Supporting Information

Synthesis of bisoxazole and bromo-substituted aryloxazoles

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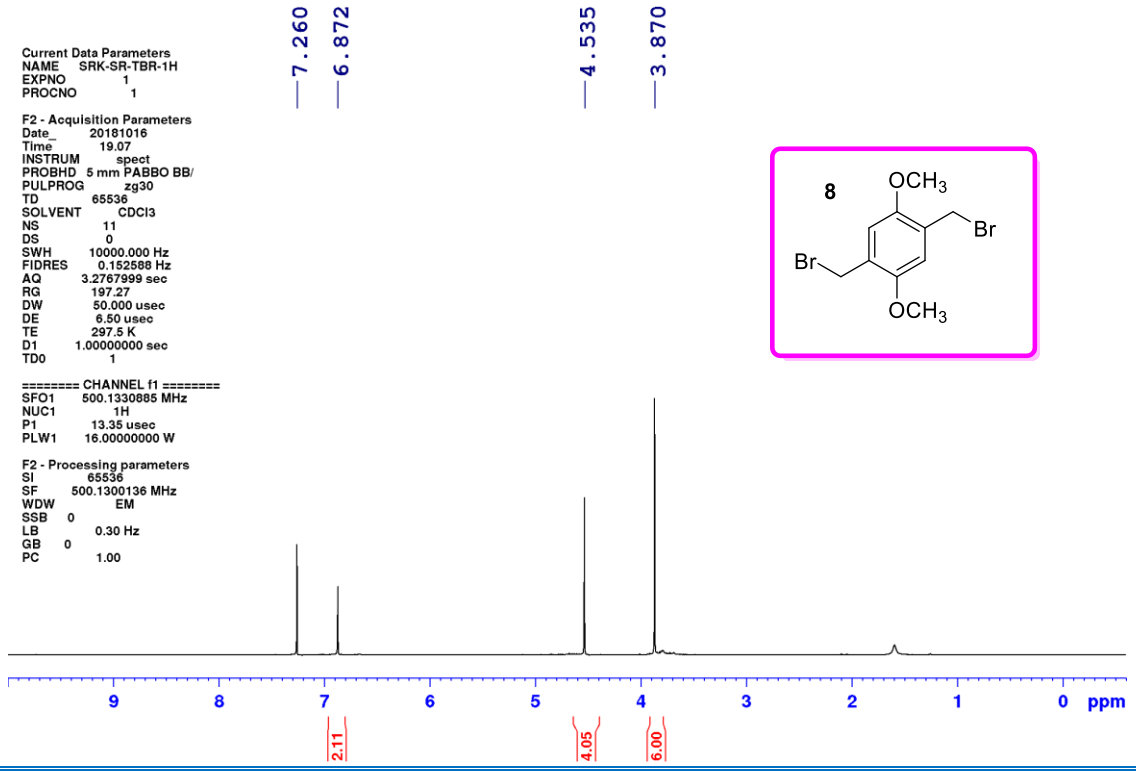
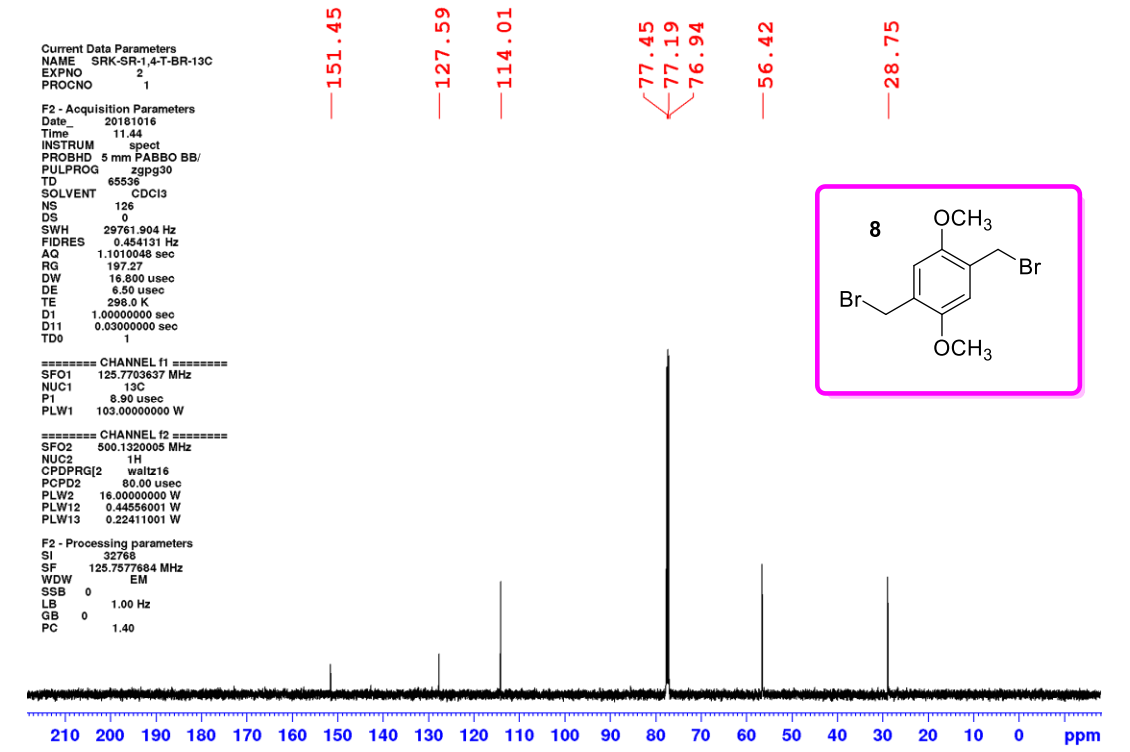
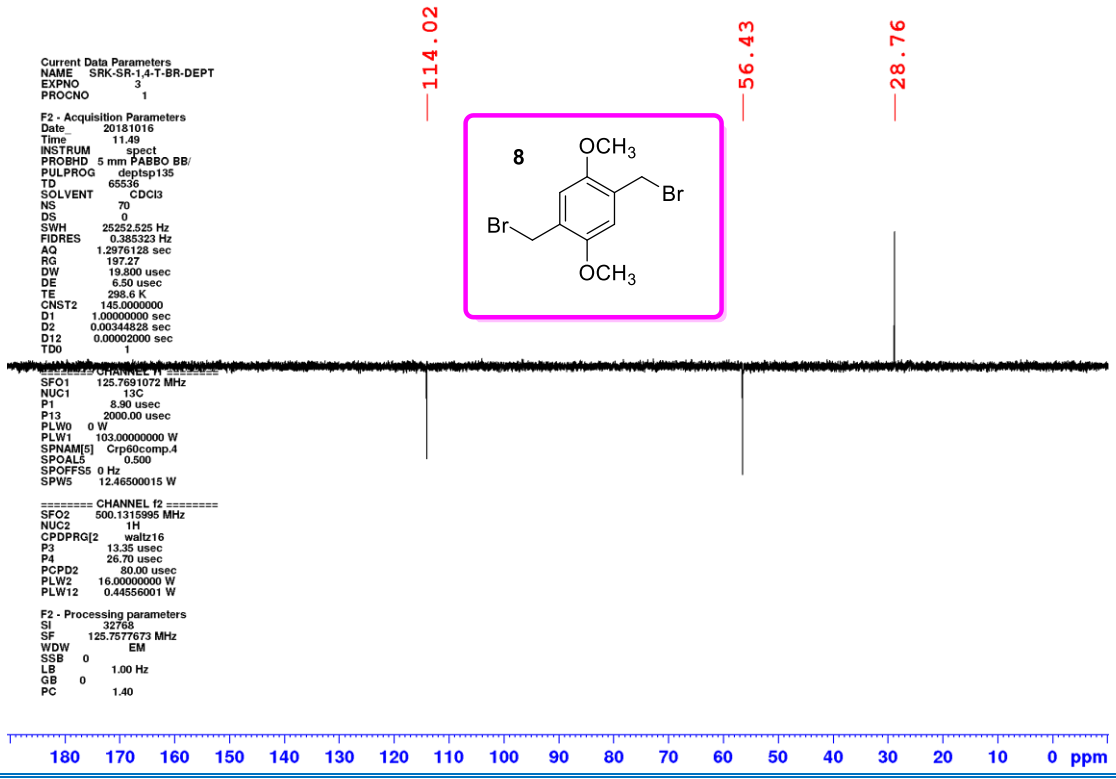
^{1}H NMR (500 MHz, $CDCl_3$) of compound 8



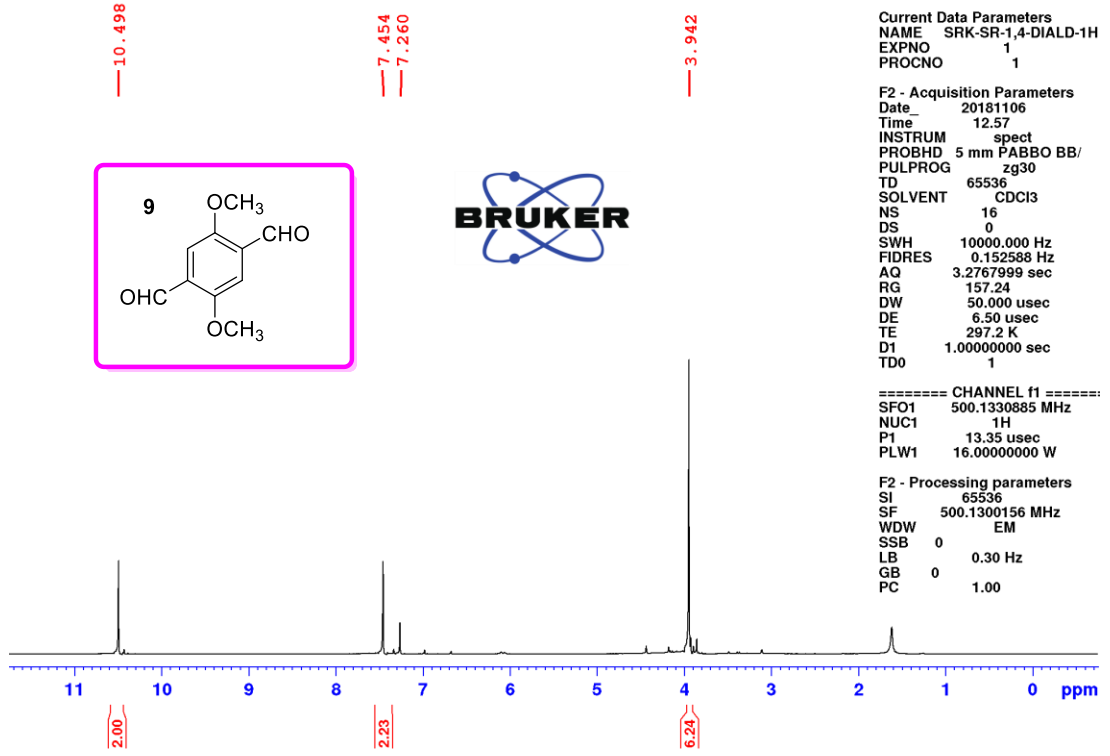
^{13}C NMR (125.7 MHz, $CDCl_3$) of compound 8



DEPT 135 NMR (125.7 MHz, $CDCl_3$) of compound 8



^1H NMR (500 MHz, $CDCl_3$) of compound 9



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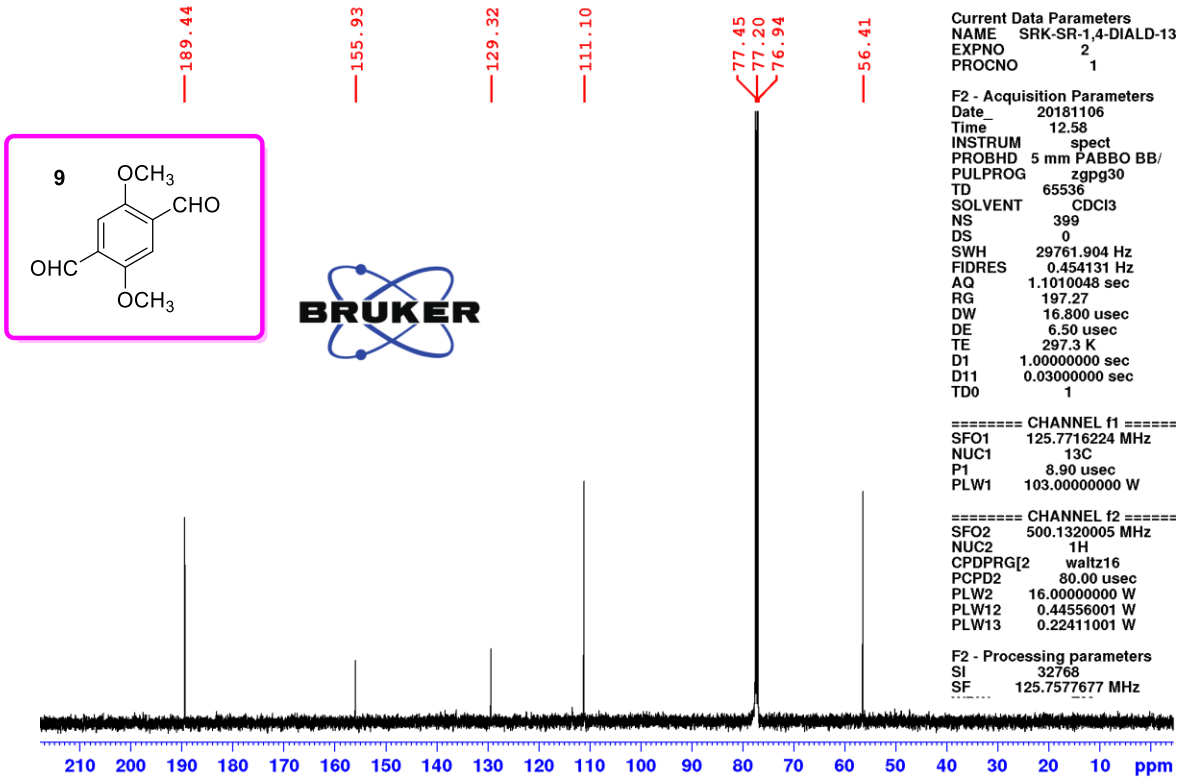

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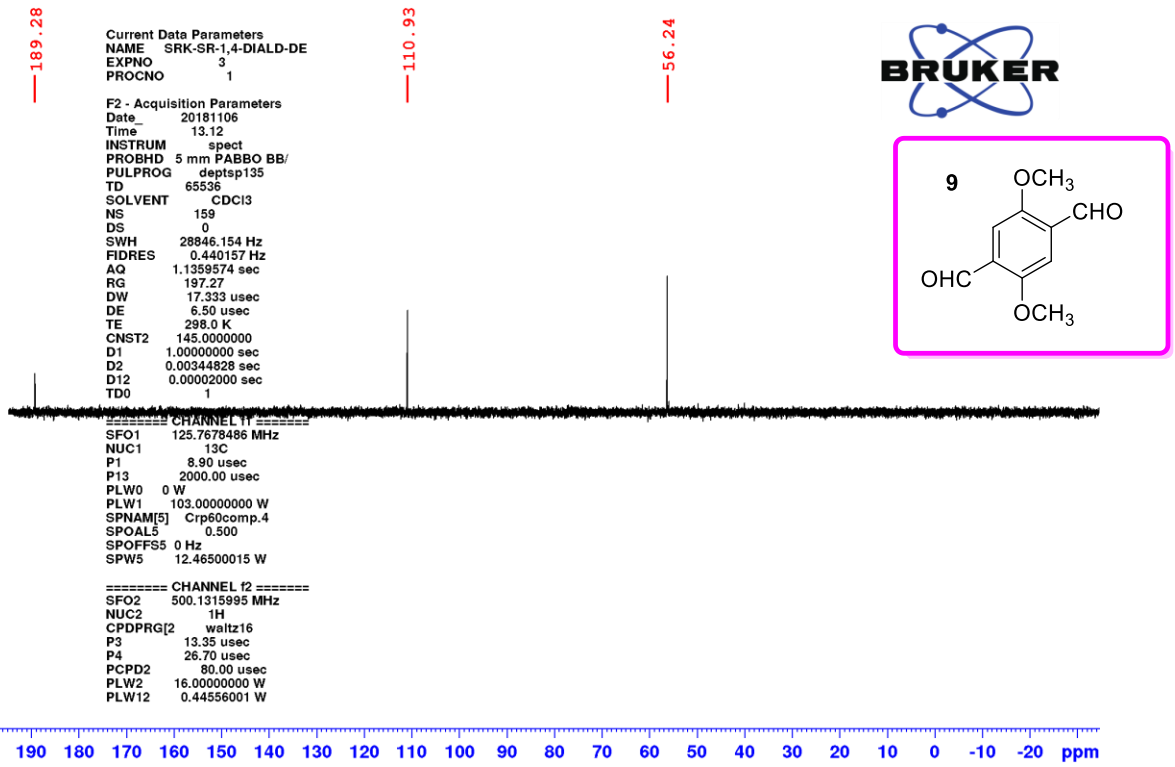
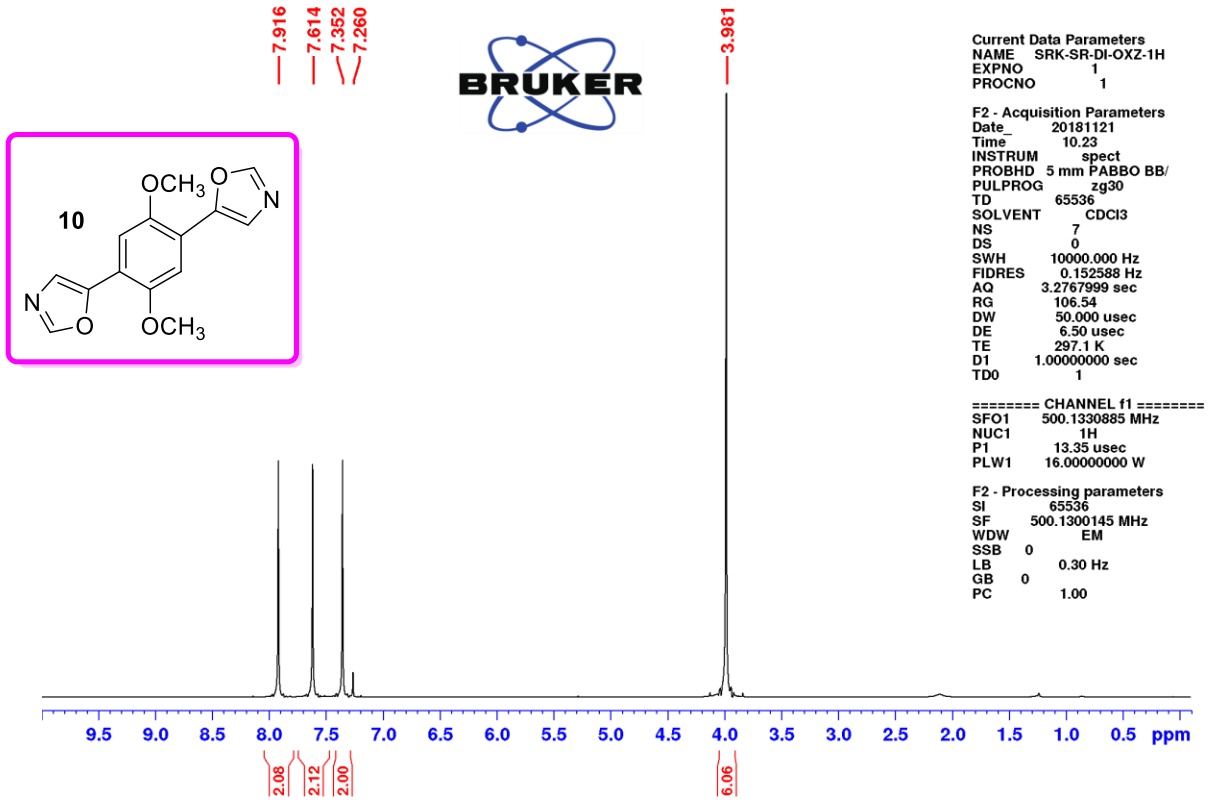


^{1}H NMR (500 MHz, $CDCl_3$) of compound 10



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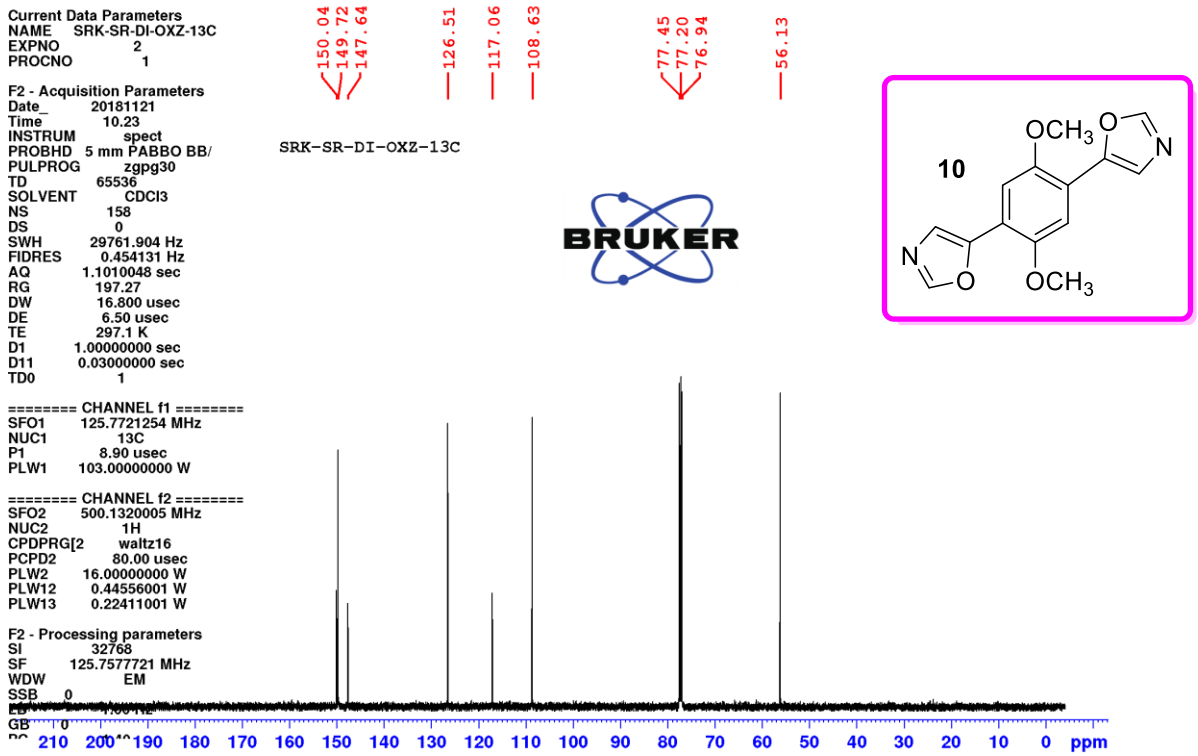

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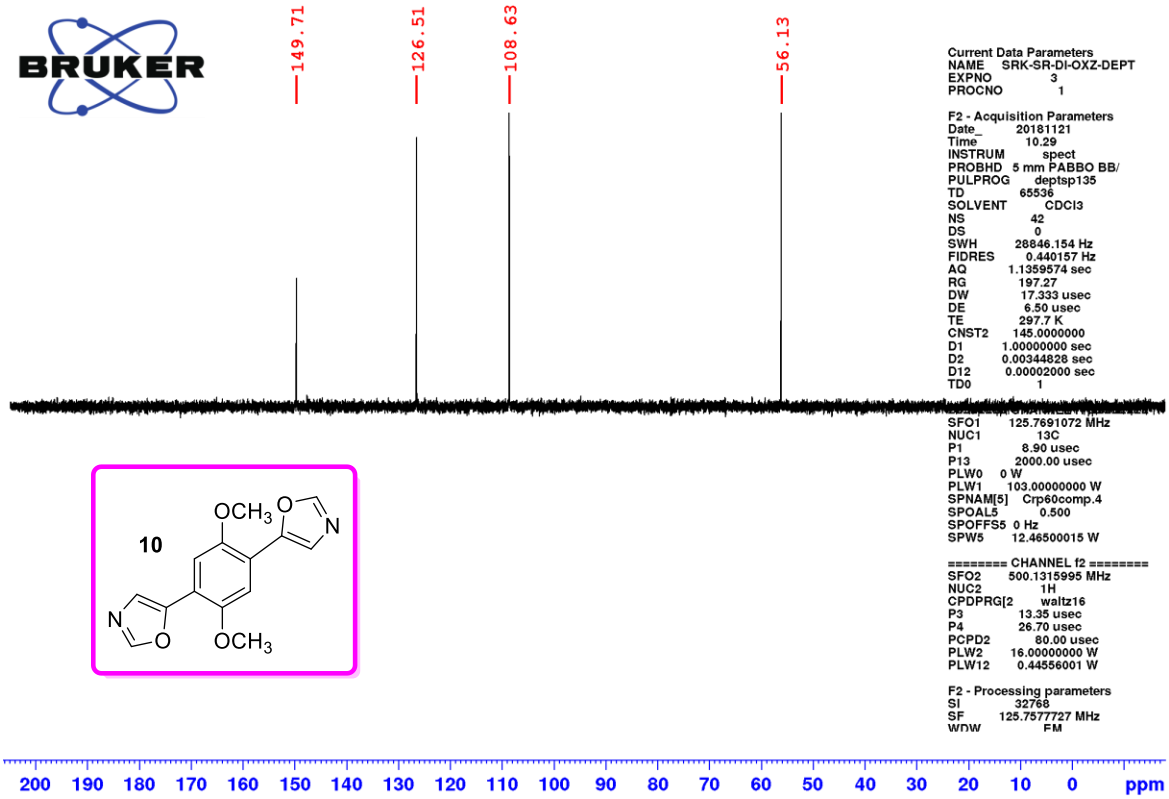
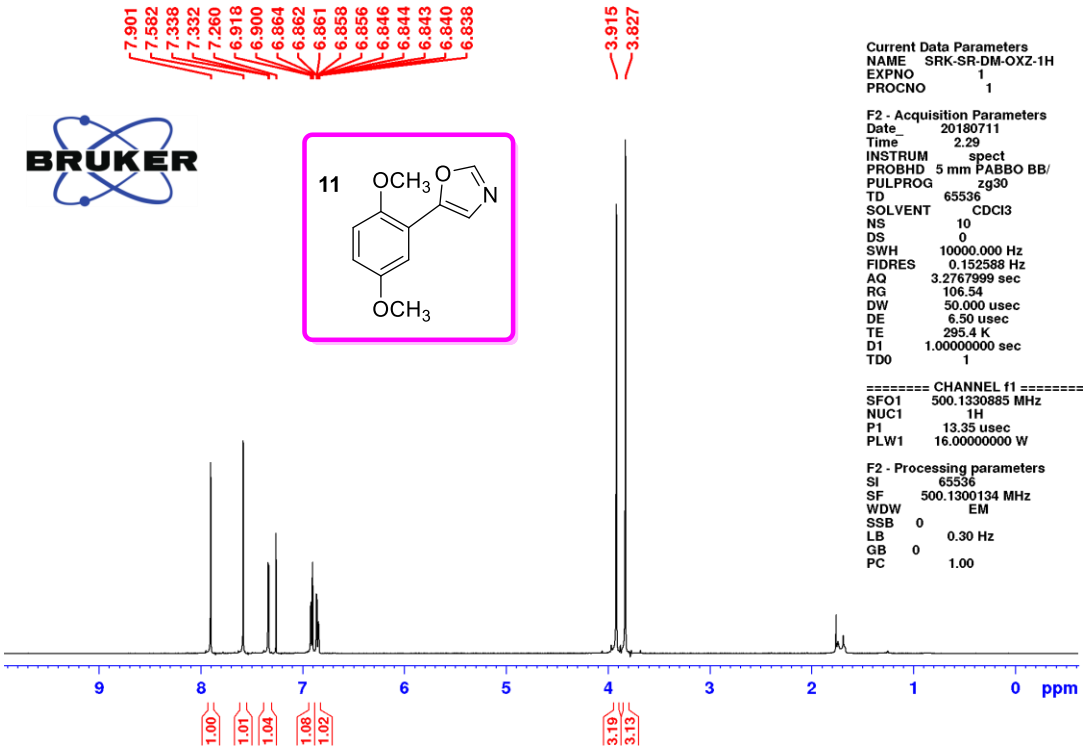
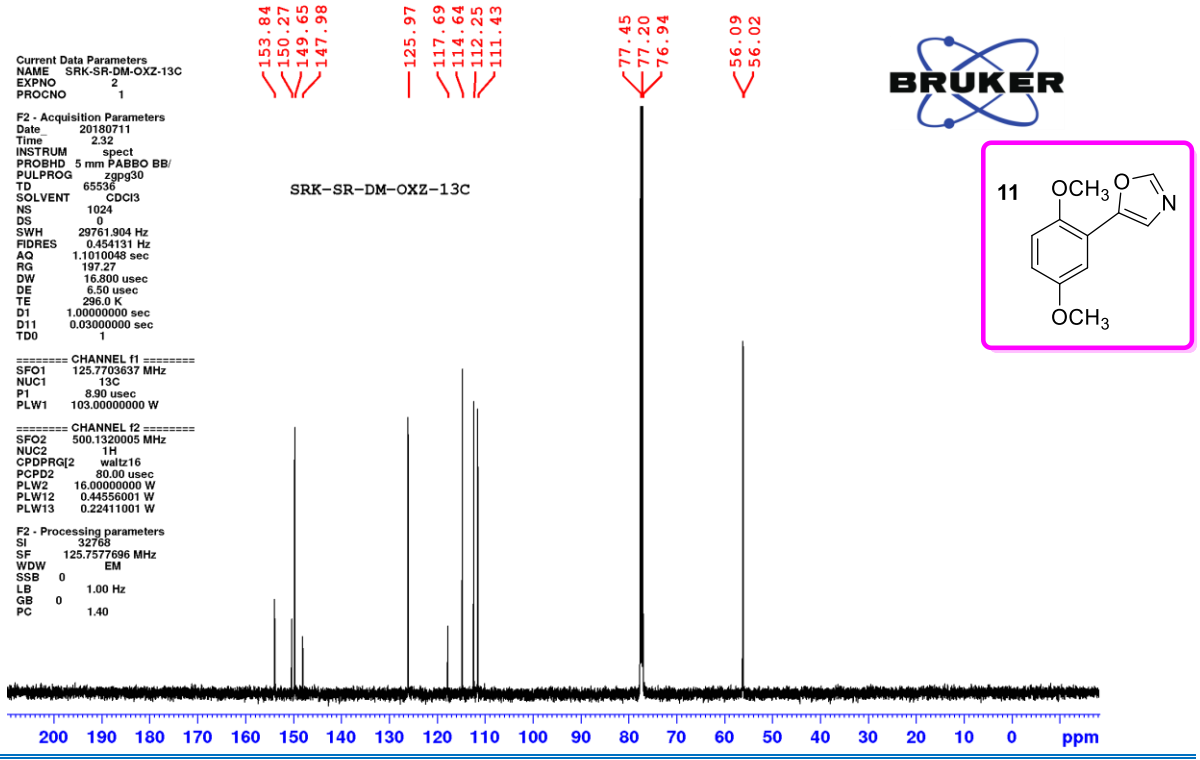


^{1}H NMR (500 MHz, $CDCl_3$) of compound 11



^{13}C NMR (125.7 MHz, $CDCl_3$) of compound 11



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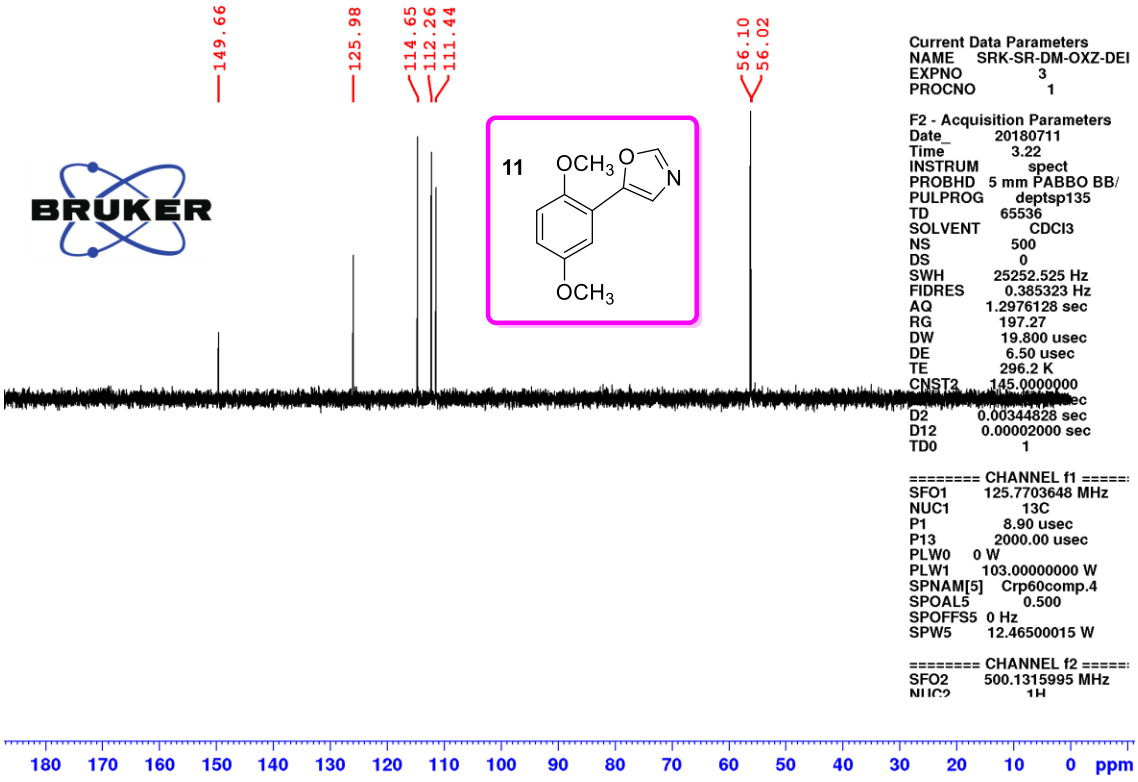
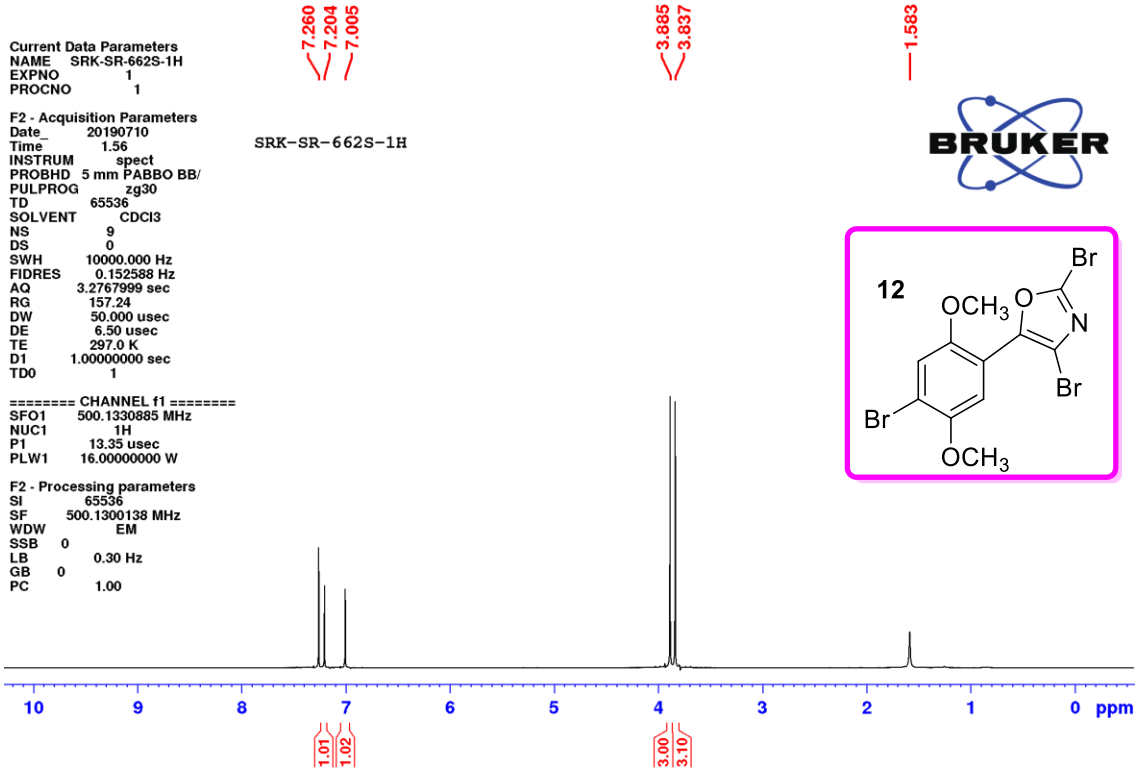
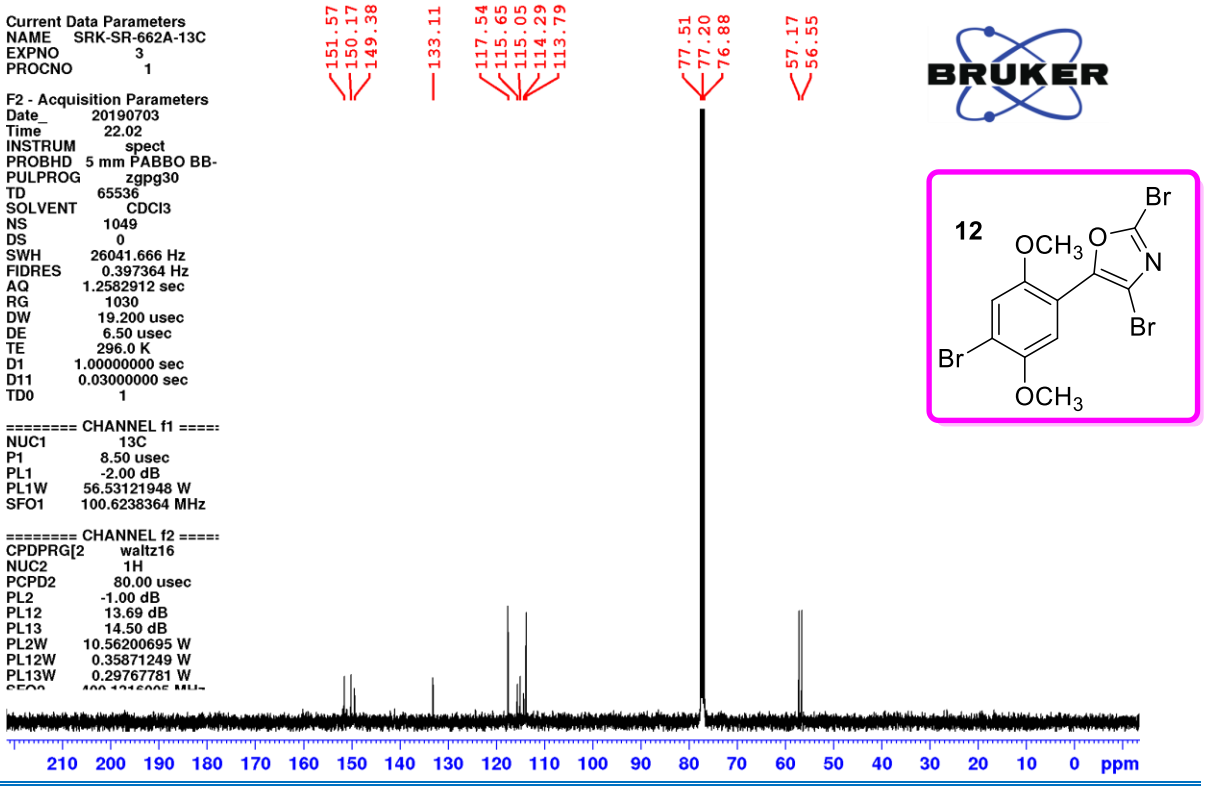


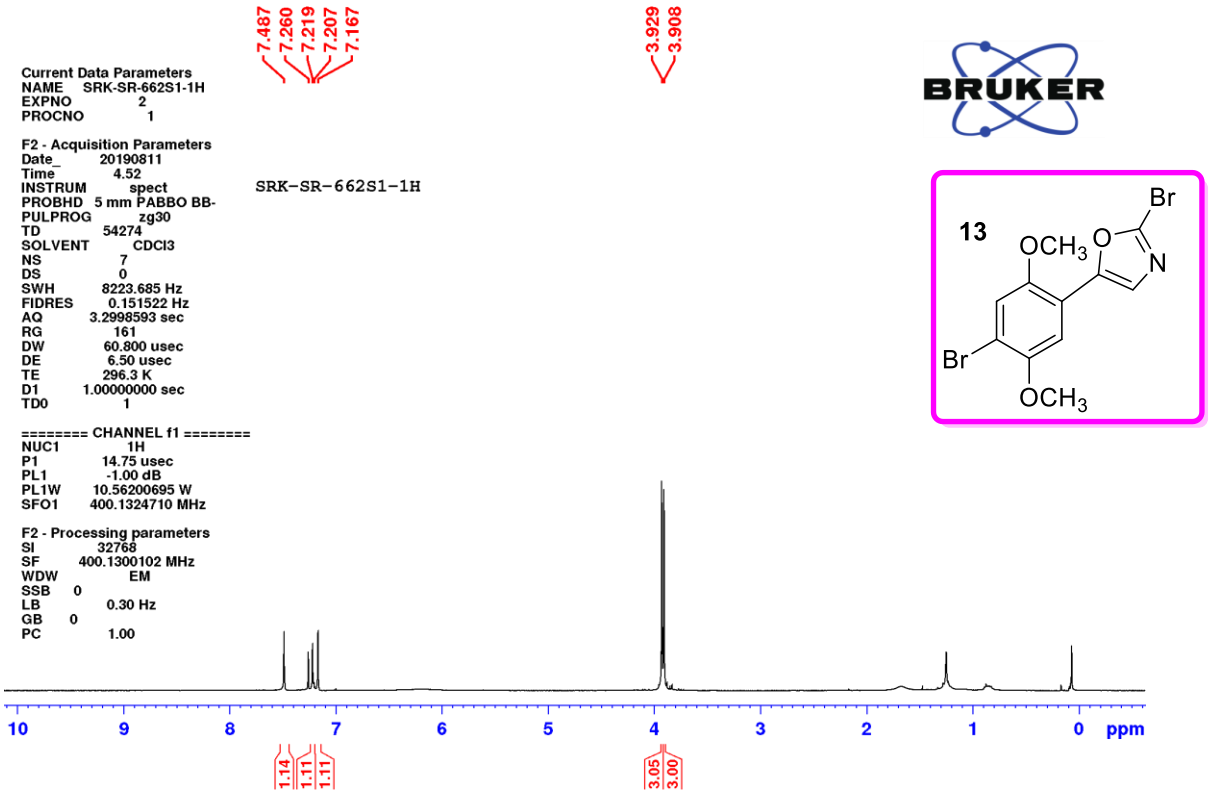
^{1}H NMR (500 MHz, $CDCl_3$) of compound 12



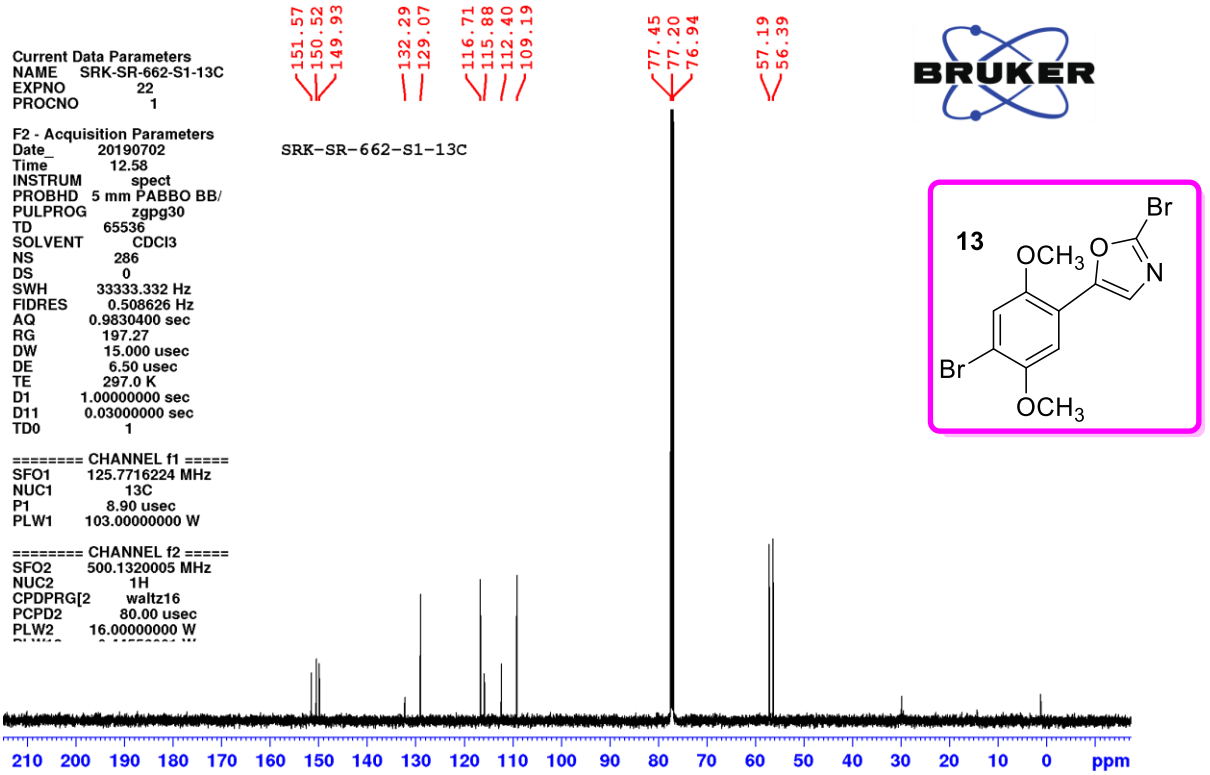
^{13}C NMR (100.6 MHz, $CDCl_3$) of compound 12



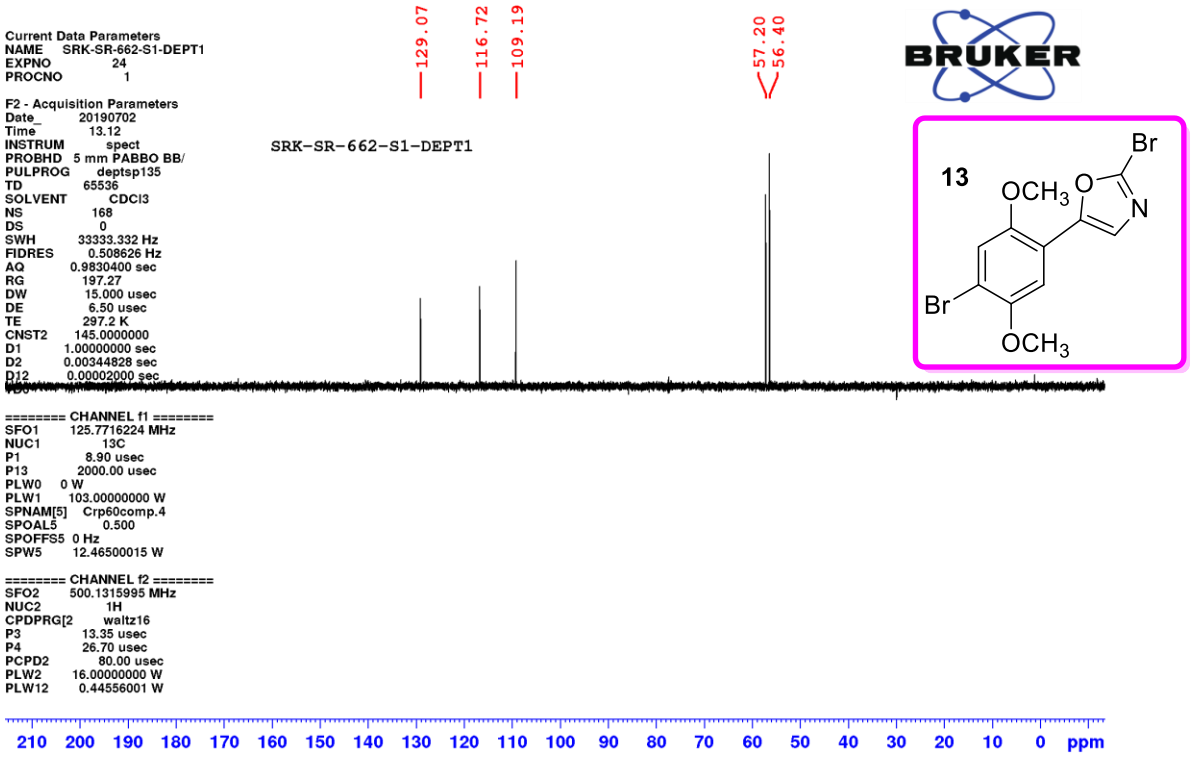
^{1}H NMR (400 MHz, $CDCl_3$) of compound 13



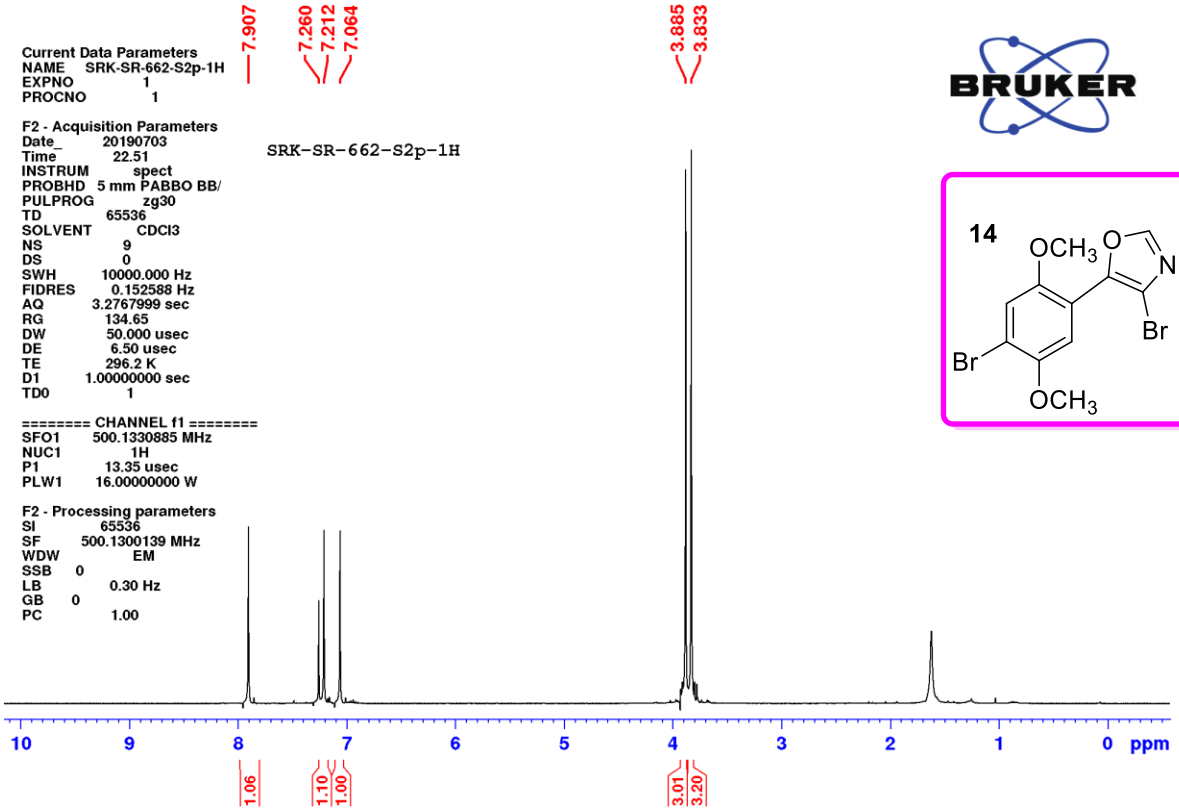
^{13}C NMR (125.7 MHz, $CDCl_3$) of compound 13



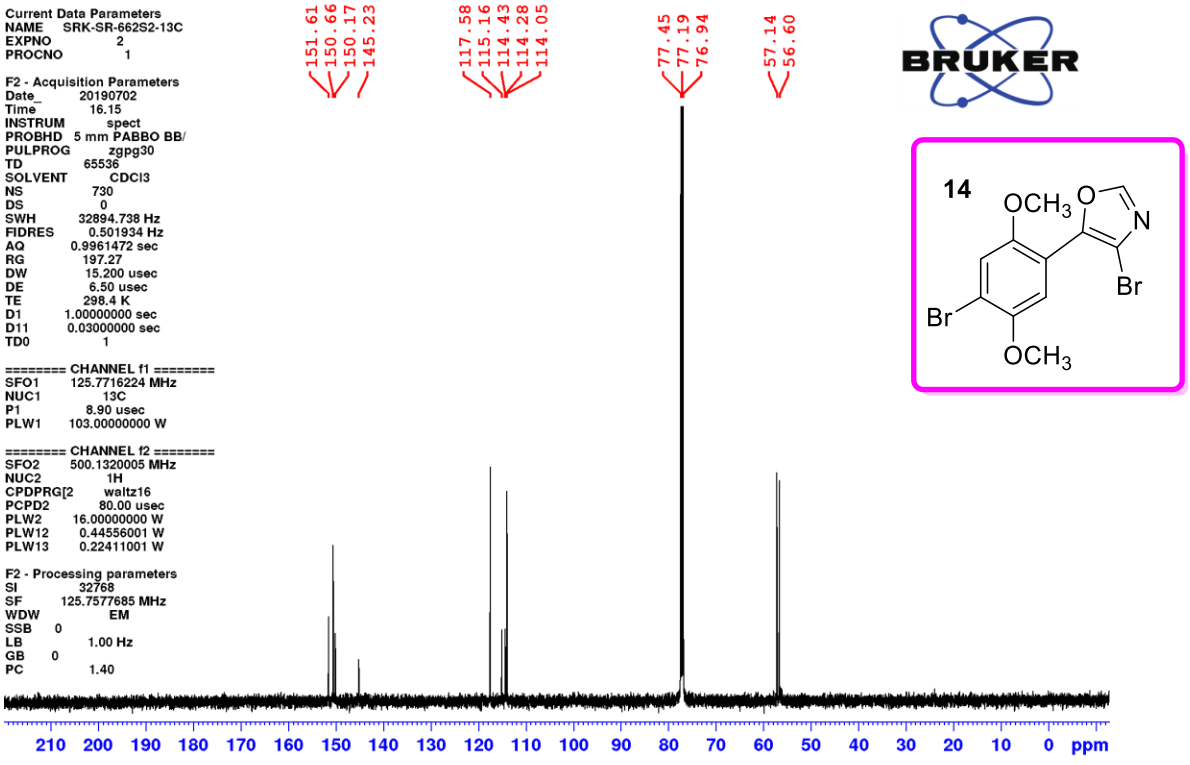
DEPT 135 NMR (125.7 MHz, $CDCl_3$) of compound 13



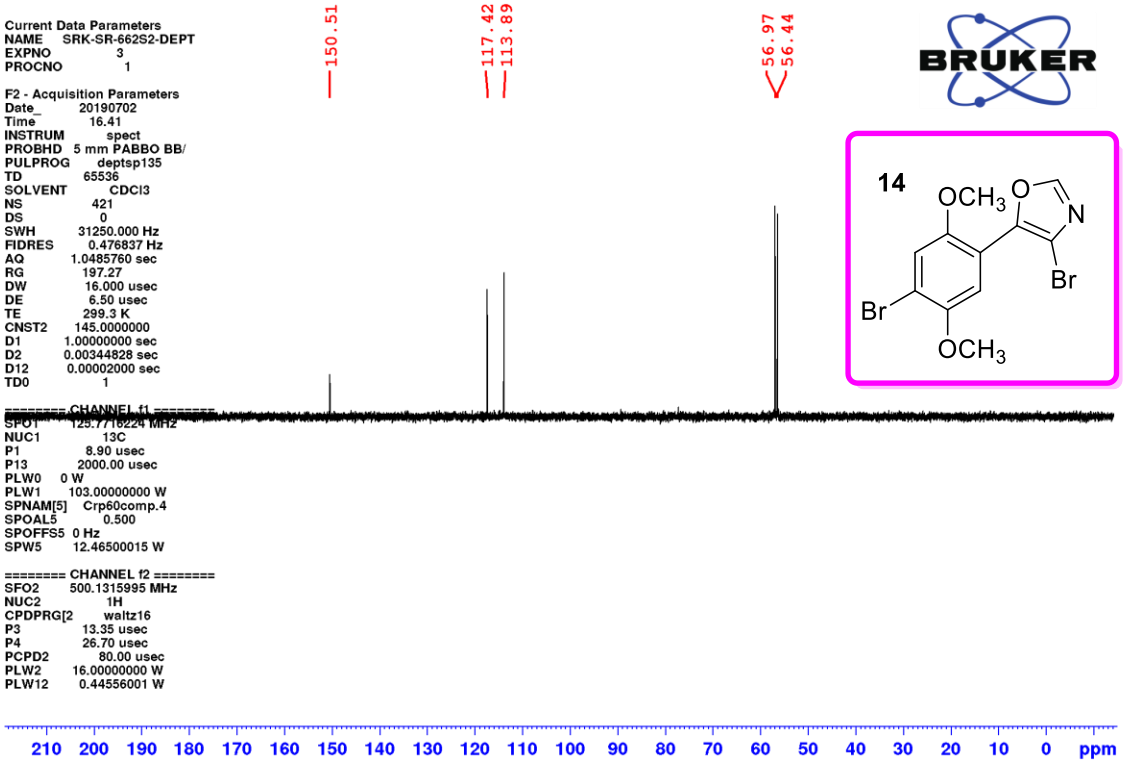
^{1}H NMR (500 MHz, $CDCl_3$) of compound 14



^{13}C NMR (125.7 MHz, $CDCl_3$) of compound 14

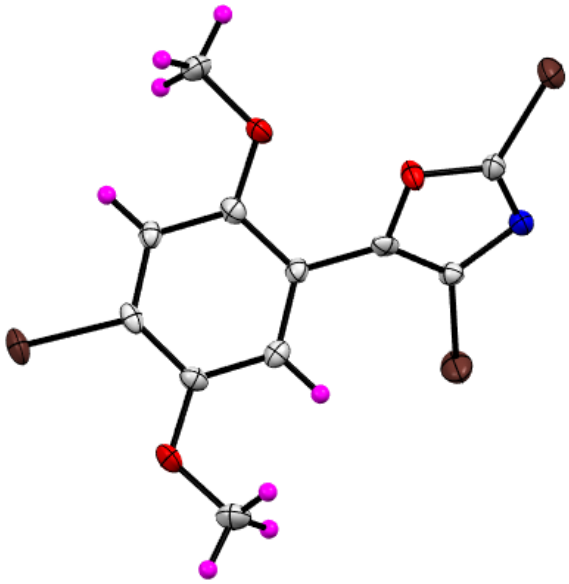


DEPT 135 NMR (125.7 MHz, $CDCl_3$) of compound 14



X-ray crystal structure and data for compounds 12(CCDC- 1984197)

1. X-ray single-crystal structure and refinement data for compound 12



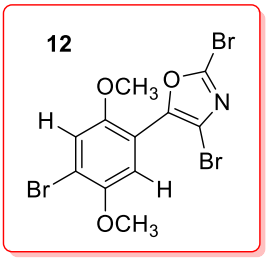


Figure S1: ORTEP representation of the compound **12** with thermal ellipsoids drawn at 30% probability level.

The X-ray structure of compound **12** was determined by single-crystal X-ray diffraction studies. Single crystals of compound **12** were obtained from EtOAc in petroleum ether solvent at room temperature. Crystal data was collected with graphite monochromatized $M_0K\alpha$ radiation (λ = 0.71073) on a Rigaku Saturn 724[1] diffractometer using ω scans at temperature 293 K. The structures were solved by direct methods using Olex-2[2] and ShelXL- 97[3] and refined by full-matrix least-square minimisation based on F^2. ORTEPs were drawn using Mercury program[4] and ORTEP-3.[5] X-ray crystallographic data and refinement parameters for compound **12** provided in below tables and are deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC No: **CCDC-1984197**. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. X-ray crystallographic data and refinement parameters for compound **12** **(CCDC 1984197)**

Identification code	srk-sr-662-br_mo
Empirical formula	$C_{11}H_8Br_3NO_3$
Formula weight	441.91
Temperature	150 K
Crystal system	orthorhombic
Space group	$Pca2_1$
Hall group	P2c -2ac
Unit cell dimensions	a = 20.6267 (8) Å^3 α = 90°
	b = 9.0594 (5) Å^3 β = 90°
	c = 7.1357 (3) Å^3 γ = 90°
Volume	1333.39 (11) Å^3
Z	4
Density (calculated)	2.201 Mg/m^3
Absorption coefficient (μ)	9.074 mm^{-1}
Absorption correction	Multi-Scan
Bond precision C–C	0.0094 A
Max. and min. transmission	1.000 and 0.522
F (000)	840.0
Crystal size	0.232 × 0.182 × 0.041 mm^3
Crystal colour, shape	Colourless, Black
Index ranges	$-23 \leq h \leq 24$, $-10 \leq k \leq 10$, $-8 \leq l \leq 8$
Theta range for data collection	4.496 to 49.96°
Reflections collected	6776
Wavelength	0.71073 Å
Independent reflections	2345 [$R_{(int)}$ = 0.0394]
Completeness to θ = 24.98°	100%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	2345/1/165

Goodness-of-fit on F^2	1.065
Final R indices [I >2sigma (I)]	R1 = 0.0290, ωR2 = 0.0560
R indices (all data)	R1 = 0.0340, ωR2 = 0.0582
Largest diff. peak and hole	0.45 and -0.36 e. $Å^{-3}$
Flack parameter	0.011 (14)

Table S2: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for srk-sr-662-s-br_mo. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br1	-1463.5(3)	-2632.1(8)	-5628.0(14)	24.79(19)
Br3	-4718.1(3)	-9505.0(9)	-1846.0(10)	29.6(2)
Br2	-4689.0(3)	-5783.9(10)	-8150.8(10)	33.6(2)
O3	-3945(2)	-7332(5)	-3340(7)	21.0(11)
O2	-2694(2)	-7657(6)	-4677(7)	23.2(12)
O1	-2848.2(18)	-1613(5)	-5836(8)	25.7(12)
N1	-4837(2)	-7717(7)	-5042(8)	20.4(15)
C10	-4514(3)	-8049(8)	-3575(10)	18.6(17)
C9	-4444(3)	-6662(8)	-5900(10)	15.7(15)
C1	-2832(3)	-3103(7)	-5596(11)	17.9(14)
C2	-3377(3)	-4000(8)	-5414(11)	17.0(15)
C11	-3469(3)	-910(8)	-5714(14)	29.1(17)
C3	-3318(3)	-5510(8)	-5102(8)	15.5(17)
C8	-3899(3)	-6432(8)	-4909(8)	16.2(16)
C5	-2156(3)	-5292(8)	-5176(9)	16.2(17)
C6	-2226(3)	-3774(8)	-5465(11)	17.5(15)
C7	-2074(3)	-8381(9)	-4622(11)	25.3(18)
C4	-2701(3)	-6167(8)	-4990(8)	16.9(17)

Table S3: Anisotropic Displacement Parameters (Å²×10³) for srk-sr-662-s-br_mo. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	20.7(3)	27.7(4)	25.9(3)	-0.5(4)	1.7(3)	-12.3(3)
Br3	22.7(3)	31.8(5)	34.3(5)	12.4(4)	3.9(4)	-4.6(3)
Br2	28.5(4)	41.7(5)	30.6(5)	15.6(4)	-11.4(4)	-6.6(4)
O3	19(2)	25(3)	19(2)	5(2)	-2(2)	-8(2)
O2	21(2)	14(3)	34(3)	3(2)	4(2)	-2(2)
O1	23(2)	15(3)	39(3)	2(3)	-1(3)	-7(2)
N1	16(3)	16(4)	29(4)	2(3)	0(3)	-1(3)
C10	14(3)	17(4)	25(4)	0(3)	3(3)	0(3)

C9	17(3)	14(4)	16(4)	0(3)	-3(3)	0(3)
C1	22(3)	13(4)	18(3)	-1(4)	1(4)	0(3)
C2	16(3)	21(4)	14(3)	-2(4)	-1(3)	2(3)
C11	32(4)	17(4)	38(4)	3(5)	1(4)	4(3)
C3	14(3)	18(4)	15(4)	1(3)	-2(2)	-1(3)
C8	19(3)	11(4)	18(4)	-1(3)	5(3)	5(3)
C5	14(3)	21(4)	14(4)	1(3)	-1(3)	-2(3)
C6	20(3)	21(4)	11(3)	0(4)	1(3)	-8(3)
C7	20(4)	21(5)	35(4)	2(4)	-3(3)	6(4)
C4	20(4)	15(4)	16(4)	-3(3)	-1(3)	-2(3)

Table S4: Bond Lengths for srk-sr-662-s-br_mo.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C6	1.886(6)	N1	C9	1.395(9)
Br3	C10	1.855(7)	C9	C8	1.345(9)
Br2	C9	1.862(7)	C1	C2	1.393(8)
O3	C10	1.352(8)	C1	C6	1.393(8)
O3	C8	1.388(8)	C2	C3	1.391(9)
O2	C7	1.438(7)	C3	C8	1.467(9)
O2	C4	1.369(9)	C3	C4	1.407(9)
O1	C1	1.362(8)	C5	C6	1.398(10)
O1	C11	1.433(7)	C5	C4	1.382(9)
N1	C10	1.277(9)			

Table S5: Bond Angles for srk-sr-662-s-br_mo.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	O3	C8	104.0(5)	C2	C3	C8	120.3(6)
C4	O2	C7	117.6(5)	C2	C3	C4	120.3(6)
C1	O1	C11	117.0(5)	C4	C3	C8	119.5(6)
C10	N1	C9	102.5(5)	O3	C8	C3	117.8(5)
O3	C10	Br3	117.2(5)	C9	C8	O3	106.0(6)
N1	C10	Br3	126.4(5)	C9	C8	C3	136.2(6)
N1	C10	O3	116.2(6)	C4	C5	C6	119.6(6)
N1	C9	Br2	120.9(4)	C1	C6	Br1	120.3(5)

C8	C9	Br2	127.9(5)	C1	C6	C5	122.1(6)
C8	C9	N1	111.2(6)	C5	C6	Br1	117.5(5)
O1	C1	C2	124.8(5)	O2	C4	C3	115.8(6)
O1	C1	C6	117.6(5)	O2	C4	C5	125.0(6)
C2	C1	C6	117.6(6)	C5	C4	C3	119.2(7)
C3	C2	C1	121.2(6)				

Table S6: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for srk-sr-662-s-br_mo.

Atom	*x*	*y*	*z*	U(eq)
H2	-3796	-3573	-5504	20
H11A	-3746	-1254	-6742	44
H11B	-3414	163	-5804	44
H11C	-3672	-1157	-4512	44
H5	-1736	-5720	-5107	19
H7A	-1848	-8220	-5811	38
H7B	-2137	-9442	-4424	38
H7C	-1816	-7974	-3593	38