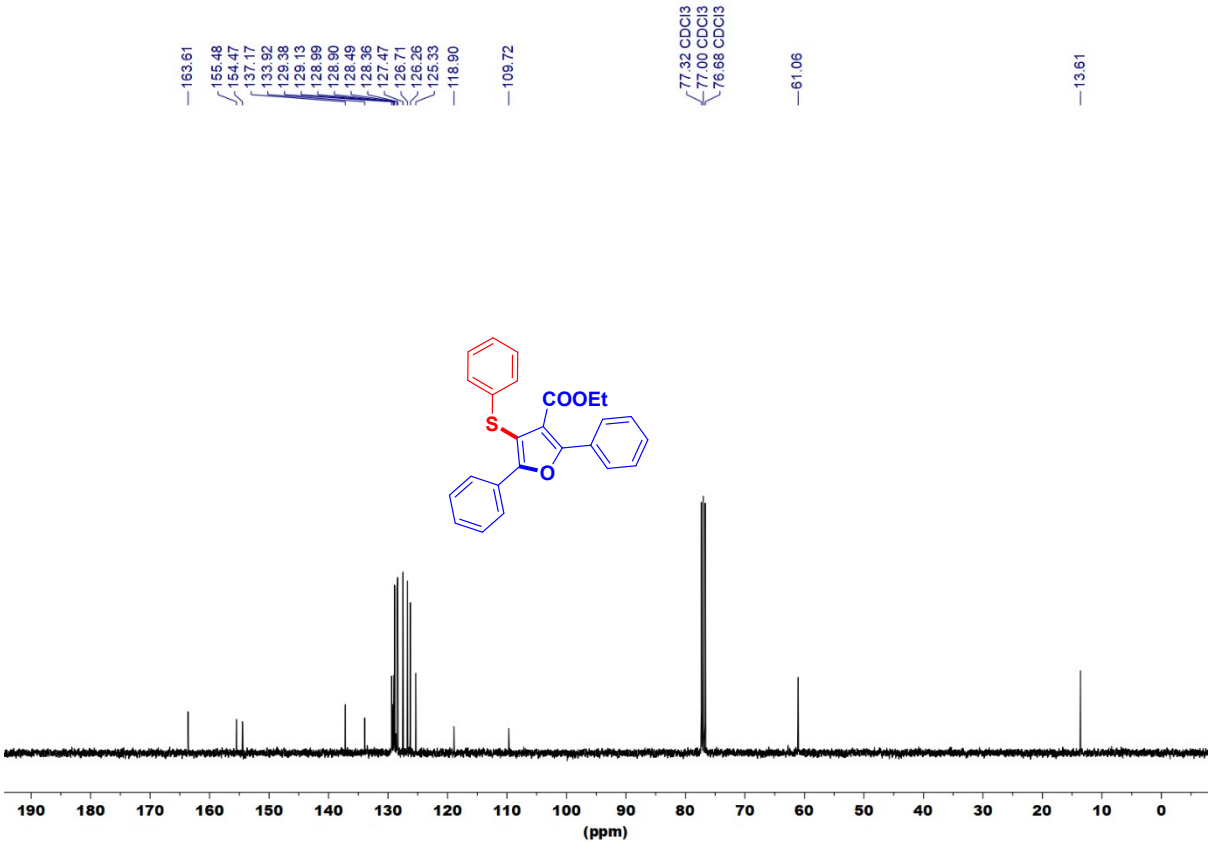

Figure S2. ^{13}C NMR spectrum of compound **3a** (101 MHz, $CDCl_3$)

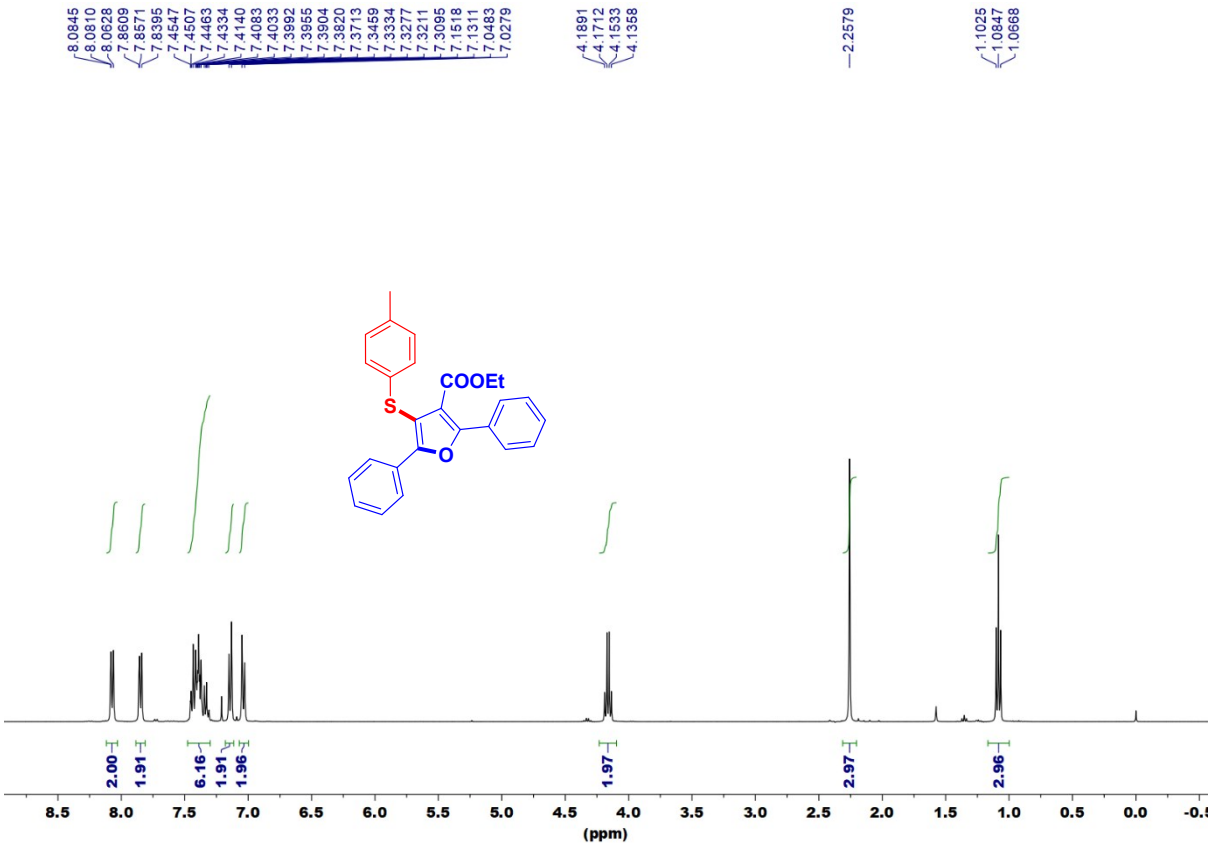

Figure S3. ^{1}H NMR spectrum of compound **3b** (400 MHz, $CDCl_3$)

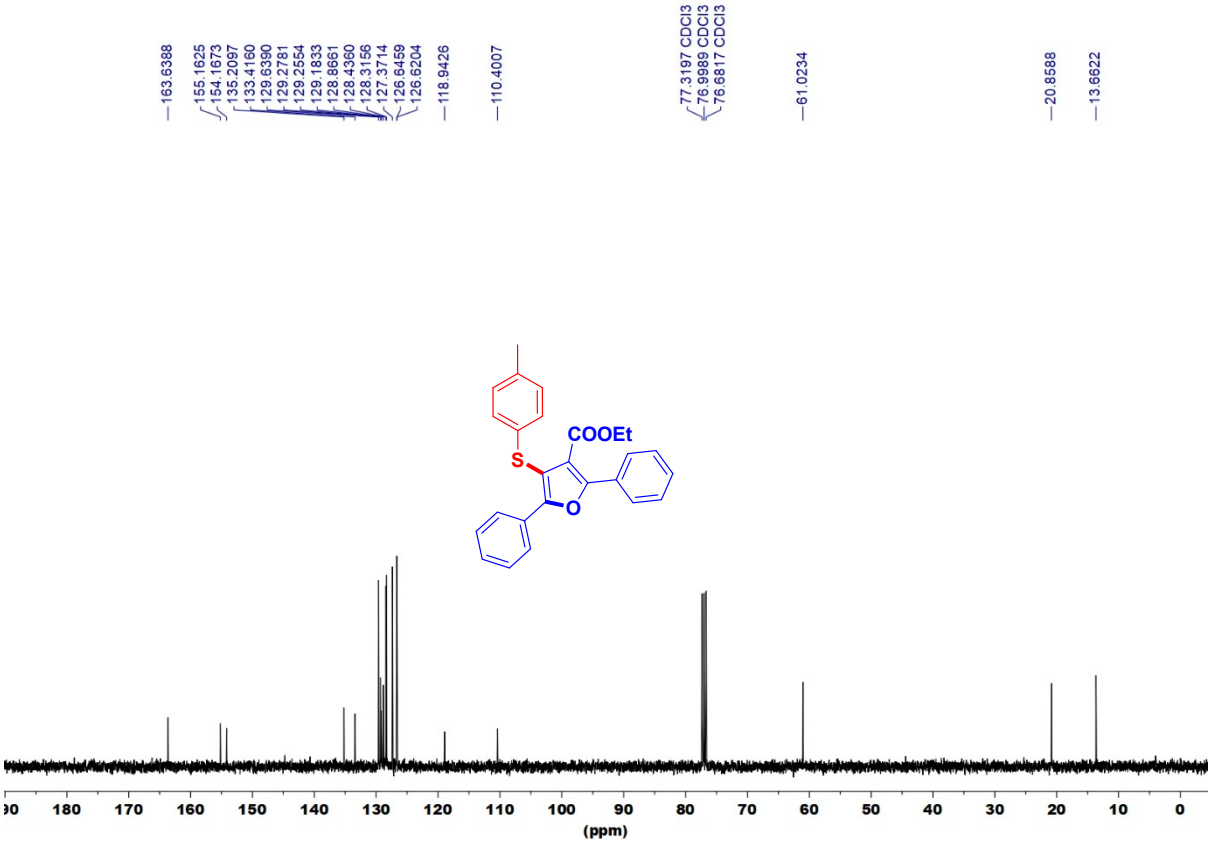

Figure S4. ^{13}C NMR spectrum of compound **3b** (101 MHz, $CDCl_3$)

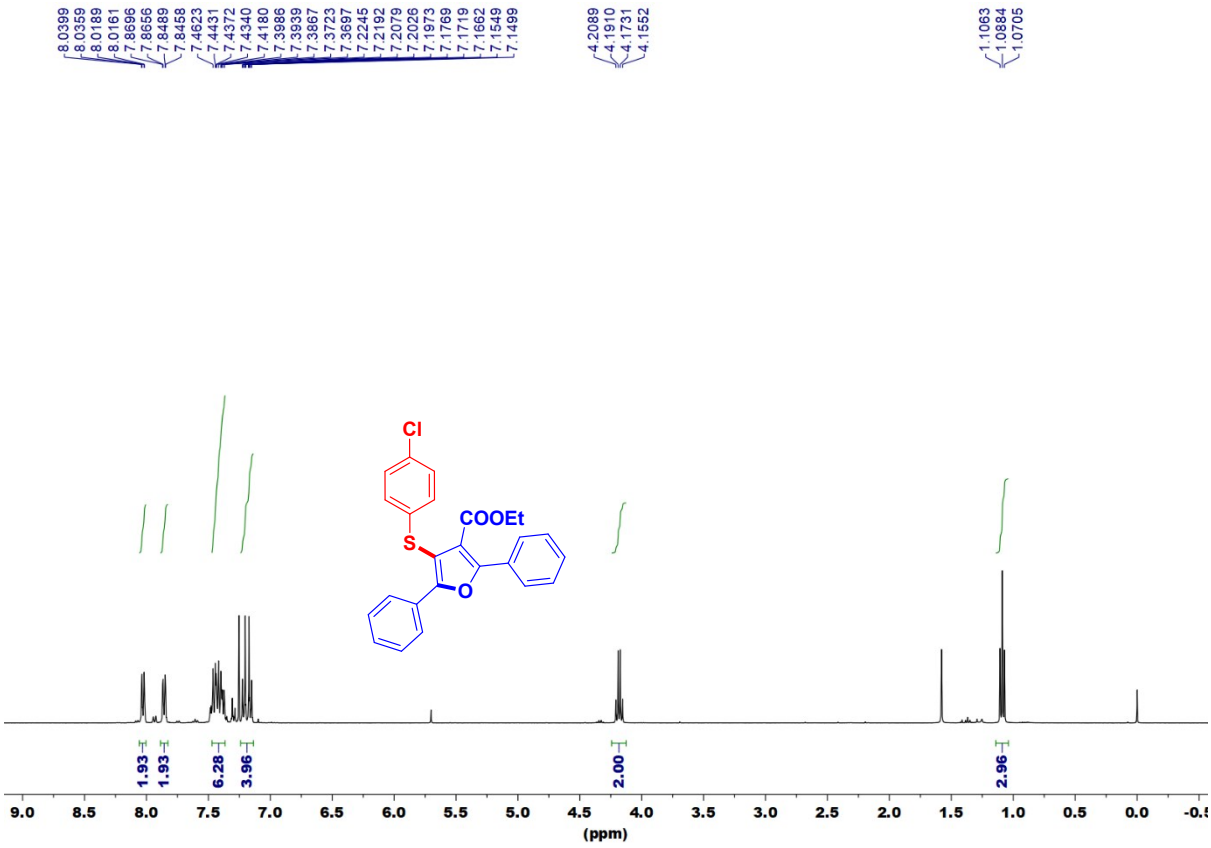

Figure S5. ^{1}H NMR spectrum of compound **3c** (400 MHz, $CDCl_3$)

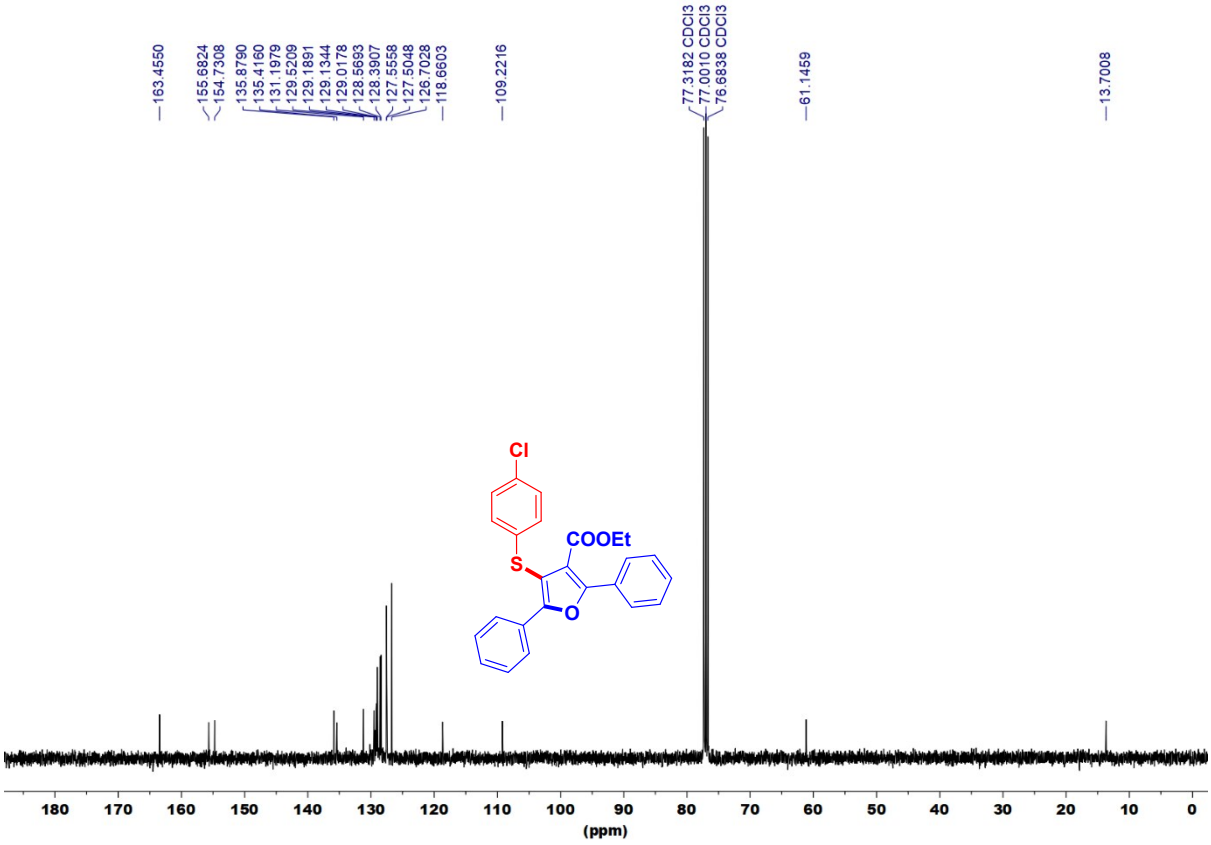

Figure S6. ^{13}C NMR spectrum of compound **3c** (101 MHz, $CDCl_3$)

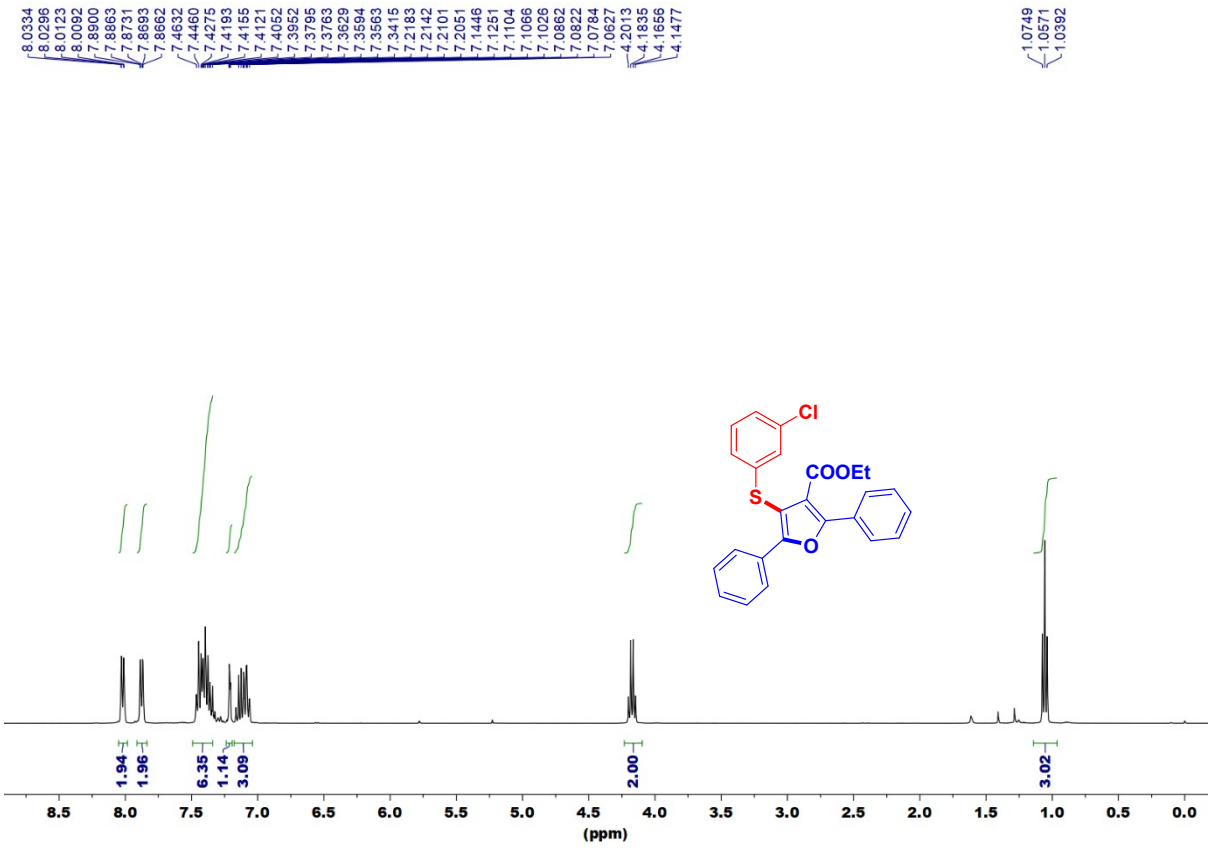

Figure S7. ^{1}H NMR spectrum of compound **3d** (400 MHz, $CDCl_3$)

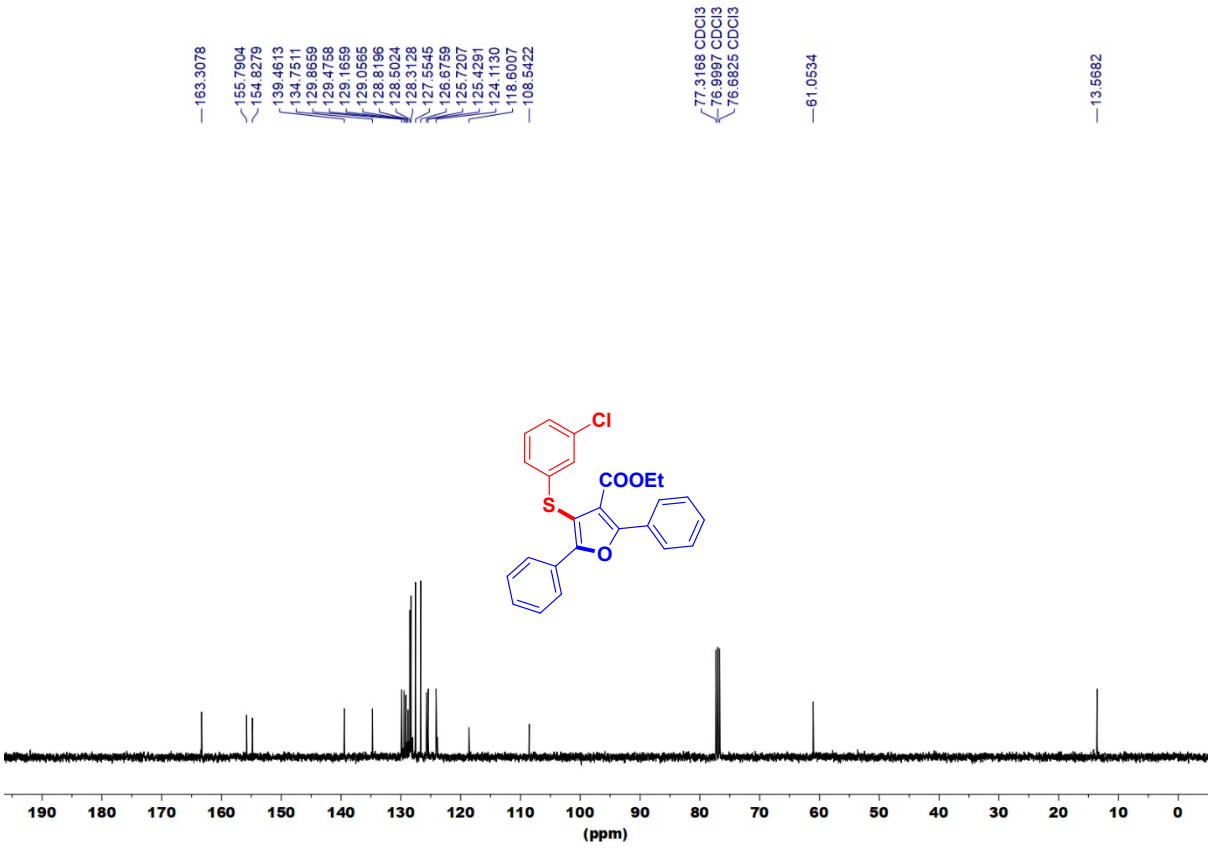

Figure S8. ^{13}C NMR spectrum of compound **3d** (101 MHz, $CDCl_3$)

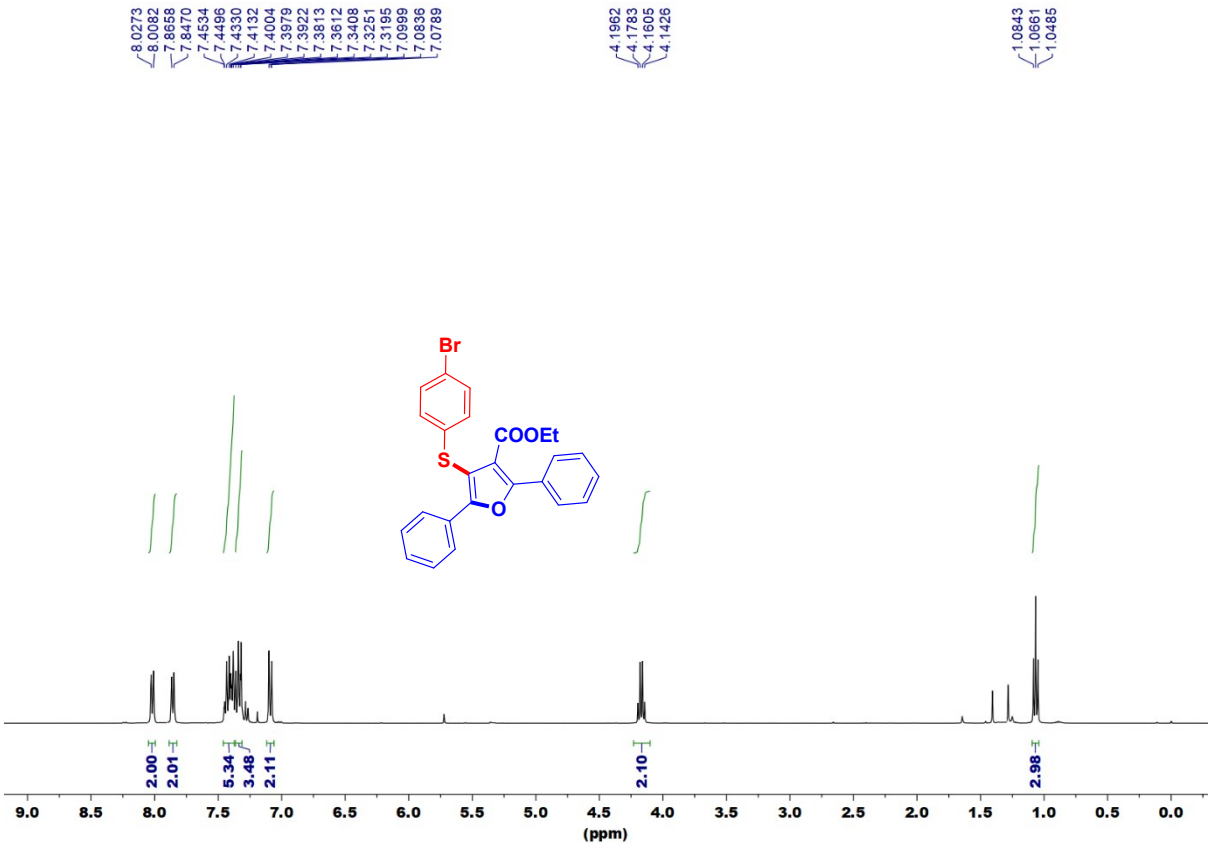

Figure S9. ^{1}H NMR spectrum of compound **3e** (400 MHz, $CDCl_3$)

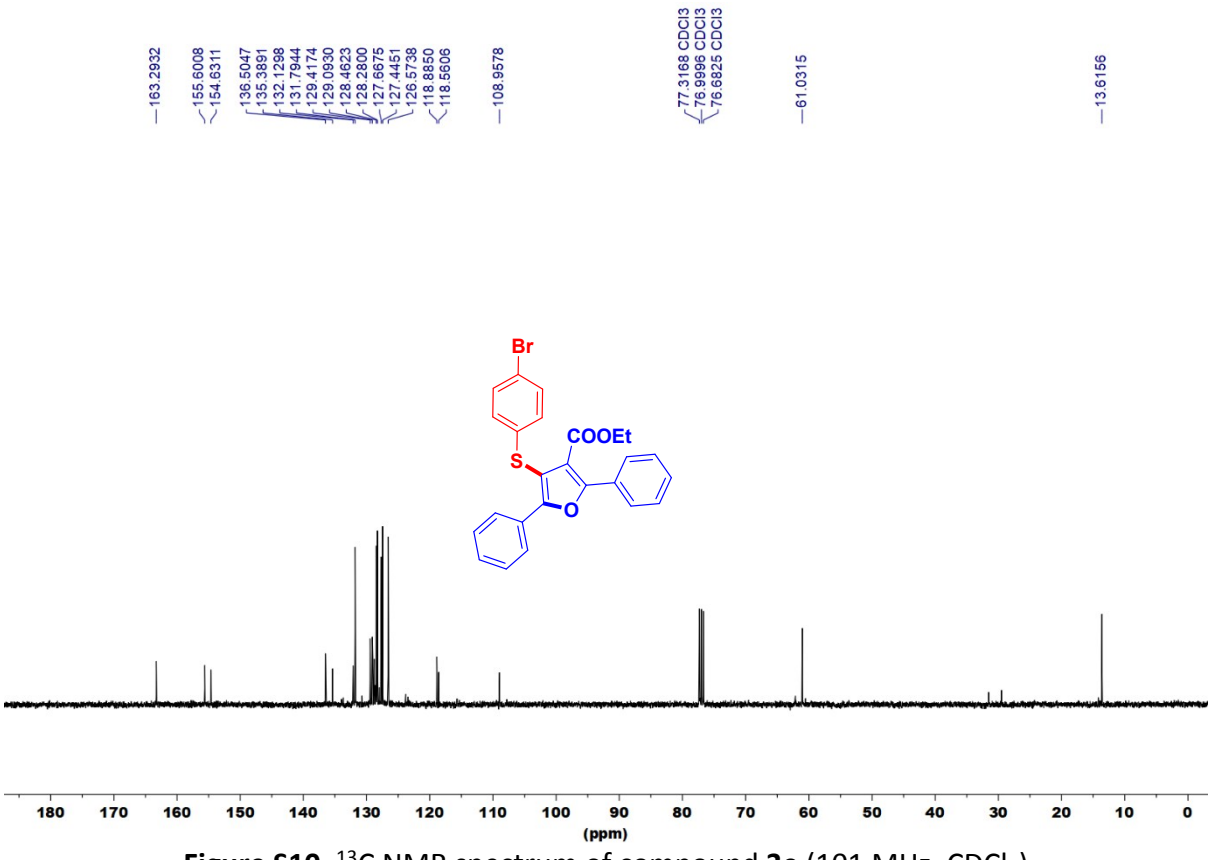

Figure S10. ^{13}C NMR spectrum of compound **3e** (101 MHz, $CDCl_3$)

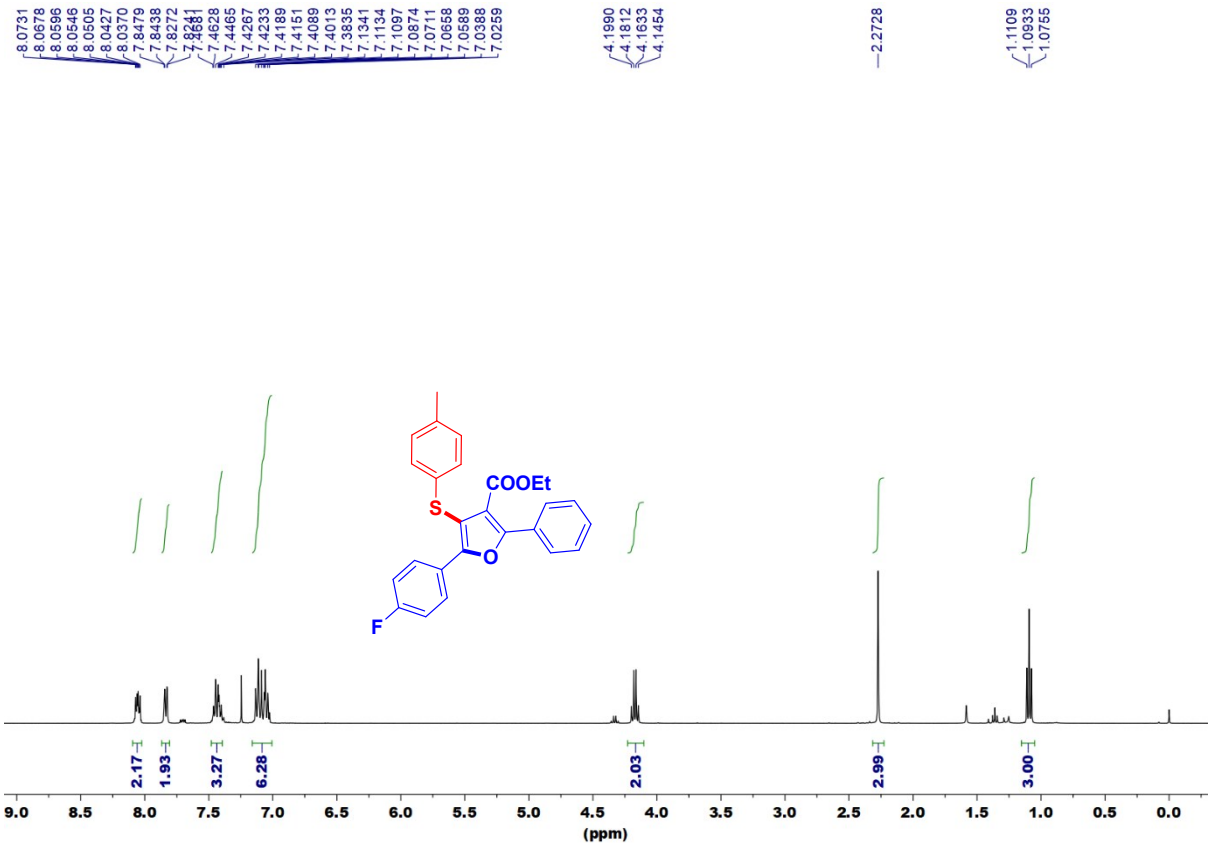

Figure S11. ^{1}H NMR spectrum of compound **3f** (400 MHz, $CDCl_3$)

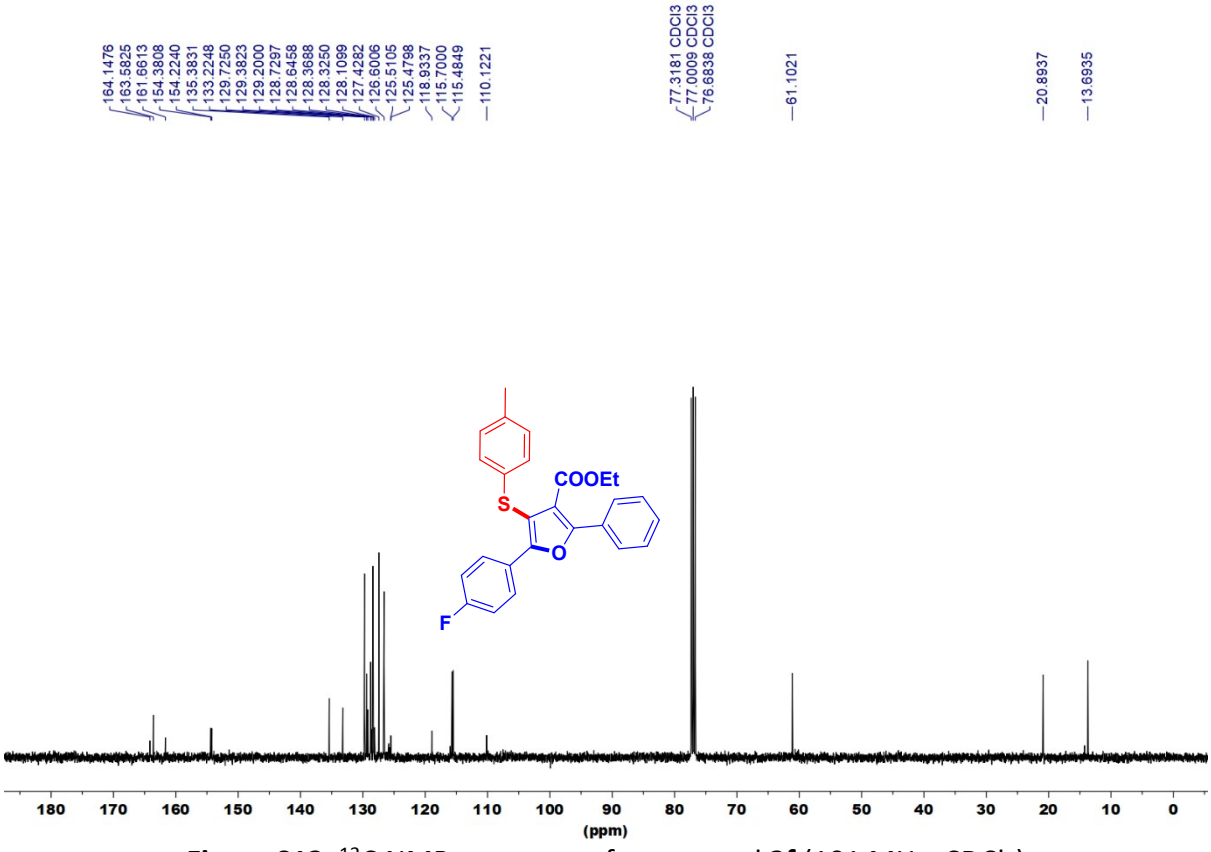

Figure S12. ^{13}C NMR spectrum of compound **3f** (101 MHz, $CDCl_3$)

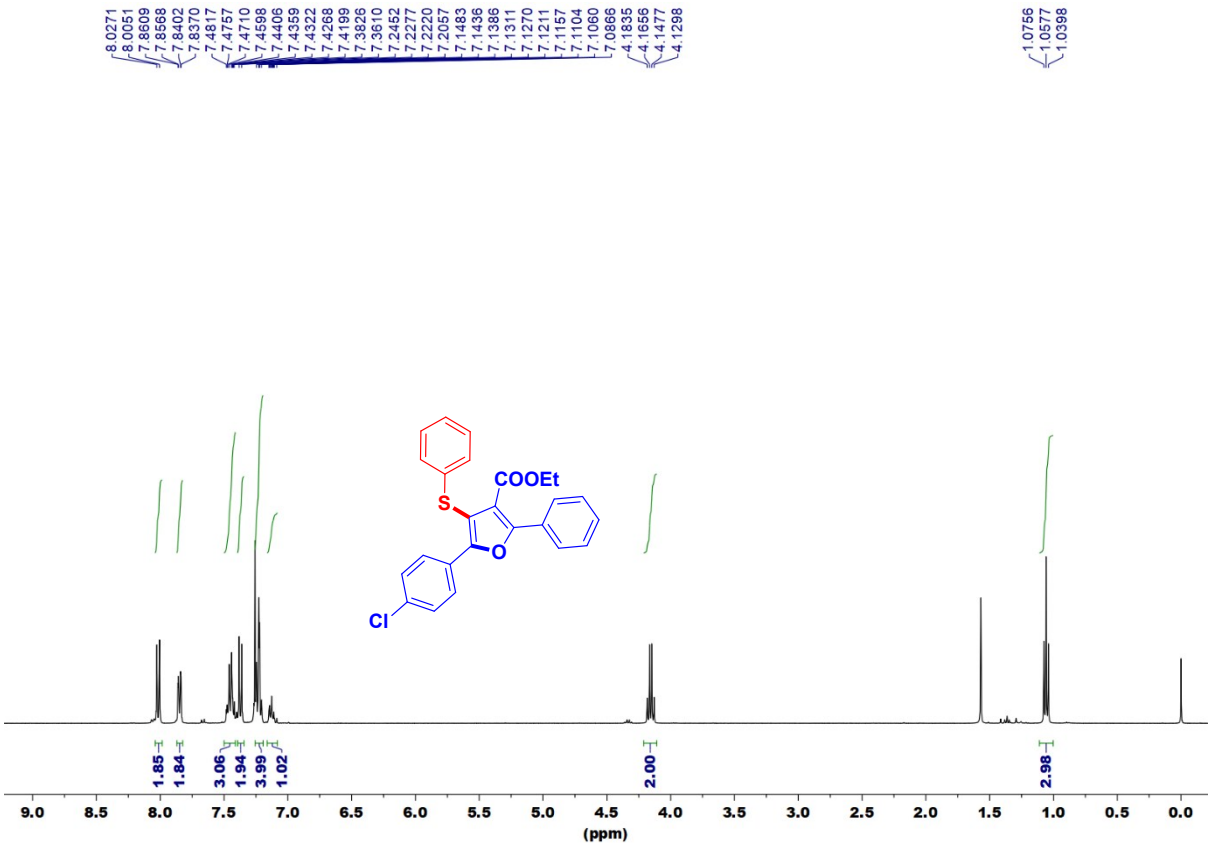

Figure S13. ^{1}H NMR spectrum of compound **3g** (400 MHz, $CDCl_3$)

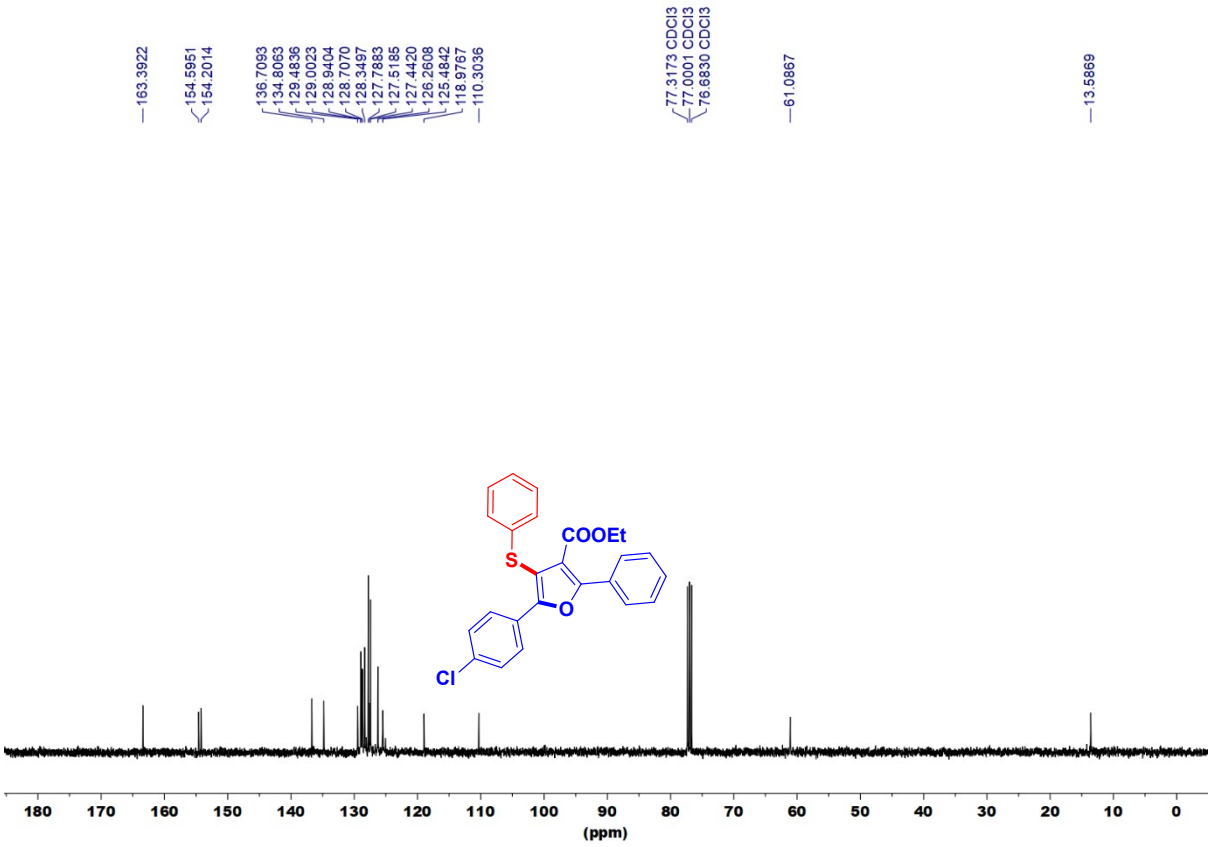

Figure S14. ^{13}C NMR spectrum of compound **3g** (101 MHz, $CDCl_3$)

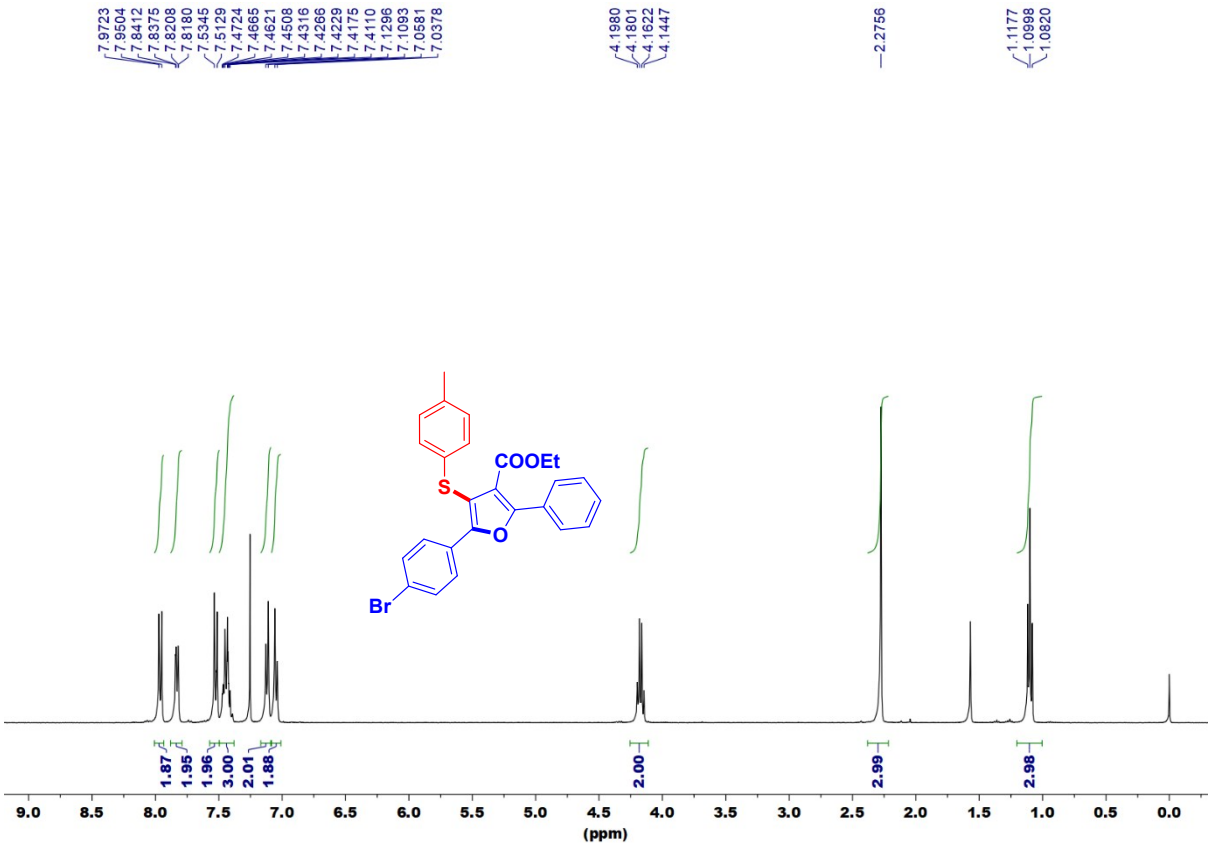

Figure S15. ^{1}H NMR spectrum of compound **3h** (400 MHz, $CDCl_3$)

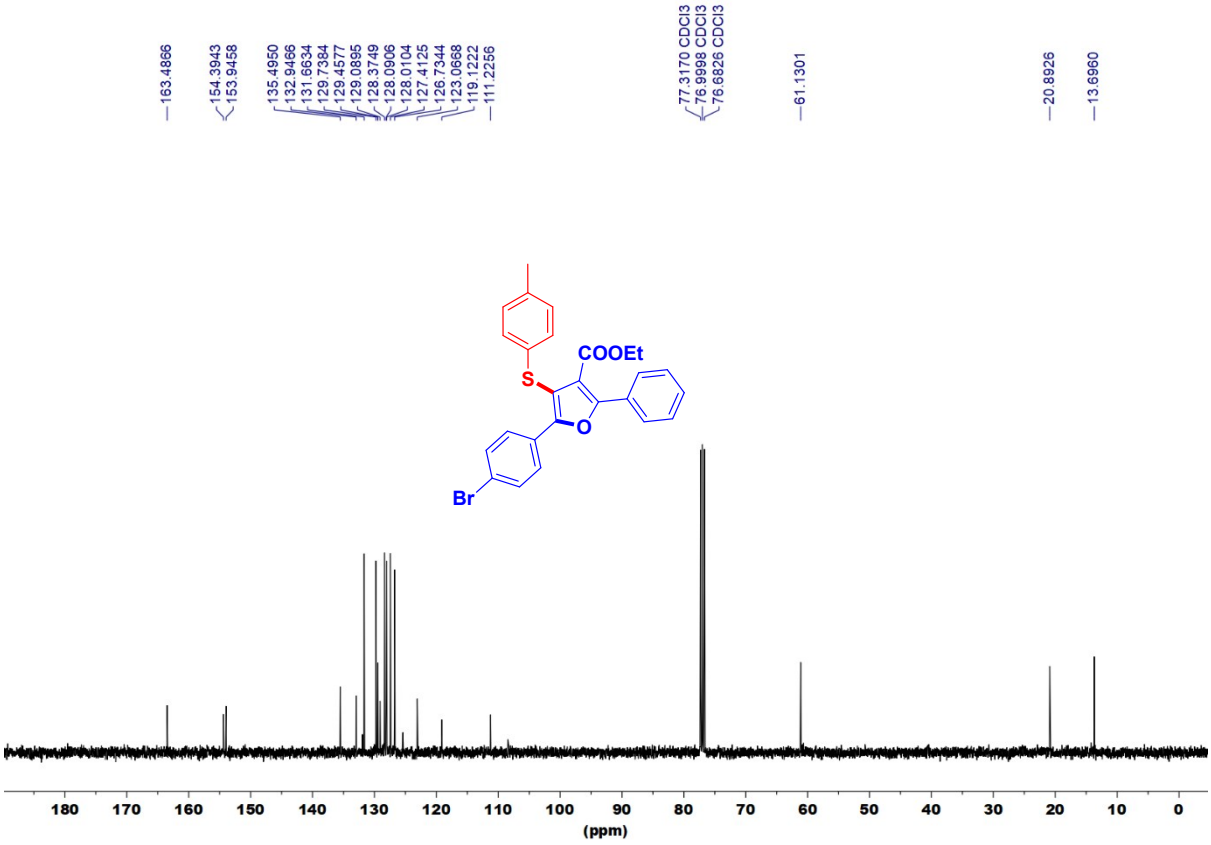

Figure S16. ^{13}C NMR spectrum of compound **3h** (101 MHz, $CDCl_3$)

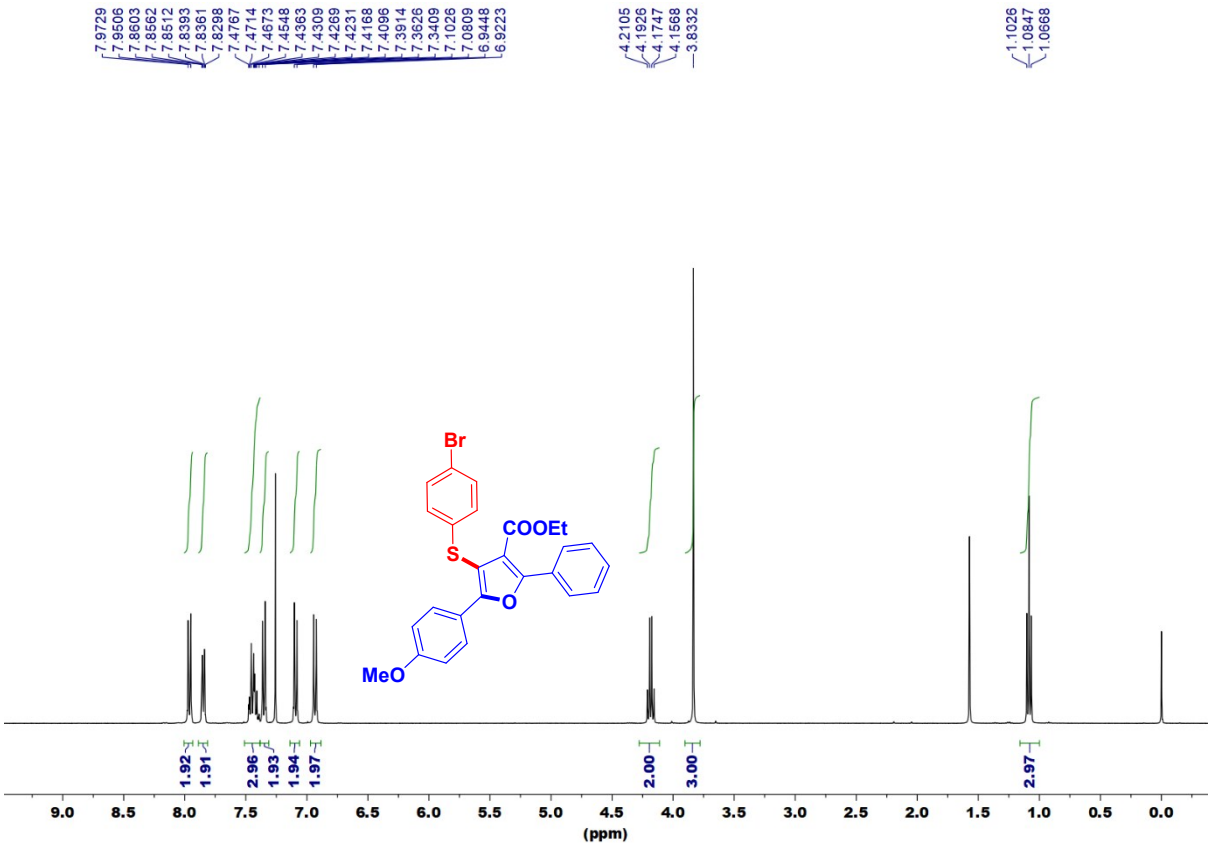

Figure S17. ^{1}H NMR spectrum of compound **3i** (400 MHz, $CDCl_3$)

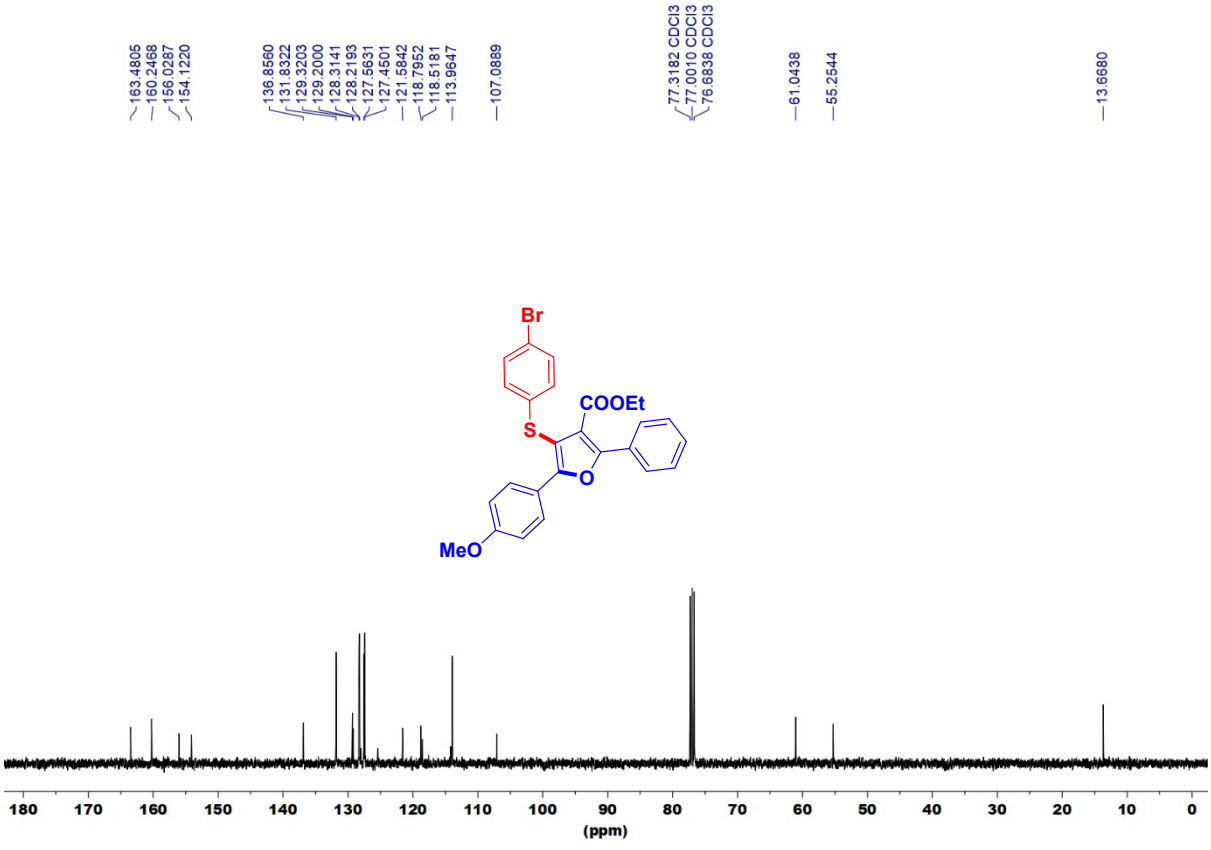

Figure S18. ^{13}C NMR spectrum of compound **3i** (101 MHz, $CDCl_3$)

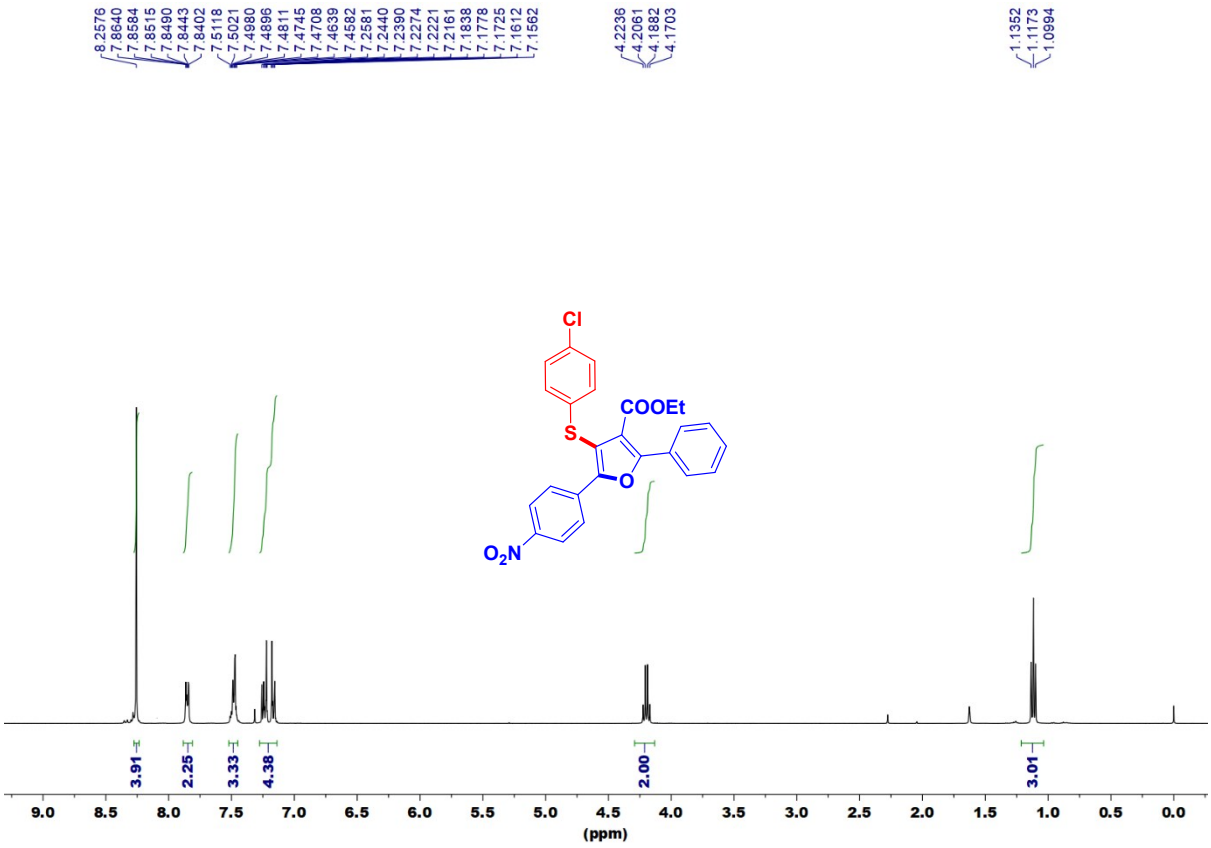

Figure S19. ^{1}H NMR spectrum of compound **3j** (400 MHz, $CDCl_3$)

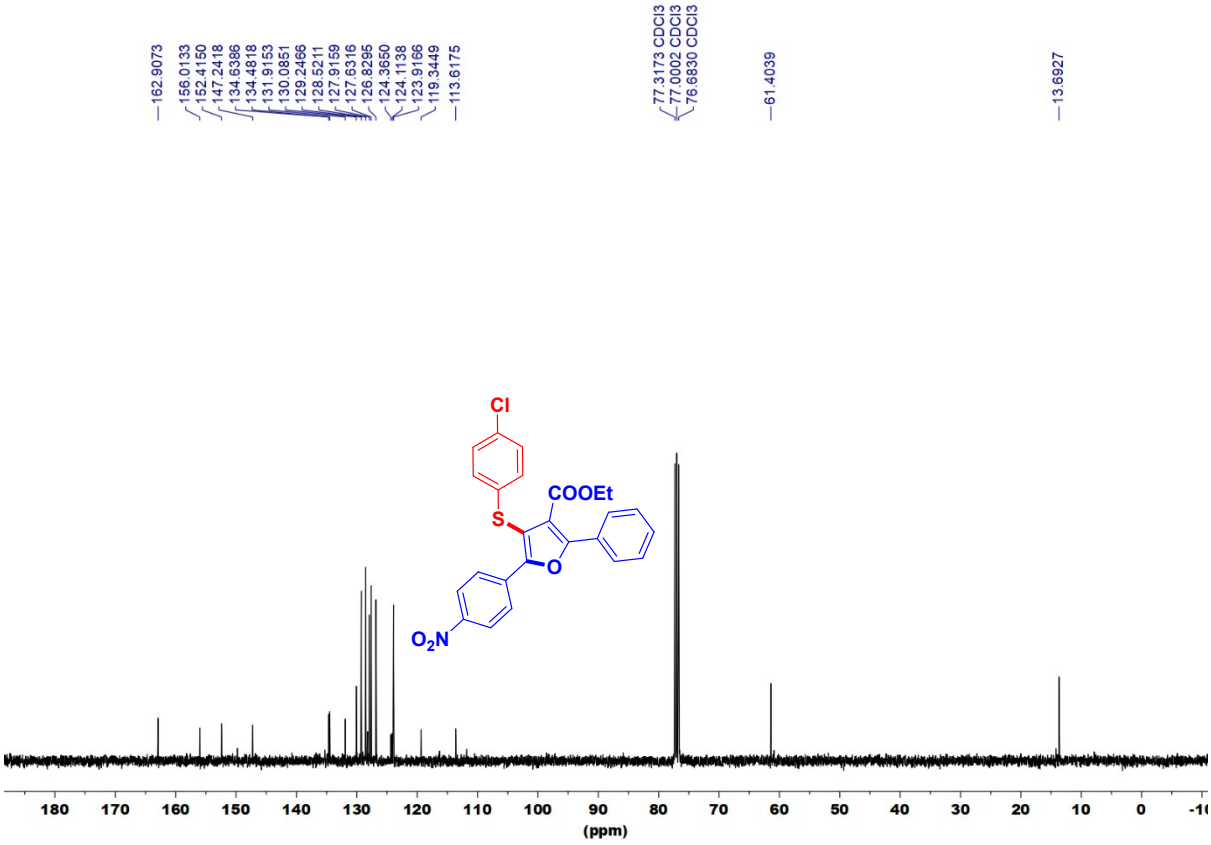

Figure S20. ^{13}C NMR spectrum of compound **3j** (101 MHz, $CDCl_3$)

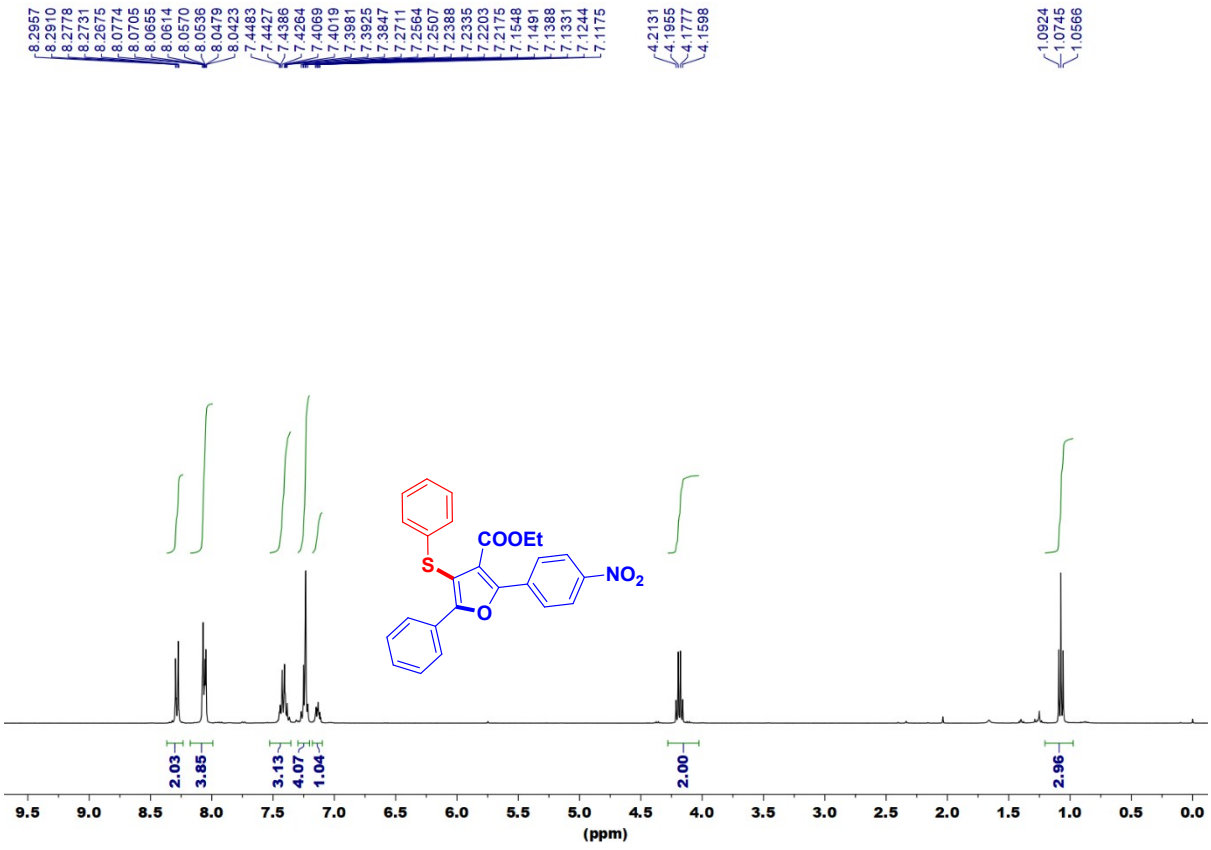

Figure S21. ^{1}H NMR spectrum of compound **3k** (400 MHz, $CDCl_3$)

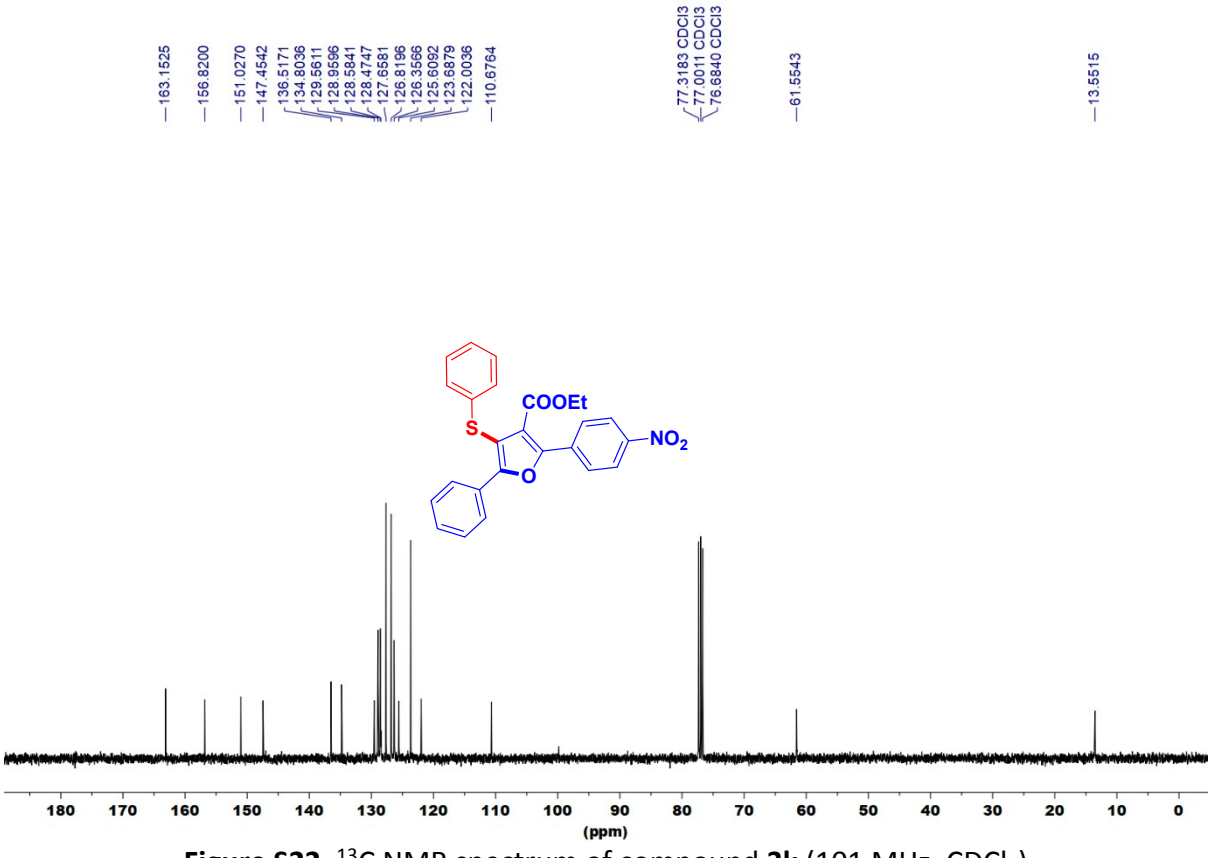

Figure S22. ^{13}C NMR spectrum of compound **3k** (101 MHz, $CDCl_3$)

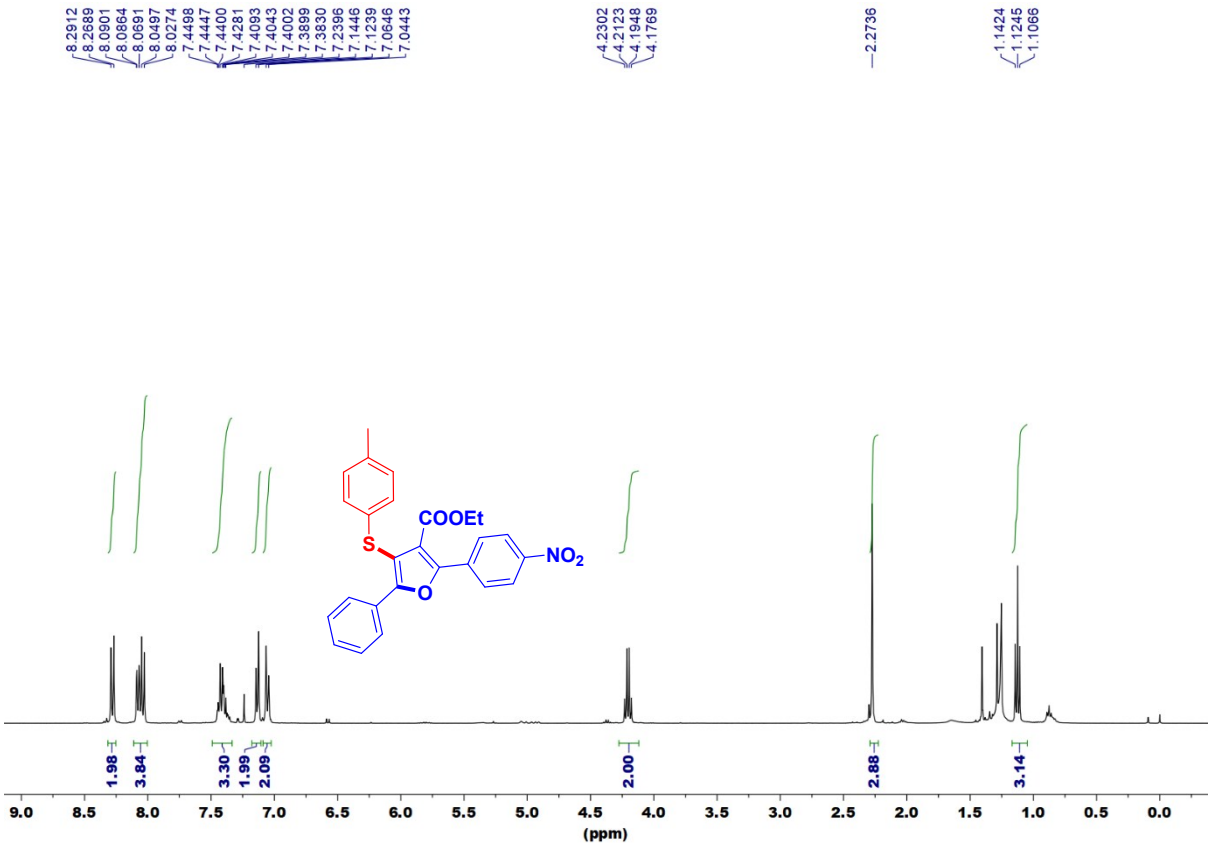

Figure S23. ^{1}H NMR spectrum of compound **3l** (400 MHz, $CDCl_3$)

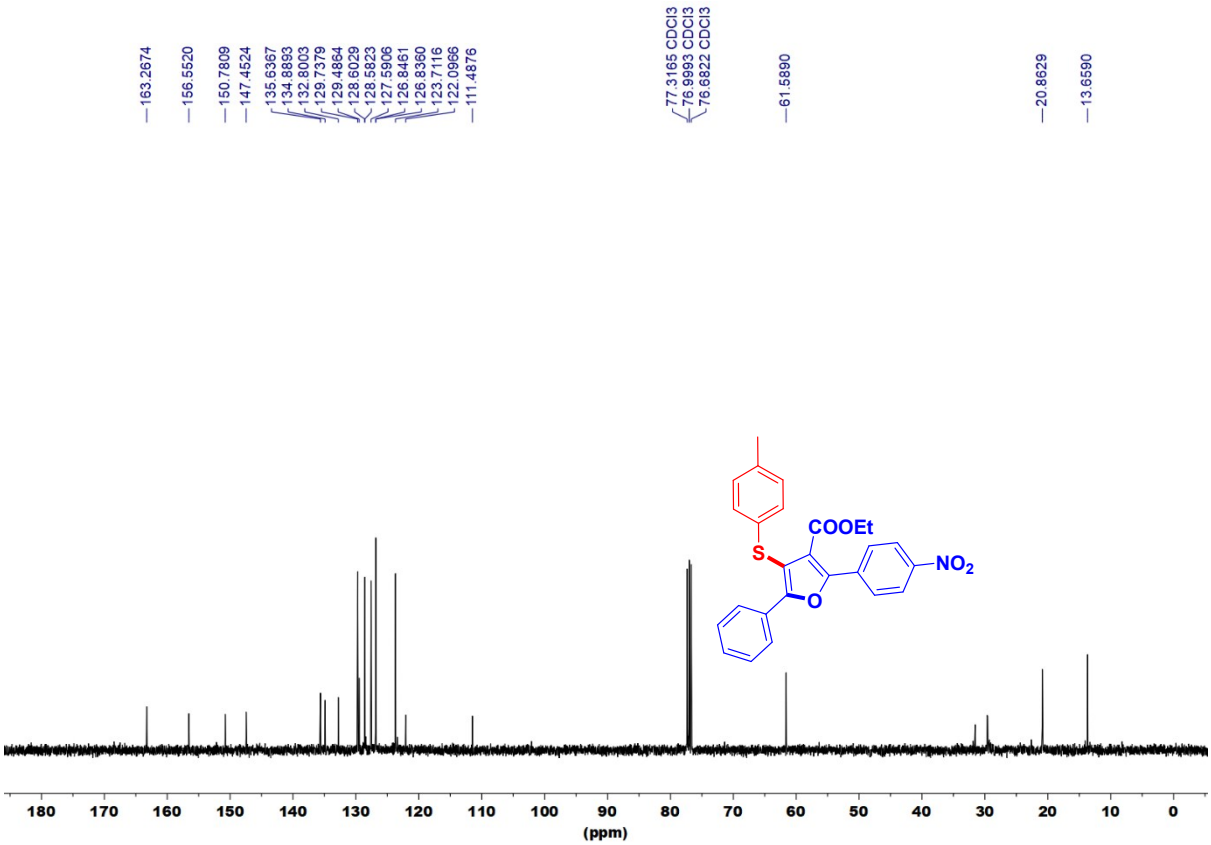

Figure S24. ^{13}C NMR spectrum of compound **3l** (101 MHz, $CDCl_3$)

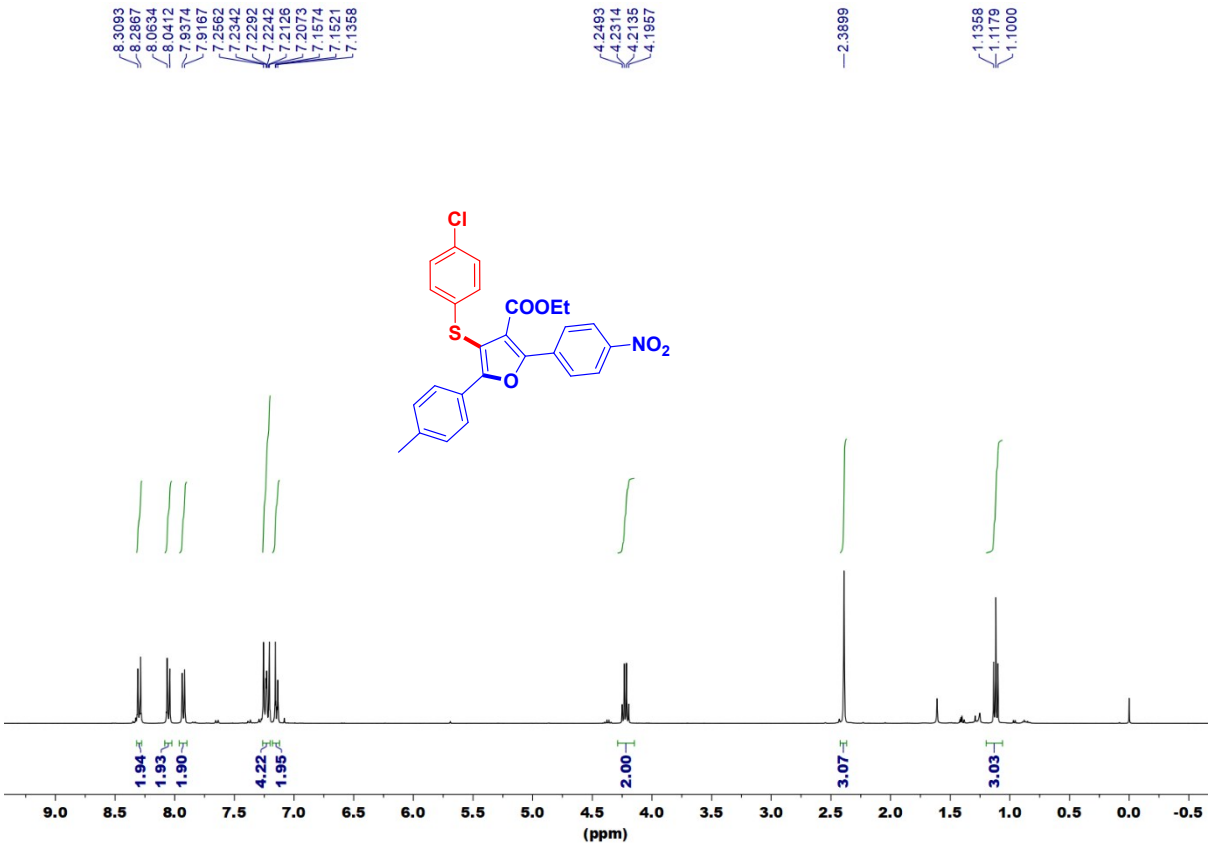

Figure S25. ^{1}H NMR spectrum of compound **3m** (400 MHz, $CDCl_3$)

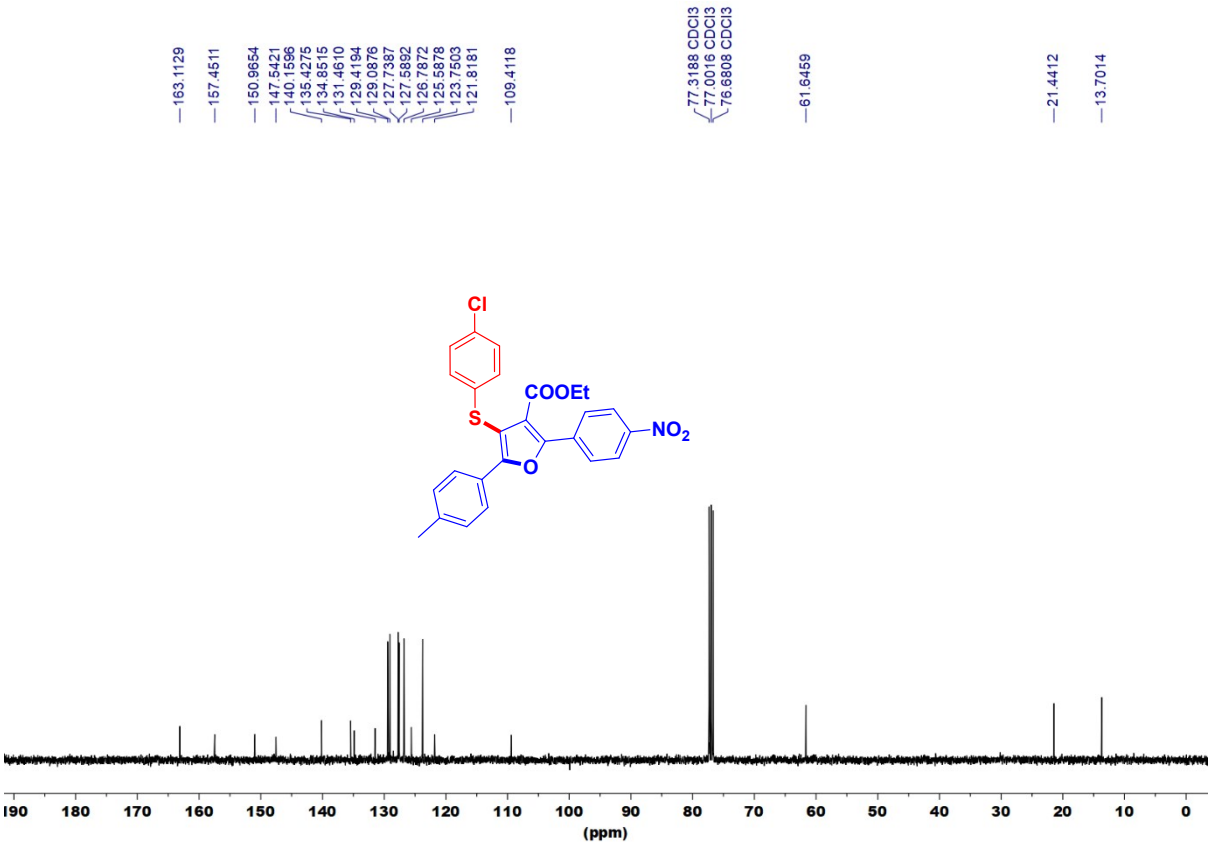

Figure S26. ^{13}C NMR spectrum of compound **3m** (101 MHz, $CDCl_3$)

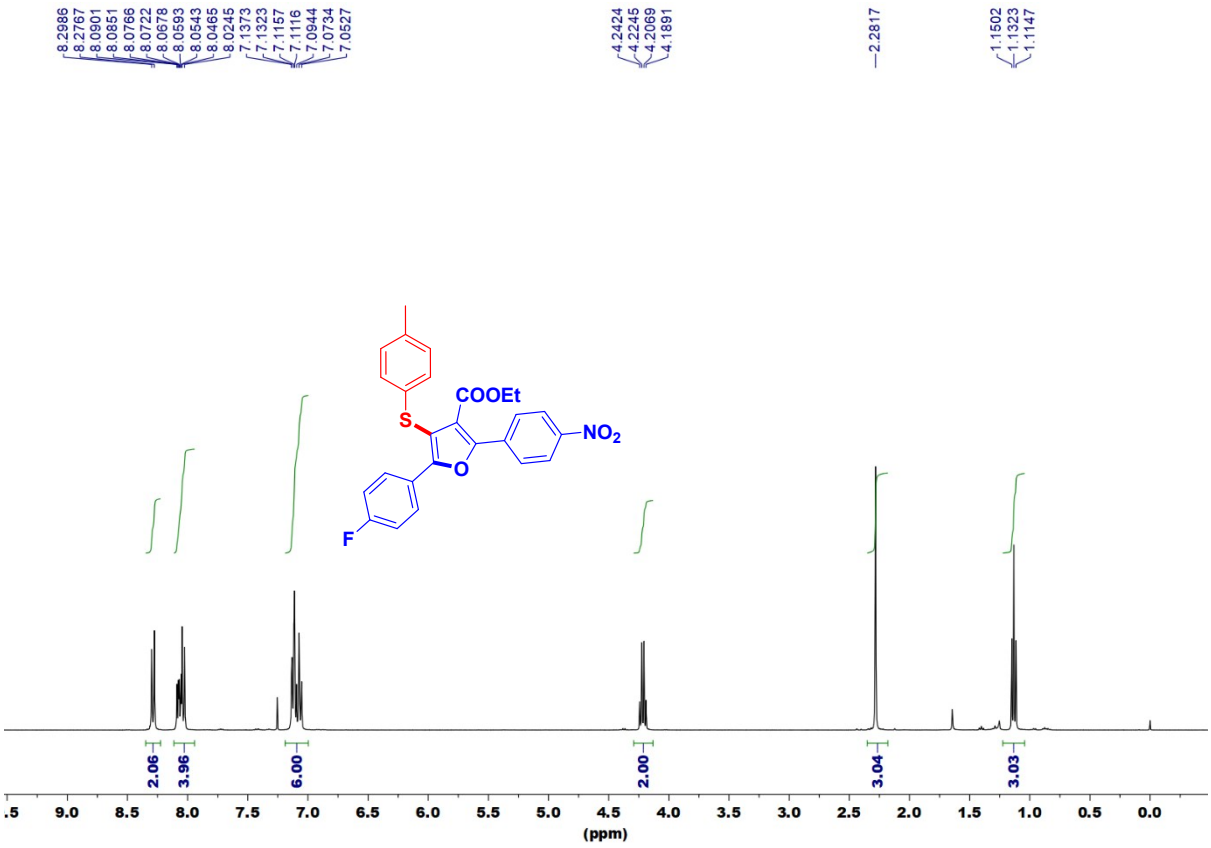

Figure S27. ^{1}H NMR spectrum of compound **3n** (400 MHz, $CDCl_3$)

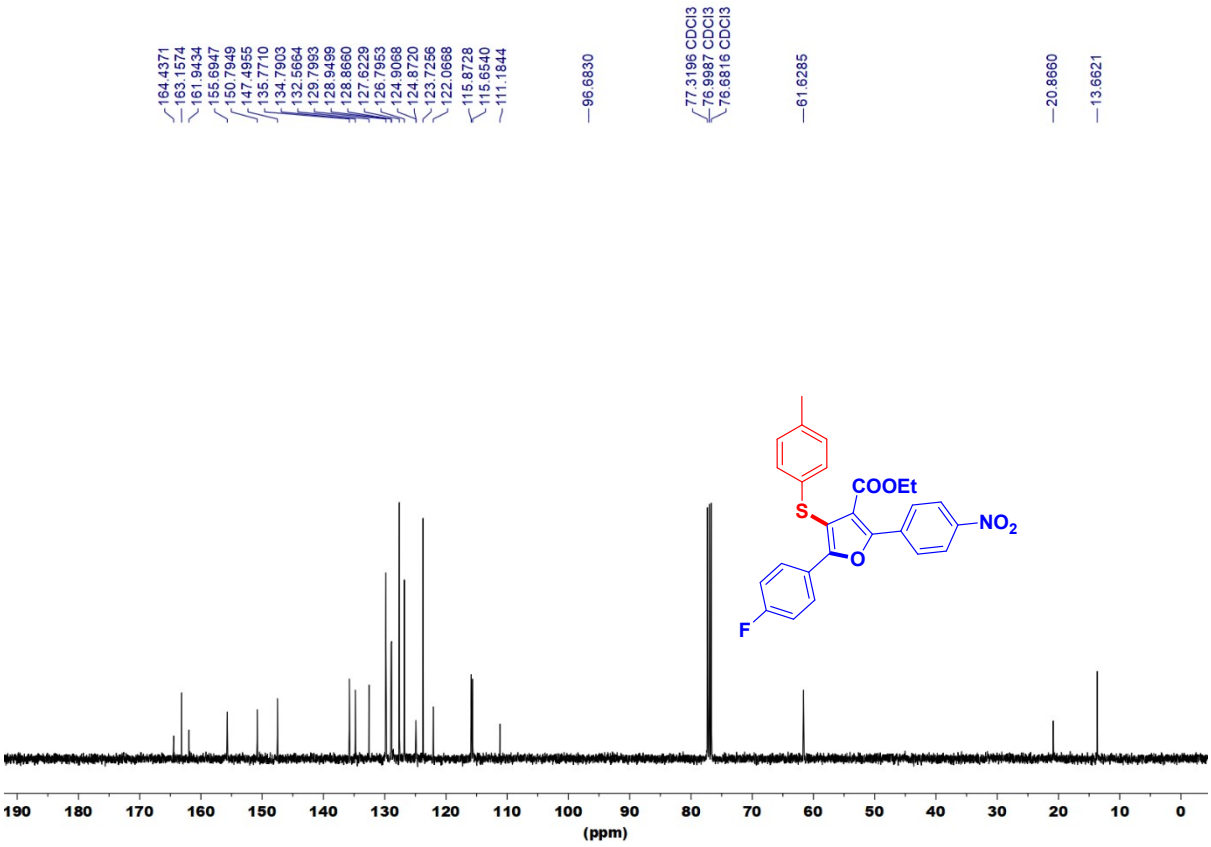

Figure S28. ^{13}C NMR spectrum of compound **3n** (101 MHz, $CDCl_3$)

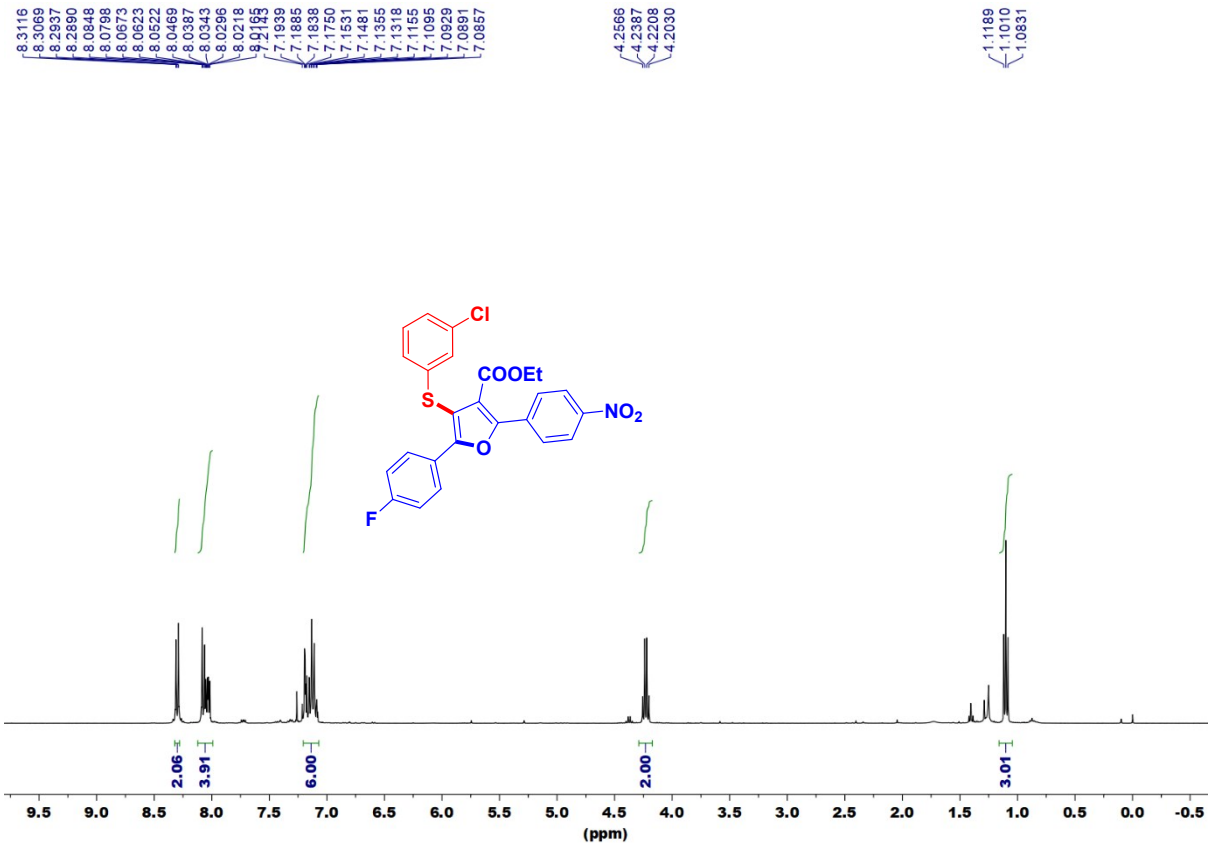

Figure S29. ^{1}H NMR spectrum of compound **3o** (400 MHz, $CDCl_3$)

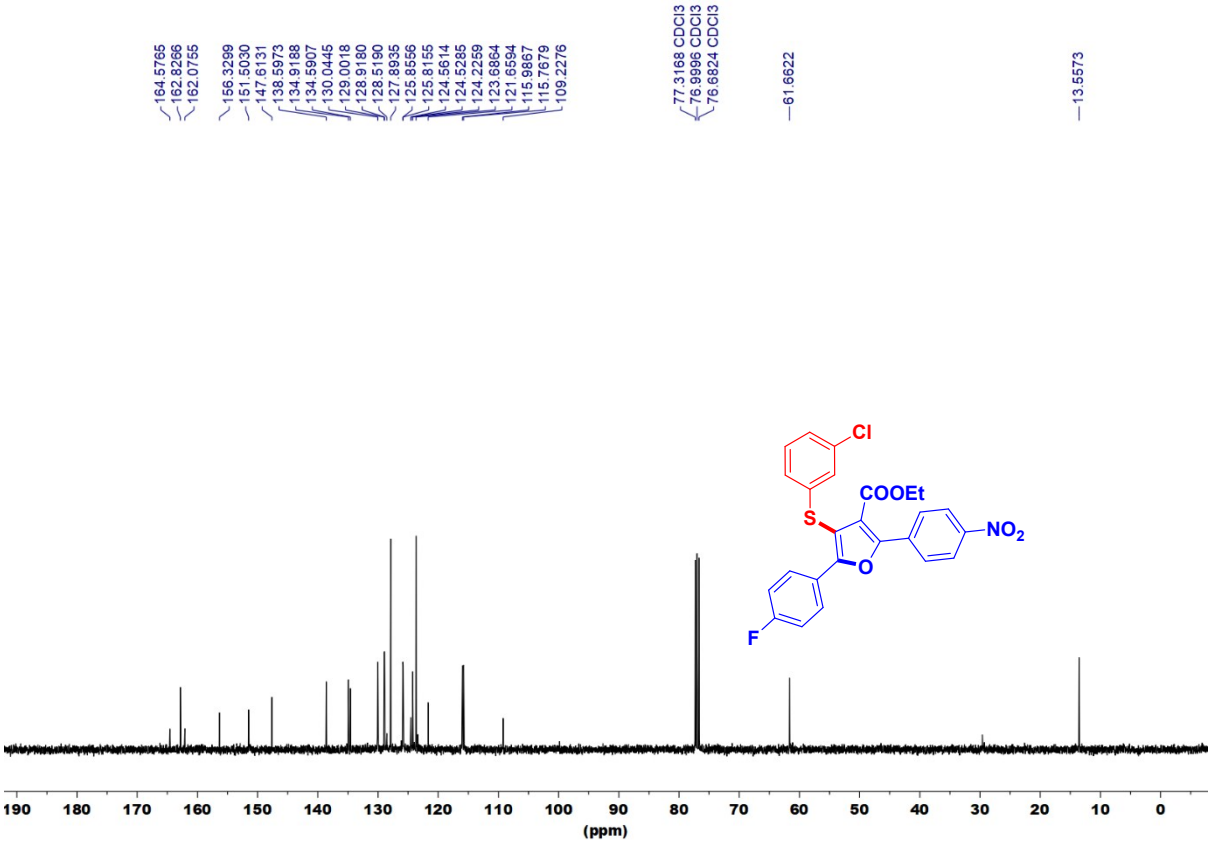

Figure S30. ^{13}C NMR spectrum of compound **3o** (101 MHz, $CDCl_3$)

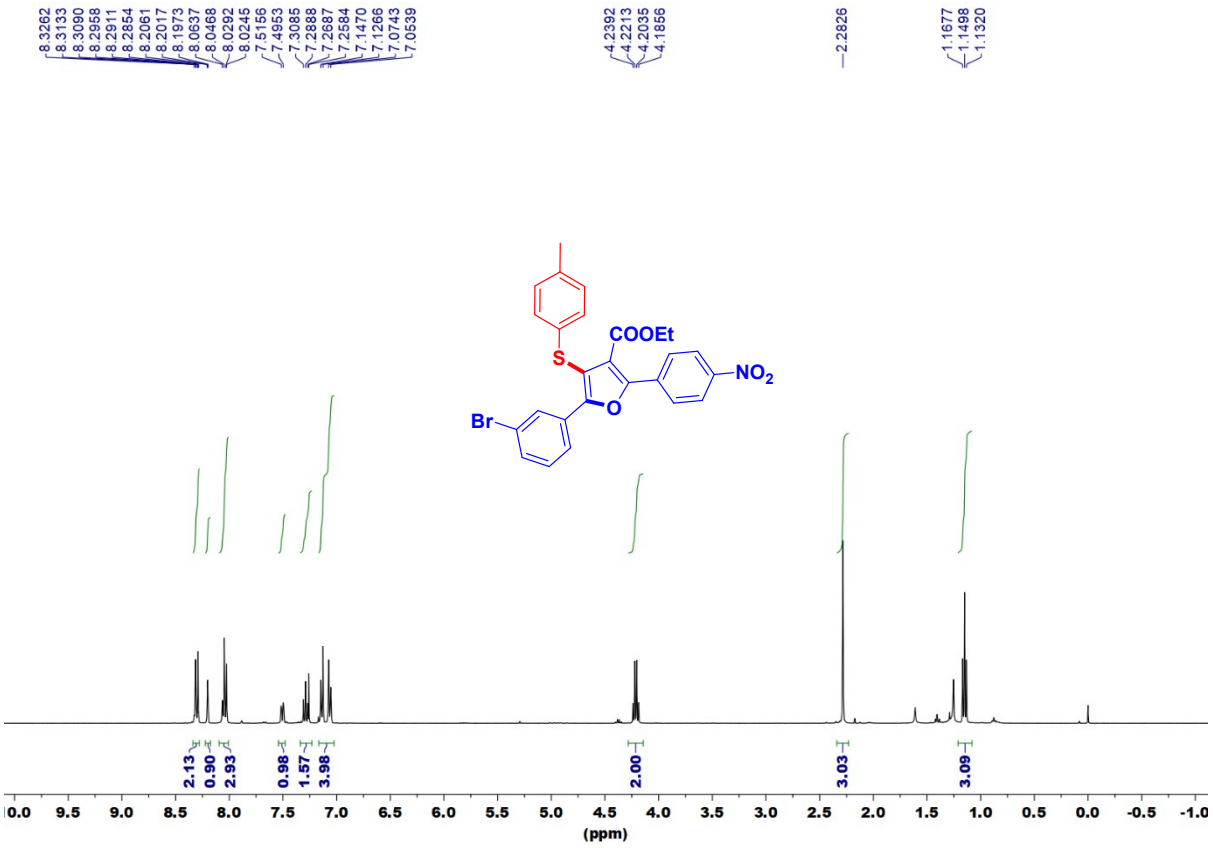

Figure S31. ^{1}H NMR spectrum of compound **3p** (400 MHz, $CDCl_3$)

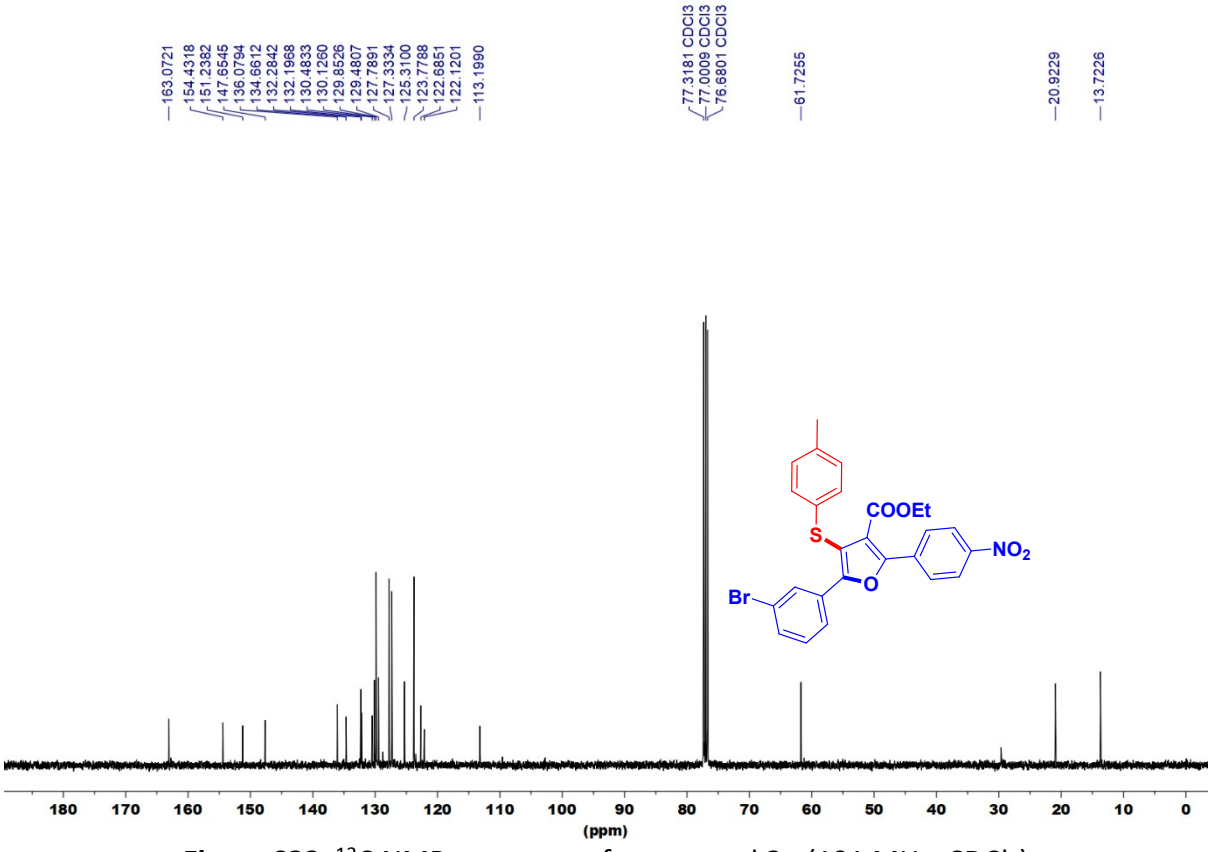

Figure S32. ^{13}C NMR spectrum of compound **3p** (101 MHz, $CDCl_3$)

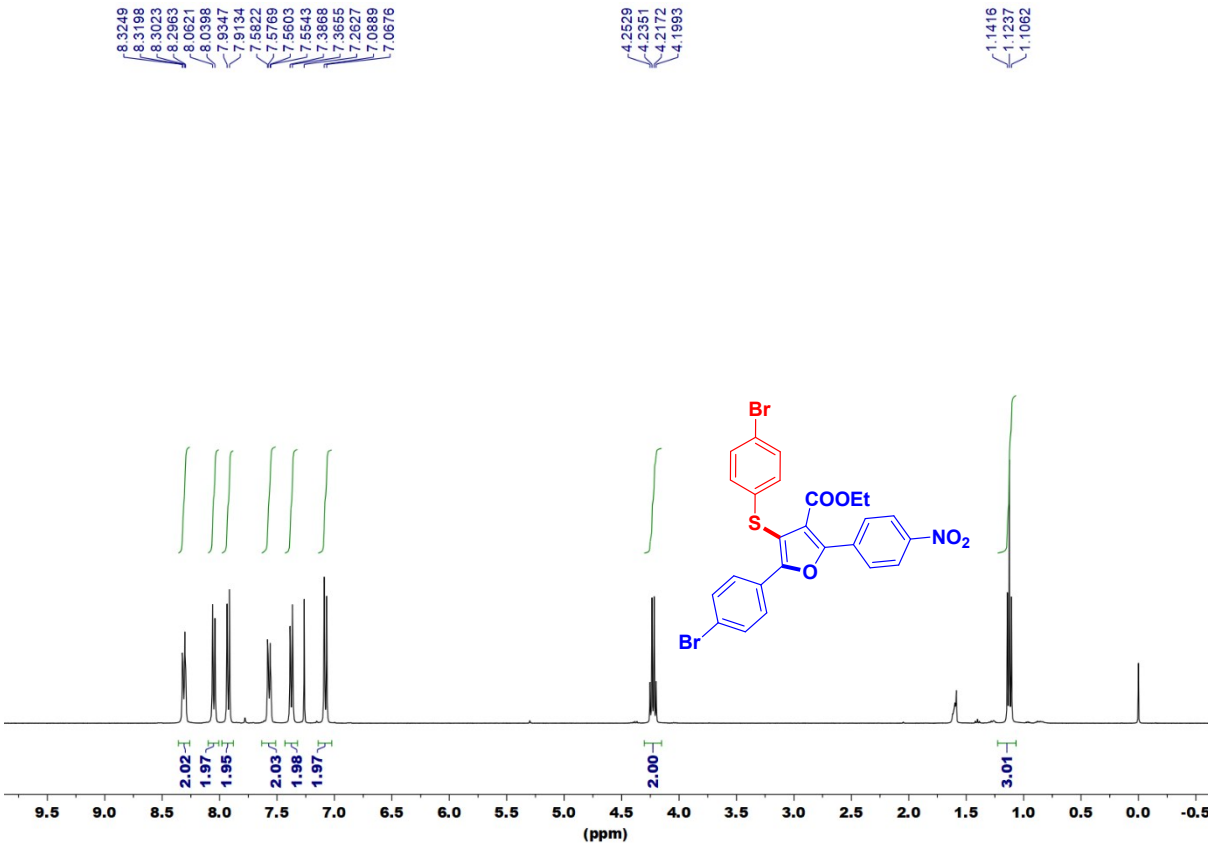

Figure S33. ^{1}H NMR spectrum of compound **3q** (400 MHz, $CDCl_3$)

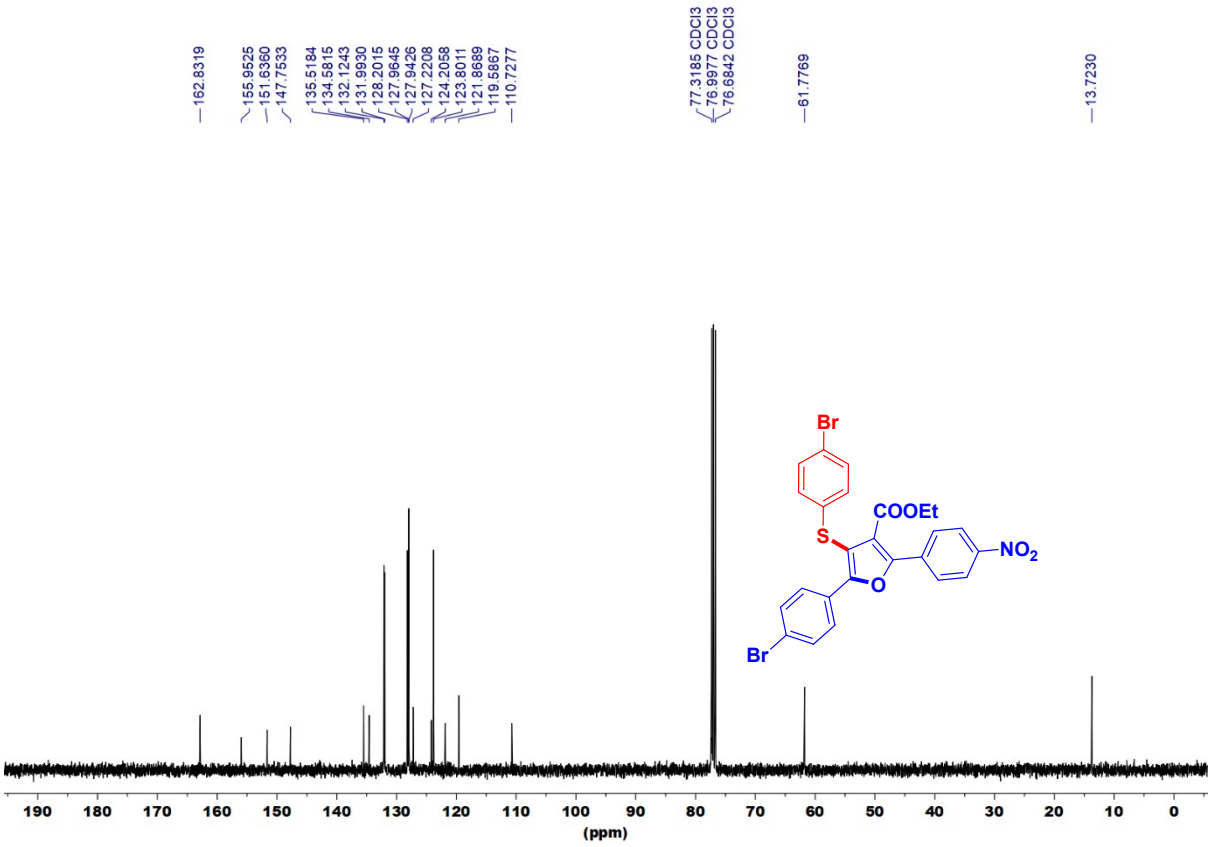

Figure S34. ^{13}C NMR spectrum of compound **3q** (101 MHz, $CDCl_3$)

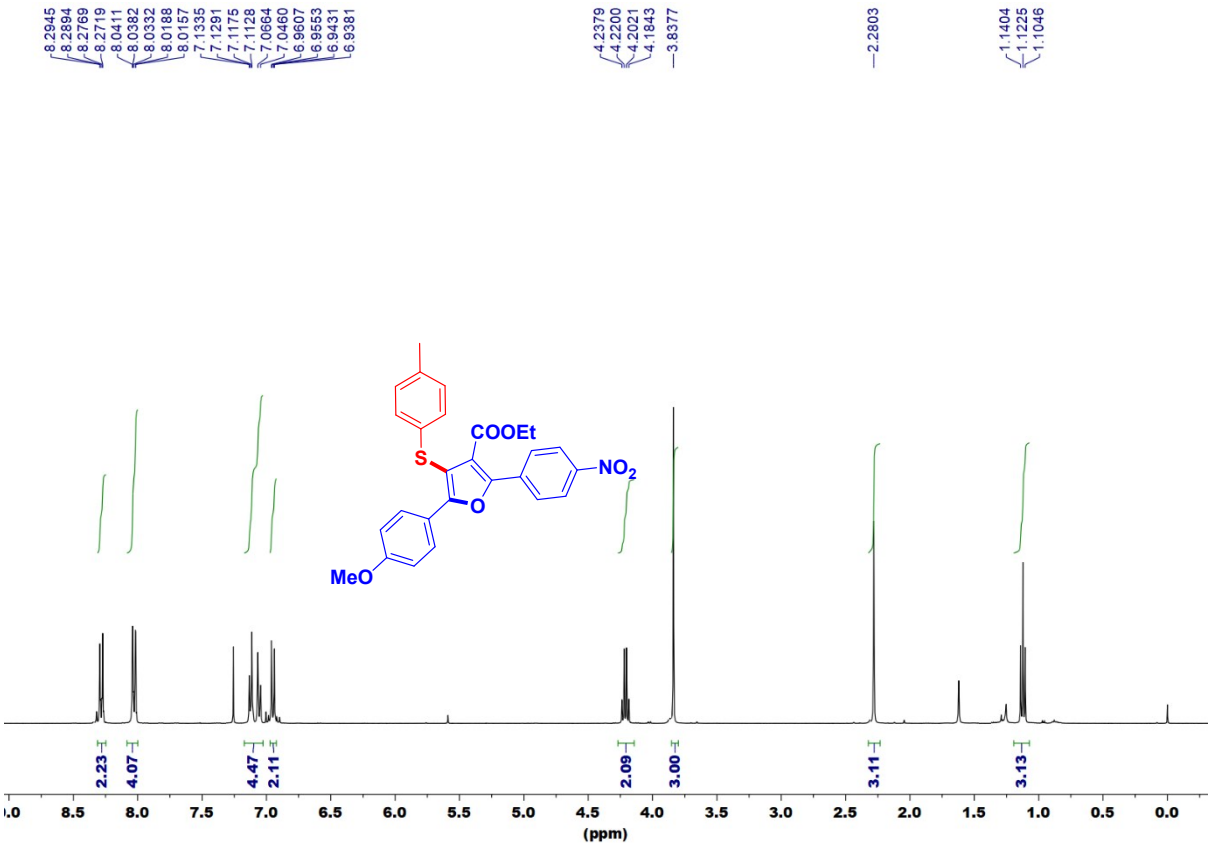

Figure S35. ^{1}H NMR spectrum of compound **3r** (400 MHz, $CDCl_3$)

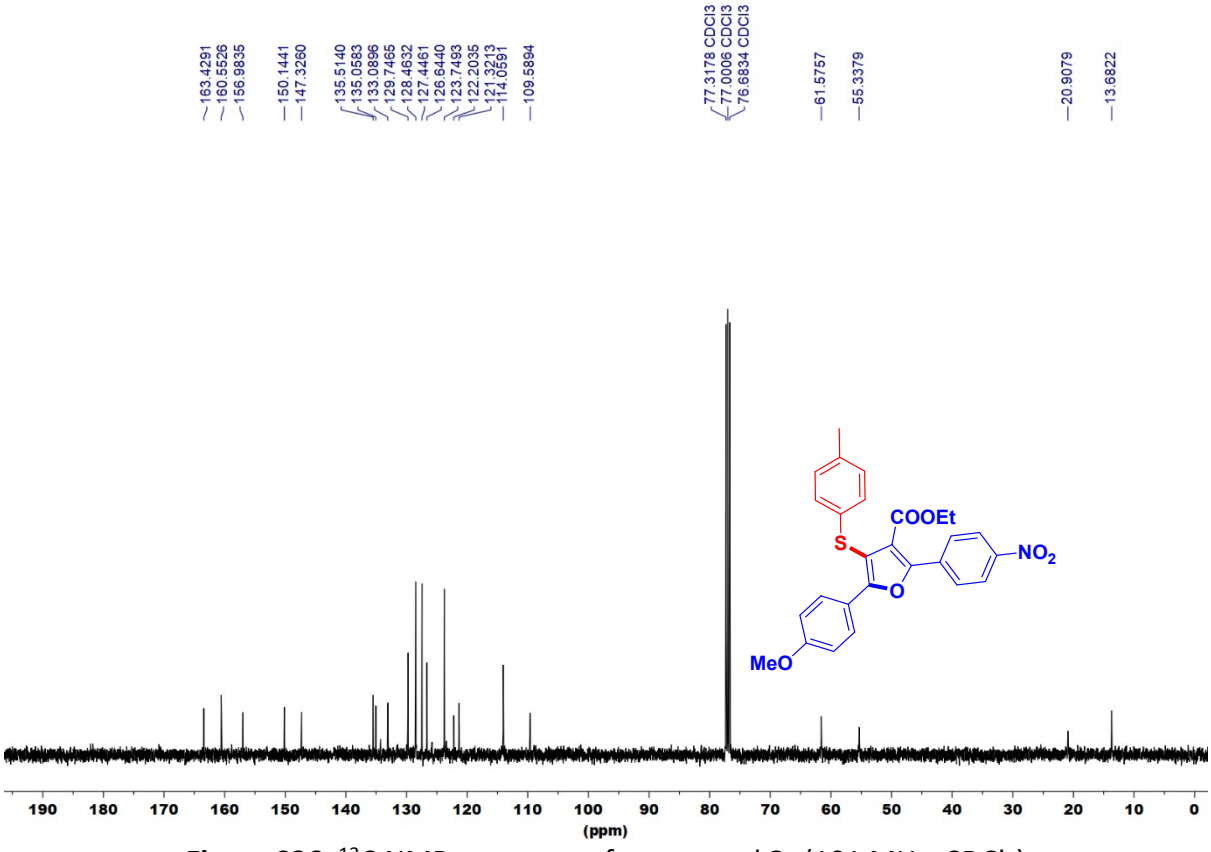

Figure S36. ^{13}C NMR spectrum of compound **3r** (101 MHz, $CDCl_3$)

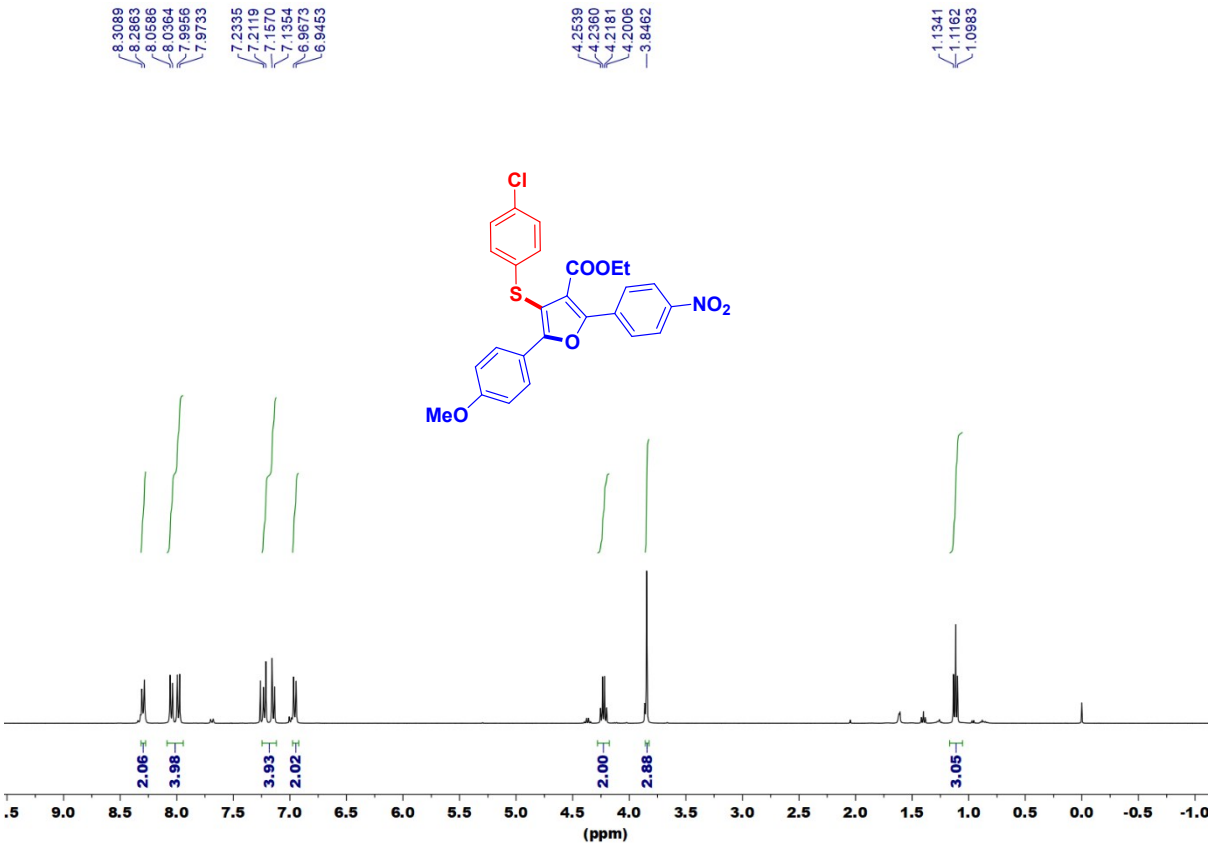

Figure S37. ^{1}H NMR spectrum of compound **3s** (400 MHz, $CDCl_3$)

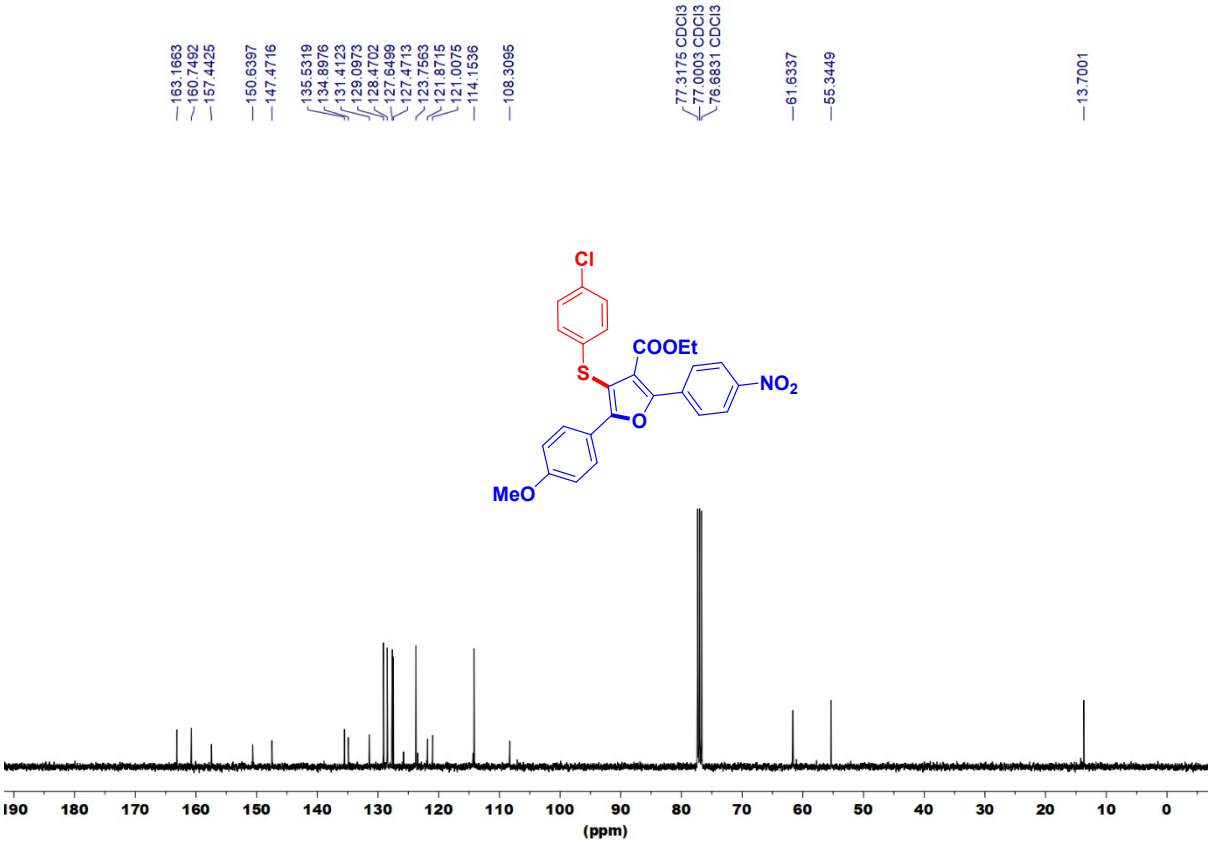

Figure S38. ^{13}C NMR spectrum of compound **3s** (101 MHz, $CDCl_3$)

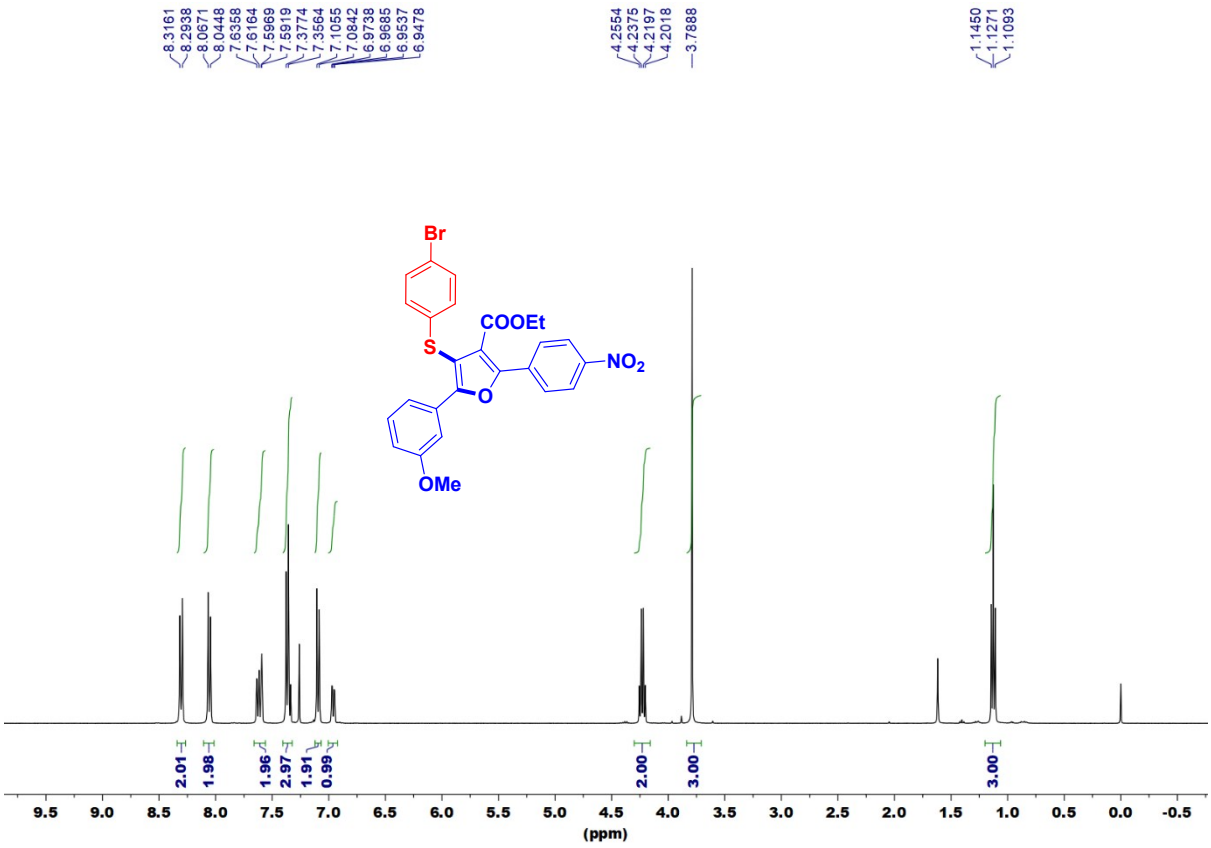

Figure S39. ^{1}H NMR spectrum of compound **3t** (400 MHz, $CDCl_3$)

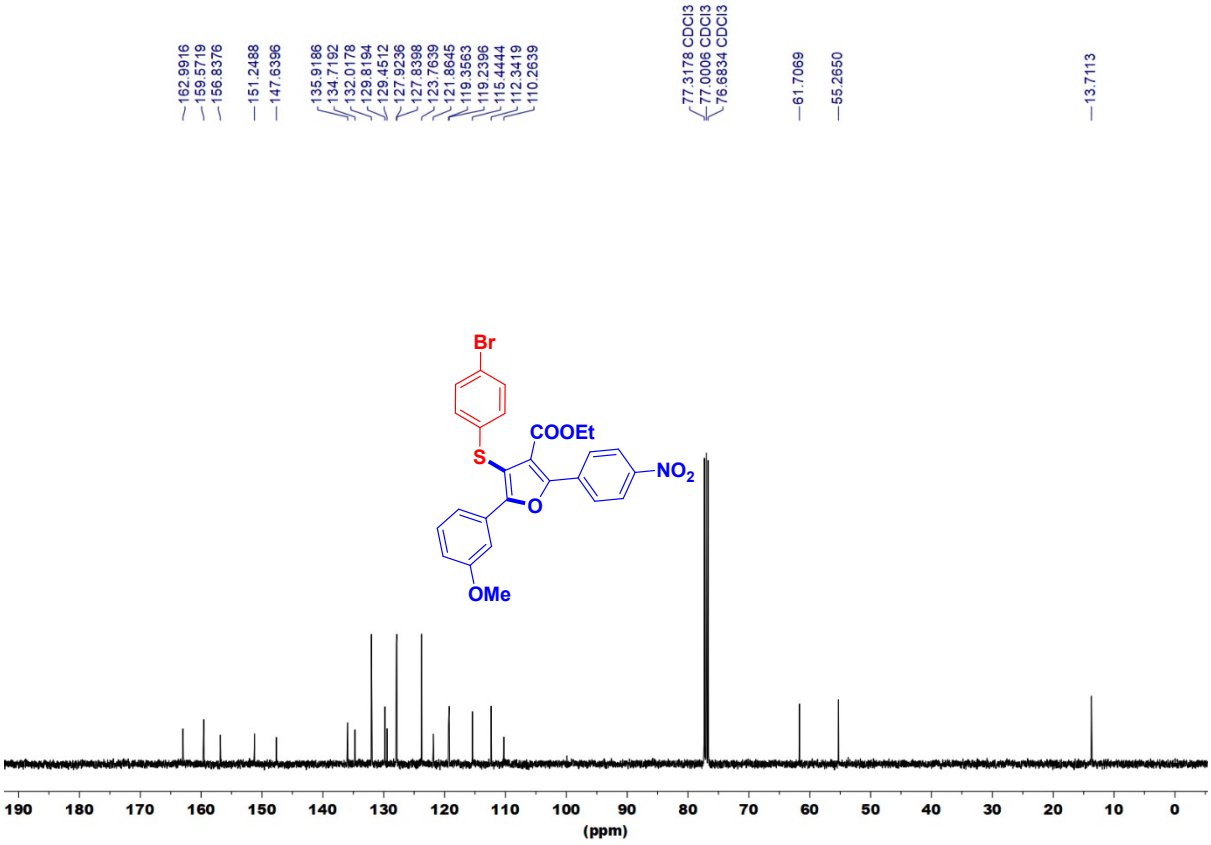

Figure S40. ^{13}C NMR spectrum of compound **3t** (101 MHz, $CDCl_3$)

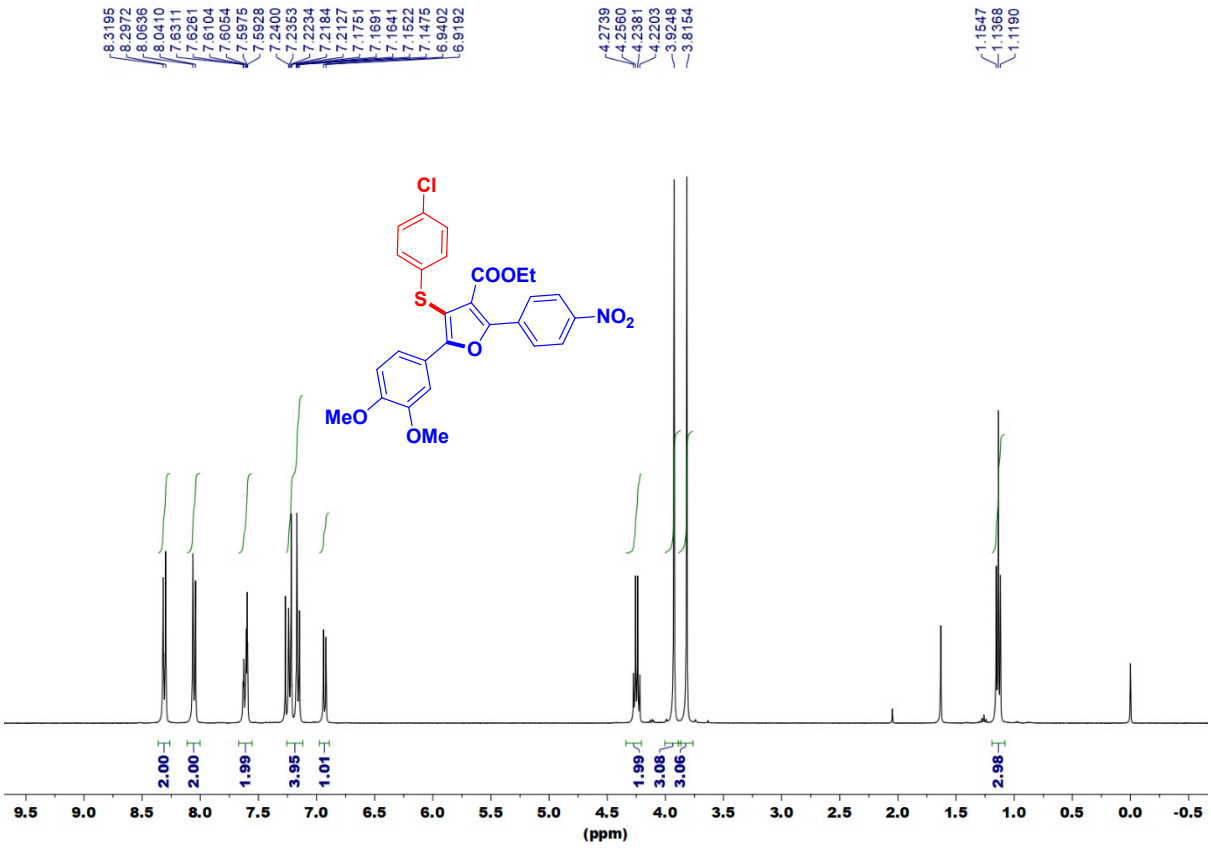

Figure S41. ^{1}H NMR spectrum of compound **3u** (400 MHz, $CDCl_3$)

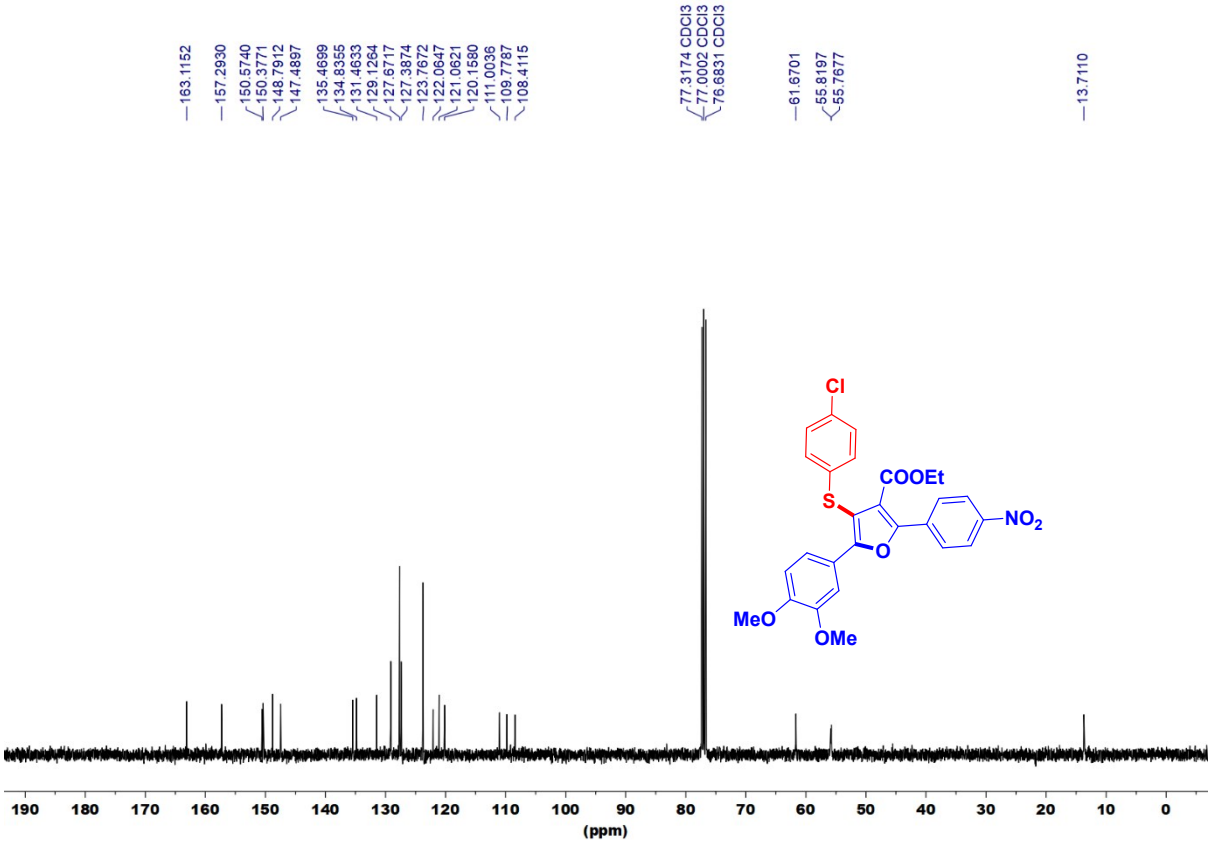

Figure S42. ^{13}C NMR spectrum of compound **3u** (101 MHz, $CDCl_3$)

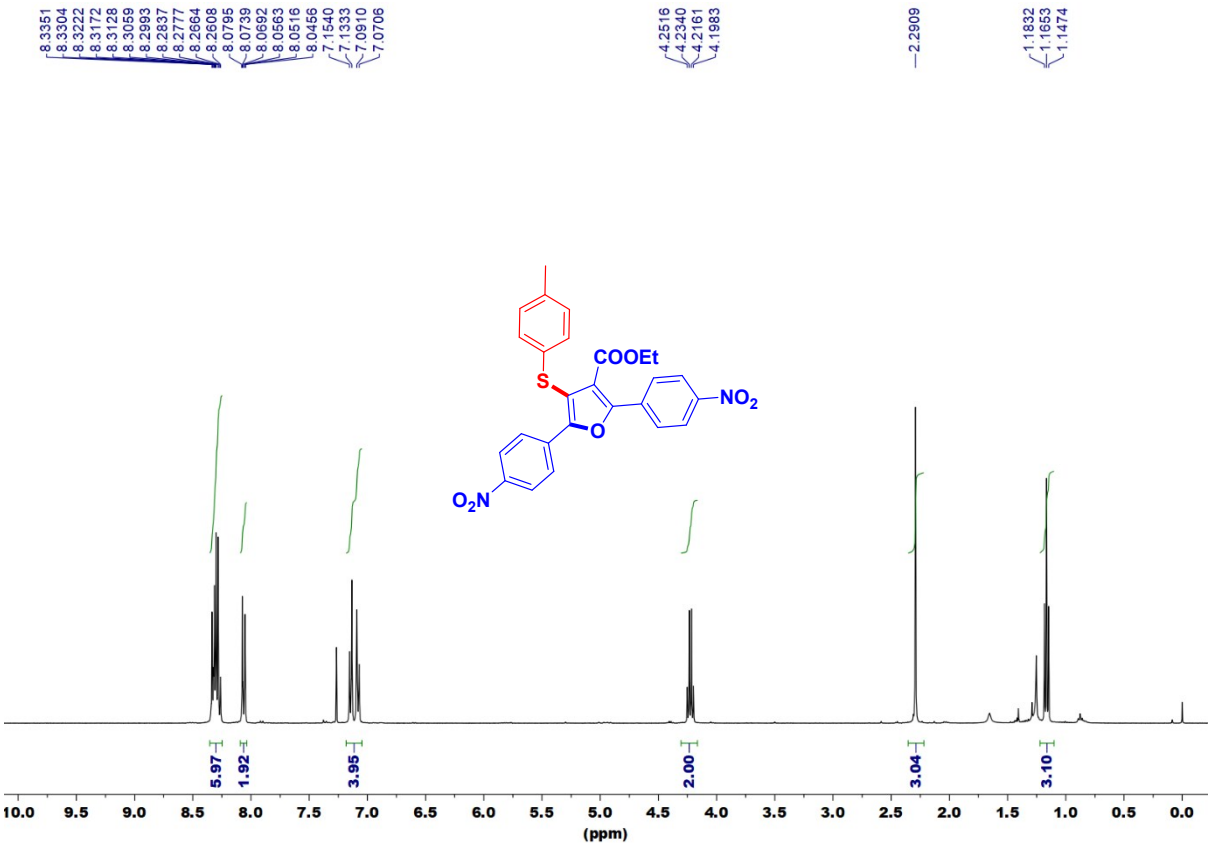

Figure S43. ^{1}H NMR spectrum of compound **3v** (400 MHz, $CDCl_3$)

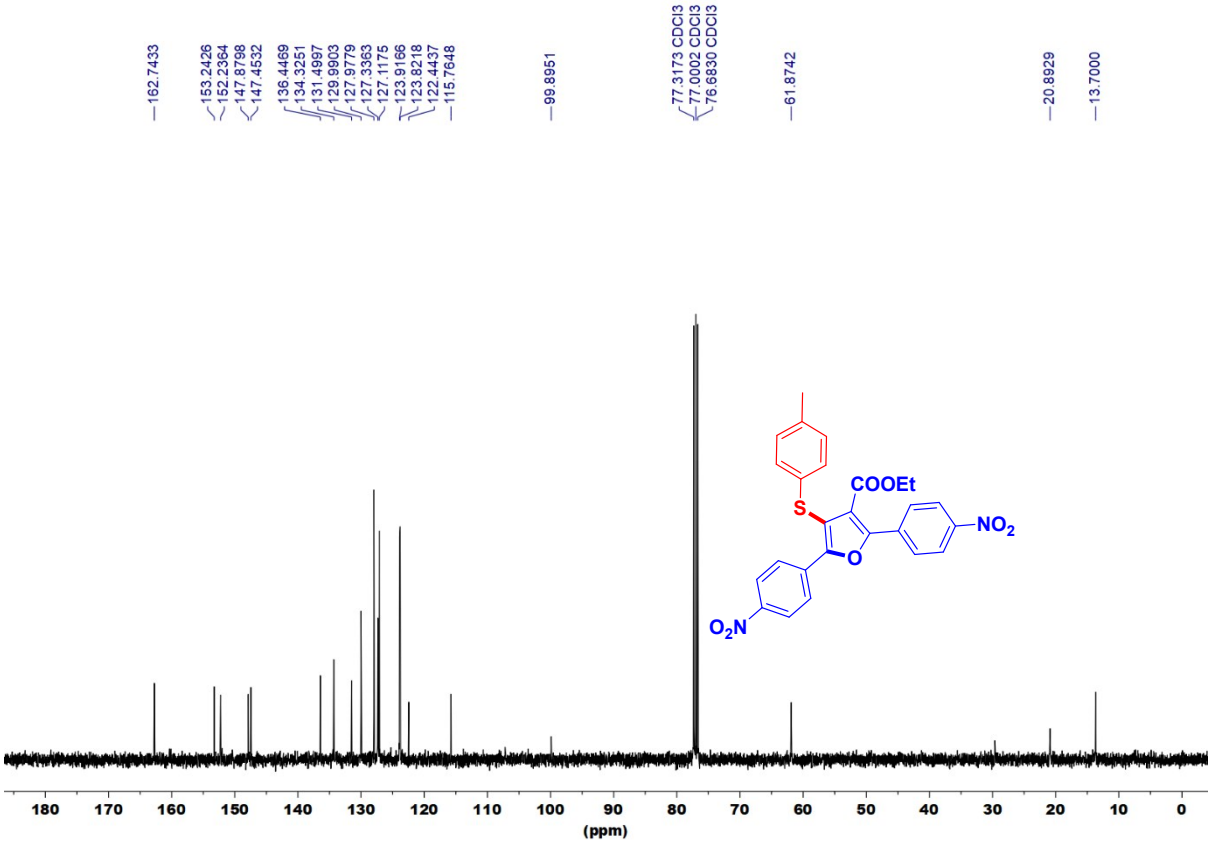

Figure S44. ^{13}C NMR spectrum of compound **3v** (101 MHz, $CDCl_3$)

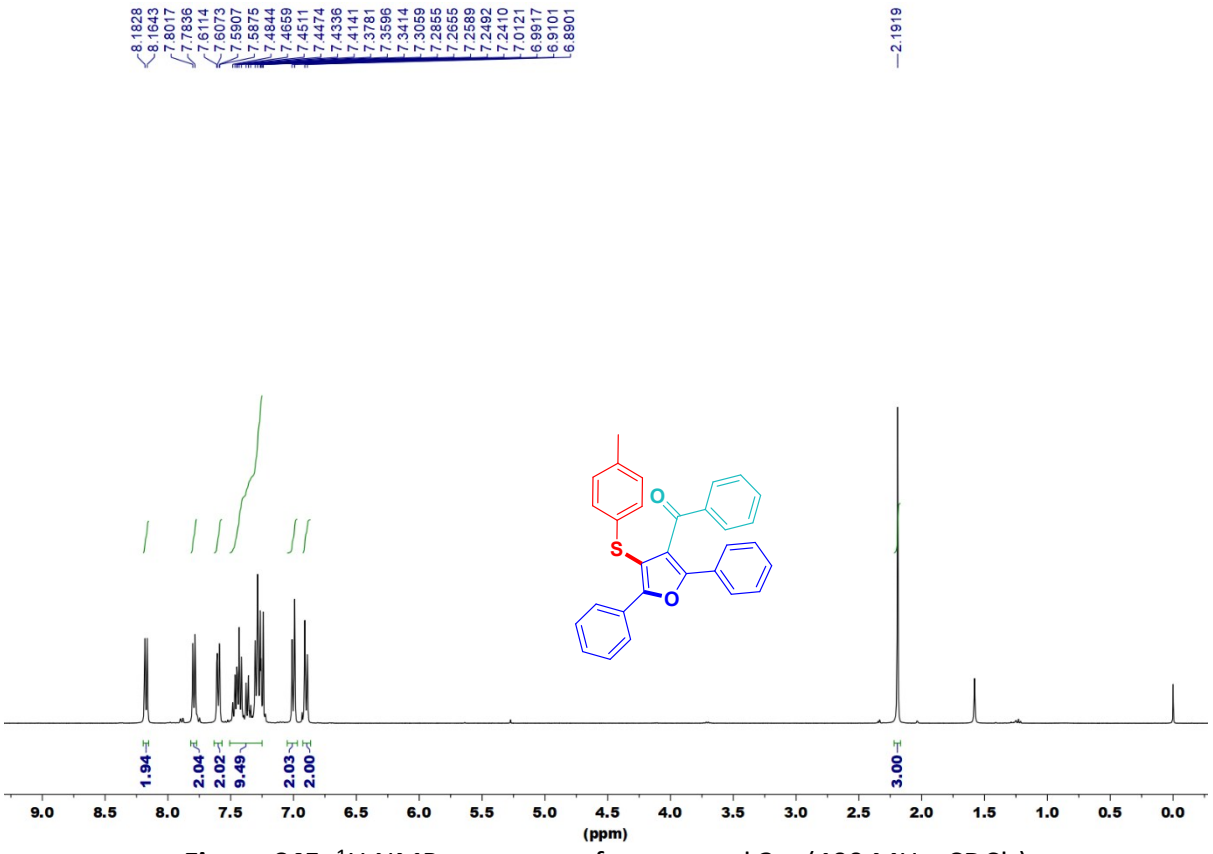

Figure S45. ^{1}H NMR spectrum of compound **3w** (400 MHz, $CDCl_3$)

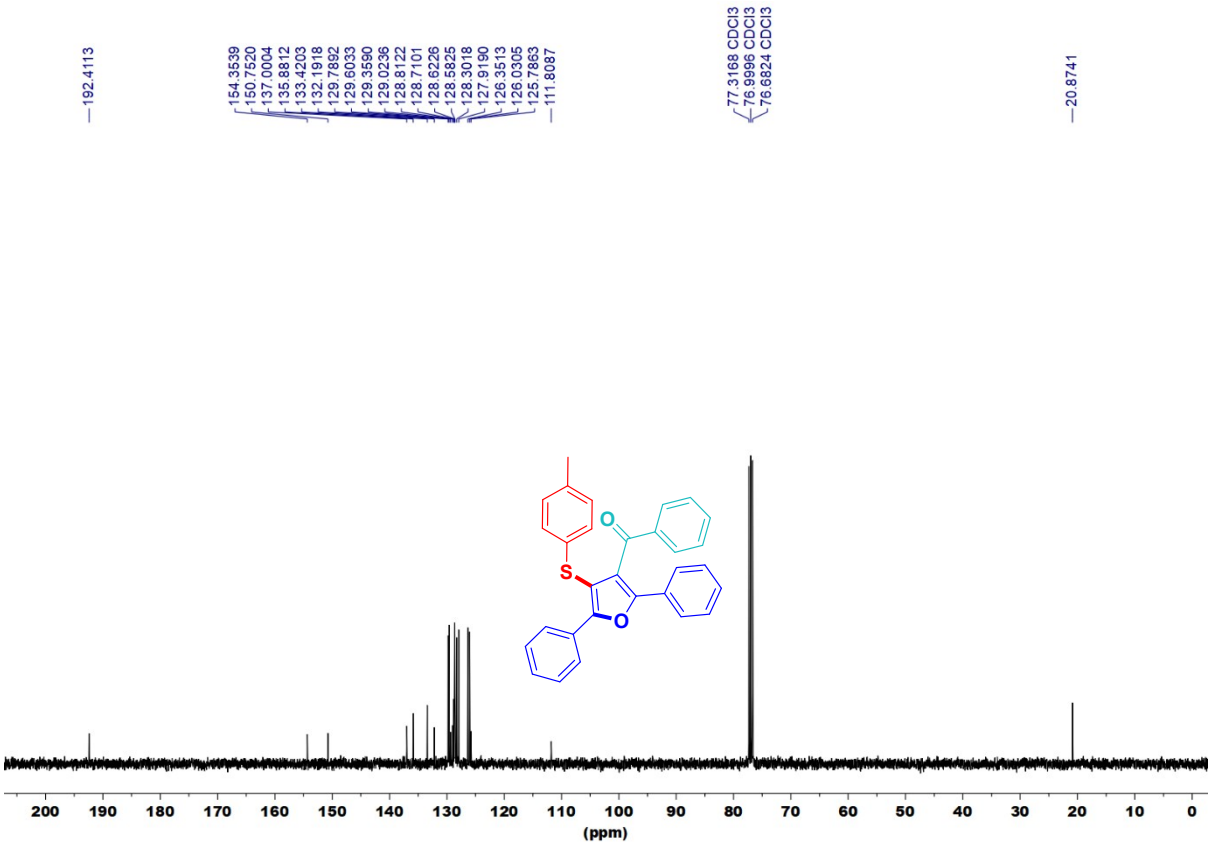

Figure S46. ^{13}C NMR spectrum of compound **3w** (101 MHz, $CDCl_3$)

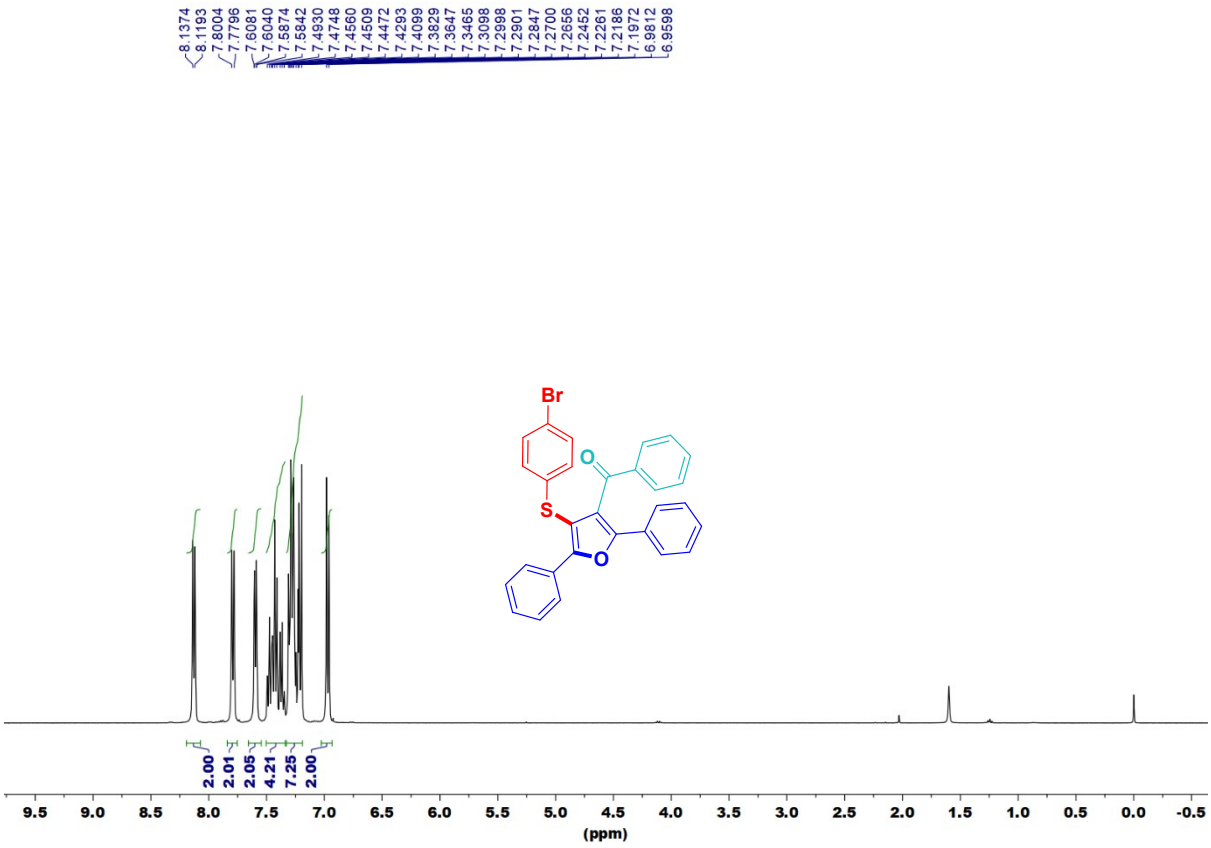

Figure S47. ^{1}H NMR spectrum of compound **3x** (400 MHz, $CDCl_3$)

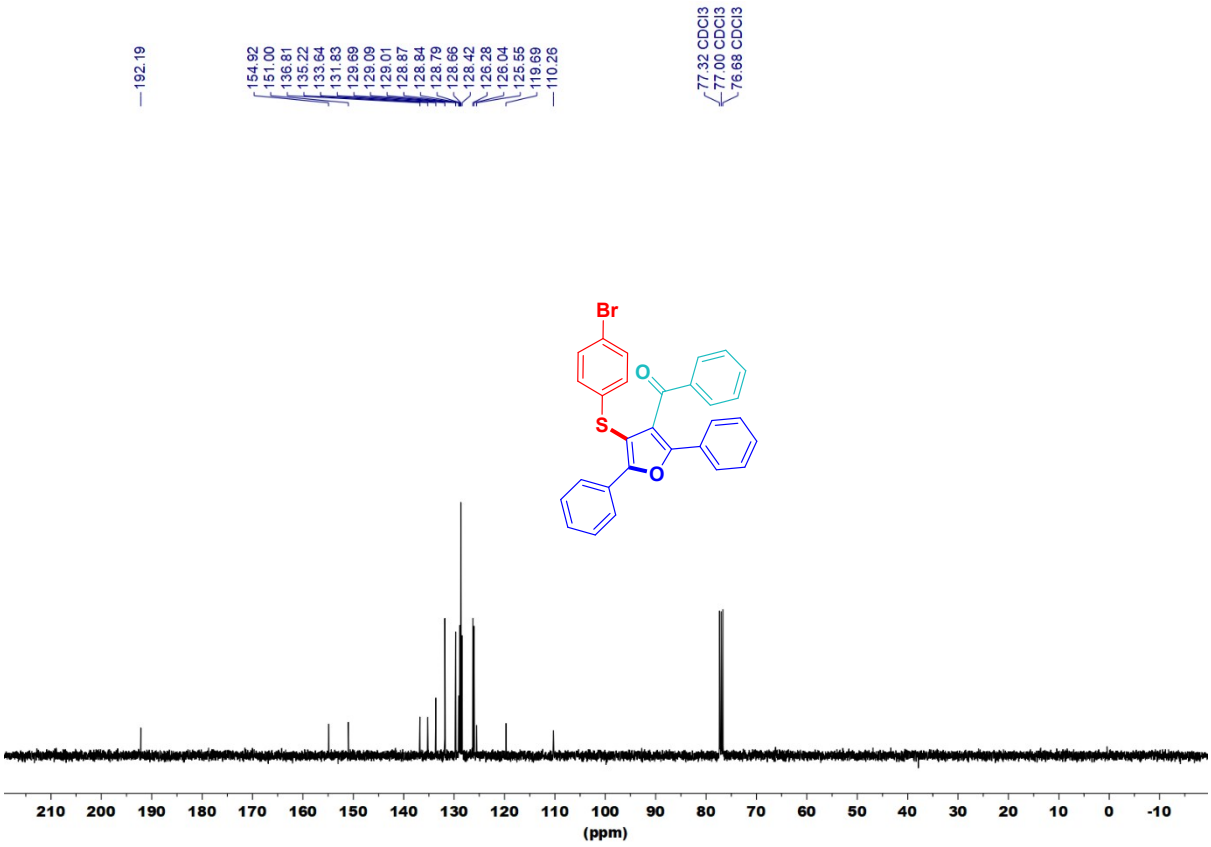

Figure S48. ^{13}C NMR spectrum of compound **3x** (101 MHz, $CDCl_3$)

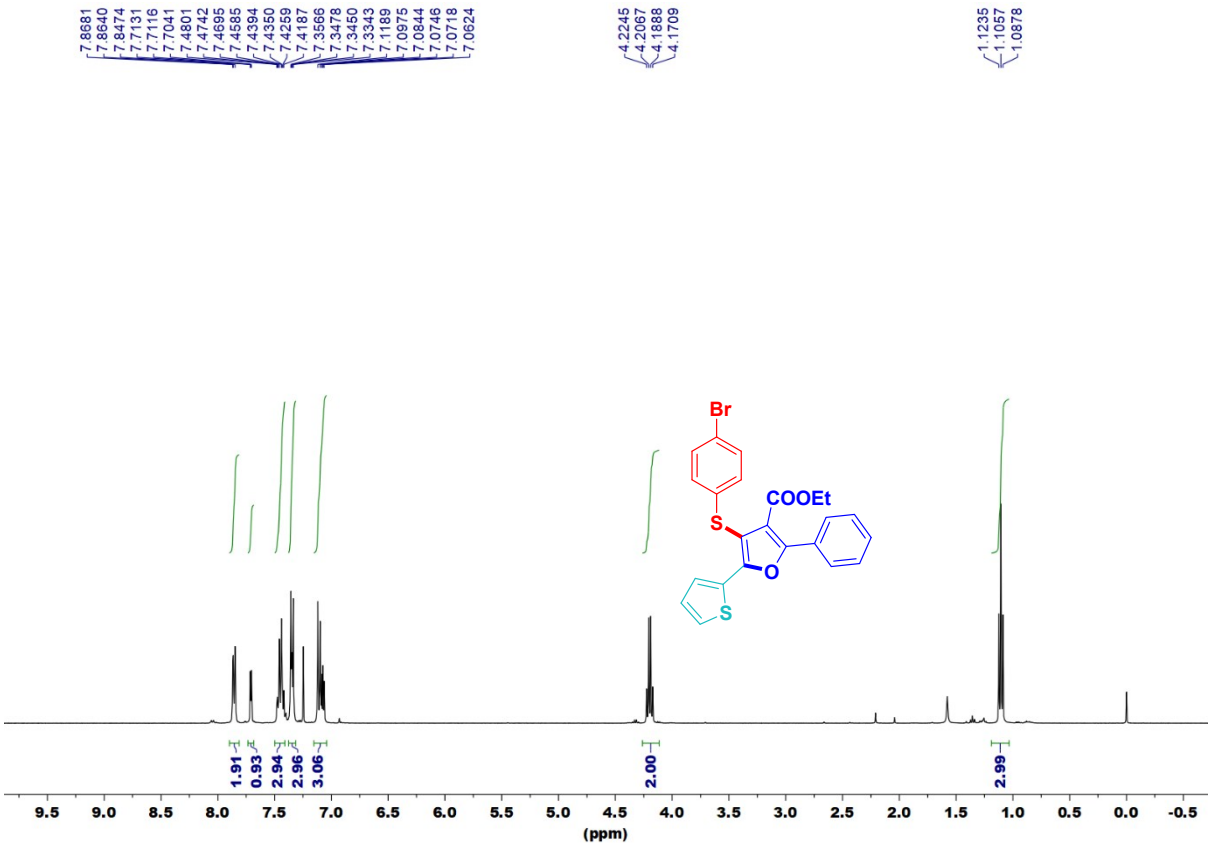

Figure S49. ^{1}H NMR spectrum of compound **3y** (400 MHz, $CDCl_3$)

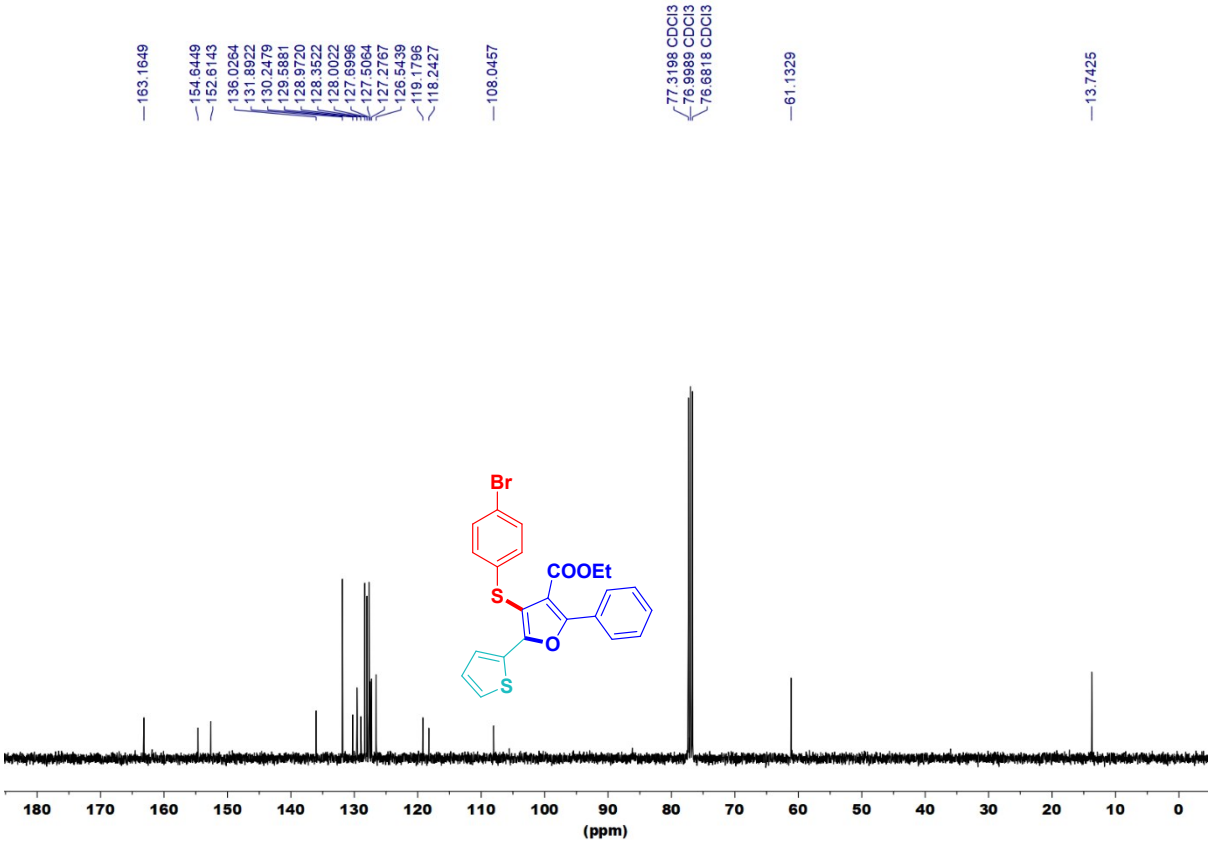

Figure S50. ^{13}C NMR spectrum of compound **3y** (101 MHz, $CDCl_3$)

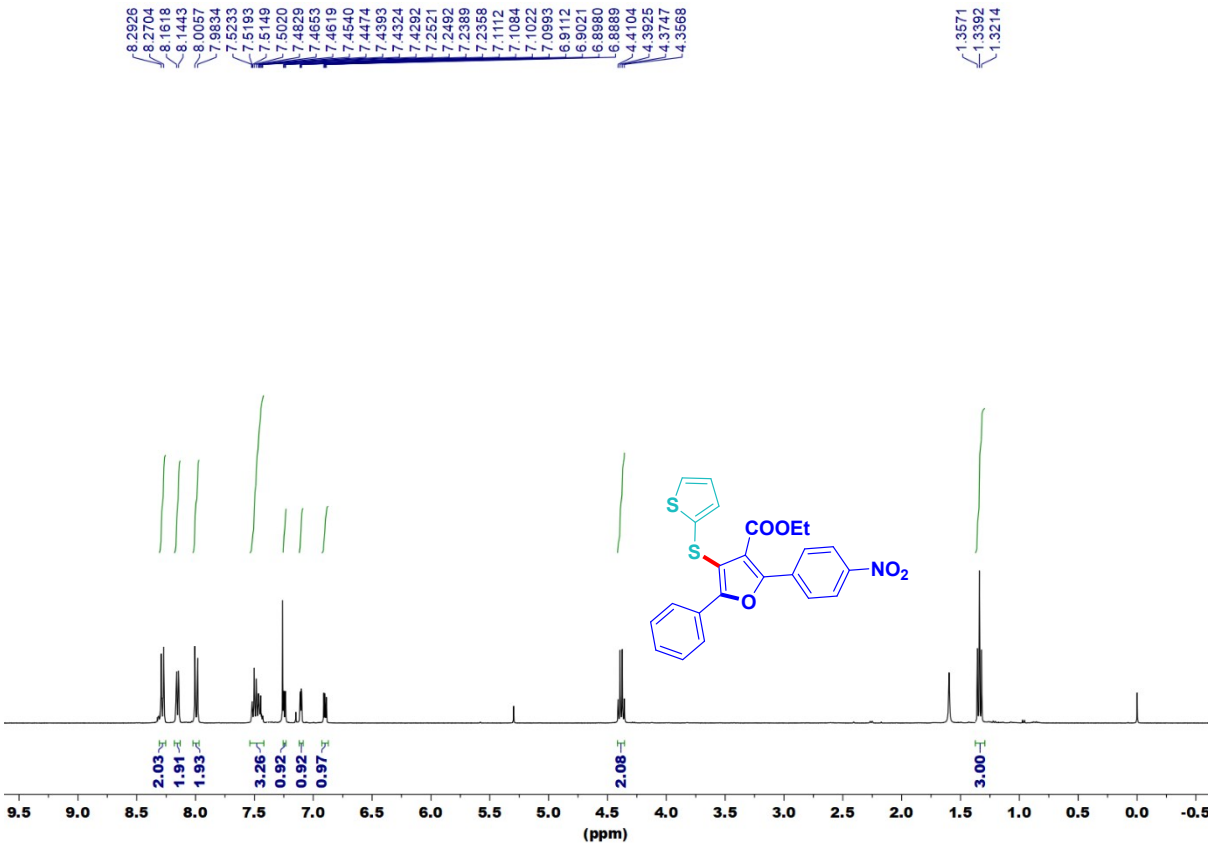

Figure S51. ^{1}H NMR spectrum of compound **3z** (400 MHz, $CDCl_3$)

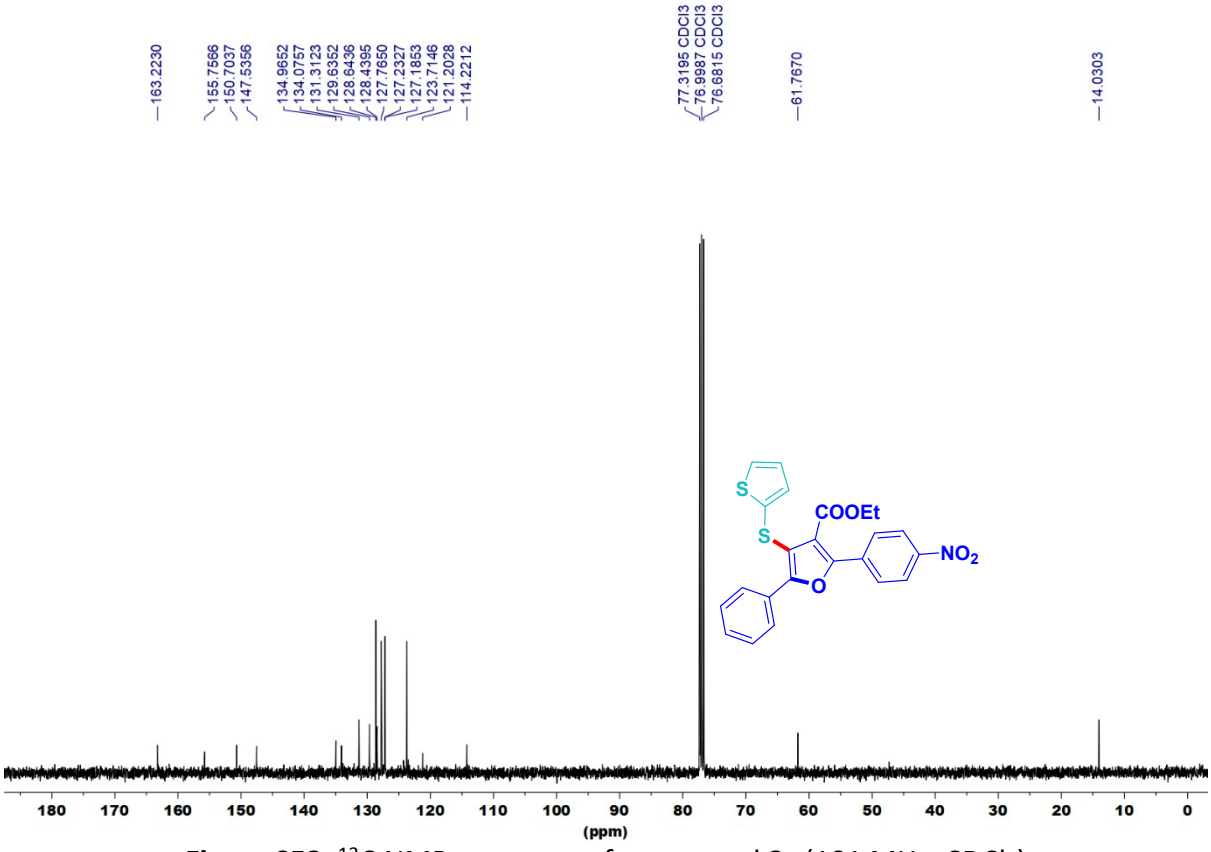

Figure S52. ^{13}C NMR spectrum of compound **3z** (101 MHz, $CDCl_3$)

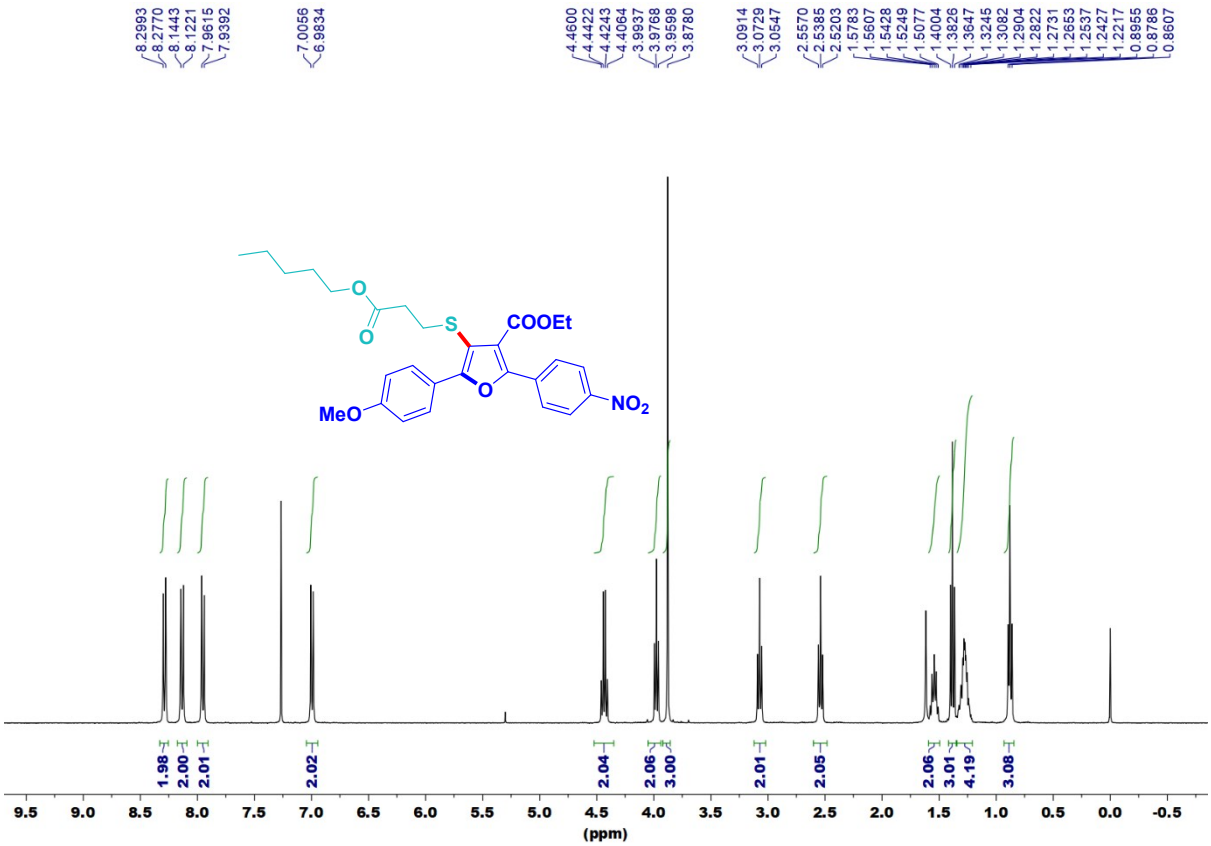

Figure S53. ^{1}H NMR spectrum of compound **3aa** (400 MHz, $CDCl_3$)

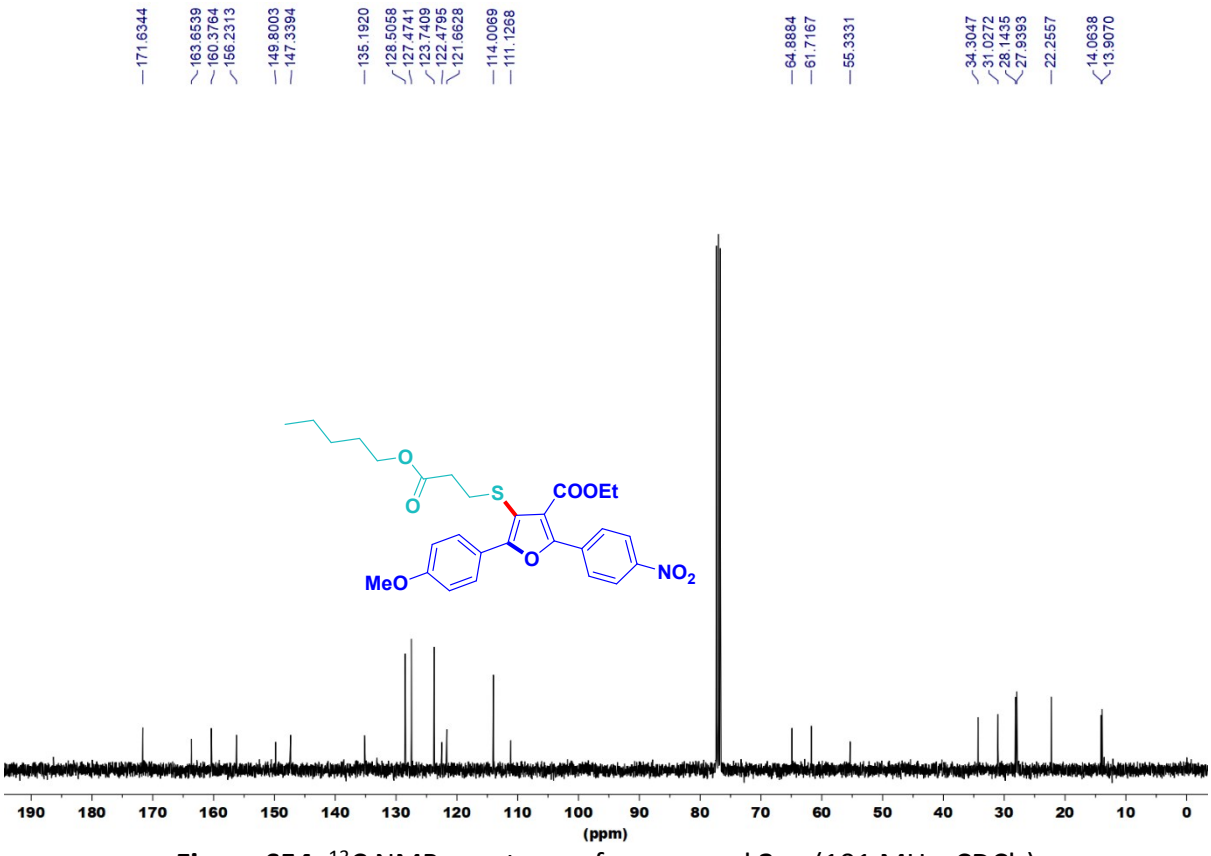

Figure S54. ^{13}C NMR spectrum of compound **3aa** (101 MHz, $CDCl_3$)

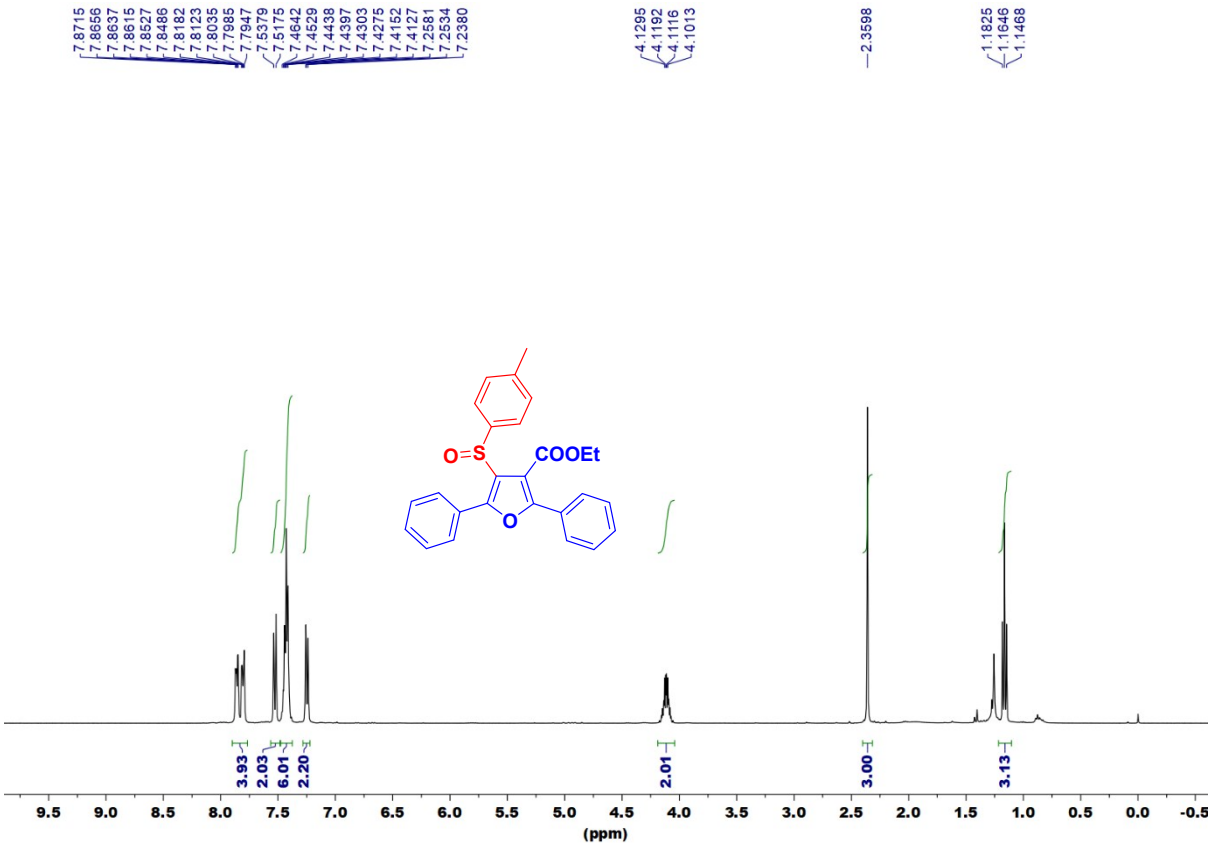

Figure S55. ^{1}H NMR spectrum of compound **4** (400 MHz, $CDCl_3$)

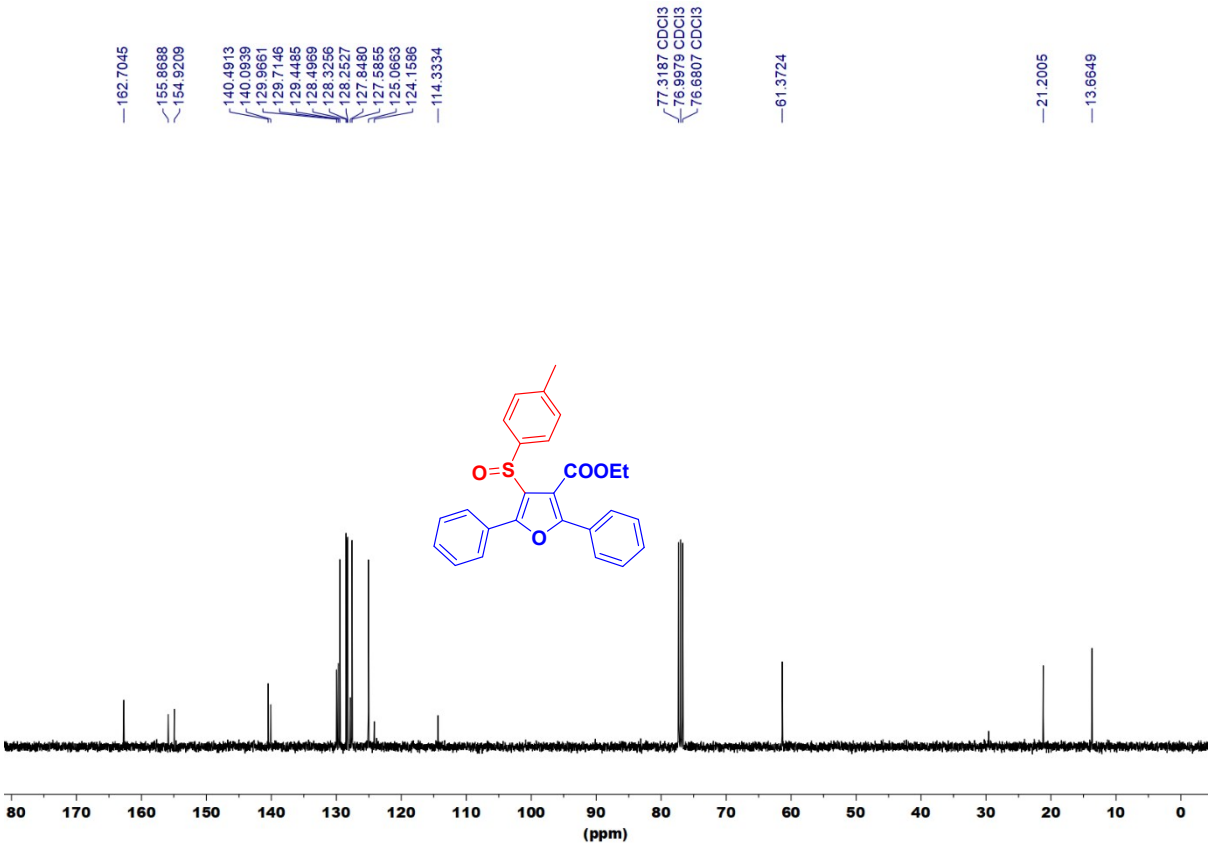

Figure S56. ^{13}C NMR spectrum of compound **4** (101 MHz, $CDCl_3$)

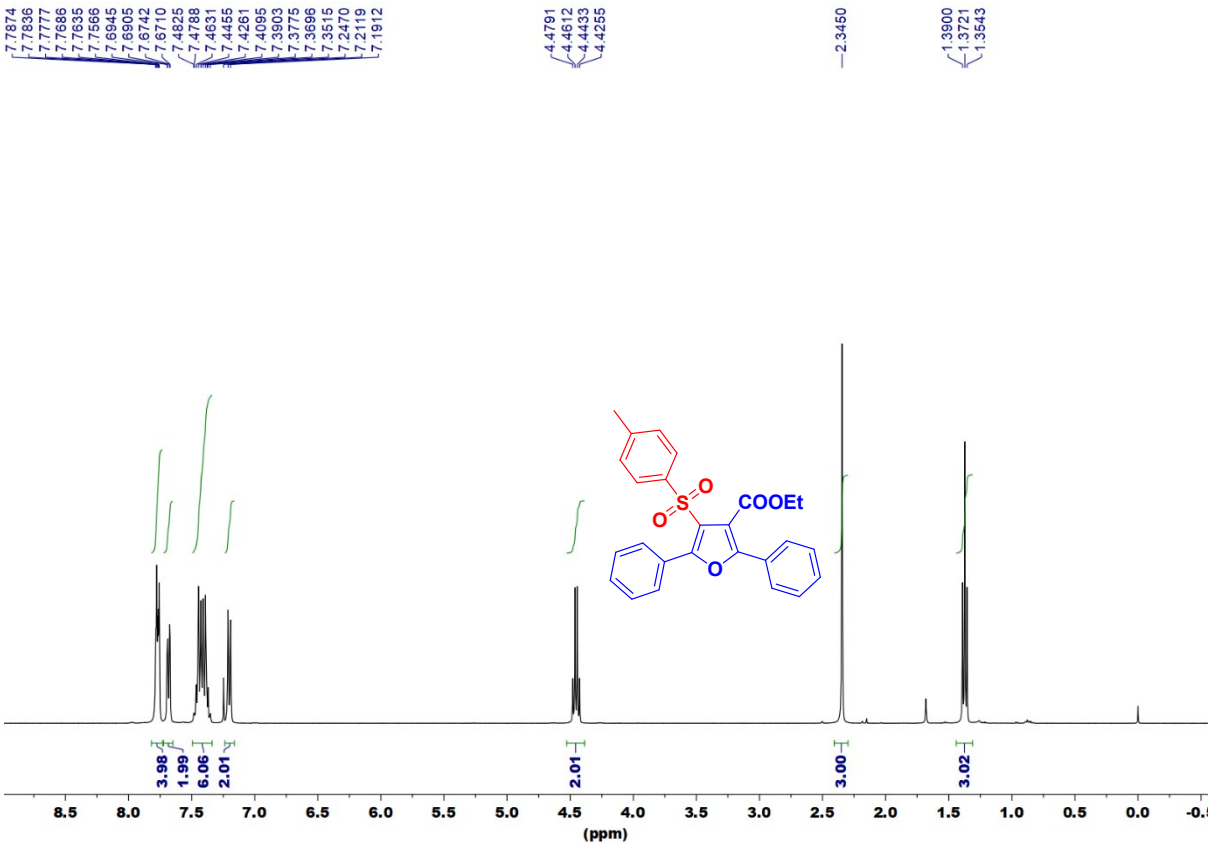

Figure S57. ^{1}H NMR spectrum of compound **5** (400 MHz, $CDCl_3$)

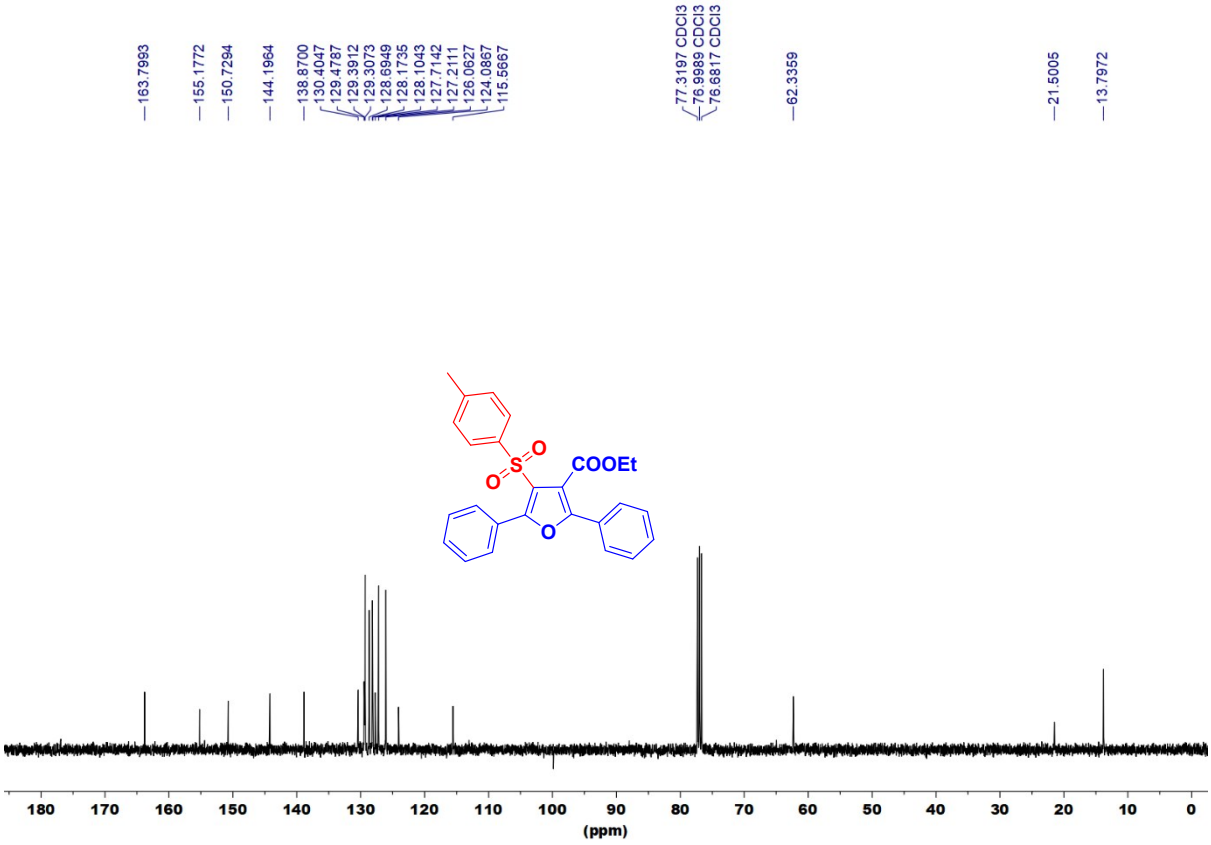

Figure S58. ^{13}C NMR spectrum of compound **5** (101 MHz, $CDCl_3$)

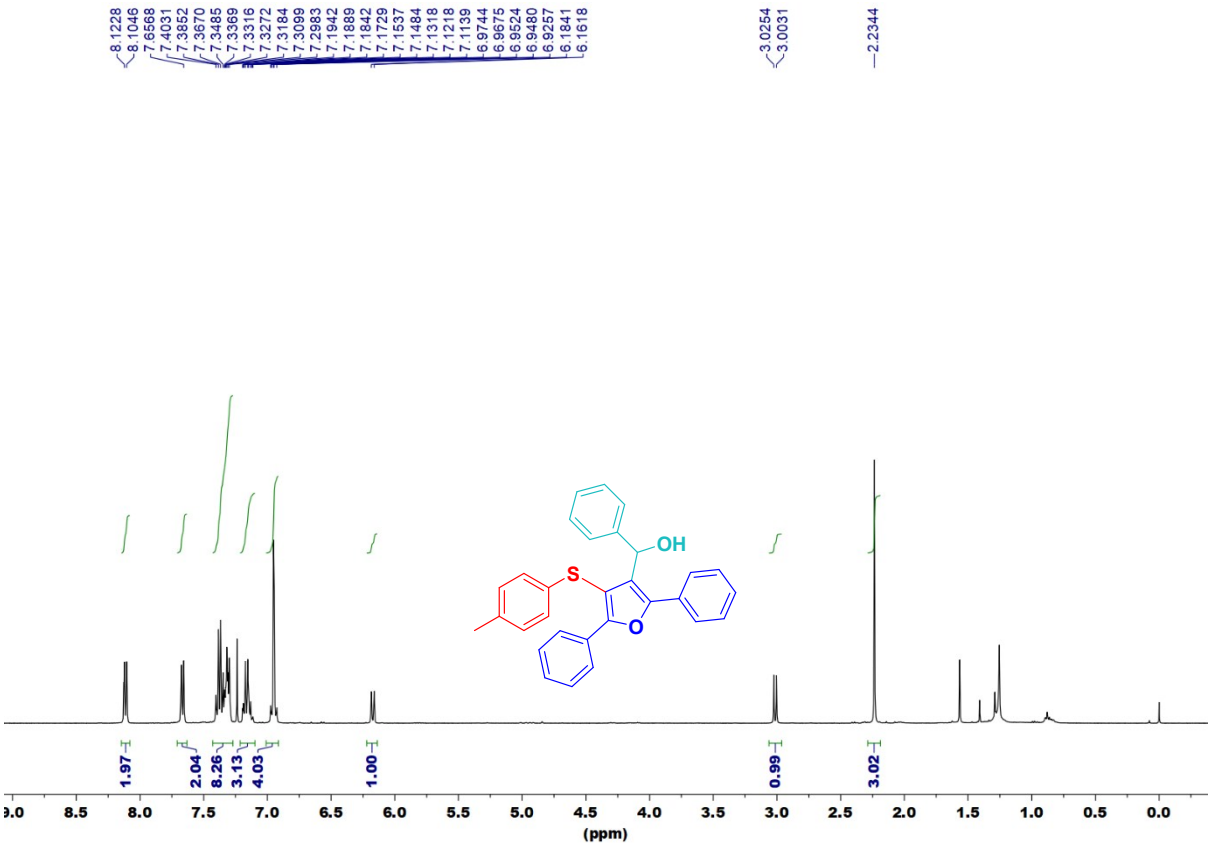

Figure S59. ^{1}H NMR spectrum of compound **6** (400 MHz, $CDCl_3$)

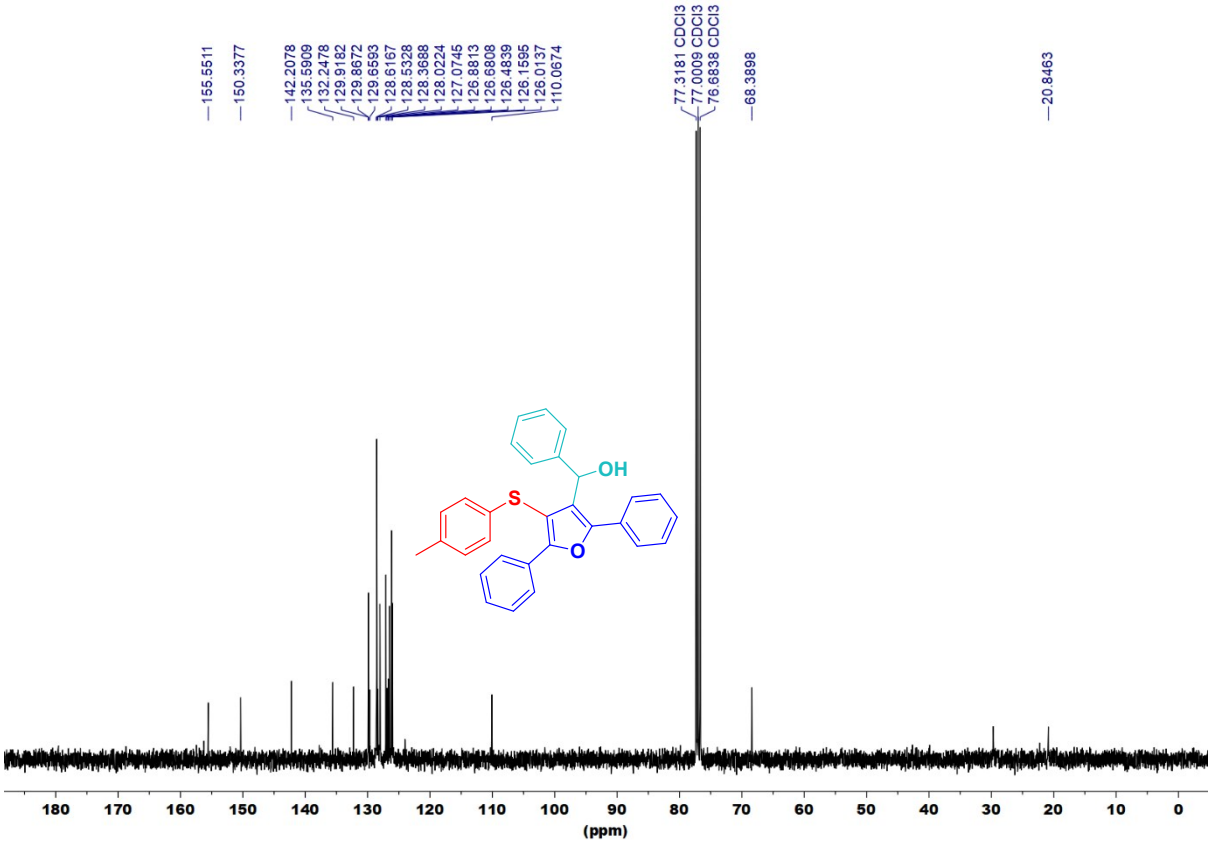

Figure S60. ^{13}C NMR spectrum of compound **6** (101 MHz, $CDCl_3$)

Sample and crystal data for compound 3b

Chemical formula	$C_{26}H_{22}O_3S$	
Formula weight	414.49 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.100 x 0.220 x 0.250 mm	
Crystal habit	clear light colourless Block	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 10.9451(3) Å	α = 90°
	b = 7.7900(2) Å	β = 95.0229(14)°
	c = 25.6813(9) Å	γ = 90°
Volume	2181.24(11) $Å^3$	
Z	4	
Density (calculated)	1.262 g/cm^3	
Absorption coefficient	0.173 mm^{-1}	
F(000)	872	

Data collection and structure refinement for compound 3b

Theta range for data collection	1.87 to 25.00°	
Index ranges	-12<=h<=13, -9<=k<=9, -30<=l<=29	
Reflections collected	10933	
Independent reflections	3834 [R(int) = 0.0231]	
Coverage of independent reflections	100.0%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9830 and 0.9580	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	3834 / 0 / 273	
Goodness-of-fit on F^2	1.046	
Final R indices	2743 data; I>2σ(I)	R1 = 0.0424, wR2 = 0.0934
	all data	R1 = 0.0694, wR2 = 0.1082
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0373P)^2+0.6798P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.216 and -0.216 $eÅ^{-3}$	
R.M.S. deviation from mean	0.032 $eÅ^{-3}$	

Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for compound 3b.

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

	x/a	y/b	z/c	U(eq)
C1	0.4903(2)	0.5450(3)	0.20684(9)	0.0622(6)
C2	0.5726(2)	0.5192(3)	0.24949(10)	0.0730(7)
C3	0.6841(2)	0.6006(3)	0.25356(10)	0.0729(7)
C4	0.7140(2)	0.7075(3)	0.21451(11)	0.0711(7)
C5	0.6332(2)	0.7335(3)	0.17112(10)	0.0617(6)
C6	0.51992(19)	0.6527(3)	0.16677(9)	0.0506(5)
C7	0.43451(19)	0.6804(3)	0.12061(9)	0.0513(5)
C8	0.3969(2)	0.7302(3)	0.03534(9)	0.0517(5)
C9	0.28623(19)	0.7301(3)	0.05592(9)	0.0516(5)
C10	0.31080(19)	0.6970(3)	0.11134(9)	0.0515(5)
C11	0.12788(18)	0.5206(3)	0.15875(8)	0.0492(5)
C12	0.1544(2)	0.3815(3)	0.12863(9)	0.0580(6)
C13	0.0839(2)	0.2344(3)	0.12920(10)	0.0634(6)
C14	0.9864(2)	0.2214(3)	0.15938(10)	0.0644(6)
C15	0.9618(2)	0.3606(4)	0.18962(11)	0.0743(7)
C16	0.0313(2)	0.5094(3)	0.18967(9)	0.0652(6)
C17	0.9090(3)	0.0597(4)	0.15837(13)	0.0971(10)
C18	0.4412(2)	0.7548(2)	0.98393(9)	0.0532(5)
C19	0.5594(2)	0.8153(3)	0.98021(10)	0.0635(6)
C20	0.6027(3)	0.8418(3)	0.93236(12)	0.0790(8)
C21	0.5294(3)	0.8094(4)	0.88749(12)	0.0881(9)
C22	0.4130(3)	0.7485(4)	0.89022(11)	0.0881(9)
C23	0.3684(2)	0.7216(3)	0.93812(10)	0.0723(7)
C24	0.1670(2)	0.7731(3)	0.02790(10)	0.0576(6)
C25	0.9522(2)	0.7253(4)	0.02515(11)	0.0790(8)
C26	0.8678(2)	0.6355(4)	0.05782(13)	0.0969(10)
O1	0.48755(12)	0.69984(18)	0.07463(6)	0.0544(4)
O2	0.15273(16)	0.8708(3)	0.99161(8)	0.0916(6)
O3	0.07603(13)	0.6908(2)	0.04776(6)	0.0671(5)
S1	0.21078(5)	0.71633(8)	0.16069(2)	0.06106(19)

Bond lengths (Å) for compound 3b

C1-C2	1.371(3)	C1-C6	1.388(3)
C1-H1	0.93	C2-C3	1.371(3)
C2-H2	0.93	C3-C4	1.366(3)
C3-H3	0.93	C4-C5	1.376(3)
C4-H4	0.93	C5-C6	1.386(3)
C5-H5	0.93	C6-C7	1.460(3)
C7-C10	1.360(3)	C7-O1	1.369(2)
C8-C9	1.364(3)	C8-O1	1.372(2)
C8-C18	1.458(3)	C9-C10	1.448(3)
C9-C24	1.472(3)	C10-S1	1.752(2)
C11-C12	1.377(3)	C11-C16	1.379(3)
C11-S1	1.773(2)	C12-C13	1.383(3)
C12-H12	0.93	C13-C14	1.376(3)
C13-H13	0.93	C14-C15	1.374(4)
C14-C17	1.517(3)	C15-C16	1.386(3)
C15-H15	0.93	C16-H16	0.93
C17-H17A	0.96	C17-H17B	0.96
C17-H17C	0.96	C18-C23	1.387(3)
C18-C19	1.388(3)	C19-C20	1.371(3)
C19-H19	0.93	C20-C21	1.369(4)
C20-H20	0.93	C21-C22	1.368(4)
C21-H21	0.93	C22-C23	1.379(4)
C22-H22	0.93	C23-H23	0.93
C24-O2	1.203(3)	C24-O3	1.324(3)
C25-O3	1.452(3)	C25-C26	1.477(4)
C25-H25A	0.97	C25-H25B	0.97
C26-H26A	0.96	C26-H26B	0.96
C26-H26C	0.96		

C2-C1-C6	120.1(2)	C2-C1-H1	120.0
C6-C1-H1	120.0	C1-C2-C3	120.8(2)
C1-C2-H2	119.6	C3-C2-H2	119.6
C4-C3-C2	119.7(2)	C4-C3-H3	120.2
C2-C3-H3	120.2	C3-C4-C5	120.4(2)
C3-C4-H4	119.8	C5-C4-H4	119.8
C4-C5-C6	120.4(2)	C4-C5-H5	119.8
C6-C5-H5	119.8	C5-C6-C1	118.7(2)
C5-C6-C7	120.2(2)	C1-C6-C7	121.13(19)
C10-C7-O1	109.23(19)	C10-C7-C6	135.5(2)
O1-C7-C6	115.27(18)	C9-C8-O1	108.92(19)

C9-C8-C18	136.7(2)	O1-C8-C18	114.36(18)
C8-C9-C10	106.63(19)	C8-C9-C24	126.1(2)
C10-C9-C24	127.0(2)	C7-C10-C9	106.57(19)
C7-C10-S1	123.84(18)	C9-C10-S1	128.42(16)
C12-C11-C16	118.9(2)	C12-C11-S1	124.07(16)
C16-C11-S1	117.04(17)	C11-C12-C13	120.1(2)
C11-C12-H12	120.0	C13-C12-H12	120.0
C14-C13-C12	121.8(2)	C14-C13-H13	119.1
C12-C13-H13	119.1	C15-C14-C13	117.4(2)
C15-C14-C17	121.9(2)	C13-C14-C17	120.7(3)
C14-C15-C16	121.7(2)	C14-C15-H15	119.1
C16-C15-H15	119.1	C11-C16-C15	120.0(2)
C11-C16-H16	120.0	C15-C16-H16	120.0
C14-C17-H17A	109.5	C14-C17-H17B	109.5
H17A-C17-H17B	109.5	C14-C17-H17C	109.5
H17A-C17-H17C	109.5	H17B-C17-H17C	109.5
C23-C18-C19	118.4(2)	C23-C18-C8	122.1(2)
C19-C18-C8	119.5(2)	C20-C19-C18	120.7(3)
C20-C19-H19	119.7	C18-C19-H19	119.7
C21-C20-C19	120.3(3)	C21-C20-H20	119.9
C19-C20-H20	119.9	C22-C21-C20	120.0(3)
C22-C21-H21	120.0	C20-C21-H21	120.0
C21-C22-C23	120.2(3)	C21-C22-H22	119.9
C23-C22-H22	119.9	C22-C23-C18	120.4(3)
C22-C23-H23	119.8	C18-C23-H23	119.8
O2-C24-O3	123.6(2)	O2-C24-C9	124.9(2)
O3-C24-C9	111.5(2)	O3-C25-C26	107.0(2)
O3-C25-H25A	110.3	C26-C25-H25A	110.3
O3-C25-H25B	110.3	C26-C25-H25B	110.3
H25A-C25-H25B	108.6	C25-C26-H26A	109.5
C25-C26-H26B	109.5	H26A-C26-H26B	109.5
C25-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C7-O1-C8	108.64(16)
C24-O3-C25	117.62(19)	C10-S1-C11	104.85(10)

Torsion angles (°) for compound 3b

C6-C1-C2-C3	0.9(4)	C1-C2-C3-C4	-0.5(4)
C2-C3-C4-C5	-0.3(4)	C3-C4-C5-C6	0.7(4)
C4-C5-C6-C1	-0.3(3)	C4-C5-C6-C7	-179.9(2)
C2-C1-C6-C5	-0.5(3)	C2-C1-C6-C7	179.1(2)
C5-C6-C7-C10	-142.7(3)	C1-C6-C7-C10	37.7(4)
C5-C6-C7-O1	35.1(3)	C1-C6-C7-O1	-144.5(2)
O1-C8-C9-C10	-0.2(2)	C18-C8-C9-C10	-179.7(2)

O1-C8-C9-C24	174.15(19)	C18-C8-C9-C24	-5.4(4)
O1-C7-C10-C9	-0.4(2)	C6-C7-C10-C9	177.5(2)
O1-C7-C10-S1	-169.02(14)	C6-C7-C10-S1	8.9(4)
C8-C9-C10-C7	0.4(2)	C24-C9-C10-C7	-173.9(2)
C8-C9-C10-S1	168.27(16)	C24-C9-C10-S1	-6.0(3)
C16-C11-C12-C13	0.7(3)	S1-C11-C12-C13	-179.37(17)
C11-C12-C13-C14	-0.1(4)	C12-C13-C14-C15	-0.6(4)
C12-C13-C14-C17	178.7(2)	C13-C14-C15-C16	0.5(4)
C17-C14-C15-C16	-178.8(2)	C12-C11-C16-C15	-0.8(3)
S1-C11-C16-C15	179.33(19)	C14-C15-C16-C11	0.1(4)
C9-C8-C18-C23	-25.8(4)	O1-C8-C18-C23	154.7(2)
C9-C8-C18-C19	153.4(2)	O1-C8-C18-C19	-26.1(3)
C23-C18-C19-C20	0.1(3)	C8-C18-C19-C20	-179.1(2)
C18-C19-C20-C21	0.3(4)	C19-C20-C21-C22	-0.8(4)
C20-C21-C22-C23	0.9(4)	C21-C22-C23-C18	-0.5(4)
C19-C18-C23-C22	0.0(3)	C8-C18-C23-C22	179.2(2)
C8-C9-C24-O2	-29.2(4)	C10-C9-C24-O2	144.0(2)
C8-C9-C24-O3	151.1(2)	C10-C9-C24-O3	-35.7(3)
C10-C7-O1-C8	0.3(2)	C6-C7-O1-C8	-178.06(17)
C9-C8-O1-C7	-0.1(2)	C18-C8-O1-C7	179.57(16)
O2-C24-O3-C25	-1.9(3)	C9-C24-O3-C25	177.9(2)
C26-C25-O3-C24	-173.3(2)	C7-C10-S1-C11	-110.40(18)
C9-C10-S1-C11	83.6(2)	C12-C11-S1-C10	7.8(2)
C16-C11-S1-C10	-172.32(17)		

Anisotropic atomic displacement parameters (Å^2) for compound 3b

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}
C1	0.0666(15)	0.0585(14)	0.0620(15)	0.0017(12)	0.0093(12)	-0.0146(11)
C2	0.0907(19)	0.0687(16)	0.0602(16)	0.0107(13)	0.0090(14)	-0.0068(14)
C3	0.0747(18)	0.0784(17)	0.0638(17)	0.0031(15)	-0.0043(13)	0.0051(14)
C4	0.0520(14)	0.0801(17)	0.0804(18)	0.0065(15)	0.0010(13)	-0.0043(13)
C5	0.0511(13)	0.0642(14)	0.0708(16)	0.0123(13)	0.0117(12)	-0.0020(11)
C6	0.0497(12)	0.0471(12)	0.0557(13)	-0.0014(11)	0.0087(10)	-0.0008(10)
C7	0.0541(13)	0.0465(12)	0.0548(13)	0.0026(11)	0.0141(11)	-0.0048(10)
C8	0.0548(13)	0.0436(11)	0.0568(14)	0.0033(11)	0.0047(11)	-0.0012(10)
C9	0.0497(12)	0.0418(11)	0.0634(15)	0.0024(11)	0.0062(10)	-0.0008(9)
C10	0.0497(13)	0.0426(11)	0.0631(15)	-0.0016(11)	0.0107(10)	-0.0068(9)
C11	0.0441(12)	0.0523(12)	0.0515(13)	0.0027(11)	0.0061(10)	0.0019(9)
C12	0.0540(13)	0.0543(13)	0.0674(15)	-0.0004(12)	0.0160(11)	-0.0008(10)
C13	0.0679(15)	0.0513(13)	0.0716(16)	-0.0014(12)	0.0102(13)	-0.0017(11)
C14	0.0571(14)	0.0603(14)	0.0750(17)	0.0149(14)	0.0007(12)	-0.0067(11)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C15	0.0615(15)	0.0805(18)	0.0851(19)	0.0131(16)	0.0296(13)	-0.0064(13)
C16	0.0631(15)	0.0673(15)	0.0684(16)	-0.0041(13)	0.0234(12)	0.0002(12)
C17	0.085(2)	0.0774(18)	0.129(3)	0.0199(18)	0.0084(18)	-0.0257(15)
C18	0.0590(14)	0.0418(12)	0.0600(14)	0.0040(11)	0.0119(11)	0.0046(10)
C19	0.0633(15)	0.0584(14)	0.0710(16)	-0.0043(13)	0.0181(12)	0.0044(11)
C20	0.0845(19)	0.0642(16)	0.095(2)	-0.0015(16)	0.0433(18)	0.0026(14)
C21	0.117(3)	0.081(2)	0.072(2)	0.0121(17)	0.0425(19)	0.0194(18)
C22	0.102(2)	0.102(2)	0.0613(18)	-0.0035(16)	0.0103(16)	0.0161(18)
C23	0.0705(17)	0.0780(17)	0.0689(17)	-0.0023(15)	0.0090(13)	-0.0005(13)
C24	0.0614(15)	0.0469(12)	0.0650(15)	0.0030(12)	0.0086(12)	0.0051(11)
C25	0.0550(15)	0.0814(18)	0.098(2)	0.0118(16)	-0.0106(14)	0.0111(13)
C26	0.0521(15)	0.104(2)	0.134(3)	0.014(2)	0.0005(16)	-0.0007(15)
O1	0.0494(8)	0.0566(9)	0.0580(9)	0.0042(8)	0.0087(7)	0.0003(7)
O2	0.0776(13)	0.0922(13)	0.1058(15)	0.0444(12)	0.0120(11)	0.0184(10)
O3	0.0483(9)	0.0669(10)	0.0843(12)	0.0169(9)	-0.0050(8)	-0.0021(8)
S1	0.0582(4)	0.0565(3)	0.0706(4)	-0.0139(3)	0.0179(3)	-0.0076(3)

Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for compound 3b

	x/a	y/b	z/c	U(eq)
H1	0.4145	0.4903	0.2048	0.075
H2	0.5526	0.4456	0.2760	0.088
H3	0.7391	0.5830	0.2828	0.088
H4	0.7895	0.7632	0.2173	0.085
H5	0.6547	0.8056	0.1446	0.074
H12	0.2197	0.3866	0.1079	0.07
H13	0.1028	0.1415	0.1086	0.076
H15	-0.1031	0.3548	0.2106	0.089
H16	0.0128	0.6017	0.2106	0.078
H17A	-0.1497	0.0688	0.1839	0.146
H17B	-0.0389	-0.0378	0.1663	0.146
H17C	-0.1332	0.0456	0.1243	0.146
H19	0.6097	0.8382	0.0105	0.076
H20	0.6822	0.8819	-0.0696	0.095
H21	0.5589	0.8289	-0.1449	0.106
H22	0.3638	0.7251	-0.1403	0.106
H23	0.2889	0.6810	-0.0603	0.087
H25A	-0.0586	0.6834	-0.0105	0.095
H25B	-0.0639	0.8478	0.0249	0.095
H26A	-0.1104	0.5162	0.0604	0.145

	x/a	y/b	z/c	U(eq)
H26B	-0.2148	0.6465	0.0422	0.145
H26C	-0.1261	0.6855	0.0921	0.145