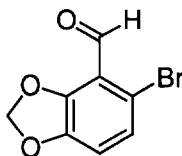
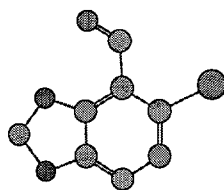


Supplemental Material:**Structure Determination of 5-bromo-benzodioxole-4-carboxaldehyde
by Single Crystal Analysis**

5-bromo-benzodioxole-4-carboxaldehyde



X-ray structure of 5-bromo-benzodioxole-4-carboxaldehyde

CRYSTAL DATAChemical formula: $C_8H_5BrO_3$

Crystal system: Orthorhombic

Space Group: $P2_12_12_1$ $a = 12.5196(7) \text{ \AA}$ $\alpha = 90^\circ$ $b = 4.0800(1) \text{ \AA}$ $\beta = 90^\circ$ $c = 15.0027(5) \text{ \AA}$ $\gamma = 90^\circ$ $Z = 4$ $d_x = 1.983 \text{ g cm}^{-3}$ $V = 766.35(5) \text{ \AA}^3$

No. of reflections for lattice parameters: 25

 θ range for lattice parameters ($^\circ$): 15.84-43.65Absorption coefficient (mm^{-1}): 7.06**EXPERIMENTAL:**CrystallizationCrystal source: $\text{CHCl}_3/\text{EtOH}$

Crystal description: Yellow plate

Crystal size (mm): 0.15 X 0.25 X 0.35

Data Collection

Temperature (K): 295

 θ_{max} ($^\circ$): 75

No. of reflections measured: 1850

No. of independent reflections: 1574

No. of observed reflections ($I > 3\sigma$): 1566Absorption correction ($T_{\text{min}}-T_{\text{max}}$): 0.66-0.99 R_{int} : 0.02**REFINEMENT**

No. of parameters refined: 109

No. of reflections used: 1566

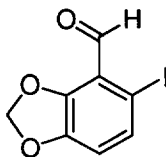
$R(F) = 0.050$ $wR(F) = 0.078$ $S = 1.69$ Weighting Scheme $w = 1/[\sigma^2(F) + 0.002F^2]$

Treatment of Hydrogen Atoms: The positions of all the hydrogen atoms were calculated from an idealized geometry with standard bond lengths and angles. They were assigned isotropic temperature factors and were included in structure factor calculations with fixed parameters.

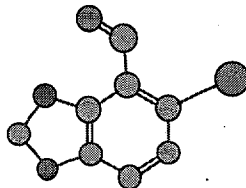
Protein Data Base Coordinates:

ATOM	1	BR1	D	1	5.293	-0.144	1.256	4.50	1.00
ATOM	2	O7	D	1	1.174	-2.435	3.782	4.50	1.00
ATOM	3	O5	D	1	1.906	-1.823	5.889	4.50	1.00
ATOM	4	C90	D	1	2.543	-1.813	1.192	4.50	1.00
ATOM	5	H90A	D	1	3.045	-1.521	0.427	4.50	1.00
ATOM	6	C2	D	1	4.659	-0.288	3.997	4.50	1.00
ATOM	7	H2A	D	1	5.454	0.243	4.078	4.50	1.00
ATOM	8	C8	D	1	2.343	-1.736	3.683	4.50	1.00
ATOM	9	C9	D	1	3.018	-1.409	2.514	4.50	1.00
ATOM	10	O9	D	1	1.574	-2.490	0.986	4.50	1.00
ATOM	11	C6	D	1	0.847	-2.474	5.186	4.50	1.00
ATOM	12	H6A	D	1	0.769	-3.384	5.481	4.50	1.00
ATOM	13	H6B	D	1	0.013	-2.027	5.348	4.50	1.00
ATOM	14	C4	D	1	2.776	-1.364	4.945	4.50	1.00
ATOM	15	C3	D	1	3.933	-0.659	5.138	4.50	1.00
ATOM	16	H3A	D	1	4.239	-0.434	6.020	4.50	1.00
ATOM	17	C1	D	1	4.214	-0.681	2.736	4.50	1.00

**Structure Determination of 5-iodo-benzodioxole-4-carboxaldehyde
by Single Crystal Analysis**



5-iodo-benzodioxole-4-carboxaldehyde



X-ray structure of 5-iodo-benzodioxole-4-carboxaldehyde

CRYSTAL DATA

Chemical formula: $C_8H_5IO_3$

Crystal system: Orthorhombic

Space Group: $P2_12_12_1$

$a = 4.2116(2) \text{ \AA}$ $\alpha = 90^\circ$

$b = 12.3896(5) \text{ \AA}$ $\beta = 90^\circ$

$c = 15.251(1) \text{ \AA}$ $\gamma = 90^\circ$

$Z = 4$ $d_x = 2.303 \text{ g cm}^{-3}$

$V = 795.76(8) \text{ \AA}^3$

No. of reflections for lattice parameters: 25

q range for lattice parameters ($^\circ$): 23.50-44.59

Absorption coefficient (mm^{-1}): 31.67

EXPERIMENTAL:

Crystallization

Crystal source: Acetone/EtOAc

Crystal description: Yellow rod

Crystal size (mm): 0.12 X 0.14 X 0.46

Data Collection

Temperature (K): 295

θ_{max} ($^\circ$): 75

No. of reflections measured: 996

No. of independent reflections: 996

No. of observed reflections ($I > 3\sigma$): 996

Absorption correction ($T_{\text{min}}-T_{\text{max}}$): 0.56-0.99

R_{int} : 0.00

REFINEMENT

No. of parameters refined: 109

No. of reflections used: 996

$R(F) = 0.097$

$wR(F) = 0.157$

$S = 1.56$

Weighting Scheme $w = 1/[\sigma^2(F) +$

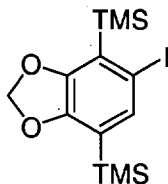
$0.01F^2]$

Treatment of Hydrogen Atoms: Positions of hydrogen atoms were calculated from an idealized geometry with standard bond lengths and angles. They were assigned isotropic temperature factors and were included in structure factor calculations with fixed parameters

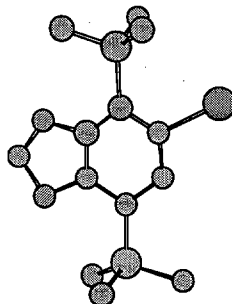
Protein Data Base Coordinates:

ATOM	1	I1	D	1	0.915	10.153	12.611	4.50	1.00
ATOM	2	O5	D	1	-0.869	13.625	17.359	4.50	1.00
ATOM	3	O7	D	1	-1.520	14.340	15.254	4.50	1.00
ATOM	4	O9'	D	1	-1.659	13.960	12.471	4.50	1.00
ATOM	5	C1	D	1	0.351	11.304	14.182	4.50	1.00
ATOM	6	C2	D	1	0.733	10.923	15.430	4.50	1.00
ATOM	7	C3	D	1	0.455	11.628	16.607	4.50	1.00
ATOM	8	C4	D	1	-0.391	12.793	16.415	4.50	1.00
ATOM	9	C6	D	1	-1.576	14.671	16.690	4.50	1.00
ATOM	10	C8	D	1	-0.737	13.174	15.135	4.50	1.00
ATOM	11	C9	D	1	-0.474	12.532	13.979	4.50	1.00
ATOM	12	C9'	D	1	-0.979	12.968	12.679	4.50	1.00
ATOM	13	H2A	D	1	1.250	10.118	15.505	4.50	1.00
ATOM	14	H3B	D	1	0.784	11.363	17.469	4.50	1.00
ATOM	15	H6B	D	1	-1.151	15.516	16.851	4.50	1.00
ATOM	16	H6A	D	1	-2.484	14.718	16.997	4.50	1.00
ATOM	17	H9'A	D	1	-0.758	12.422	11.920	4.50	1.00

Structure Determination of 4,7-bistrimethylsilyl-5-iodobenzodioxole
by Single Crystal Analysis



4,7-bistrimethylsilyl-5-iodobenzodioxole



X-ray structure of 4,7-bistrimethylsilyl-5-iodobenzodioxole

CRYSTAL DATA

Chemical formula: $C_{13}H_{21}ISi_2O_2$

Crystal system: Monoclinic

Space Group: $P2_1$

$a = 6.7263(6) \text{ \AA}$ $\alpha = 90^\circ$

$b = 11.6797(7) \text{ \AA}$ $\beta = 103.052(8)^\circ$

$c = 11.767(1) \text{ \AA}$ $\gamma = 90^\circ$

$Z = 2$ $d_x = 1.447 \text{ g cm}^{-3}$

$V = 900.6(1) \text{ \AA}^3$

No. of reflections for lattice parameters: 25

θ range for lattice parameters ($^\circ$): 18.85-43.02

Absorption coefficient (mm^{-1}): 15.39

EXPERIMENTAL:

Crystallization

Crystal source: MeOH/Water

Crystal description: Pale-yellow plate

Crystal size (mm): 0.03 X 0.25 X 0.43

Data Collection

Temperature (K): 295

θ_{max} ($^\circ$): 75

No. of reflections measured: 2124

No. of independent reflections: 1956

No. of observed reflections ($I > 3\sigma$): 1857

Absorption correction ($T_{\text{min}}-T_{\text{max}}$): 0.17-1.00

R_{int} : 0.041

REFINEMENT

No. of parameters refined: 152

No. of reflections used: 1857

 $R(F) = 0.109$ $wR(F) = 0.146$ $S = 2.10$ Weighting Scheme $w = 1/[\sigma^2(F) + 0.003F^2]$

Treatment of Hydrogen Atoms: Positions of hydrogen atoms were calculated from an idealized geometry with standard bond lengths and angles. They were assigned isotropic temperature factors and were included in structure factor calculations with fixed parameters.

Protein Data Base Coordinates:

ATOM	1	I1	D	1	-0.265	5.004	10.751	4.50	1.00
ATOM	2	SI2	D	1	1.789	3.121	8.432	4.50	1.00
ATOM	3	SI8	D	1	3.146	3.061	15.008	4.50	1.00
ATOM	4	O4	D	1	3.999	1.603	10.245	4.50	1.00
ATOM	5	O6	D	1	4.541	1.567	12.492	4.50	1.00
ATOM	6	C1	D	1	1.385	3.793	11.276	4.50	1.00
ATOM	7	C2	D	1	2.132	3.101	10.317	4.50	1.00
ATOM	8	C3	D	1	3.127	2.461	10.862	4.50	1.00
ATOM	9	C5	D	1	4.890	1.114	11.164	4.50	1.00
ATOM	10	C7	D	1	3.409	2.360	12.217	4.50	1.00
ATOM	11	C8	D	1	2.689	3.091	13.196	4.50	1.00
ATOM	12	C9	D	1	1.626	3.834	12.650	4.50	1.00
ATOM	13	C21	D	1	0.047	2.681	8.011	4.50	1.00
ATOM	14	C22	D	1	2.338	4.746	7.754	4.50	1.00
ATOM	15	C23	D	1	2.781	1.967	7.582	4.50	1.00
ATOM	16	C81	D	1	2.225	4.426	15.888	4.50	1.00
ATOM	17	C82	D	1	2.706	1.375	15.723	4.50	1.00
ATOM	18	C83	D	1	4.962	3.286	15.243	4.50	1.00
ATOM	19	H21A	D	1	-0.057	2.730	7.057	4.50	1.00
ATOM	20	H21B	D	1	-0.211	1.809	8.317	4.50	1.00
ATOM	21	H21C	D	1	-0.509	3.344	8.427	4.50	1.00
ATOM	22	H22C	D	1	3.269	4.914	7.920	4.50	1.00
ATOM	23	H22A	D	1	2.173	4.762	6.808	4.50	1.00
ATOM	24	H22B	D	1	1.809	5.423	8.182	4.50	1.00
ATOM	25	H23A	D	1	2.621	2.009	6.636	4.50	1.00
ATOM	26	H23B	D	1	3.708	2.149	7.758	4.50	1.00
ATOM	27	H23C	D	1	2.560	1.091	7.906	4.50	1.00
ATOM	28	H81A	D	1	1.283	4.293	15.759	4.50	1.00
ATOM	29	H81C	D	1	2.489	5.258	15.487	4.50	1.00
ATOM	30	H81B	D	1	2.420	4.448	16.828	4.50	1.00
ATOM	31	H82B	D	1	2.893	1.360	16.665	4.50	1.00
ATOM	32	H82C	D	1	1.768	1.222	15.581	4.50	1.00
ATOM	33	H82A	D	1	3.212	0.687	15.285	4.50	1.00
ATOM	34	H83B	D	1	5.271	4.097	14.832	4.50	1.00
ATOM	35	H83C	D	1	5.203	3.287	16.173	4.50	1.00
ATOM	36	H83A	D	1	5.367	2.532	14.808	4.50	1.00
ATOM	37	H51	D	1	5.763	1.419	10.948	4.50	1.00
ATOM	38	H52	D	1	4.872	0.164	11.143	4.50	1.00
ATOM	39	H9	D	1	1.073	4.361	13.215	4.50	1.00