

Supporting Information

Synthesis of bisoxazole and bromo-substituted aryloxazoles

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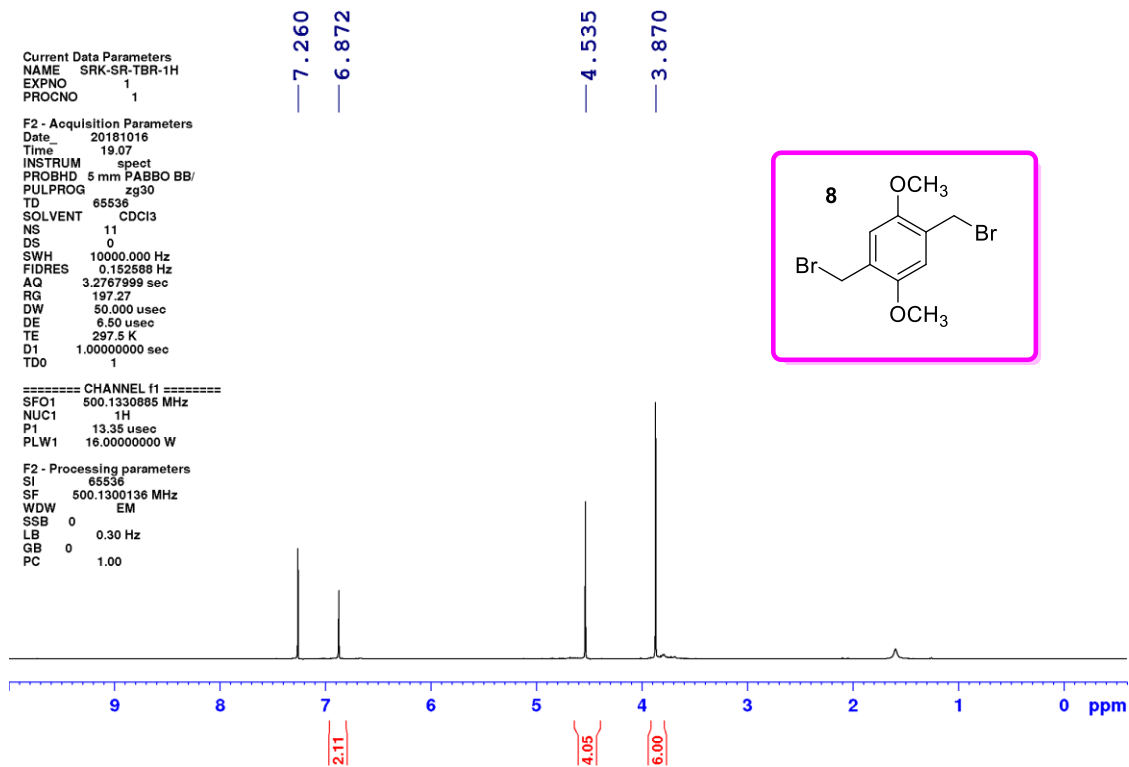
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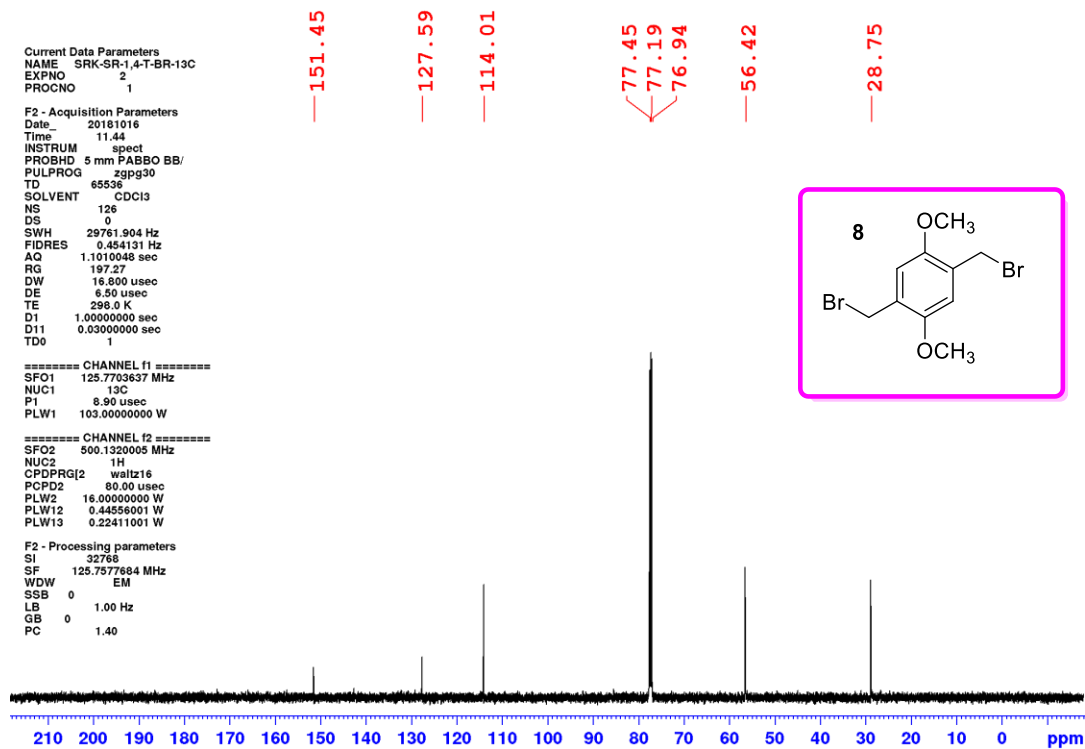
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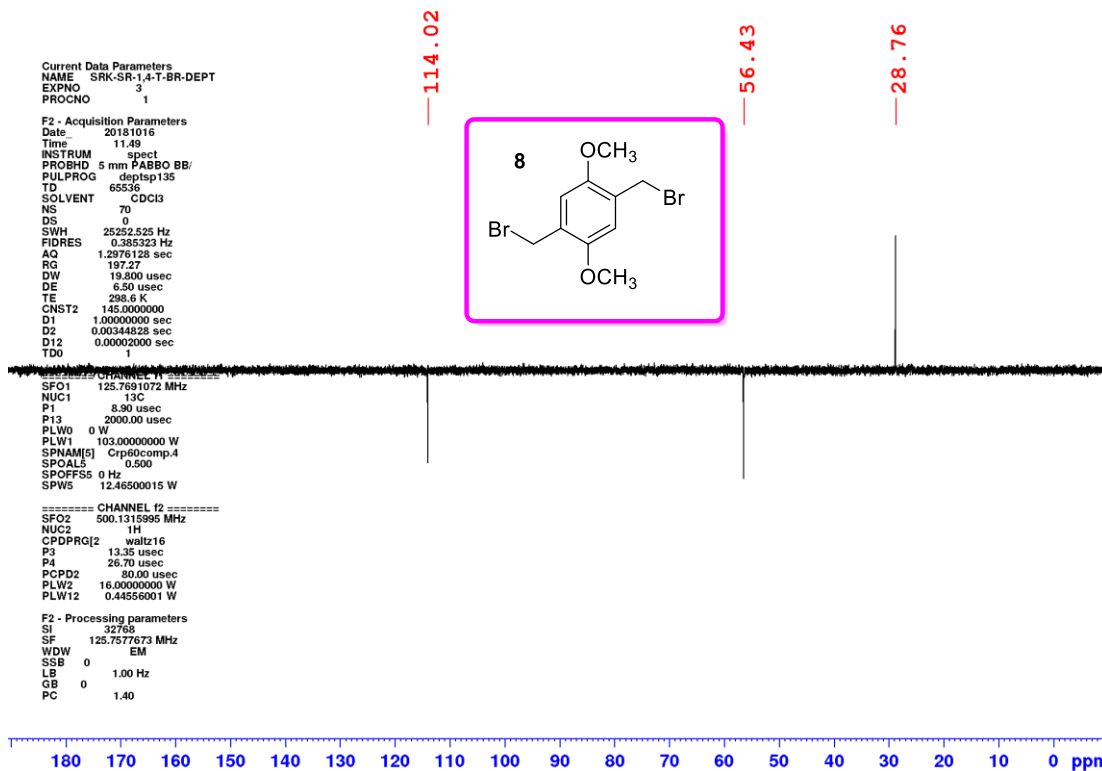
¹H NMR (500 MHz, CDCl₃) of compound **8**



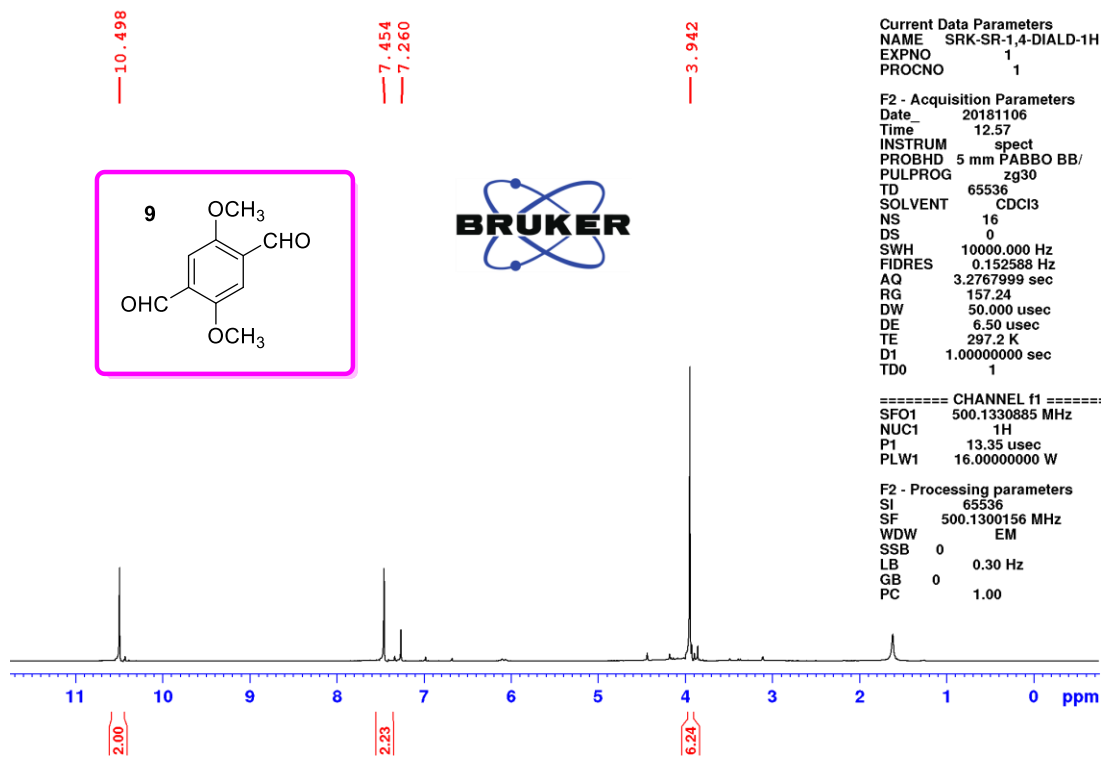
¹³C NMR (125.7 MHz, CDCl₃) of compound **8**



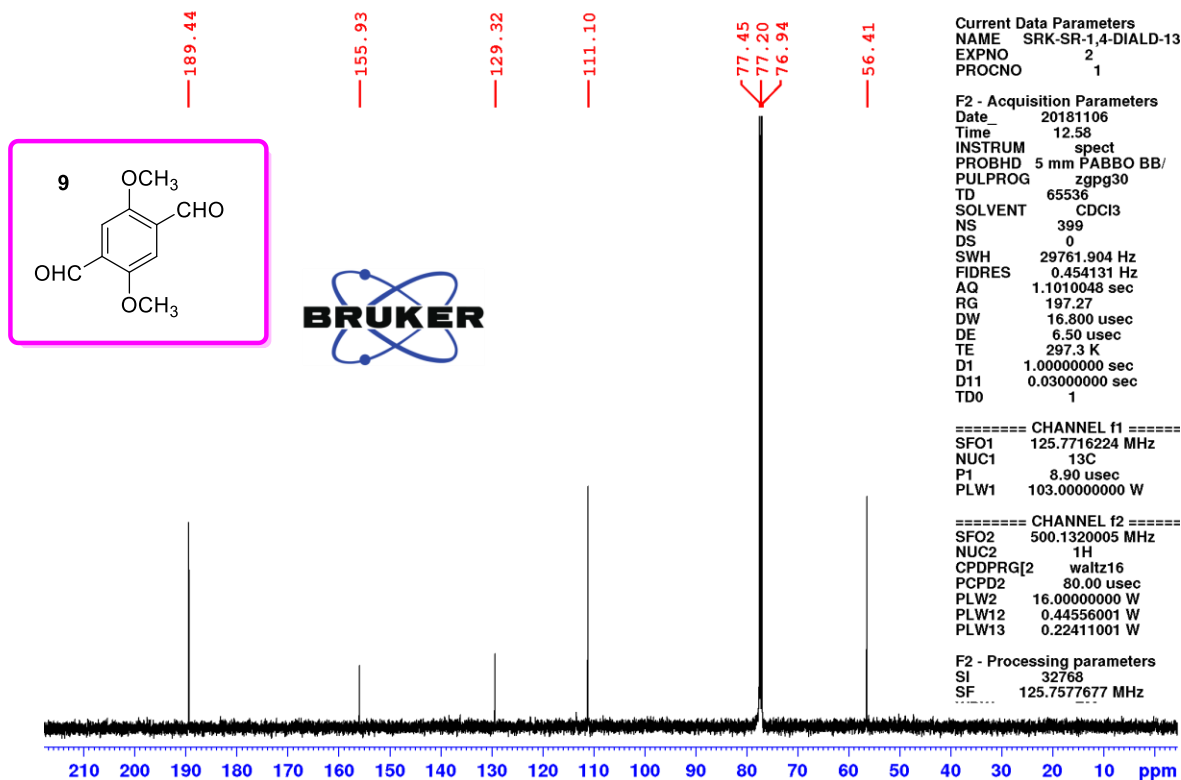
DEPT 135 NMR (125.7 MHz, CDCl₃) of compound **8**



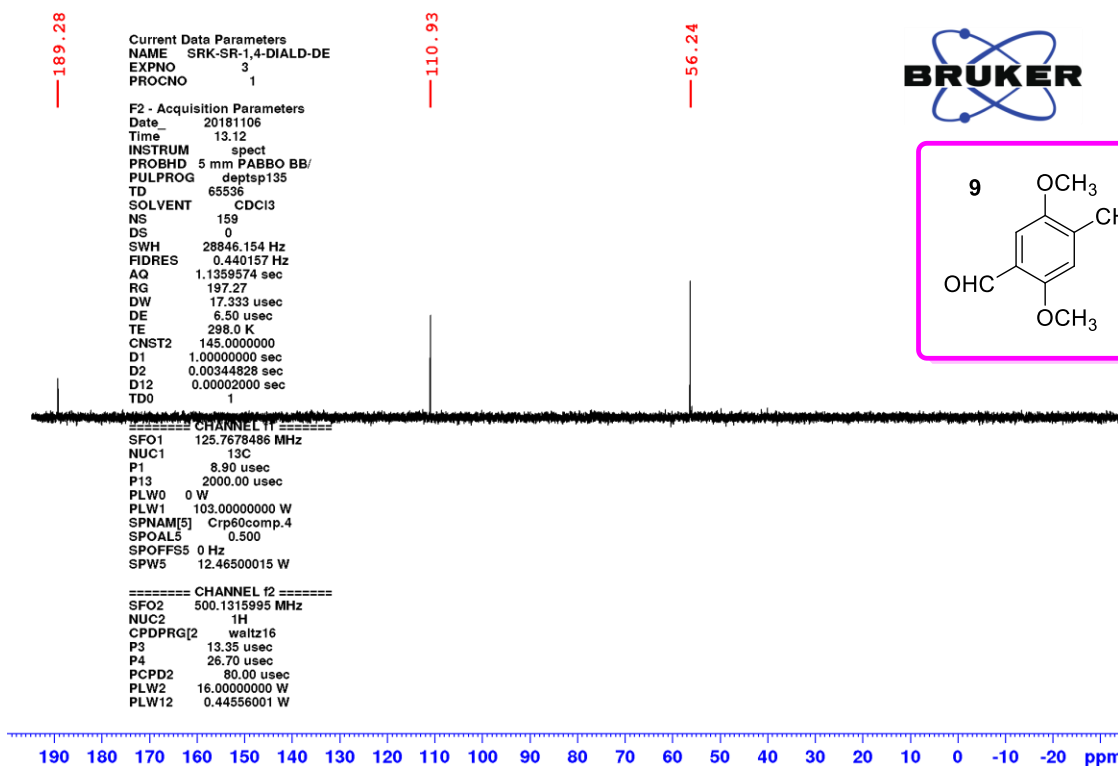
¹H NMR (500 MHz, CDCl₃) of compound **9**



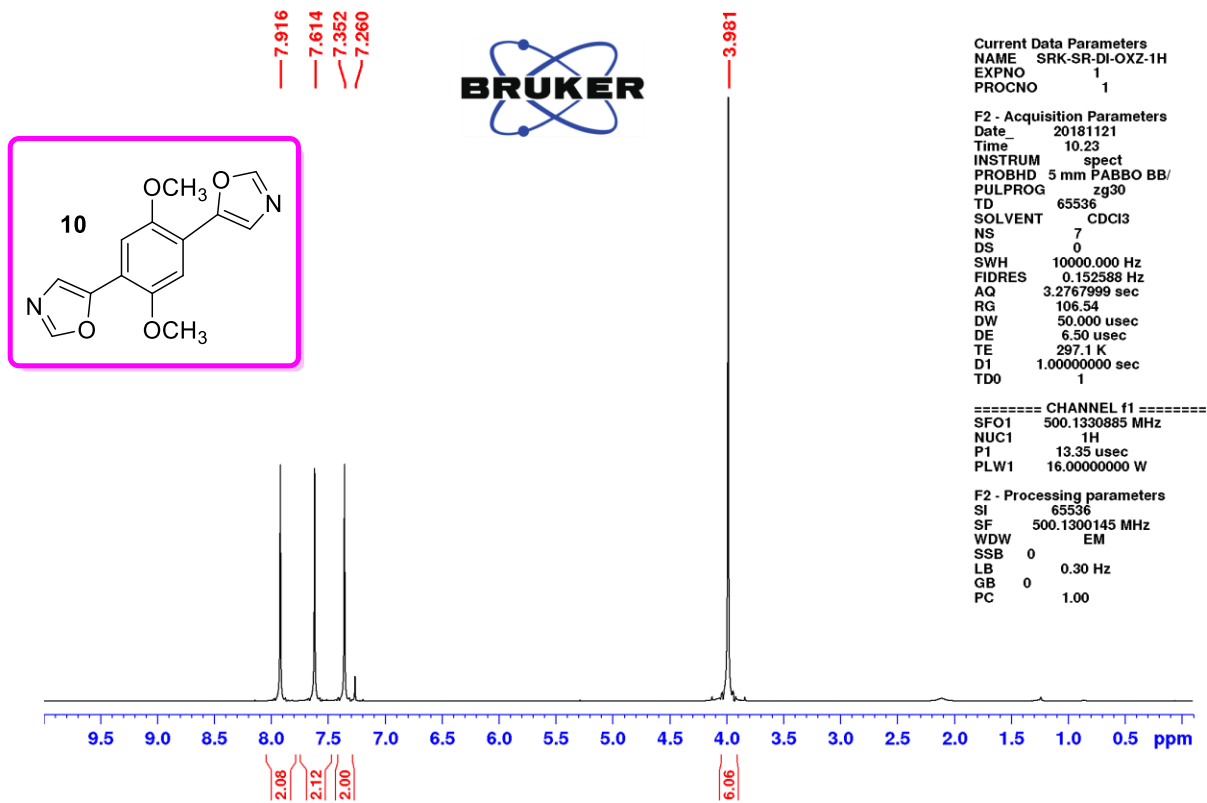
¹³C NMR (125.7 MHz, CDCl₃) of compound **9**



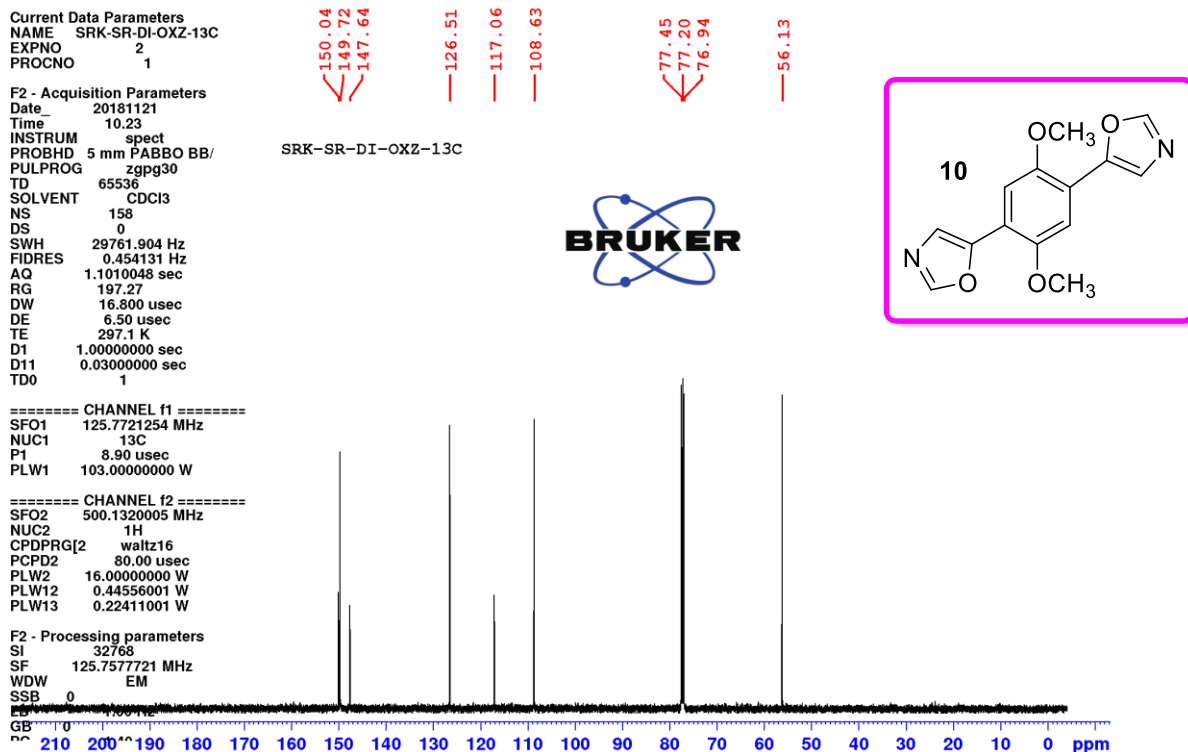
DEPT 135 NMR (125.7 MHz, CDCl₃) of compound **9**



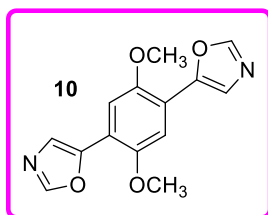
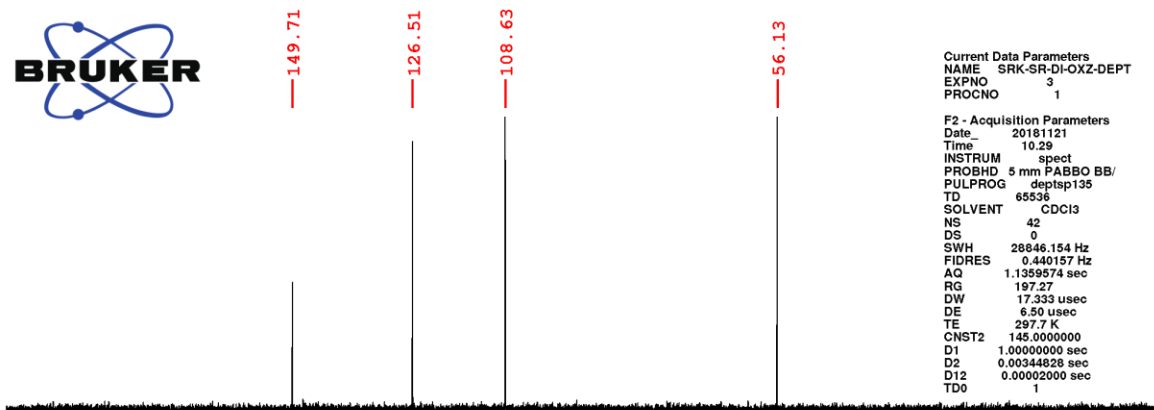
¹H NMR (500 MHz, CDCl₃) of compound **10**



¹³C NMR (125.7 MHz, CDCl₃) of compound **10**



DEPT 135 NMR (125.7 MHz, CDCl₃) of compound **10**



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 PROCNO 1

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 FIDRES 0.440157 Hz
 AQ 1.1359574 sec
 RG 197.27
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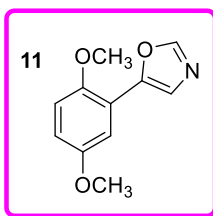
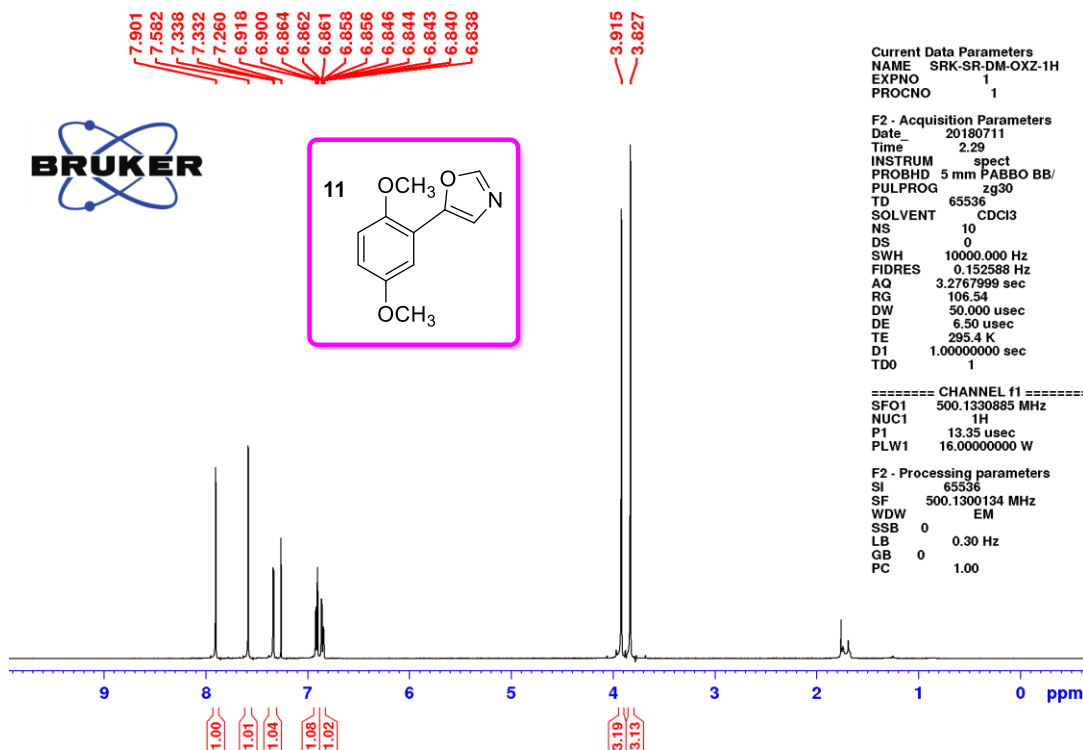
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 SPOALS 0.500
 SPOFFS 0 Hz
 SPW5 12.46500015 W

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 PLW12 0.44556001 W

F2 - Processing parameters
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 WDW FM

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¹H NMR (500 MHz, CDCl₃) of compound **11**



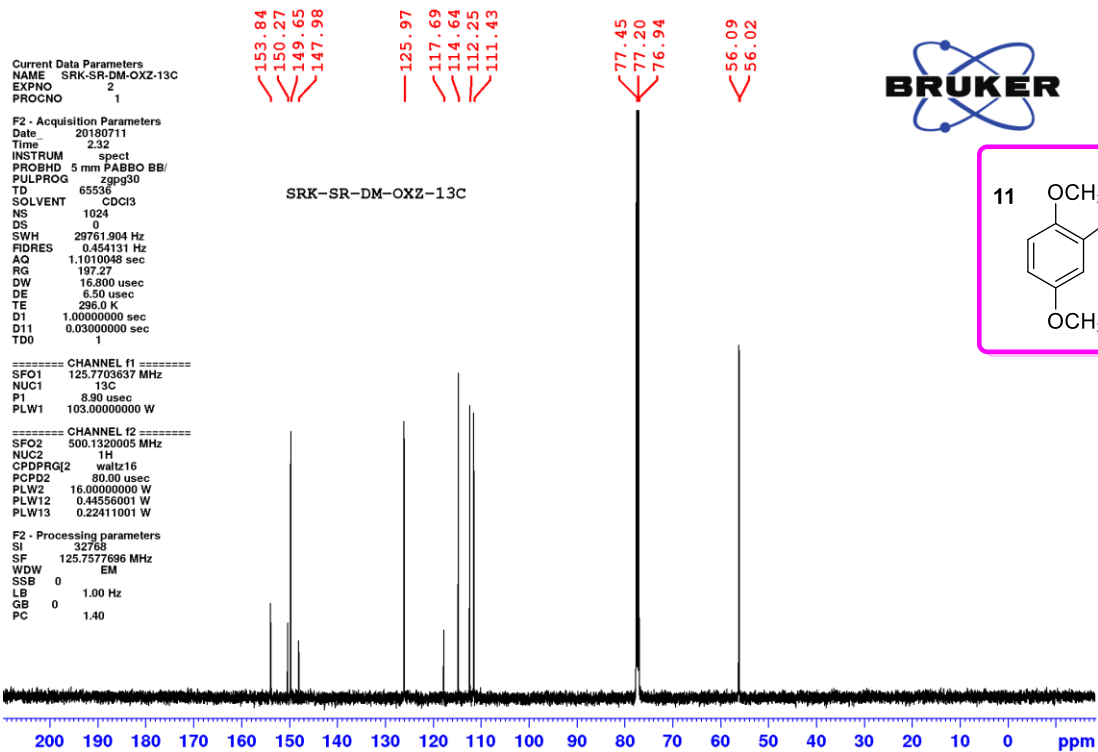
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 RG 106.54
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 DE 6.50 usec
 TE 295.4 K
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 TD0 1

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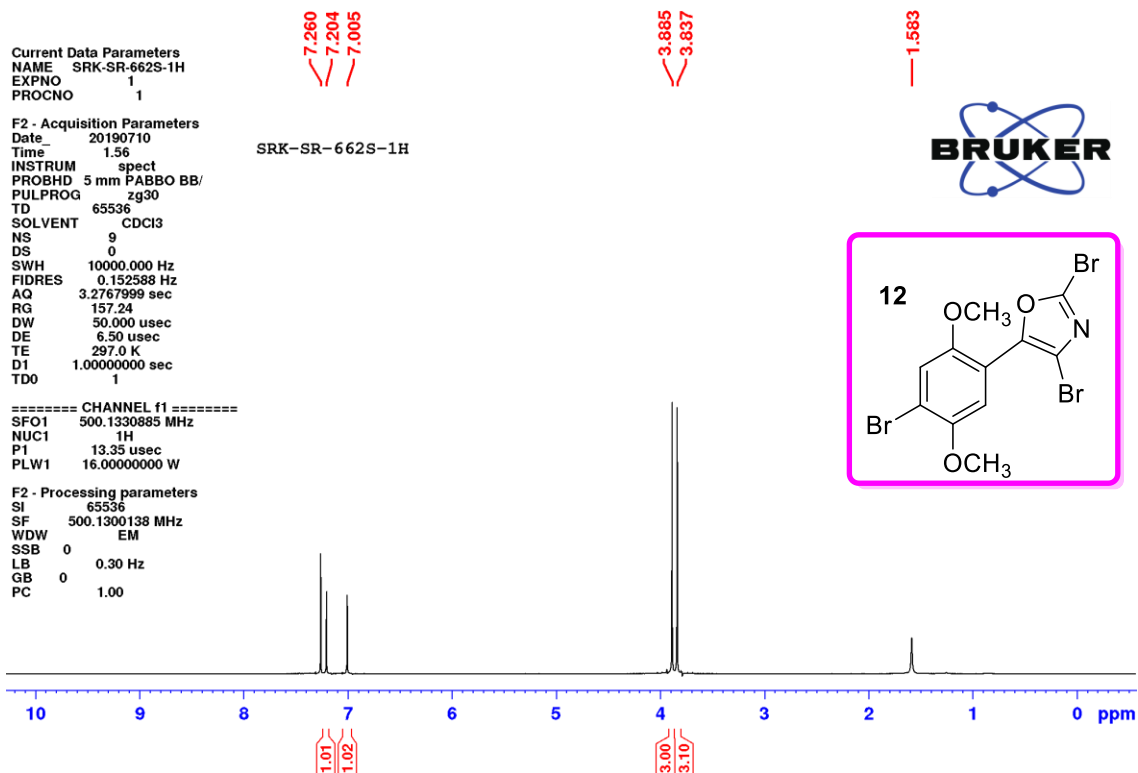
¹³C NMR (125.7 MHz, CDCl₃) of compound **11**



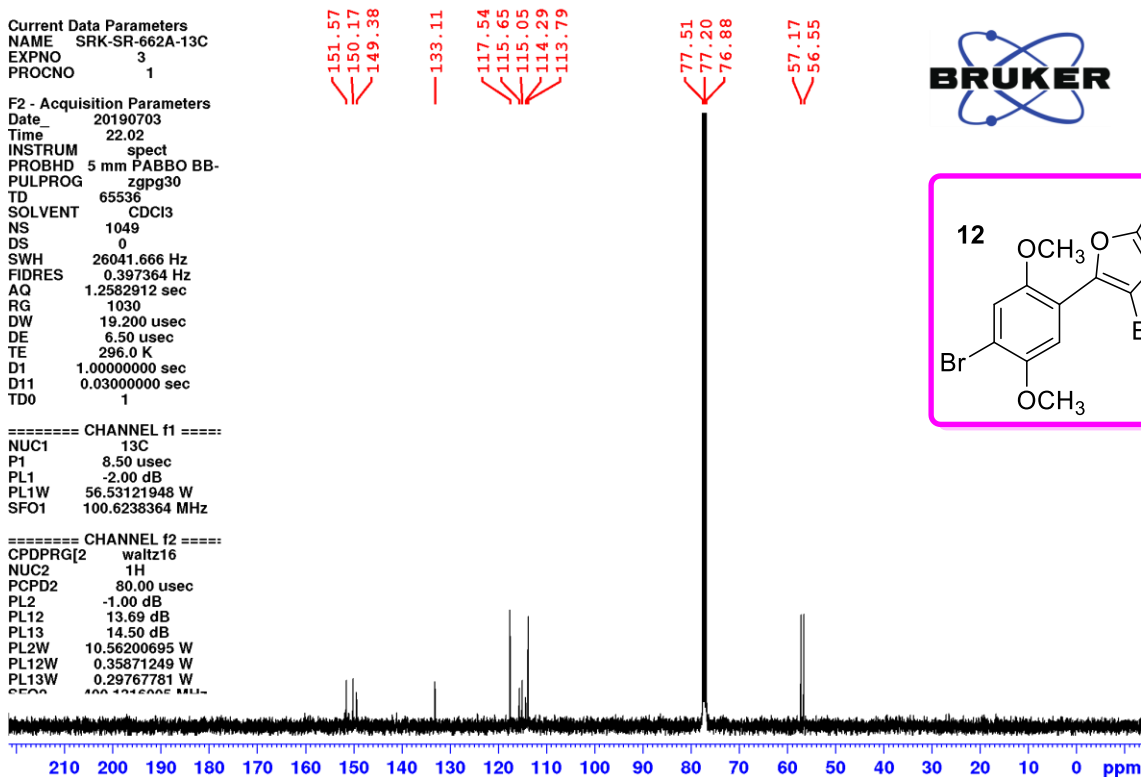
DEPT 135 NMR (125.7 MHz, CDCl₃) of compound **11**



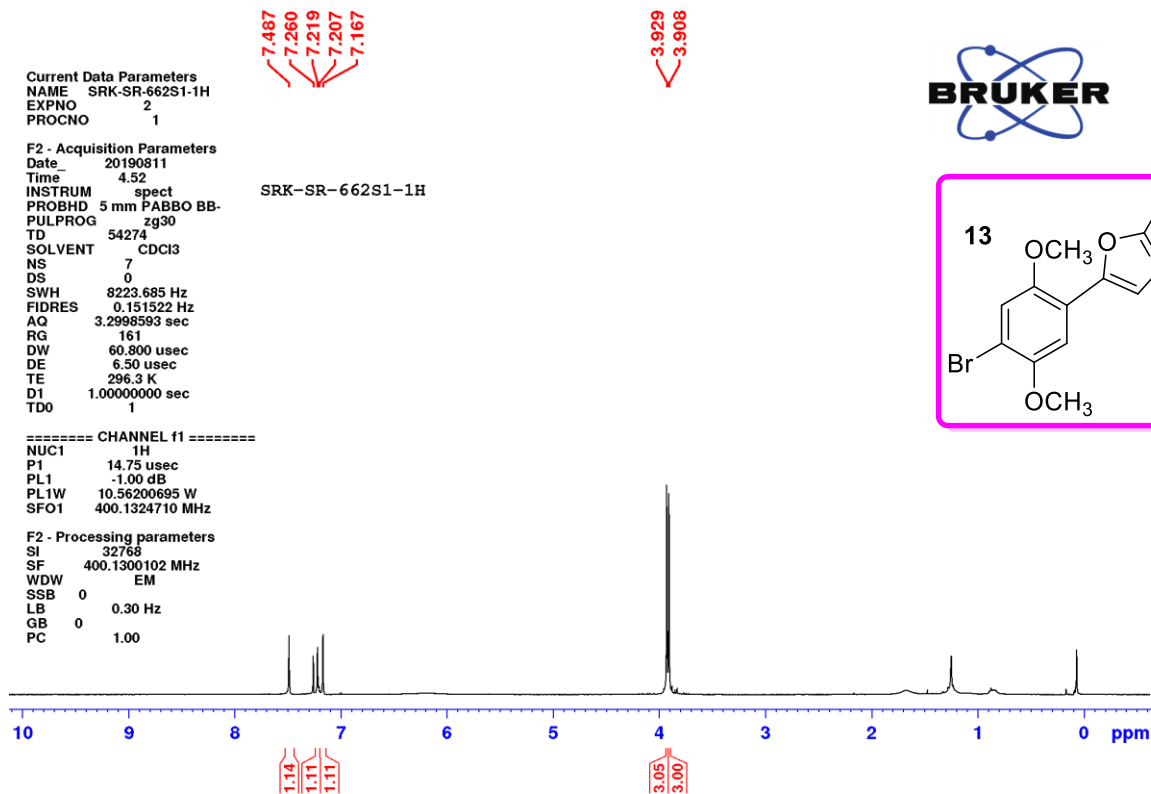
¹H NMR (500 MHz, CDCl₃) of compound 12



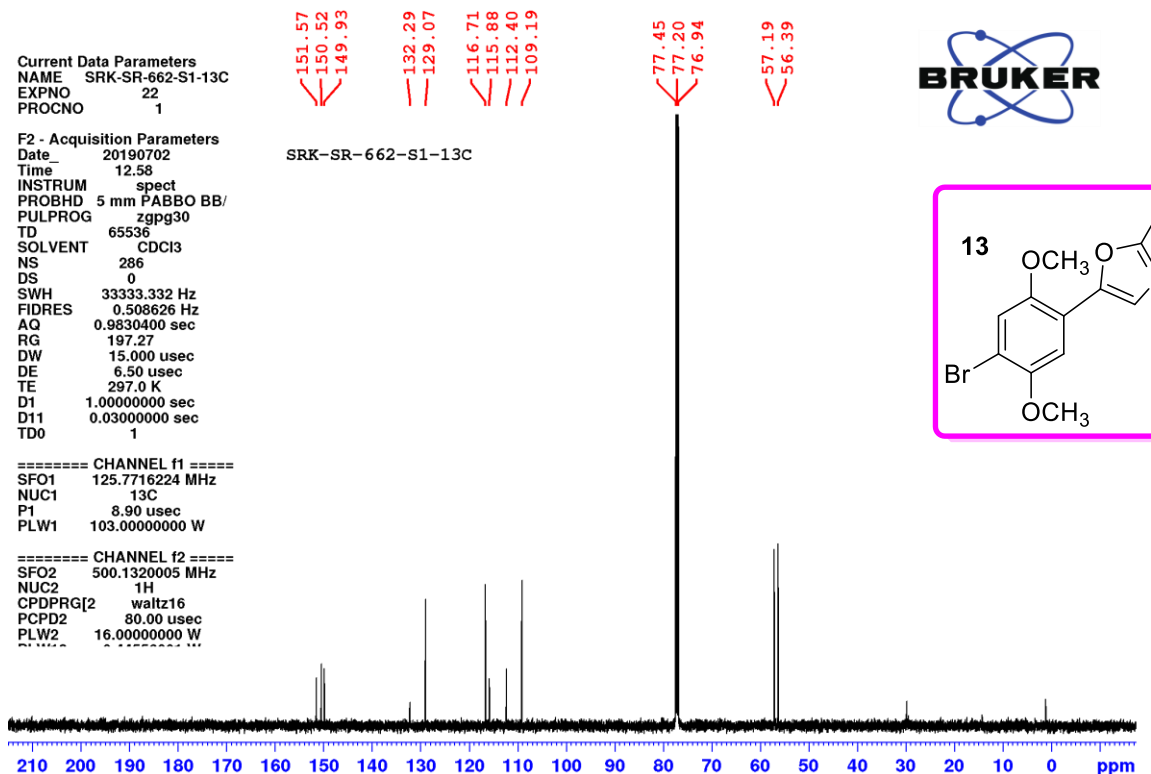
¹³C NMR (100.6 MHz, CDCl₃) of compound 12



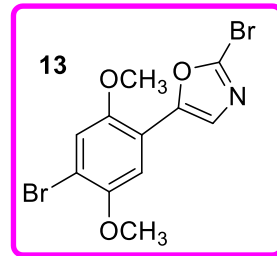
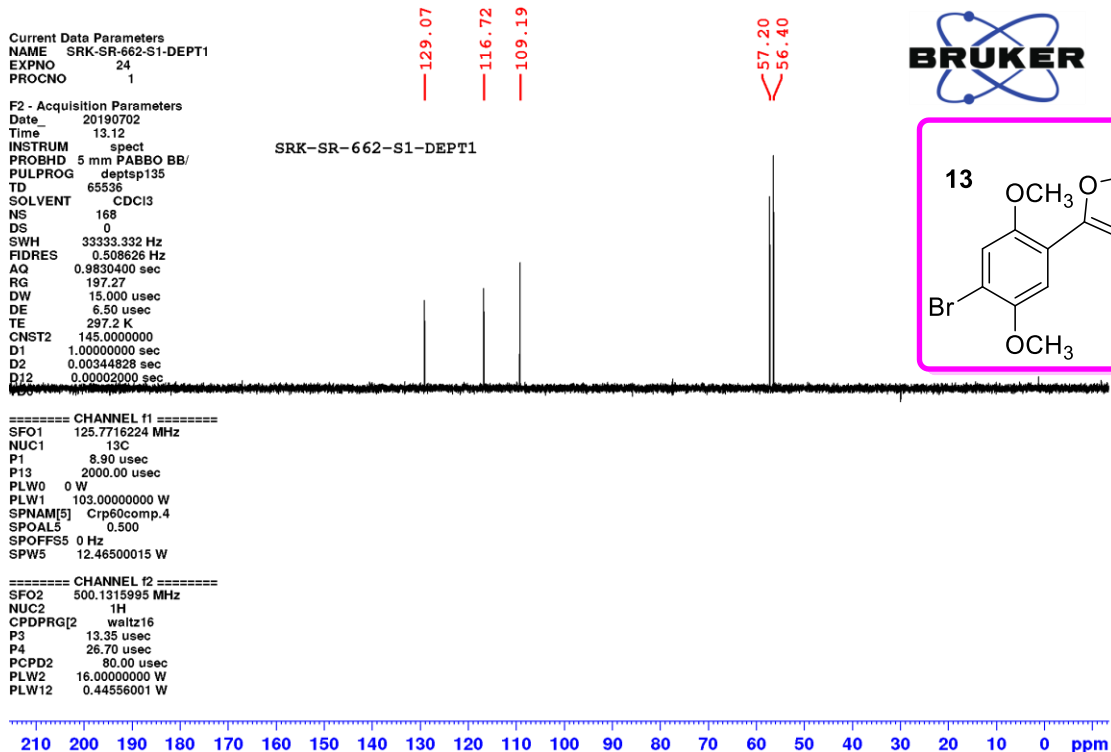
¹H NMR (400 MHz, CDCl₃) of compound **13**



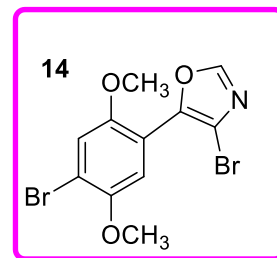
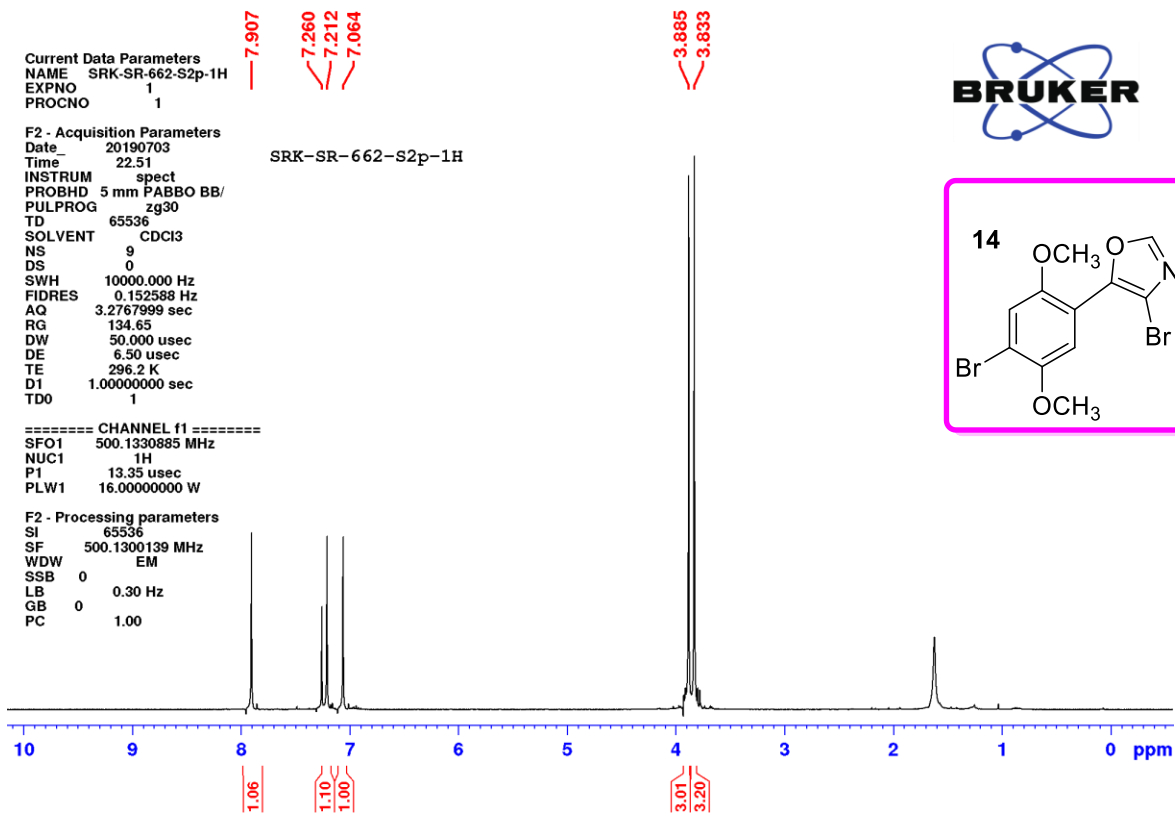
¹³C NMR (125.7 MHz, CDCl₃) of compound **13**



DEPT 135 NMR (125.7 MHz, CDCl₃) of compound **13**



¹H NMR (500 MHz, CDCl₃) of compound **14**



¹³C NMR (125.7 MHz, CDCl₃) of compound **14**

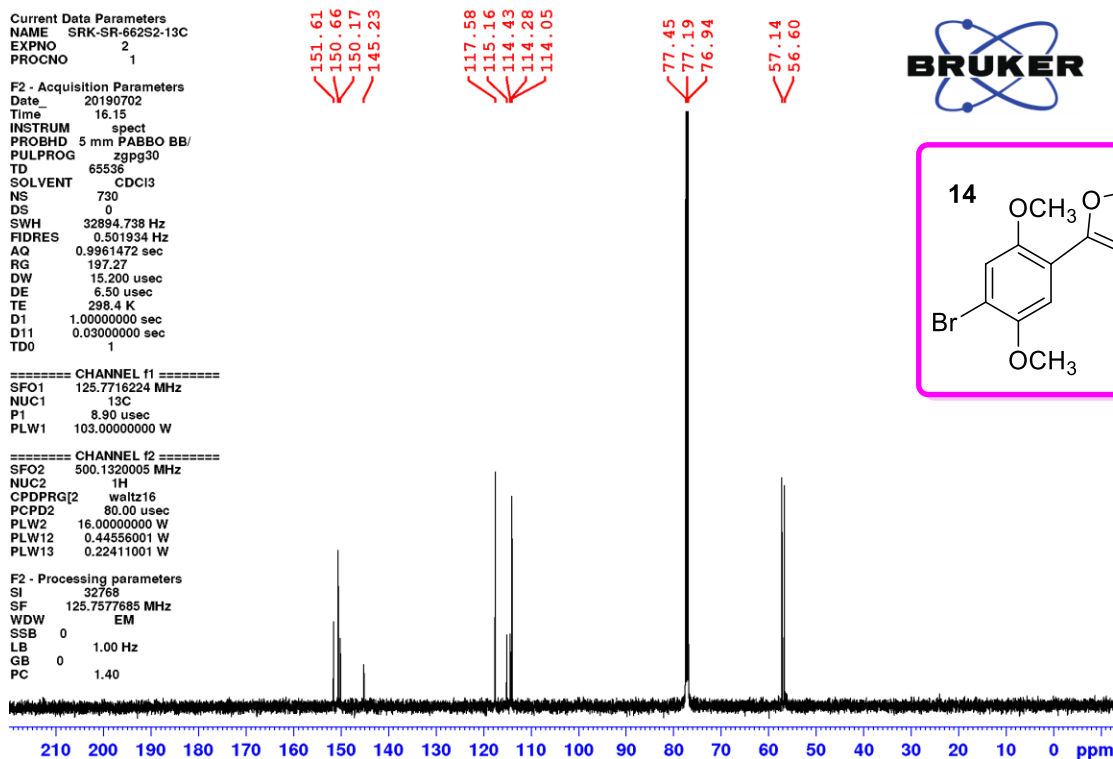
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NUC2 1H
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F2 - Processing parameters
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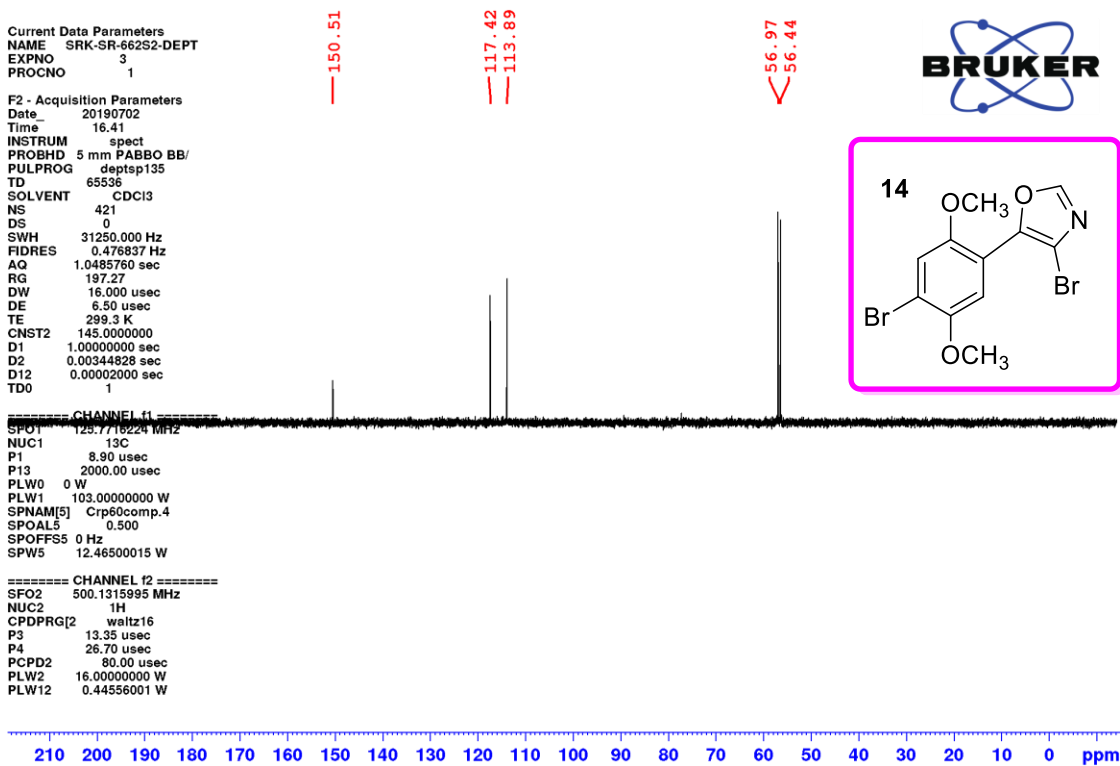
DEPT 135 NMR (125.7 MHz, CDCl₃) of compound **14**

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SOLVENT CDCl₃
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FIDRES 0.476837 Hz
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RG 197.27
DW 16.000 usec
DE 6.50 usec
TE 299.3 K
CNST2 145.0000000
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D12 0.00002000 sec
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P13 2000.00 usec
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PLW1 103.00000000 W
SPNAM[5] Crp60comp.4
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SPOFFS5 0 Hz
SPW5 12.46500015 W

===== CHANNEL f2 =====
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CPDPRG[2] waltz16
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P4 26.70 usec
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.44556001 W



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

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

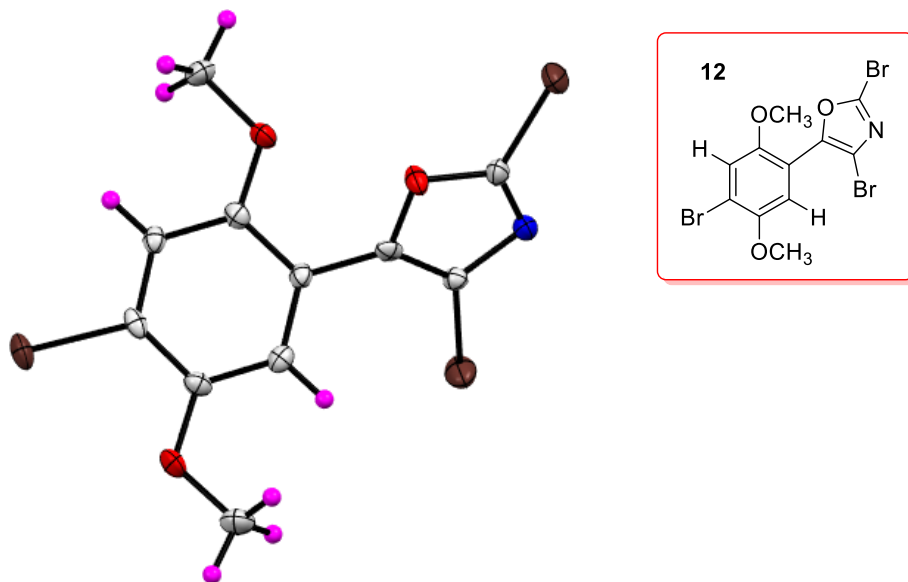


Figure S1: ORTEP representation of the compound **12** with thermal ellipsoids drawn at 30% probability level.

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 MoK α radiation ($\lambda = 0.71073$) on a Rigaku Saturn 724¹ diffractometer using ω scans at temperature 293 K. The structures were solved by direct methods using Olex-2² and ShelXL-97³ and refined by full-matrix least-square minimisation based on F^2 . ORTEPs were drawn using Mercury program⁴ 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 ₈ Br ₃ NO 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 Å
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 ≤ h ≤ 24, -10 ≤ k ≤ 10, -8 ≤ l ≤ 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 [$I > 2\sigma(I)$]	$R1 = 0.0290$, $\omega R2 = 0.0560$
R indices (all data)	$R1 = 0.0340$, $\omega R2 = 0.0582$
Largest diff. peak and hole	0.45 and -0.36 e. \AA^{-3}
Flack parameter	0.011 (14)

Table S2: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for srk-sr-662-s-br_mo. U_{eq} is defined as 1/3 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 ($\text{\AA}^2 \times 10^3$) for srk-sr-662-s-br_mo. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

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 ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) 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