Supporting Information

for

SYNTHESIS AND ANTIFUNGAL ACTIVITIES OF PYRIDINE BIOISOSTERES OF A BISMUTH HETEROCYCLE DERIVED FROM DIPHENYL SULFONE

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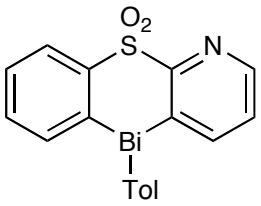

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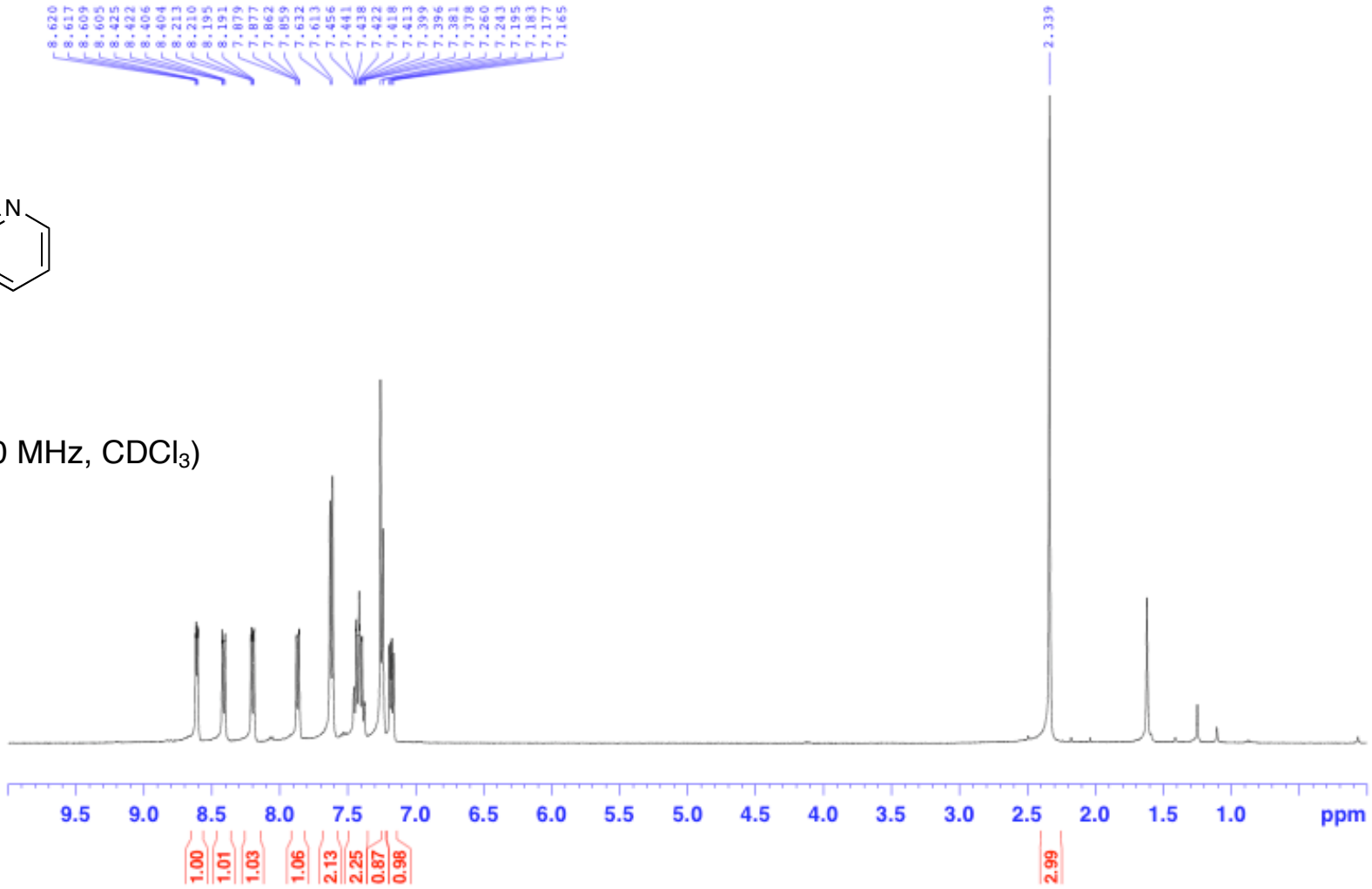

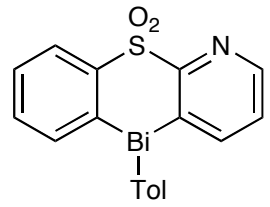

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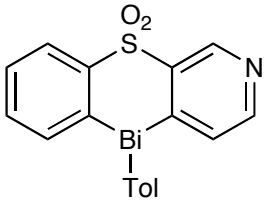

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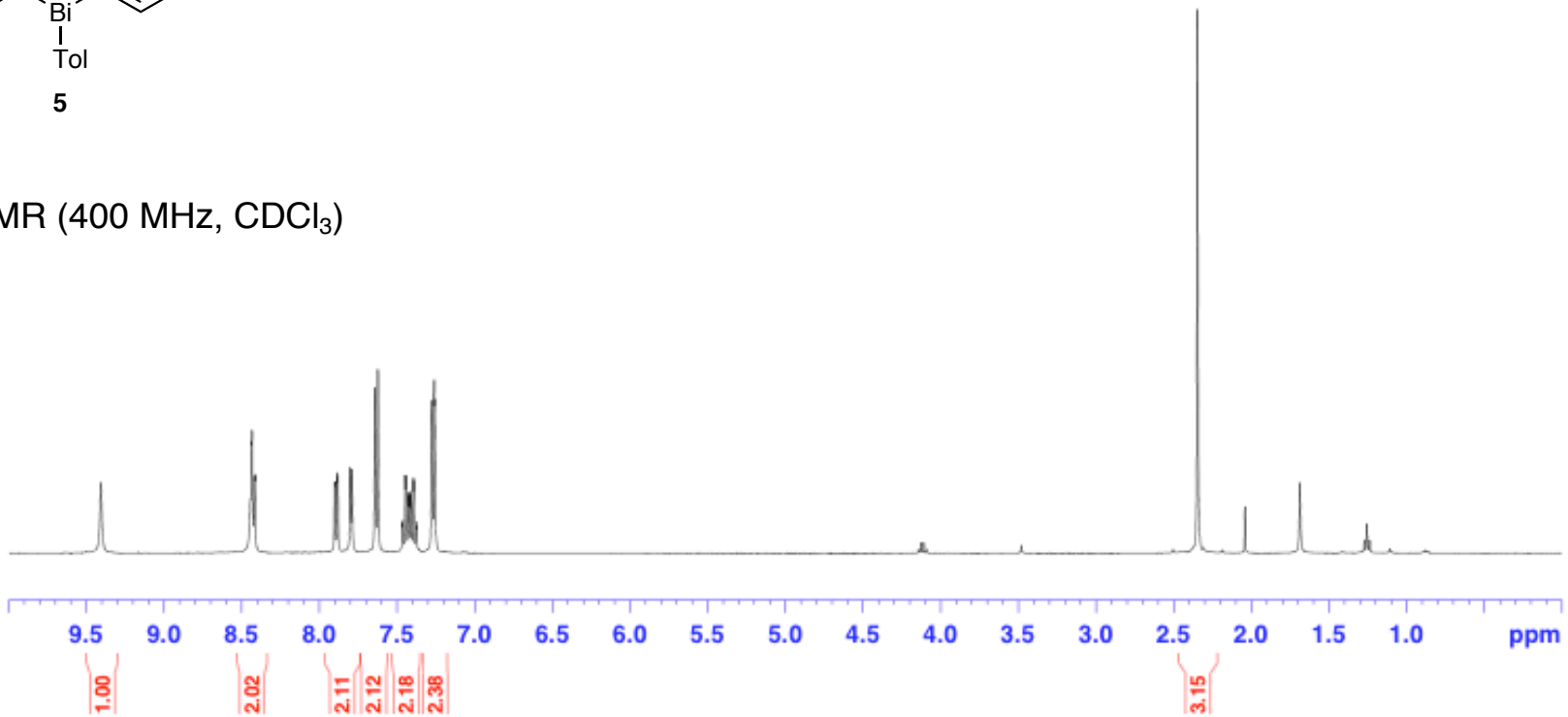

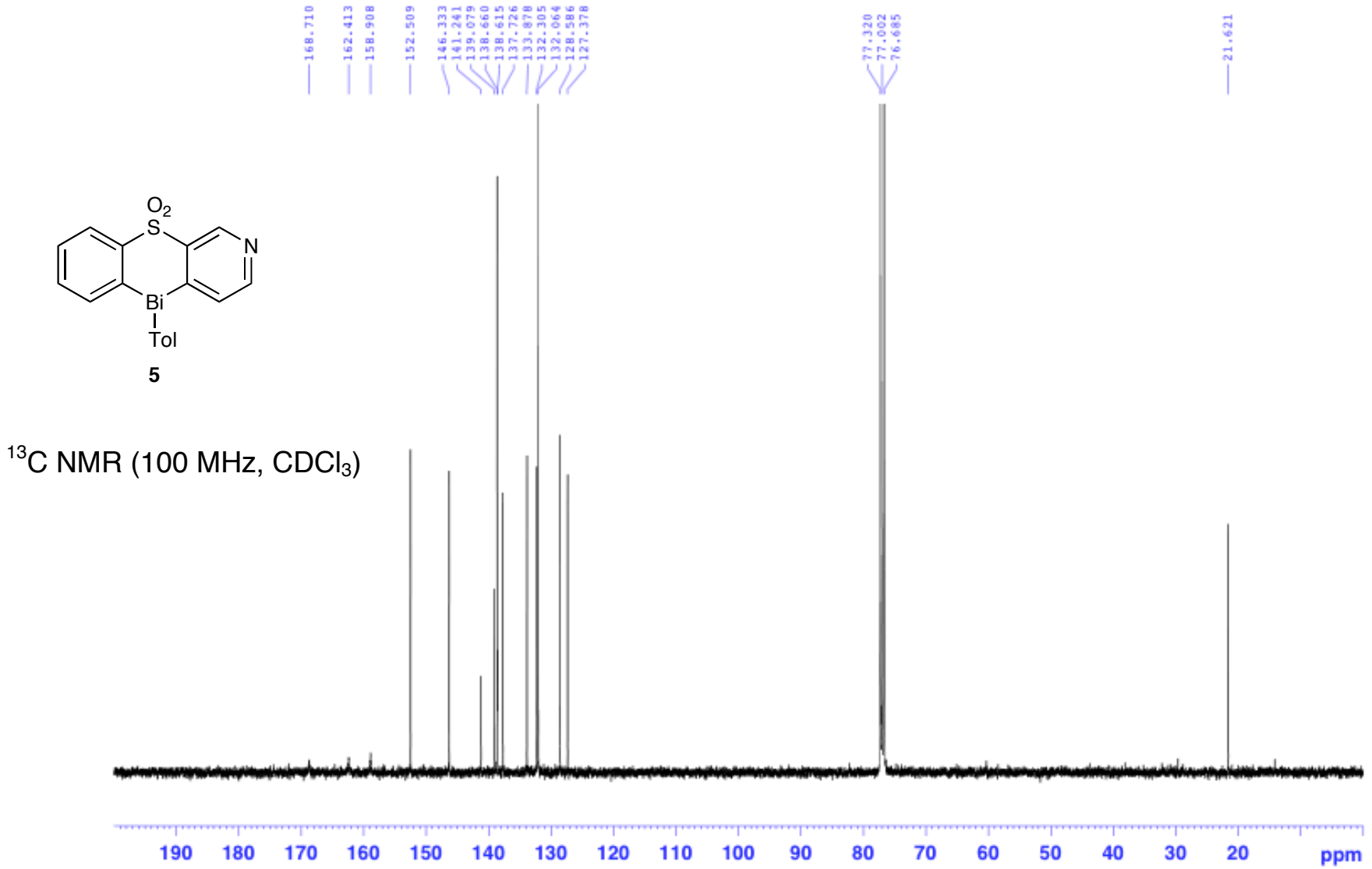

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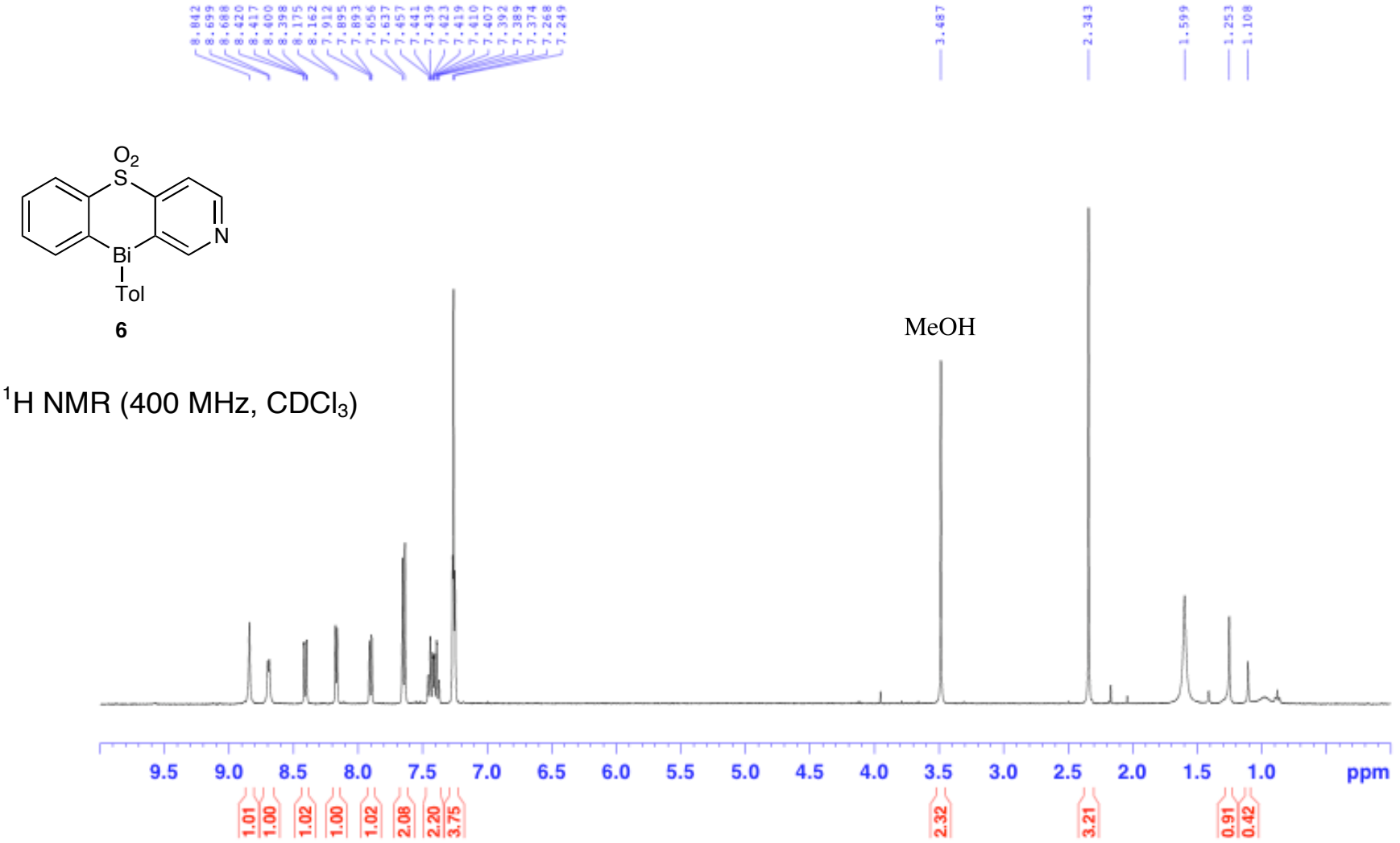

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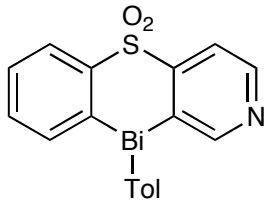

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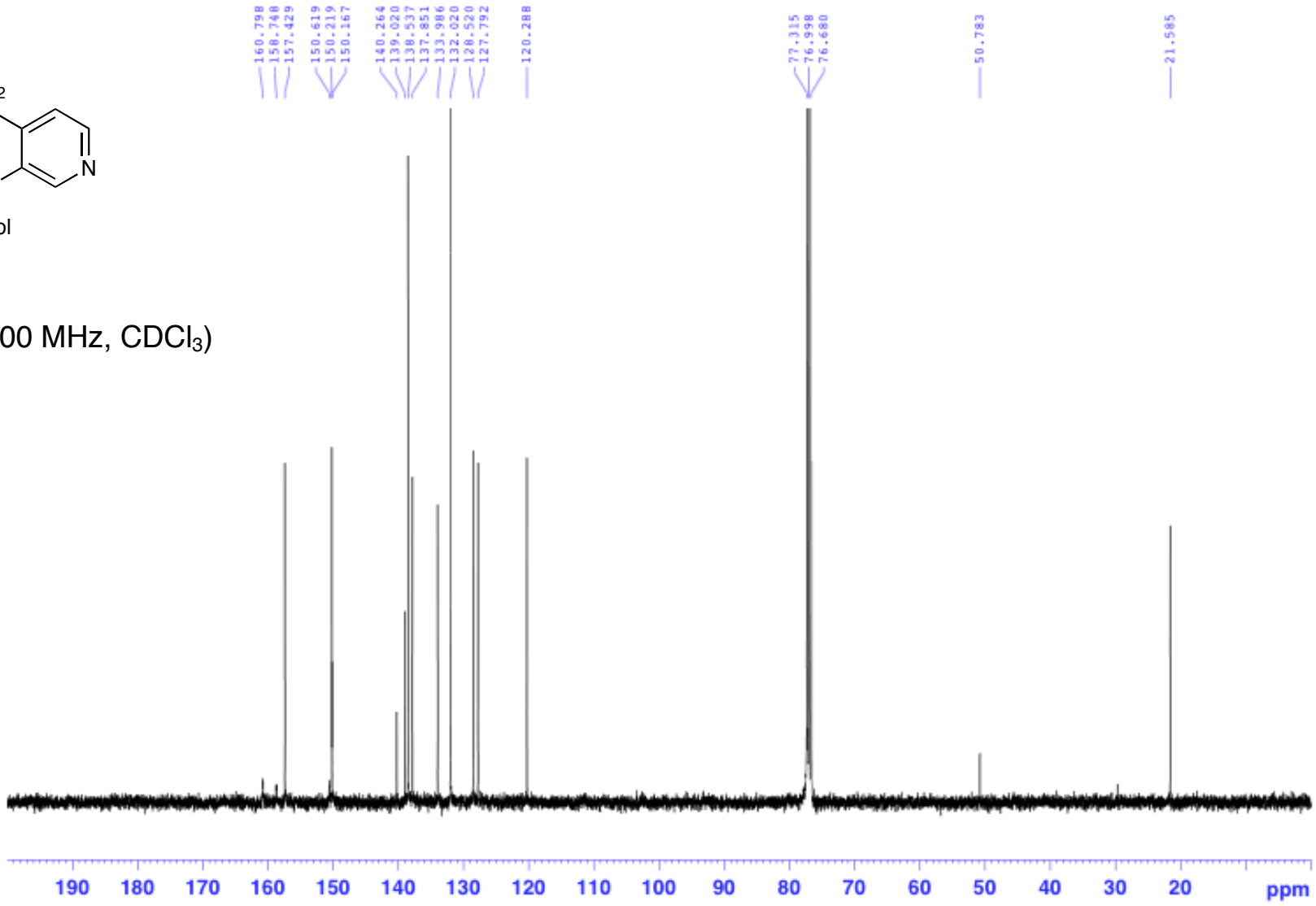

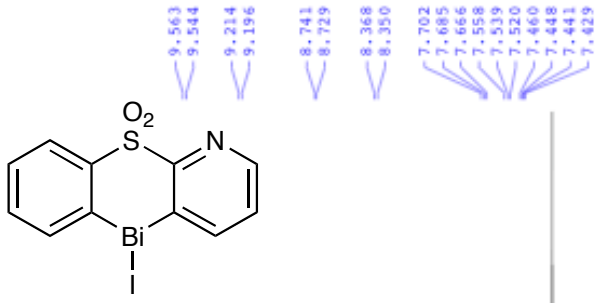

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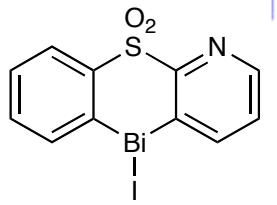

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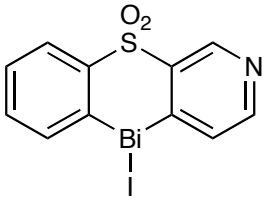

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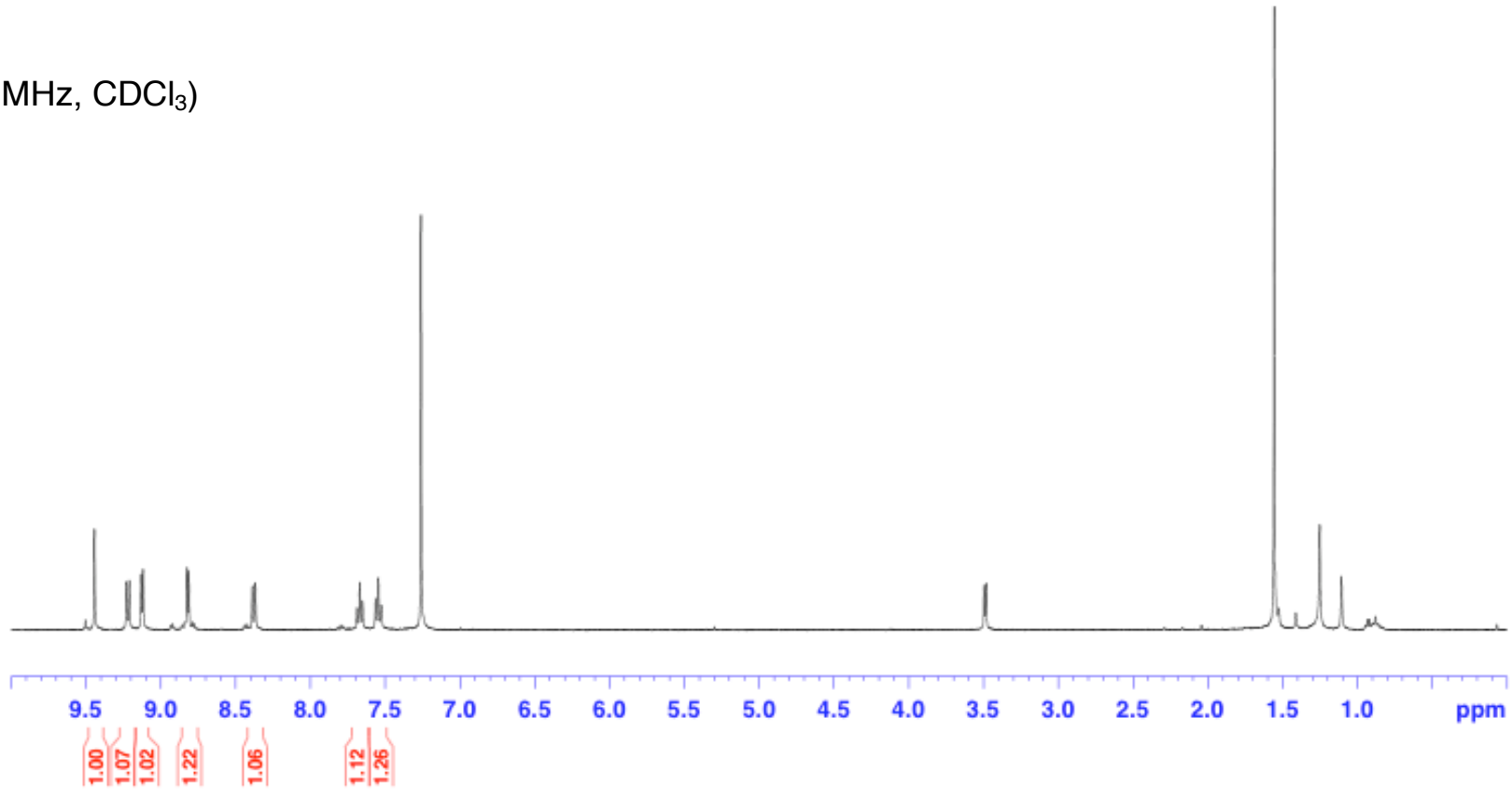
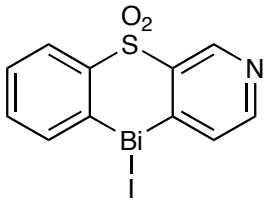
^{1}H NMR (400 MHz, $CDCl_3$)





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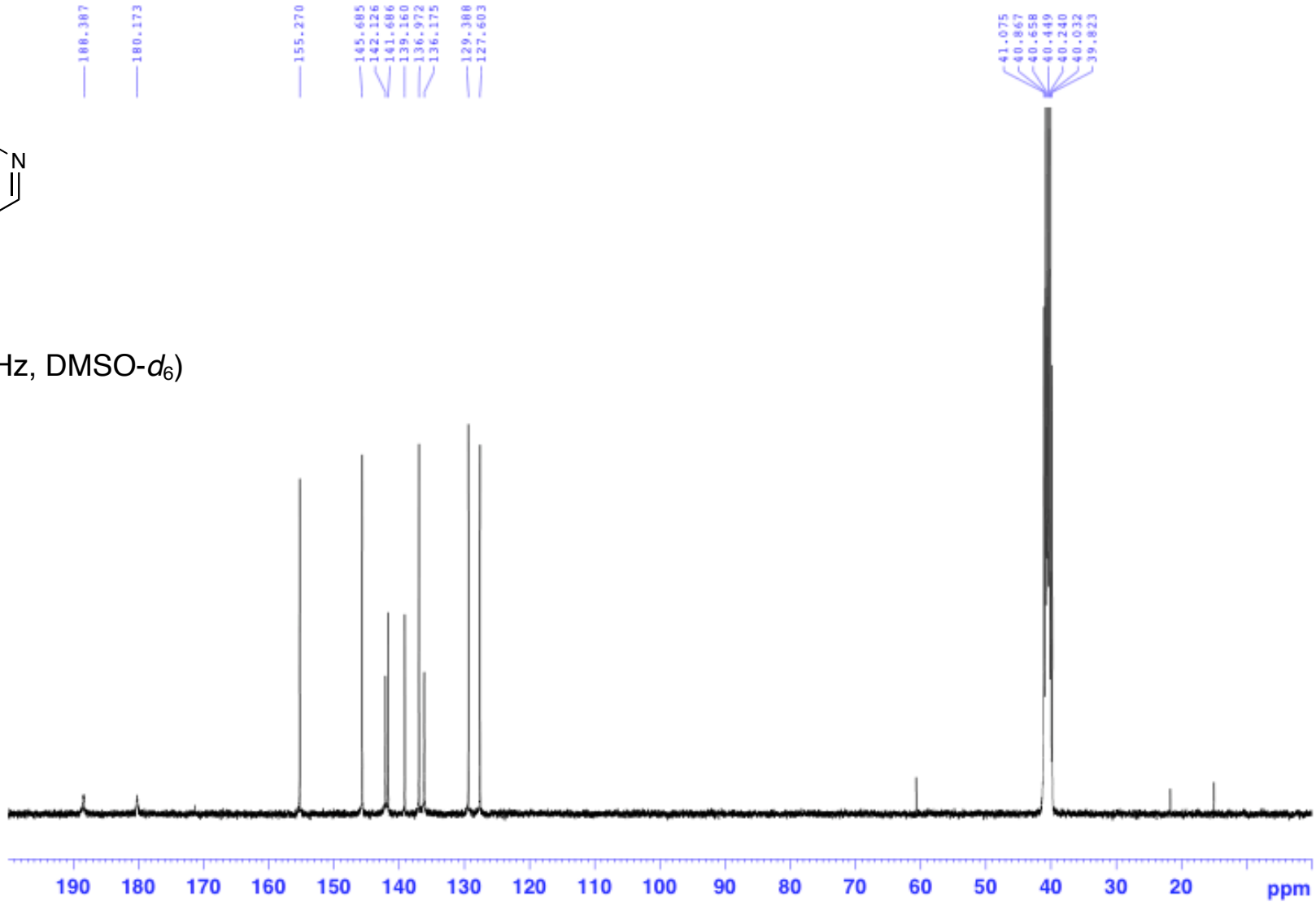
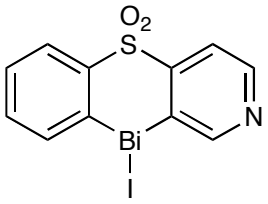
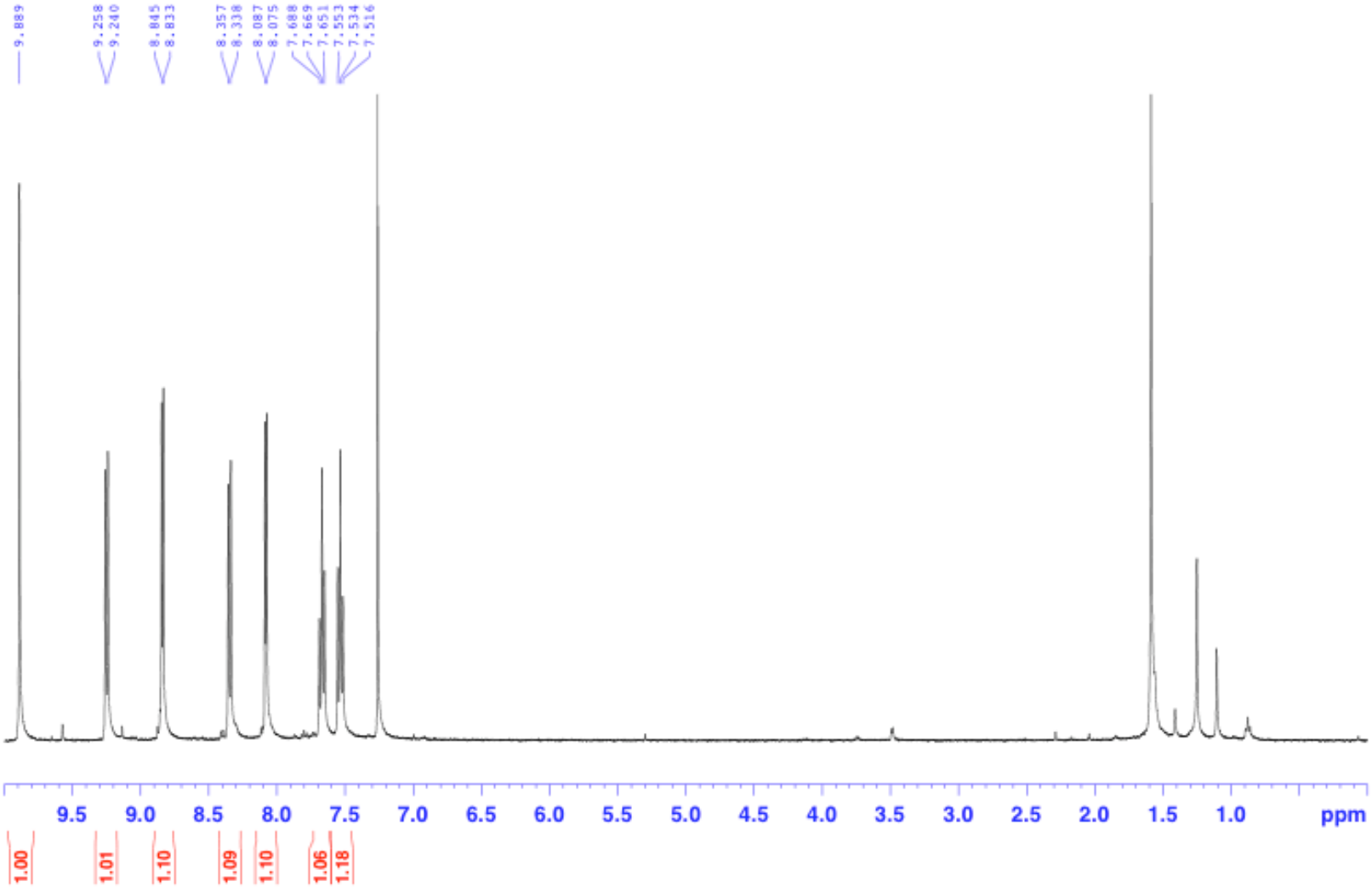
^{13}C NMR (100 MHz, DMSO-d_6)

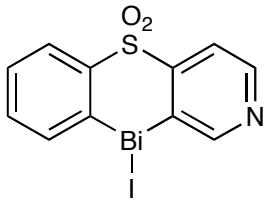




9

1H NMR
(400 MHz,
$CDCl_3$)





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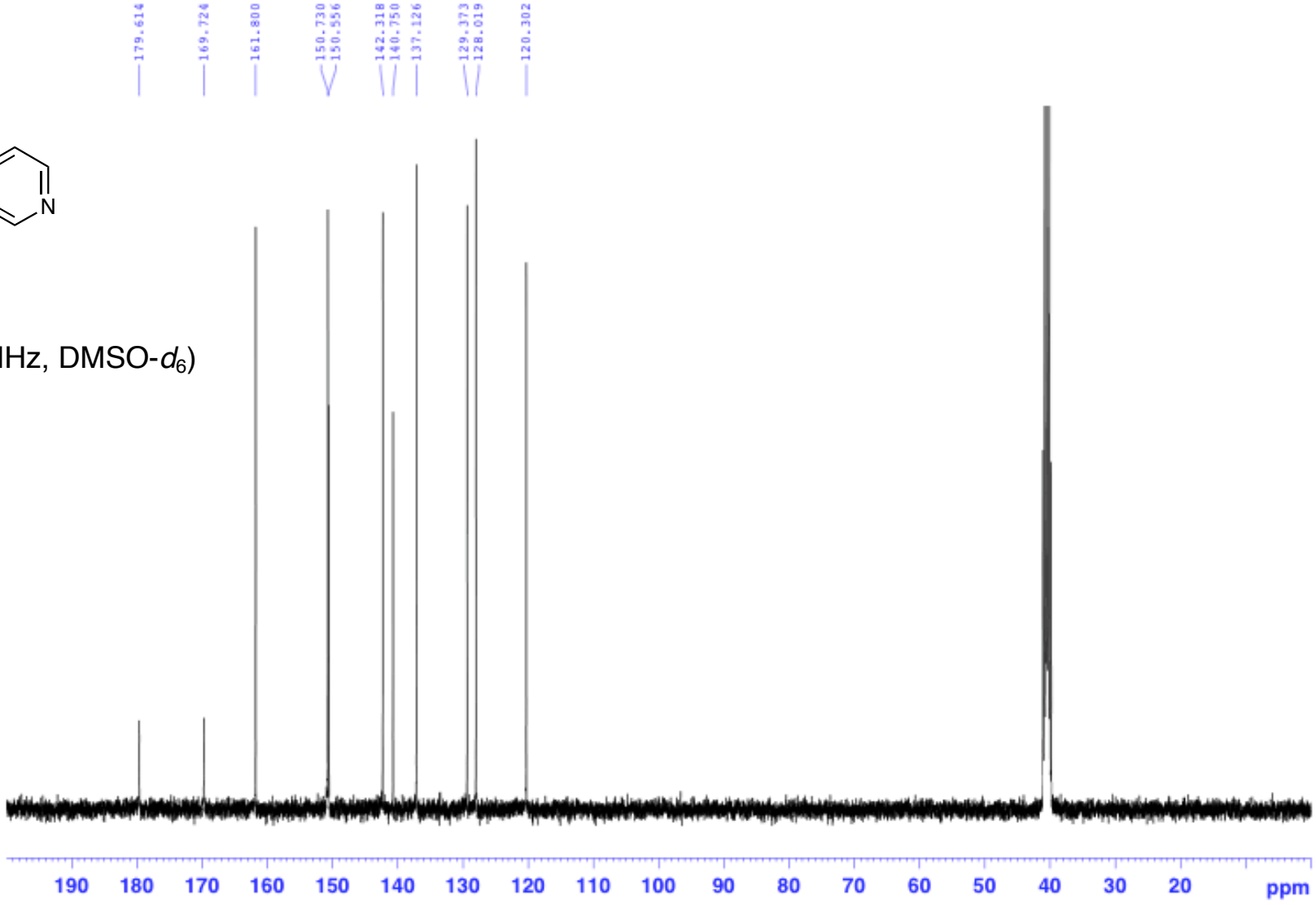
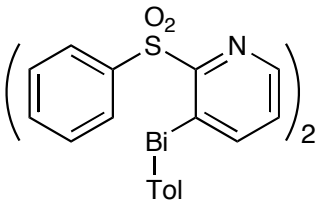
^{13}C NMR (100 MHz, DMSO-d_6)





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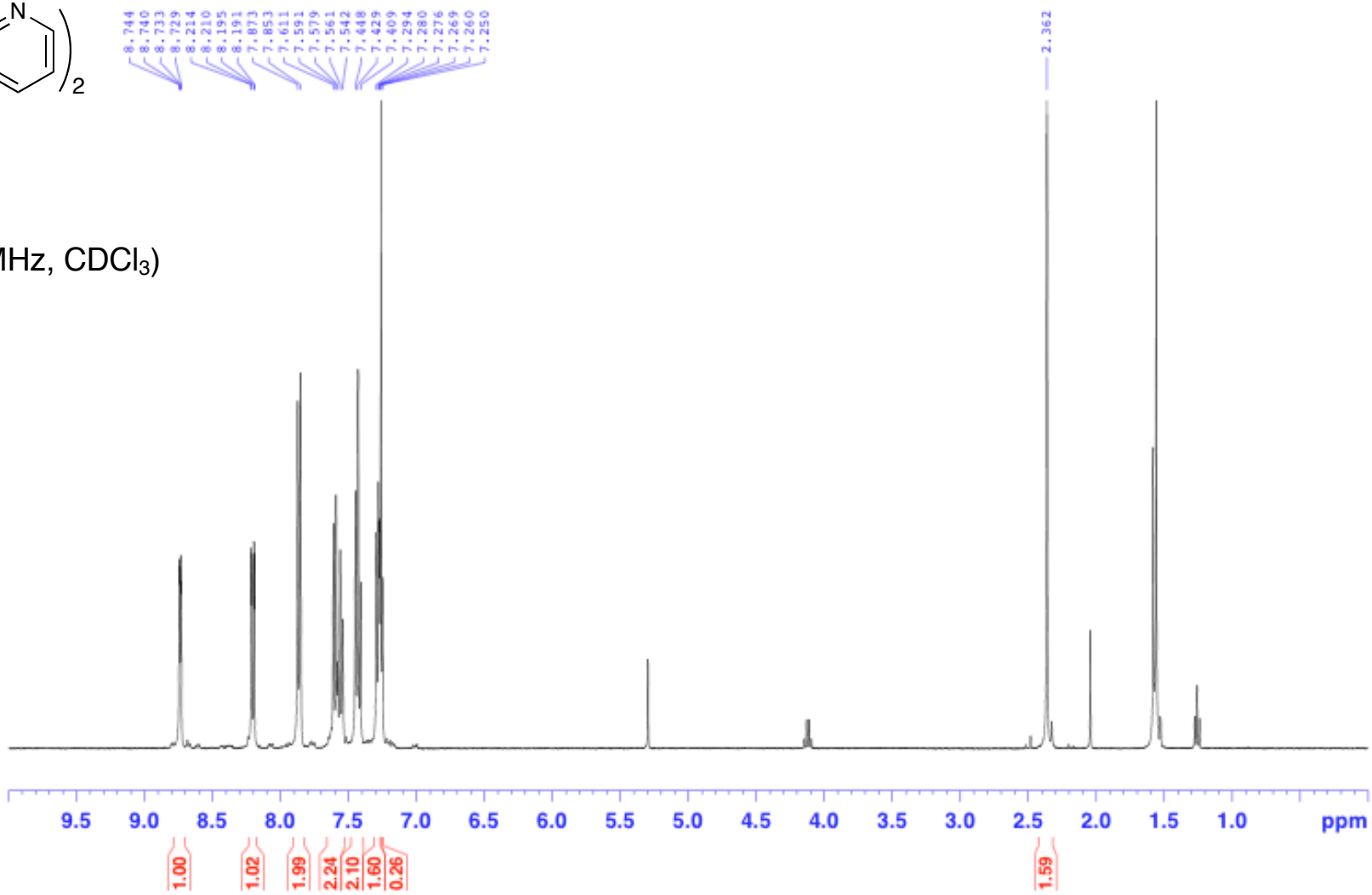
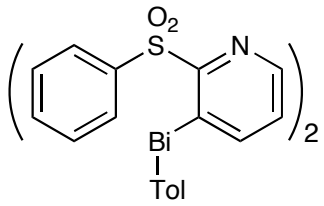
^{1}H NMR (400 MHz, $CDCl_3$)





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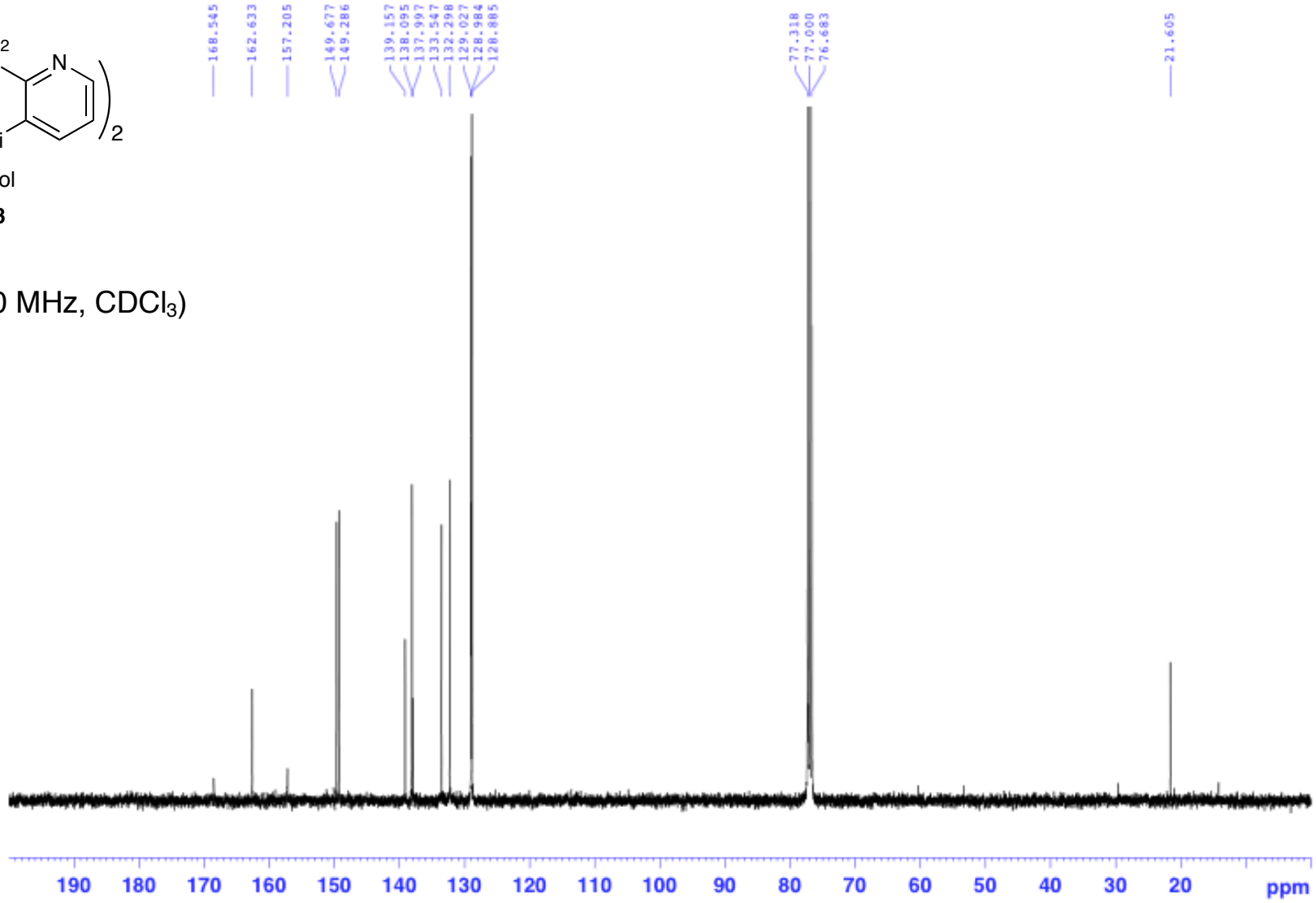

X-Ray Structure Report

for

compound **9**

Experimental

Data Collection

A colorless unknown crystal of $C_{11}H_7BiINO_2S$ having approximate dimensions of 0.200 x 0.200 x 0.150 mm was mounted on a glass fiber. All measurements were made on a Rigaku Mercury70 diffractometer using graphite monochromated Mo-Kα radiation.

The crystal-to-detector distance was 55.01 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 8.403(2) Å
b = 7.854(2) Å β = 94.689(3)°
c = 9.726(2) Å
V = 639.8(3) Å^3

For Z = 2 and F.W. = 553.13, the calculated density is 2.871 g/cm^3. Based on the reflection conditions of:

0k0: k = 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$P2_1$ (#4)

The data were collected at a temperature of -119 ± 1°C to a maximum 2θ value of 55.0°. A total of 1080 oscillation images were collected. A sweep of data was done using ω scans from -65.0 to 115.0° in 0.50° step, at χ=45.0° and ϕ = 0.0°. The exposure rate was 40.0 [sec./°]. The detector swing angle was 25.00°. A second sweep was performed using ω scans from -65.0 to 115.0° in 0.50° step, at χ=45.0° and ϕ = 90.0°. The exposure rate was 40.0 [sec./°]. The detector swing angle was 25.00°. Another sweep was performed using ω scans from -65.0 to 115.0° in 0.50° step, at χ=45.0° and ϕ = 180.0°. The exposure rate was 40.0 [sec./°]. The detector swing angle was 25.00°. The crystal-to-detector distance was 55.01 mm. Readout was performed in the 0.137 mm pixel mode.

Data Reduction

Of the 6217 reflections were collected, where 2845 were unique (R_{int} = 0.0527); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).[1]

The linear absorption coefficient, m, for Mo-Kα radiation is 163.181 cm^{-1}. A numerical absorption correction was applied which resulted in transmission factors ranging from 0.037 to 0.086. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 2845 observed reflections and 154 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0331$$

$$wR2 = [\; \Sigma \; (\; w \; (Fo^2 - Fc^2)^2 \;) / \; \Sigma \; w(Fo^2)^2 \;]^{1/2} = 0.0640$$

The goodness of fit[4] was 0.80. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.23 and -2.02 $e/Å^3$, respectively. The final Flack parameter[5] was 0.039(9),

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10] crystallographic software package except for refinement, which was performed using SHELXL Version 2016/6[11].

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998-2015). Tokyo 196-8666, Japan.

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C. and Guagliardi, A. (1993). J. Appl. Cryst. 26, 343-350.

(3) Least Squares function minimized: (SHELXL Version 2016/6)

$\Sigma w(F_o^2 - F_c^2)^2$ where w = Least Squares weights.

(4) Goodness of fit is defined as:

$[\Sigma w(F_o^2 - F_c^2)^2/(N_o - N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(5) Parsons, S. and Flack, H. (2004), Acta Cryst. A60, s61.

(6) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) CrystalStructure 4.2.5: Crystal Structure Analysis Package, Rigaku Corporation (2000-2017). Tokyo 196-8666, Japan.

(11) SHELXL Version 2016/6: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{11}H_7BiINO_2S$
Formula Weight	553.13
Crystal Color, Habit	colorless, unknown
Crystal Dimensions	0.200 x 0.200 x 0.150 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 8.403(2) Å b = 7.854(2) Å c = 9.726(2) Å β = 94.689(3)° V = 639.8(3) Å^3
Space Group	$P2_1$ (#4)
Z value	2
D_{calc}	2.871 g/cm^3
F_{000}	496.00
μ(MoKα)	163.181 cm^{-1}

B. Intensity Measurements

Diffractometer	Mercury70	
Radiation	MoKα (λ = 0.71075 Å)	graphite monochromated
Voltage, Current	50kV, 40mA	
Temperature	-119.8°C	
Detector Aperture	70.0 x 70.0 mm	

Data Images	1080 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-65.0 –115.0°
Exposure Rate	40.0 sec./°
Detector Swing Angle	25.00°
ω oscillation Range (χ=45.0, ϕ=90.0)	-65.0 –115.0°
Exposure Rate	40.0 sec./°
Detector Swing Angle	25.00°
w oscillation Range (χ=45.0, ϕ=180.0)	-65.0 –115.0°
Exposure Rate	40.0 sec./°
Detector Swing Angle	25.00°
Detector Position	55.01 mm
Pixel Size	0.137 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 6217 Unique: 2845 (R_{int} = 0.0527) Parsons quotients (Flack x parameter): 809
Corrections	Lorentz-polarization Absorption (trans. factors: 0.037–0.086)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$

Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0077 \cdot P)^2 + 0.0000 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	2845
No. Variables	154
Reflection/Parameter Ratio	18.47
Residuals: R1 ($I>2.00\sigma(I)$)	0.0331
Residuals: R (All reflections)	0.0374
Residuals: wR2 (All reflections)	0.0640
Goodness of Fit Indicator	0.799
Flack parameter (Parsons' quotients = 809)	0.039(9)
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	1.23 $e/Å^3$
Minimum peak in Final Diff. Map	-2.02 $e/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Bi1	0.21706(6)	0.70503(7)	0.10586(5)	1.282(10)
I1	0.04391(13)	0.80381(13)	-0.14590(10)	1.90(2)
S1	0.2727(5)	0.8907(5)	0.4097(4)	1.50(7)
O1	0.3362(10)	0.719(2)	0.3817(10)	2.3(2)
O2	0.3058(13)	0.9643(14)	0.5440(11)	2.3(2)
N1	0.4820(13)	1.205(2)	0.0842(11)	1.9(2)
C1	0.3365(16)	0.9638(17)	0.1505(15)	1.0(2)
C2	0.4028(18)	1.0627(18)	0.0532(16)	1.6(3)
C3	0.4865(17)	1.2634(19)	0.2162(16)	2.0(3)
C4	0.4190(16)	1.1751(18)	0.3201(14)	1.4(3)
C5	0.3446(16)	1.0234(18)	0.2815(15)	1.0(2)
C6	0.0201(16)	0.7994(17)	0.2372(14)	1.2(2)
C7	-0.1387(16)	0.7852(19)	0.1990(16)	1.8(3)
C8	-0.2496(17)	0.846(2)	0.2834(16)	1.9(3)
C9	-0.2051(18)	0.925(2)	0.4069(16)	2.1(3)
C10	-0.0437(18)	0.9441(19)	0.4482(16)	1.8(3)
C11	0.0655(16)	0.8779(19)	0.3633(15)	1.2(3)

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H2	0.39103	1.02727	-0.04048	1.904
H3	0.53782	1.36898	0.23777	2.371
H4	0.42353	1.21614	0.41217	1.654
H7	-0.17322	0.73325	0.11348	2.178
H8	-0.36000	0.83226	0.25579	2.268
H9	-0.28379	0.96622	0.46335	2.486
H10	-0.00957	1.00061	0.53179	2.160

Table 3. Anisotropic displacement parameters

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Bi1	0.0174(3)	0.0141(2)	0.0180(3)	0.0015(3)	0.0056(2)	0.0003(3)
I1	0.0293(6)	0.0239(6)	0.0186(6)	0.0013(5)	-0.0002(5)	-0.0028(5)
S1	0.019(2)	0.027(2)	0.0116(19)	-0.0006(18)	0.0011(16)	0.0057(17)
O1	0.024(6)	0.035(6)	0.029(6)	0.010(8)	-0.006(5)	0.007(7)
O2	0.028(6)	0.050(8)	0.009(6)	0.001(6)	-0.000(5)	0.001(5)
N1	0.027(7)	0.030(6)	0.017(6)	-0.014(9)	0.001(5)	0.002(8)
C1	0.006(7)	0.015(7)	0.015(8)	0.000(6)	0.000(6)	-0.004(6)
C2	0.030(9)	0.018(8)	0.013(8)	-0.004(7)	0.004(7)	-0.003(6)
C3	0.023(9)	0.031(10)	0.021(9)	-0.006(7)	-0.001(7)	0.003(7)
C4	0.019(8)	0.022(10)	0.011(7)	-0.001(7)	-0.002(6)	-0.000(6)
C5	0.006(7)	0.018(8)	0.014(8)	-0.005(6)	-0.003(6)	-0.004(6)
C6	0.021(8)	0.008(7)	0.016(7)	-0.001(7)	0.008(6)	-0.004(6)
C7	0.018(8)	0.024(9)	0.025(9)	-0.003(7)	-0.007(7)	-0.006(7)
C8	0.010(8)	0.032(10)	0.029(10)	-0.002(7)	-0.000(7)	-0.002(7)
C9	0.028(10)	0.026(9)	0.026(10)	0.003(8)	0.007(8)	0.004(8)
C10	0.032(10)	0.022(8)	0.015(8)	0.002(7)	0.012(7)	-0.002(7)
C11	0.010(8)	0.021(8)	0.017(8)	-0.001(6)	0.004(6)	0.004(6)

The general temperature factor expression:

$$\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Bi1	I1	2.8518(12)	Bi1	C1	2.293(14)
Bi1	C6	2.294(14)	S1	O1	1.485(16)
S1	O2	1.435(11)	S1	C5	1.769(15)
S1	C11	1.766(14)	N1	C2	1.32(2)
N1	C3	1.362(19)	C1	C2	1.38(2)
C1	C5	1.35(2)	C3	C4	1.39(2)
C4	C5	1.383(19)	C6	C7	1.360(19)
C6	C11	1.398(19)	C7	C8	1.38(2)
C8	C9	1.38(2)	C9	C10	1.39(2)
C10	C11	1.39(2)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C2	H2	0.950	C3	H3	0.950
C4	H4	0.950	C7	H7	0.950
C8	H8	0.950	C9	H9	0.950
C10	H10	0.950			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
I1	Bi1	C1	96.1(3)	I1	Bi1	C6	92.8(3)
C1	Bi1	C6	86.1(5)	O1	S1	O2	119.2(6)
O1	S1	C5	105.0(7)	O1	S1	C11	105.2(6)
O2	S1	C5	110.6(7)	O2	S1	C11	111.6(7)
C5	S1	C11	103.9(7)	C2	N1	C3	118.4(13)
Bi1	C1	C2	124.4(10)	Bi1	C1	C5	118.2(10)
C2	C1	C5	117.4(13)	N1	C2	C1	122.9(14)
N1	C3	C4	122.5(14)	C3	C4	C5	115.9(13)
S1	C5	C1	117.8(11)	S1	C5	C4	119.3(11)
C1	C5	C4	122.7(13)	Bi1	C6	C7	123.9(10)
Bi1	C6	C11	118.3(9)	C7	C6	C11	117.8(13)
C6	C7	C8	120.4(14)	C7	C8	C9	121.8(13)
C8	C9	C10	119.3(14)	C9	C10	C11	117.8(14)
S1	C11	C6	116.2(11)	S1	C11	C10	121.0(11)
C6	C11	C10	122.8(13)				

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C2	H2	118.5	C1	C2	H2	118.5
N1	C3	H3	118.8	C4	C3	H3	118.8
C3	C4	H4	122.1	C5	C4	H4	122.1
C6	C7	H7	119.8	C8	C7	H7	119.8
C7	C8	H8	119.1	C9	C8	H8	119.1
C8	C9	H9	120.4	C10	C9	H9	120.3
C9	C10	H10	121.1	C11	C10	H10	121.1

Table 8. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
I1	Bi1	C1	C2	-43.3(9)	I1	Bi1	C1	C5	137.5(8)
I1	Bi1	C6	C7	37.2(9)	I1	Bi1	C6	C11	-142.0(8)
C1	Bi1	C6	C7	133.2(10)	C1	Bi1	C6	C11	-46.1(9)
C6	Bi1	C1	C2	-135.7(10)	C6	Bi1	C1	C5	45.1(9)
O1	S1	C5	C1	43.9(10)	O1	S1	C5	C4	-130.4(9)
O1	S1	C11	C6	-45.9(11)	O1	S1	C11	C10	134.6(10)
O2	S1	C5	C1	173.7(8)	O2	S1	C5	C4	-0.6(12)
O2	S1	C11	C6	-176.7(9)	O2	S1	C11	C10	3.9(13)
C5	S1	C11	C6	64.1(11)	C5	S1	C11	C10	-115.4(11)
C11	S1	C5	C1	-66.4(10)	C11	S1	C5	C4	119.4(10)
C2	N1	C3	C4	4(2)	C3	N1	C2	C1	-6(2)
Bi1	C1	C2	N1	-174.4(9)	Bi1	C1	C5	S1	3.7(15)
Bi1	C1	C5	C4	177.7(8)	C2	C1	C5	S1	-175.6(11)
C2	C1	C5	C4	-1.5(19)	C5	C1	C2	N1	5(2)
N1	C3	C4	C5	-1(2)	C3	C4	C5	S1	173.6(10)
C3	C4	C5	C1	-0.4(19)	Bi1	C6	C7	C8	-179.8(8)
Bi1	C6	C11	S1	-1.6(15)	Bi1	C6	C11	C10	177.9(8)
C7	C6	C11	S1	179.1(11)	C7	C6	C11	C10	-1(2)
C11	C6	C7	C8	-0(2)	C6	C7	C8	C9	1(2)
C7	C8	C9	C10	-0(2)	C8	C9	C10	C11	-1(2)
C9	C10	C11	S1	-178.2(12)	C9	C10	C11	C6	2(2)

Table 9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Bi1	S1	3.294(4)	Bi1	O1	2.788(9)
O1	C1	2.959(19)	O1	C6	2.970(16)
O2	C4	2.954(18)	O2	C10	3.013(18)
N1	C5	2.72(2)	C1	C3	2.72(2)
C1	C11	3.27(2)	C2	C4	2.73(2)
C5	C6	3.244(19)	C6	C9	2.79(2)
C7	C10	2.78(2)	C8	C11	2.710(19)

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Bi1	H2	3.303	Bi1	H7	3.294
I1	H2	3.486	I1	H7	3.279
S1	H4	2.852	S1	H10	2.872
O2	H4	2.596	O2	H10	2.659
N1	H4	3.268	C1	H4	3.261
C2	H3	3.156	C3	H2	3.160
C5	H2	3.187	C5	H3	3.209
C6	H8	3.225	C6	H10	3.300
C7	H9	3.261	C8	H10	3.254
C9	H7	3.258	C10	H8	3.244
C11	H7	3.229	C11	H9	3.242
H3	H4	2.347	H7	H8	2.311
H8	H9	2.320	H9	H10	2.361

Table 11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Bi1	$N1^{1}$	3.252(11)	O1	$C4^{2}$	3.434(16)
O1	$C9^{3}$	3.34(2)	O2	$C3^{2}$	3.211(18)
O2	$C4^{2}$	3.429(17)	O2	$C8^{4}$	3.484(19)
N1	$Bi1^{5}$	3.252(11)	N1	$C1^{5}$	3.50(2)
N1	$C2^{5}$	3.29(2)	C1	$N1^{1}$	3.50(2)
C2	$N1^{1}$	3.29(2)	C3	$O2^{6}$	3.211(18)
C4	$O1^{6}$	3.434(16)	C4	$O2^{6}$	3.429(17)
C8	$O2^{3}$	3.484(19)	C9	$O1^{4}$	3.34(2)

Symmetry Operators:

(1) -X+1,Y+1/2-1,-Z	(2) -X+1,Y+1/2-1,-Z+1
(3) -X,Y+1/2-1,-Z+1	(4) -X,Y+1/2,-Z+1
(5) -X+1,Y+1/2,-Z	(6) -X+1,Y+1/2,-Z+1

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
I1	H7[1]	3.550	I1	H10[2]	3.491
S1	H4[3]	3.267	S1	H8[4]	3.568
S1	H9[5]	3.554	O1	H3[6]	3.573
O1	H4[3]	2.727	O1	H8[4]	3.053
O1	H9[5]	2.551	O1	H10[5]	3.399
O2	H3[3]	2.517	O2	H4[3]	2.999
O2	H8[7]	3.494	O2	H9[4]	3.599
N1	H2[8]	2.795	N1	H7[1]	3.109
N1	H8[4]	3.570	N1	H8[1]	3.526
C1	H7[1]	3.519	C1	H8[4]	2.862
C2	H3[9]	3.287	C2	H7[1]	2.763
C2	H8[4]	3.239	C3	H2[8]	2.926
C4	H8[4]	3.358	C4	H9[4]	3.210
C4	H9[7]	3.369	C5	H8[4]	2.929
C5	H9[4]	3.490	C6	H10[5]	3.255
C7	H2[10]	3.231	C7	H10[5]	3.588
C8	H2[10]	3.576	C8	H4[5]	3.556
C9	H4[5]	3.112	C10	H10[5]	3.515
C11	H10[5]	3.181	H2	N1[9]	2.795
H2	C3[9]	2.926	H2	C7[1]	3.231
H2	C8[1]	3.576	H2	H3[9]	2.403
H2	H7[1]	2.502	H2	H8[1]	3.178
H3	O1[11]	3.573	H3	O2[12]	2.517
H3	C2[8]	3.287	H3	H2[8]	2.403
H4	S1[12]	3.267	H4	O1[12]	2.727
H4	O2[12]	2.999	H4	C8[7]	3.556
H4	C9[7]	3.112	H4	H8[7]	3.439
H4	H9[4]	3.154	H4	H9[7]	2.633
H7	I1[10]	3.550	H7	N1[10]	3.109
H7	C1[10]	3.519	H7	C2[10]	2.763
H7	H2[10]	2.502	H8	S1[13]	3.568
H8	O1[13]	3.053	H8	O2[5]	3.494
H8	N1[13]	3.570	H8	N1[10]	3.526
H8	C1[13]	2.862	H8	C2[13]	3.239
H8	C4[13]	3.358	H8	C5[13]	2.929
H8	H2[10]	3.178	H8	H4[5]	3.439
H9	S1[7]	3.554	H9	O1[7]	2.551
H9	O2[13]	3.599	H9	C4[13]	3.210
H9	C4[5]	3.369	H9	C5[13]	3.490
H9	H4[13]	3.154	H9	H4[5]	2.633
H10	I1[14]	3.491	H10	O1[7]	3.399
H10	C6[7]	3.255	H10	C7[7]	3.588
H10	C10[7]	3.515	H10	C11[7]	3.181

Symmetry Operators:

(1) -X,Y+1/2,-Z
(2) X,Y,Z-1
(3) -X+1,Y+1/2-1,-Z+1
(4) X+1,Y,Z
(5) -X,Y+1/2-1,-Z+1
(6) X,Y-1,Z
(7) -X,Y+1/2,-Z+1
(8) -X+1,Y+1/2,-Z
(9) -X+1,Y+1/2-1,-Z
(10) -X,Y+1/2-1,-Z
(11) X,Y+1,Z
(12) -X+1,Y+1/2,-Z+1
(13) X-1,Y,Z
(14) X,Y,Z+1