Experimental data for the X-ray diffraction study of 2

Empirical Formula	$C_{35}H_{78}N_5Si_4YO$
Formula Weight	786.28
Crystal Color	colorless
Habit	plates
Crystal Dimensions	0.17 X 0.15 X 0.10 mm
Crystal System	monoclinic
Lattice Parameters	a = 10.023(1) Å b = 18.636(2) Å c = 12.370(1) Å β = 101.087(1)° V = 2267.4(4) Å^3
Space Group	$P2_1$ (#4)
Z value	2
D_{calc}	1.152 g/cm^3
F_{000}	852.00
μ(MoKα)	14.24 cm^{-1}
μ	2.72 mm^{-1}
Temperature	-160 °C
$2\theta_{max}$	49.5°
Total reflections	10290
Independent reflections	6857 (R_{int} = 0.035)
No. Observations (I>3.00σ(I))	3958
No. Variables	414
Reflection/Parameter Ratio	9.56
Residuals: R; Rw; Rall	0.066; 0.059; 0.066
Goodness of Fit Indicator	1.08
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.71 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.72 e$^-$/Å^3
Absorption	Tmax = 1.00; Tmin = 0.14
p-factor	0.0300
Detector Position	60.00 mm
Exposure Time	20 seconds per frame.

Table 1. Atomic coordinates and B_{iso}/B_{eq} for 2

atom	x	y	z	B_{eq}
Y(1)	0.85564(7)	0.2196	-0.02794(5)	1.17(1)
Si(1)	0.5391(2)	0.1594(1)	-0.1578(2)	1.86(5)
Si(2)	0.7970(2)	0.0718(1)	-0.1529(2)	1.70(5)
Si(3)	0.7739(2)	0.3615(1)	0.1432(2)	2.00(5)
Si(4)	0.6772(2)	0.3659(1)	-0.1022(2)	1.95(5)
O(1)	0.8513(5)	0.1606(3)	0.1117(4)	1.7(1)
N(1)	1.1057(5)	0.2248(4)	0.0805(4)	1.4(1)
N(2)	1.2704(6)	0.3270(3)	0.3379(5)	1.8(1)
N(3)	1.0155(7)	0.2513(3)	-0.1631(5)	1.8(1)
N(4)	0.7109(6)	0.1476(3)	-0.1355(5)	1.4(1)
N(5)	0.7655(6)	0.3274(3)	0.0153(5)	1.7(1)
C(1)	0.9247(8)	0.1285(4)	0.1997(6)	1.3(2)
C(2)	1.0645(8)	0.1224(4)	0.2072(6)	1.4(2)
C(3)	1.1454(7)	0.0899(4)	0.2997(6)	1.4(2)
C(4)	1.0888(8)	0.0640(4)	0.3844(6)	1.6(2)
C(5)	0.9485(8)	0.0687(4)	0.3752(6)	1.7(2)
C(6)	0.8623(8)	0.1005(4)	0.2853(6)	1.6(2)
C(7)	0.7098(8)	0.1055(4)	0.2787(6)	1.9(2)
C(8)	0.6655(9)	0.1826(5)	0.2806(7)	2.8(2)
C(9)	0.6663(9)	0.0679(6)	0.3780(8)	3.3(2)
C(10)	0.6324(9)	0.0688(6)	0.1727(7)	2.6(2)
C(11)	1.1746(8)	0.0291(4)	0.4889(6)	1.8(2)
C(12)	1.1370(9)	-0.0484(5)	0.4961(7)	2.9(2)
C(13)	1.1467(9)	0.0691(5)	0.5890(7)	2.9(2)
C(14)	1.3270(9)	0.0339(5)	0.4876(7)	2.8(2)
C(15)	1.1313(7)	0.1466(4)	0.1150(6)	1.5(2)
C(16)	1.1170(8)	0.2729(4)	0.1767(6)	1.8(2)
C(17)	1.2548(8)	0.2704(4)	0.2568(6)	1.6(2)
C(18)	1.1552(9)	0.3352(4)	0.3938(6)	2.3(2)
C(19)	1.1182(10)	0.2716(5)	0.4568(7)	3.0(2)
C(20)	1.4010(9)	0.3160(5)	0.4161(7)	2.7(2)
C(21)	1.437(1)	0.3745(5)	0.5015(8)	4.0(3)
C(22)	1.1989(8)	0.2462(4)	0.0069(6)	2.0(2)
C(23)	1.1521(7)	0.2233(6)	-0.1105(5)	2.1(2)
C(24)	1.0138(8)	0.3317(4)	-0.1694(6)	2.0(2)
C(25)	1.1128(9)	0.3679(5)	-0.2308(8)	3.1(2)
C(26)	0.9861(7)	0.2195(6)	-0.2757(5)	2.1(2)
C(27)	0.8522(8)	0.2401(5)	-0.3472(6)	2.5(2)
C(28)	0.7735(9)	0.0411(5)	-0.2972(7)	2.7(2)
C(29)	0.7766(9)	-0.0055(5)	-0.0643(8)	2.8(2)
C(30)	0.4404(8)	0.0781(5)	-0.1423(7)	2.3(2)
C(31)	0.4681(9)	0.1987(4)	-0.2963(7)	2.8(2)
C(32)	0.4912(9)	0.3729(5)	-0.1135(8)	3.0(2)
C(33)	0.7370(10)	0.4561(5)	-0.1359(8)	3.5(2)
C(34)	0.6050(9)	0.3746(5)	0.1823(7)	2.6(2)
C(35)	0.8698(9)	0.4474(5)	0.1624(8)	3.4(2)
H(1)	0.9088	0.0490	0.4327	1.9991
H(2)	1.2405	0.0858	0.3036	1.7455
H(3)	1.0567	0.2337	-0.3126	2.6465
H(4)	0.9874	0.1687	-0.2678	2.6465
H(5)	0.9248	0.3457	-0.2041	2.5146
H(6)	1.0324	0.3493	-0.0958	2.5146
H(7)	1.1491	0.1725	-0.1126	2.4872

H(8)	1.2167	0.2401	-0.1518	2.4872
H(9)	1.2071	0.2970	0.0089	2.3082
H(10)	1.2852	0.2252	0.0339	2.3082
H(11)	1.1018	0.3208	0.1506	2.2050
H(12)	1.0480	0.2599	0.2163	2.2050
H(13)	1.3251	0.2747	0.2154	1.9858
H(14)	1.2627	0.2255	0.2938	1.9858
H(15)	1.0983	0.1171	0.0529	1.8020
H(16)	1.2264	0.1398	0.1375	1.8020
H(17)	1.1749	0.3740	0.4441	2.8162
H(18)	1.0774	0.3468	0.3392	2.8162
H(19)	1.3953	0.2716	0.4532	3.3263
H(20)	1.4714	0.3131	0.3748	3.3263
H(21)	1.5213	0.3642	0.5477	4.8774
H(22)	1.4417	0.4193	0.4658	4.8774
H(23)	1.3678	0.3772	0.5451	4.8774
H(24)	1.0416	0.2831	0.4883	3.6242
H(25)	1.0971	0.2320	0.4084	3.6242
H(26)	1.1930	0.2597	0.5137	3.6242
H(27)	1.3772	0.0139	0.5536	3.4350
H(28)	1.3463	0.0085	0.4260	3.4350
H(29)	1.3521	0.0830	0.4827	3.4350
H(30)	1.1978	0.0479	0.6536	3.5320
H(31)	1.1725	0.1179	0.5848	3.5320
H(32)	1.0526	0.0663	0.5907	3.5320
H(33)	1.0427	-0.0520	0.4981	3.4686
H(34)	1.1551	-0.0734	0.4339	3.4686
H(35)	1.1885	-0.0686	0.5614	3.4686
H(36)	0.5709	0.0707	0.3702	4.0128
H(37)	0.6947	0.0194	0.3803	4.0128
H(38)	0.7087	0.0916	0.4440	4.0128
H(39)	0.7089	0.2041	0.3473	3.4120
H(40)	0.6900	0.2070	0.2199	3.4120
H(41)	0.5698	0.1842	0.2747	3.4120
H(42)	0.5376	0.0712	0.1711	3.1330
H(43)	0.6536	0.0920	0.1102	3.1330
H(44)	0.6596	0.0197	0.1728	3.1330
H(45)	0.6832	-0.0190	-0.0772	3.3798
H(46)	0.8294	-0.0445	-0.0817	3.3798
H(47)	0.8051	0.0076	0.0105	3.3798
H(48)	0.3470	0.0894	-0.1551	2.7980
H(49)	0.4577	0.0431	-0.1935	2.7980
H(50)	0.4682	0.0599	-0.0694	2.7980
H(51)	0.6800	0.0311	-0.3242	3.2581
H(52)	0.8032	0.0772	-0.3411	3.2581
H(53)	0.8250	-0.0016	-0.3009	3.2581
H(54)	0.5080	0.2443	-0.3025	3.3661
H(55)	0.4873	0.1677	-0.3519	3.3661
H(56)	0.3722	0.2040	-0.3039	3.3661
H(57)	1.2029	0.3536	-0.1987	3.6625
H(58)	1.0930	0.3533	-0.3057	3.6625
H(59)	1.1044	0.4182	-0.2259	3.6625
H(60)	0.8316	0.4550	-0.1338	4.1948
H(61)	0.6912	0.4695	-0.2083	4.1948
H(62)	0.7163	0.4902	-0.0846	4.1948
H(63)	0.4725	0.4080	-0.0619	3.5444

H(64)	0.4507	0.3872	-0.1855	3.5444
H(65)	0.4561	0.3280	-0.0967	3.5444
H(66)	0.8494	0.2906	-0.3583	2.9754
H(67)	0.8423	0.2166	-0.4164	2.9754
H(68)	0.7796	0.2263	-0.3121	2.9754
H(69)	0.9594	0.4405	0.1512	3.9814
H(70)	0.8250	0.4821	0.1106	3.9814
H(71)	0.8719	0.4653	0.2350	3.9814
H(72)	0.6174	0.3942	0.2546	3.0619
H(73)	0.5519	0.4066	0.1318	3.0619
H(74)	0.5597	0.3297	0.1808	3.0619
H(75)	0.6901	0.3352	-0.1610	2.3578
H(76)	0.8232	0.3280	0.1939	2.4209
H(77)	0.8906	0.0846	-0.1332	2.0675
H(78)	0.5212	0.1930	-0.1040	2.2516

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters for 2

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Y(1)	0.0152(4)	0.0148(3)	0.0144(3)	0.0008(4)	0.0031(2)	0.0006(4)
Si(1)	0.022(1)	0.021(1)	0.025(1)	-0.0002(10)	-0.0028(10)	-0.0018(9)
Si(2)	0.020(1)	0.021(1)	0.024(1)	-0.0027(10)	0.0028(9)	-0.0021(9)
Si(3)	0.023(1)	0.024(1)	0.030(1)	0.001(1)	0.0066(10)	-0.0026(10)
Si(4)	0.022(1)	0.019(1)	0.033(1)	0.000(1)	0.005(1)	0.0012(10)
O(1)	0.022(3)	0.019(3)	0.025(3)	0.003(2)	0.007(2)	0.012(2)
N(1)	0.016(3)	0.024(3)	0.016(3)	-0.001(4)	0.005(2)	0.002(4)
N(2)	0.019(4)	0.023(4)	0.025(4)	-0.004(3)	0.000(3)	0.001(3)
N(3)	0.025(4)	0.022(4)	0.021(3)	0.003(3)	0.002(3)	0.001(3)
N(4)	0.020(4)	0.009(3)	0.025(4)	-0.007(3)	0.002(3)	0.002(3)
N(5)	0.024(4)	0.016(3)	0.028(4)	0.007(3)	0.013(3)	0.008(3)
C(1)	0.019(5)	0.015(4)	0.014(4)	0.002(3)	0.001(3)	-0.000(3)
C(2)	0.020(5)	0.014(4)	0.020(4)	0.001(3)	0.004(3)	-0.002(3)
C(3)	0.014(4)	0.014(4)	0.024(4)	0.003(3)	0.003(3)	0.002(3)
C(4)	0.025(5)	0.016(4)	0.016(4)	-0.000(3)	0.001(3)	-0.001(3)
C(5)	0.025(5)	0.017(4)	0.020(4)	-0.001(4)	0.001(3)	0.001(3)
C(6)	0.017(4)	0.018(4)	0.023(4)	-0.004(3)	0.001(3)	-0.003(3)
C(7)	0.021(5)	0.026(5)	0.026(5)	-0.001(4)	0.007(4)	0.003(3)
C(8)	0.027(5)	0.045(6)	0.036(5)	0.001(4)	0.013(4)	-0.005(4)
C(9)	0.027(5)	0.060(7)	0.041(6)	-0.006(5)	0.014(4)	0.022(5)
C(10)	0.021(5)	0.044(6)	0.031(5)	-0.014(5)	0.002(4)	-0.004(4)
C(11)	0.020(5)	0.024(5)	0.021(4)	0.006(4)	-0.002(3)	0.006(3)
C(12)	0.045(6)	0.025(5)	0.035(5)	-0.001(4)	-0.003(4)	0.010(4)
C(13)	0.039(6)	0.044(6)	0.025(5)	-0.001(5)	0.003(4)	0.007(4)
C(14)	0.028(6)	0.051(6)	0.024(5)	0.011(4)	-0.002(4)	0.006(4)
C(15)	0.010(4)	0.025(5)	0.021(4)	0.004(3)	0.001(3)	-0.005(3)
C(16)	0.023(5)	0.025(5)	0.022(4)	0.000(4)	0.005(3)	0.002(3)
C(17)	0.014(4)	0.027(5)	0.019(4)	-0.004(3)	-0.003(3)	-0.001(3)
C(18)	0.038(6)	0.028(5)	0.021(4)	-0.001(4)	0.003(4)	-0.005(4)
C(19)	0.044(6)	0.047(6)	0.024(5)	-0.008(5)	0.011(4)	-0.002(4)
C(20)	0.035(6)	0.037(6)	0.029(5)	-0.005(4)	0.001(4)	0.007(4)
C(21)	0.054(7)	0.037(6)	0.051(6)	-0.010(5)	-0.013(5)	-0.004(5)
C(22)	0.021(5)	0.033(5)	0.021(4)	-0.000(3)	0.008(3)	0.009(3)
C(23)	0.023(4)	0.038(4)	0.020(4)	-0.002(5)	0.010(3)	0.005(5)
C(24)	0.019(5)	0.035(5)	0.022(4)	-0.004(4)	-0.002(4)	0.006(3)
C(25)	0.030(5)	0.031(5)	0.057(6)	-0.009(4)	0.008(4)	0.008(5)
C(26)	0.036(5)	0.029(4)	0.021(4)	-0.004(5)	0.014(3)	0.004(5)
C(27)	0.032(5)	0.045(7)	0.021(4)	-0.006(4)	0.009(4)	-0.001(4)
C(28)	0.039(6)	0.036(5)	0.025(5)	0.008(4)	0.003(4)	-0.010(4)
C(29)	0.033(6)	0.025(5)	0.050(6)	0.007(4)	0.009(5)	-0.002(4)
C(30)	0.015(5)	0.032(5)	0.038(5)	-0.003(4)	-0.000(4)	0.002(4)
C(31)	0.029(5)	0.032(6)	0.039(5)	-0.007(4)	-0.006(4)	0.004(4)
C(32)	0.029(6)	0.032(5)	0.045(6)	0.003(4)	-0.007(4)	0.011(4)
C(33)	0.042(6)	0.027(5)	0.061(7)	-0.006(5)	0.006(5)	0.014(5)
C(34)	0.029(5)	0.038(6)	0.034(5)	-0.002(4)	0.015(4)	-0.004(4)
C(35)	0.038(6)	0.041(6)	0.053(6)	-0.004(5)	0.018(5)	-0.026(5)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å) for 2

atom	atom	distance	atom	atom	distance
Y(1)	O(1)	2.055(5)	Y(1)	N(1)	2.607(5)
Y(1)	N(3)	2.596(7)	Y(1)	N(4)	2.221(6)
Y(1)	N(5)	2.307(6)	Si(1)	N(4)	1.705(6)
Si(1)	C(30)	1.840(9)	Si(1)	C(31)	1.873(9)
Si(2)	N(4)	1.691(7)	Si(2)	C(28)	1.845(8)
Si(2)	C(29)	1.844(9)	Si(3)	N(5)	1.692(6)
Si(3)	C(34)	1.865(10)	Si(3)	C(35)	1.858(10)
Si(4)	N(5)	1.707(6)	Si(4)	C(32)	1.847(10)
Si(4)	C(33)	1.859(9)	O(1)	C(1)	1.333(8)
N(1)	C(15)	1.53(1)	N(1)	C(16)	1.476(10)
N(1)	C(22)	1.479(9)	N(2)	C(17)	1.442(9)
N(2)	C(18)	1.46(1)	N(2)	C(20)	1.485(10)
N(3)	C(23)	1.493(9)	N(3)	C(24)	1.500(10)
N(3)	C(26)	1.491(9)	C(1)	C(2)	1.39(1)
C(1)	C(6)	1.43(1)	C(2)	C(3)	1.406(10)
C(2)	C(15)	1.50(1)	C(3)	C(4)	1.37(1)
C(4)	C(5)	1.39(1)	C(4)	C(11)	1.551(10)
C(5)	C(6)	1.40(1)	C(6)	C(7)	1.52(1)
C(7)	C(8)	1.50(1)	C(7)	C(9)	1.55(1)
C(7)	C(10)	1.55(1)	C(11)	C(12)	1.50(1)
C(11)	C(13)	1.52(1)	C(11)	C(14)	1.53(1)
C(16)	C(17)	1.54(1)	C(18)	C(19)	1.50(1)
C(20)	C(21)	1.51(1)	C(22)	C(23)	1.50(1)
C(24)	C(25)	1.52(1)	C(26)	C(27)	1.51(1)

Table 4. Bond Lengths(Å) for 2

atom	atom	distance	atom	atom	distance
Si(1)	H(78)	0.95	Si(2)	H(77)	0.95
Si(3)	H(76)	0.95	Si(4)	H(75)	0.95
C(3)	H(2)	0.95	C(5)	H(1)	0.95
C(8)	H(39)	0.95	C(8)	H(40)	0.95
C(8)	H(41)	0.95	C(9)	H(36)	0.94
C(9)	H(37)	0.95	C(9)	H(38)	0.95
C(10)	H(42)	0.95	C(10)	H(43)	0.95
C(10)	H(44)	0.96	C(12)	H(33)	0.95
C(12)	H(34)	0.95	C(12)	H(35)	0.95
C(13)	H(30)	0.95	C(13)	H(31)	0.95
C(13)	H(32)	0.95	C(14)	H(27)	0.95
C(14)	H(28)	0.95	C(14)	H(29)	0.95
C(15)	H(15)	0.95	C(15)	H(16)	0.95
C(16)	H(11)	0.95	C(16)	H(12)	0.95
C(17)	H(13)	0.95	C(17)	H(14)	0.95
C(18)	H(17)	0.95	C(18)	H(18)	0.95
C(19)	H(24)	0.95	C(19)	H(25)	0.95
C(19)	H(26)	0.95	C(20)	H(19)	0.95
C(20)	H(20)	0.95	C(21)	H(21)	0.95
C(21)	H(22)	0.95	C(21)	H(23)	0.96
C(22)	H(9)	0.95	C(22)	H(10)	0.95
C(23)	H(7)	0.95	C(23)	H(8)	0.95
C(24)	H(5)	0.95	C(24)	H(6)	0.95
C(25)	H(57)	0.95	C(25)	H(58)	0.95
C(25)	H(59)	0.94	C(26)	H(3)	0.95
C(26)	H(4)	0.95	C(27)	H(66)	0.95
C(27)	H(67)	0.95	C(27)	H(68)	0.95
C(28)	H(51)	0.95	C(28)	H(52)	0.95
C(28)	H(53)	0.95	C(29)	H(45)	0.95
C(29)	H(46)	0.95	C(29)	H(47)	0.95
C(30)	H(48)	0.94	C(30)	H(49)	0.95
C(30)	H(50)	0.95	C(31)	H(54)	0.95
C(31)	H(55)	0.95	C(31)	H(56)	0.95
C(32)	H(63)	0.96	C(32)	H(64)	0.94
C(32)	H(65)	0.95	C(33)	H(60)	0.94
C(33)	H(61)	0.96	C(33)	H(62)	0.95
C(34)	H(72)	0.95	C(34)	H(73)	0.95
C(34)	H(74)	0.95	C(35)	H(69)	0.94
C(35)	H(70)	0.96	C(35)	H(71)	0.95

Table 5. Bond Angles (deg) for 2

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Y(1)	N(1)	76.2(2)	O(1)	Y(1)	N(3)	141.1(2)
O(1)	Y(1)	N(4)	93.6(2)	O(1)	Y(1)	N(5)	101.4(2)
N(1)	Y(1)	N(3)	70.8(2)	N(1)	Y(1)	N(4)	141.5(2)
N(1)	Y(1)	N(5)	103.2(2)	N(3)	Y(1)	N(4)	99.5(2)
N(3)	Y(1)	N(5)	105.6(2)	N(4)	Y(1)	N(5)	115.2(2)
N(4)	Si(1)	C(30)	115.1(3)	N(4)	Si(1)	C(31)	113.1(4)
C(30)	Si(1)	C(31)	107.4(4)	Y(1)	Si(2)	N(4)	42.3(2)
Y(1)	Si(2)	C(28)	136.1(3)	Y(1)	Si(2)	C(29)	114.9(3)
N(4)	Si(2)	C(28)	114.2(3)	N(4)	Si(2)	C(29)	117.3(4)
C(28)	Si(2)	C(29)	109.0(4)	N(5)	Si(3)	C(34)	114.0(4)
N(5)	Si(3)	C(35)	112.0(4)	C(34)	Si(3)	C(35)	109.1(4)
N(5)	Si(4)	C(32)	116.4(4)	N(5)	Si(4)	C(33)	115.7(4)
C(32)	Si(4)	C(33)	106.5(4)	Y(1)	O(1)	C(1)	146.0(5)
Y(1)	N(1)	C(15)	101.7(4)	Y(1)	N(1)	C(16)	110.7(4)
Y(1)	N(1)	C(22)	110.6(4)	C(15)	N(1)	C(16)	111.8(5)
C(15)	N(1)	C(22)	109.7(6)	C(16)	N(1)	C(22)	111.9(6)
C(17)	N(2)	C(18)	114.6(6)	C(17)	N(2)	C(20)	108.5(6)
C(18)	N(2)	C(20)	112.6(6)	Y(1)	N(3)	C(23)	105.5(4)
Y(1)	N(3)	C(24)	105.0(5)	Y(1)	N(3)	C(26)	118.4(5)
C(23)	N(3)	C(24)	111.9(6)	C(23)	N(3)	C(26)	105.5(6)
C(24)	N(3)	C(26)	110.5(6)	Y(1)	N(4)	Si(1)	122.8(3)
Y(1)	N(4)	Si(2)	106.9(3)	Si(1)	N(4)	Si(2)	127.7(4)
Y(1)	N(5)	Si(3)	126.3(3)	Y(1)	N(5)	Si(4)	109.3(3)
Si(3)	N(5)	Si(4)	124.2(4)	O(1)	C(1)	C(2)	118.8(7)
O(1)	C(1)	C(6)	121.2(7)	C(2)	C(1)	C(6)	120.0(6)
C(1)	C(2)	C(3)	120.4(7)	C(1)	C(2)	C(15)	121.1(6)
C(3)	C(2)	C(15)	118.5(7)	C(2)	C(3)	C(4)	120.9(7)
C(3)	C(4)	C(5)	118.4(7)	C(3)	C(4)	C(11)	122.6(7)
C(5)	C(4)	C(11)	119.0(7)	C(4)	C(5)	C(6)	123.4(7)
C(1)	C(6)	C(5)	116.9(7)	C(1)	C(6)	C(7)	121.2(6)
C(5)	C(6)	C(7)	122.0(7)	C(6)	C(7)	C(8)	110.8(7)
C(6)	C(7)	C(9)	111.4(6)	C(6)	C(7)	C(10)	110.7(7)
C(8)	C(7)	C(9)	106.9(7)	C(8)	C(7)	C(10)	109.4(7)
C(9)	C(7)	C(10)	107.5(7)	C(4)	C(11)	C(12)	110.4(6)
C(4)	C(11)	C(13)	108.3(7)	C(4)	C(11)	C(14)	111.2(7)
C(12)	C(11)	C(13)	109.7(7)	C(12)	C(11)	C(14)	108.6(7)
C(13)	C(11)	C(14)	108.6(6)	N(1)	C(15)	C(2)	115.1(6)
N(1)	C(16)	C(17)	114.9(6)	N(2)	C(17)	C(16)	113.0(6)
N(2)	C(18)	C(19)	117.2(7)	N(2)	C(20)	C(21)	114.7(8)
N(1)	C(22)	C(23)	113.7(6)	N(3)	C(23)	C(22)	114.3(7)
N(3)	C(24)	C(25)	117.9(7)	N(3)	C(26)	C(27)	116.1(7)

Table 6. Bond Angles (deg) for 2

atom	atom	atom	angle	atom	atom	atom	angle
N(4)	Si(1)	H(75)	106.9	C(30)	Si(1)	H(75)	106.9
C(31)	Si(1)	H(75)	107.0	N(4)	Si(2)	H(76)	105.0
C(28)	Si(2)	H(76)	105.1	C(29)	Si(2)	H(76)	105.1
N(5)	Si(3)	H(78)	107.2	C(34)	Si(3)	H(78)	107.2
C(35)	Si(3)	H(78)	106.9	N(5)	Si(4)	H(77)	105.8
C(32)	Si(4)	H(77)	105.5	C(33)	Si(4)	H(77)	105.9
C(2)	C(3)	H(2)	119.6	C(4)	C(3)	H(2)	119.5
C(4)	C(5)	H(1)	118.4	C(6)	C(5)	H(1)	118.2
C(7)	C(8)	H(39)	109.3	C(7)	C(8)	H(40)	108.9
C(7)	C(8)	H(41)	109.1	H(39)	C(8)	H(40)	109.9
H(39)	C(8)	H(41)	110.0	H(40)	C(8)	H(41)	109.6
C(7)	C(9)	H(36)	109.3	C(7)	C(9)	H(37)	109.1
C(7)	C(9)	H(38)	108.8	H(36)	C(9)	H(37)	110.4
H(36)	C(9)	H(38)	109.7	H(37)	C(9)	H(38)	109.6
C(7)	C(10)	H(42)	109.6	C(7)	C(10)	H(43)	109.6
C(7)	C(10)	H(44)	109.0	H(42)	C(10)	H(43)	110.1
H(42)	C(10)	H(44)	109.2	H(43)	C(10)	H(44)	109.3
C(11)	C(12)	H(33)	109.3	C(11)	C(12)	H(34)	109.7
C(11)	C(12)	H(35)	109.4	H(33)	C(12)	H(34)	109.4
H(33)	C(12)	H(35)	109.3	H(34)	C(12)	H(35)	109.7
C(11)	C(13)	H(30)	109.1	C(11)	C(13)	H(31)	109.4
C(11)	C(13)	H(32)	109.3	H(30)	C(13)	H(31)	109.7
H(30)	C(13)	H(32)	109.7	H(31)	C(13)	H(32)	109.7
C(11)	C(14)	H(27)	109.4	C(11)	C(14)	H(28)	109.6
C(11)	C(14)	H(29)	109.4	H(27)	C(14)	H(28)	109.7
H(27)	C(14)	H(29)	109.3	H(28)	C(14)	H(29)	109.4
N(1)	C(15)	H(15)	108.2	N(1)	C(15)	H(16)	108.4
C(2)	C(15)	H(15)	107.7	C(2)	C(15)	H(16)	107.9
H(15)	C(15)	H(16)	109.5	N(1)	C(16)	H(11)	108.3
N(1)	C(16)	H(12)	108.0	C(17)	C(16)	H(11)	108.2
C(17)	C(16)	H(12)	108.1	H(11)	C(16)	H(12)	109.2
N(2)	C(17)	H(13)	108.8	N(2)	C(17)	H(14)	108.7
C(16)	C(17)	H(13)	108.5	C(16)	C(17)	H(14)	108.6
H(13)	C(17)	H(14)	109.3	N(2)	C(18)	H(17)	107.8
N(2)	C(18)	H(18)	107.5	C(19)	C(18)	H(17)	107.5
C(19)	C(18)	H(18)	107.2	H(17)	C(18)	H(18)	109.3
C(18)	C(19)	H(24)	109.5	C(18)	C(19)	H(25)	109.5
C(18)	C(19)	H(26)	109.3	H(24)	C(19)	H(25)	109.5
H(24)	C(19)	H(26)	109.5	H(25)	C(19)	H(26)	109.6
N(2)	C(20)	H(19)	107.8	N(2)	C(20)	H(20)	108.1
C(21)	C(20)	H(19)	108.5	C(21)	C(20)	H(20)	108.4
H(19)	C(20)	H(20)	109.2	C(20)	C(21)	H(21)	109.9
C(20)	C(21)	H(22)	109.6	C(20)	C(21)	H(23)	109.3
H(21)	C(21)	H(22)	109.8	H(21)	C(21)	H(23)	109.2
H(22)	C(21)	H(23)	108.9	N(1)	C(22)	H(9)	108.4
N(1)	C(22)	H(10)	108.3	C(23)	C(22)	H(9)	108.5
C(23)	C(22)	H(10)	108.4	H(9)	C(22)	H(10)	109.5
N(3)	C(23)	H(7)	108.4	N(3)	C(23)	H(8)	108.2
C(22)	C(23)	H(7)	108.3	C(22)	C(23)	H(8)	108.0
H(7)	C(23)	H(8)	109.6	N(3)	C(24)	H(5)	107.4
N(3)	C(24)	H(6)	107.3	C(25)	C(24)	H(5)	107.4
C(25)	C(24)	H(6)	107.4	H(5)	C(24)	H(6)	109.3

C(24)	C(25)	H(57)	109.0	C(24)	C(25)	H(58)	109.1
C(24)	C(25)	H(59)	109.5	H(57)	C(25)	H(58)	109.3
H(57)	C(25)	H(59)	109.8	H(58)	C(25)	H(59)	110.0
N(3)	C(26)	H(3)	107.8	N(3)	C(26)	H(4)	107.7
C(27)	C(26)	H(3)	107.9	C(27)	C(26)	H(4)	107.8
H(3)	C(26)	H(4)	109.3	C(26)	C(27)	H(66)	109.6
C(26)	C(27)	H(67)	109.8	C(26)	C(27)	H(68)	109.6
H(66)	C(27)	H(67)	109.3	H(66)	C(27)	H(68)	109.1
H(67)	C(27)	H(68)	109.3	Si(2)	C(28)	H(51)	109.5
Si(2)	C(28)	H(52)	109.8	Si(2)	C(28)	H(53)	109.6
H(51)	C(28)	H(52)	109.5	H(51)	C(28)	H(53)	109.1
H(52)	C(28)	H(53)	109.3	Si(2)	C(29)	H(45)	109.0
Si(2)	C(29)	H(46)	109.5	Si(2)	C(29)	H(47)	109.5
H(45)	C(29)	H(46)	109.4	H(45)	C(29)	H(47)	109.5
H(46)	C(29)	H(47)	110.0	Si(1)	C(30)	H(48)	109.5
Si(1)	C(30)	H(49)	109.0	Si(1)	C(30)	H(50)	109.0
H(48)	C(30)	H(49)	110.2	H(48)	C(30)	H(50)	109.8
H(49)	C(30)	H(50)	109.3	Si(1)	C(31)	H(54)	109.4
Si(1)	C(31)	H(55)	109.4	Si(1)	C(31)	H(56)	109.2
H(54)	C(31)	H(55)	109.9	H(54)	C(31)	H(56)	109.4
H(55)	C(31)	H(56)	109.6	Si(4)	C(32)	H(63)	108.8
Si(4)	C(32)	H(64)	109.7	Si(4)	C(32)	H(65)	109.5
H(63)	C(32)	H(64)	109.4	H(63)	C(32)	H(65)	109.2
H(64)	C(32)	H(65)	110.3	Si(4)	C(33)	H(60)	109.8
Si(4)	C(33)	H(61)	109.1	Si(4)	C(33)	H(62)	109.5
H(60)	C(33)	H(61)	109.3	H(60)	C(33)	H(62)	110.1
H(61)	C(33)	H(62)	109.0	Si(3)	C(34)	H(72)	109.4
Si(3)	C(34)	H(73)	109.4	Si(3)	C(34)	H(74)	109.5
H(72)	C(34)	H(73)	109.4	H(72)	C(34)	H(74)	109.4
H(73)	C(34)	H(74)	109.6	Si(3)	C(35)	H(69)	110.3
Si(3)	C(35)	H(70)	109.4	Si(3)	C(35)	H(71)	109.8
H(69)	C(35)	H(70)	109.2	H(69)	C(35)	H(71)	109.7
H(70)	C(35)	H(71)	108.4				

Table 7. Torsion Angles (deg) for 2

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Y(1)	O(1)	C(1)	C(2)	-9(1)	Y(1)	O(1)	C(1)	C(6)	171.0(6)
Y(1)	N(1)	C(15)	C(2)	-74.9(6)	Y(1)	N(1)	C(16)	C(17)	170.5(5)
Y(1)	N(1)	C(22)	C(23)	-30.2(8)	Y(1)	N(3)	C(23)	C(22)	-51.0(8)
Y(1)	N(3)	C(24)	C(25)	172.1(5)	Y(1)	N(3)	C(26)	C(27)	62.6(9)
Y(1)	N(4)	Si(1)	C(30)	-131.9(4)	Y(1)	N(4)	Si(1)	C(31)	104.1(4)
Y(1)	N(4)	Si(2)	C(28)	-132.9(4)	Y(1)	N(4)	Si(2)	C(29)	97.9(4)
Y(1)	N(5)	Si(3)	C(34)	-118.2(5)	Y(1)	N(5)	Si(3)	C(35)	117.2(5)
Y(1)	N(5)	Si(4)	C(32)	113.0(4)	Y(1)	N(5)	Si(4)	C(33)	-120.7(4)
Si(1)	N(4)	Y(1)	Si(2)	163.0(6)	Si(1)	N(4)	Y(1)	O(1)	89.1(4)
Si(1)	N(4)	Y(1)	N(1)	161.3(3)	Si(1)	N(4)	Y(1)	N(3)	-127.6(4)
Si(1)	N(4)	Y(1)	N(5)	-15.3(4)	Si(1)	N(4)	Si(2)	C(28)	65.1(6)
Si(1)	N(4)	Si(2)	C(29)	-64.1(6)	Si(2)	Y(1)	O(1)	C(1)	100.5(8)
Si(2)	Y(1)	N(1)	C(15)	-33.7(4)	Si(2)	Y(1)	N(1)	C(16)	-152.7(5)
Si(2)	Y(1)	N(1)	C(22)	82.8(5)	Si(2)	Y(1)	N(3)	C(23)	-89.2(5)
Si(2)	Y(1)	N(3)	C(24)	152.5(4)	Si(2)	Y(1)	N(3)	C(26)	28.6(5)
Si(2)	Y(1)	N(5)	Si(3)	126.1(3)	Si(2)	Y(1)	N(5)	Si(4)	-49.8(5)
Si(2)	N(4)	Y(1)	O(1)	-73.9(3)	Si(2)	N(4)	Y(1)	N(1)	-1.7(5)
Si(2)	N(4)	Y(1)	N(3)	69.3(3)	Si(2)	N(4)	Y(1)	N(5)	-178.4(3)
Si(2)	N(4)	Si(1)	C(30)	27.5(6)	Si(2)	N(4)	Si(1)	C(31)	-96.6(5)
Si(3)	N(5)	Y(1)	O(1)	28.0(4)	Si(3)	N(5)	Y(1)	N(1)	-50.3(4)
Si(3)	N(5)	Y(1)	N(3)	-123.8(4)	Si(3)	N(5)	Y(1)	N(4)	127.5(4)
Si(3)	N(5)	Si(4)	C(32)	-62.9(6)	Si(3)	N(5)	Si(4)	C(33)	63.3(6)
Si(4)	N(5)	Y(1)	O(1)	-147.9(3)	Si(4)	N(5)	Y(1)	N(1)	133.9(3)
Si(4)	N(5)	Y(1)	N(3)	60.4(3)	Si(4)	N(5)	Y(1)	N(4)	-48.3(4)
Si(4)	N(5)	Si(3)	C(34)	57.0(6)	Si(4)	N(5)	Si(3)	C(35)	-67.5(6)
O(1)	Y(1)	Si(2)	N(4)	105.7(3)	O(1)	Y(1)	Si(2)	C(28)	-179.7(4)
O(1)	Y(1)	Si(2)	C(29)	1.8(4)	O(1)	Y(1)	N(1)	C(15)	45.4(4)
O(1)	Y(1)	N(1)	C(16)	-73.6(5)	O(1)	Y(1)	N(1)	C(22)	161.9(6)
O(1)	Y(1)	N(3)	C(23)	-9.8(6)	O(1)	Y(1)	N(3)	C(24)	-128.2(4)
O(1)	Y(1)	N(3)	C(26)	107.9(6)	O(1)	C(1)	C(2)	C(3)	178.9(6)
O(1)	C(1)	C(2)	C(15)	-4(1)	O(1)	C(1)	C(6)	C(5)	-179.0(6)
O(1)	C(1)	C(6)	C(7)	0(1)	N(1)	Y(1)	Si(2)	N(4)	178.8(3)
N(1)	Y(1)	Si(2)	C(28)	-106.6(4)	N(1)	Y(1)	Si(2)	C(29)	74.9(4)
N(1)	Y(1)	O(1)	C(1)	-12.3(8)	N(1)	Y(1)	N(3)	C(23)	23.6(5)
N(1)	Y(1)	N(3)	C(24)	-94.7(4)	N(1)	Y(1)	N(3)	C(26)	141.4(6)
N(1)	C(15)	C(2)	C(1)	56.4(9)	N(1)	C(15)	C(2)	C(3)	-126.7(7)
N(1)	C(16)	C(17)	N(2)	169.4(6)	N(1)	C(22)	C(23)	N(3)	58.4(10)
N(3)	Y(1)	Si(2)	N(4)	-112.6(3)	N(3)	Y(1)	Si(2)	C(28)	-38.0(4)
N(3)	Y(1)	Si(2)	C(29)	143.5(4)	N(3)	Y(1)	O(1)	C(1)	20.1(10)
N(3)	Y(1)	N(1)	C(15)	-113.7(4)	N(3)	Y(1)	N(1)	C(16)	127.3(5)
N(3)	Y(1)	N(1)	C(22)	2.8(5)	N(4)	Y(1)	Si(2)	C(28)	74.6(5)
N(4)	Y(1)	Si(2)	C(29)	-103.9(4)	N(4)	Y(1)	O(1)	C(1)	130.1(8)
N(4)	Y(1)	N(1)	C(15)	-32.7(5)	N(4)	Y(1)	N(1)	C(16)	-151.7(5)
N(4)	Y(1)	N(1)	C(22)	83.7(6)	N(4)	Y(1)	N(3)	C(23)	-117.8(5)
N(4)	Y(1)	N(3)	C(24)	123.8(4)	N(4)	Y(1)	N(3)	C(26)	-0.1(6)
N(4)	Si(2)	Y(1)	N(5)	2.6(4)	N(5)	Y(1)	Si(2)	C(28)	77.2(5)
N(5)	Y(1)	Si(2)	C(29)	-101.3(4)	N(5)	Y(1)	O(1)	C(1)	-113.3(8)
N(5)	Y(1)	N(1)	C(15)	144.1(4)	N(5)	Y(1)	N(1)	C(16)	25.2(5)
N(5)	Y(1)	N(1)	C(22)	-99.4(5)	N(5)	Y(1)	N(3)	C(23)	122.5(5)
N(5)	Y(1)	N(3)	C(24)	4.2(5)	N(5)	Y(1)	N(3)	C(26)	-119.7(5)
C(1)	C(2)	C(3)	C(4)	0(1)	C(1)	C(6)	C(5)	C(4)	0(1)

C(1)	C(6)	C(7)	C(8)	-64.2(9)	C(1)	C(6)	C(7)	C(9)	177.0(7)
C(1)	C(6)	C(7)	C(10)	57.5(10)	C(2)	C(1)	C(6)	C(5)	1(1)
C(2)	C(1)	C(6)	C(7)	-179.2(7)	C(2)	C(3)	C(4)	C(5)	1(1)
C(2)	C(3)	C(4)	C(11)	-178.8(7)	C(2)	C(15)	N(1)	C(16)	43.3(8)
C(2)	C(15)	N(1)	C(22)	168.1(6)	C(3)	C(2)	C(1)	C(6)	-1(1)
C(3)	C(4)	C(5)	C(6)	-1(1)	C(3)	C(4)	C(11)	C(12)	-115.7(9)
C(3)	C(4)	C(11)	C(13)	124.2(8)	C(3)	C(4)	C(11)	C(14)	4(1)
C(4)	C(3)	C(2)	C(15)	-177.3(7)	C(4)	C(5)	C(6)	C(7)	-179.3(7)
C(5)	C(4)	C(11)	C(12)	63.6(10)	C(5)	C(4)	C(11)	C(13)	-56.5(9)
C(5)	C(4)	C(11)	C(14)	-175.8(7)	C(5)	C(6)	C(7)	C(8)	115.5(8)
C(5)	C(6)	C(7)	C(9)	-3(1)	C(5)	C(6)	C(7)	C(10)	-122.8(8)
C(6)	C(1)	C(2)	C(15)	175.7(7)	C(6)	C(5)	C(4)	C(11)	178.7(7)
C(15)	N(1)	C(16)	C(17)	57.9(8)	C(15)	N(1)	C(22)	C(23)	81.1(8)
C(16)	N(1)	C(22)	C(23)	-154.1(7)	C(16)	C(17)	N(2)	C(18)	48.7(9)
C(16)	C(17)	N(2)	C(20)	175.3(6)	C(17)	N(2)	C(18)	C(19)	59.5(9)
C(17)	N(2)	C(20)	C(21)	175.6(7)	C(17)	C(16)	N(1)	C(22)	-65.6(8)
C(18)	N(2)	C(20)	C(21)	-56.5(10)	C(19)	C(18)	N(2)	C(20)	-65.0(9)
C(22)	C(23)	N(3)	C(24)	62.6(9)	C(22)	C(23)	N(3)	C(26)	-177.1(7)
C(23)	N(3)	C(24)	C(25)	58.1(8)	C(23)	N(3)	C(26)	C(27)	-179.6(7)
C(24)	N(3)	C(26)	C(27)	-58.5(9)	C(25)	C(24)	N(3)	C(26)	-59.2(8)

Figure 1. ^{1}H-^{1}H correlation spectra of 2 (500 MHz, d_8-toluene, 233 K).

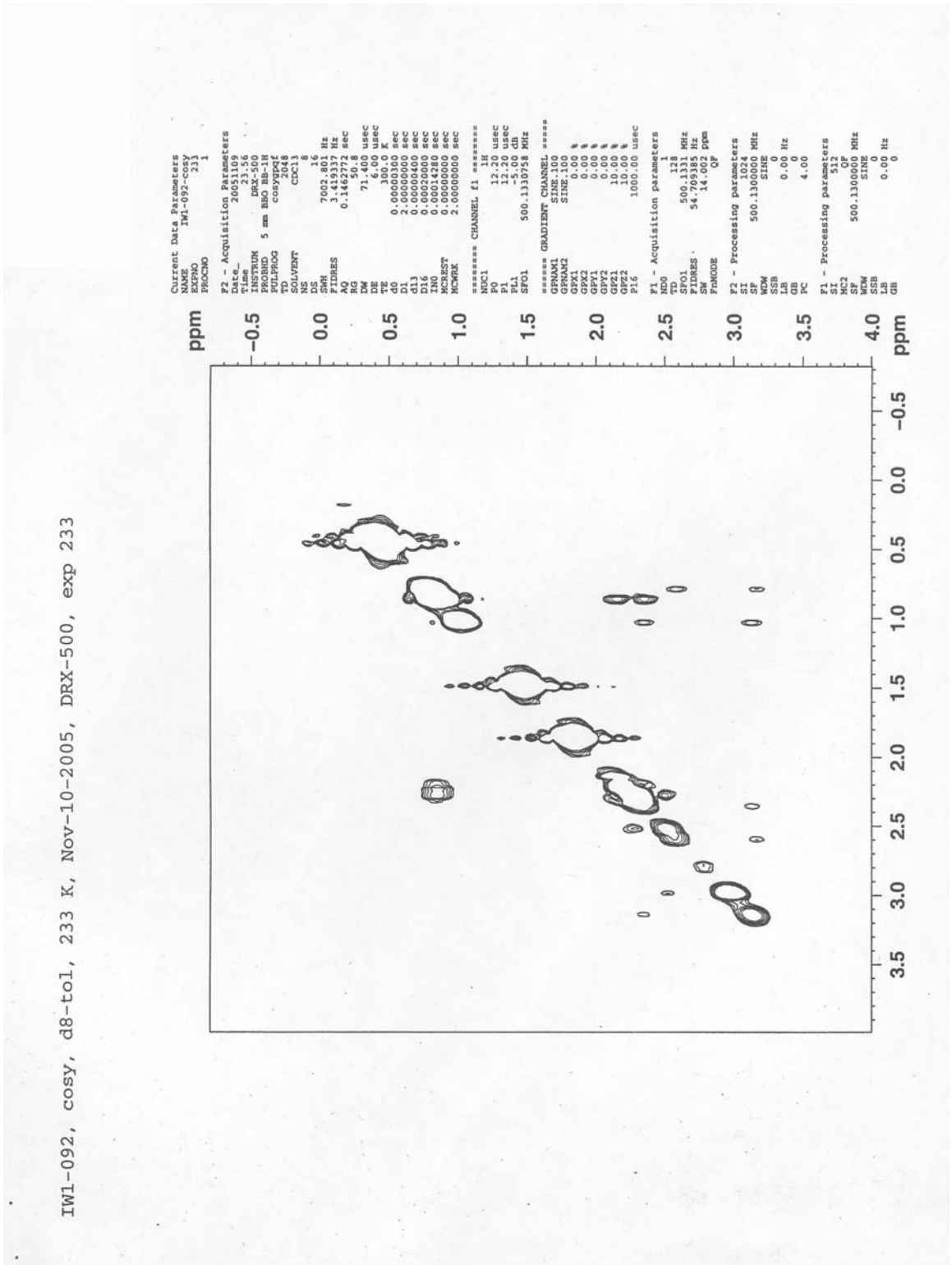

Figure 2. ^{1}H-^{1}H correlation spectra of 2 (500 MHz, d_8-toluene, 253 K).

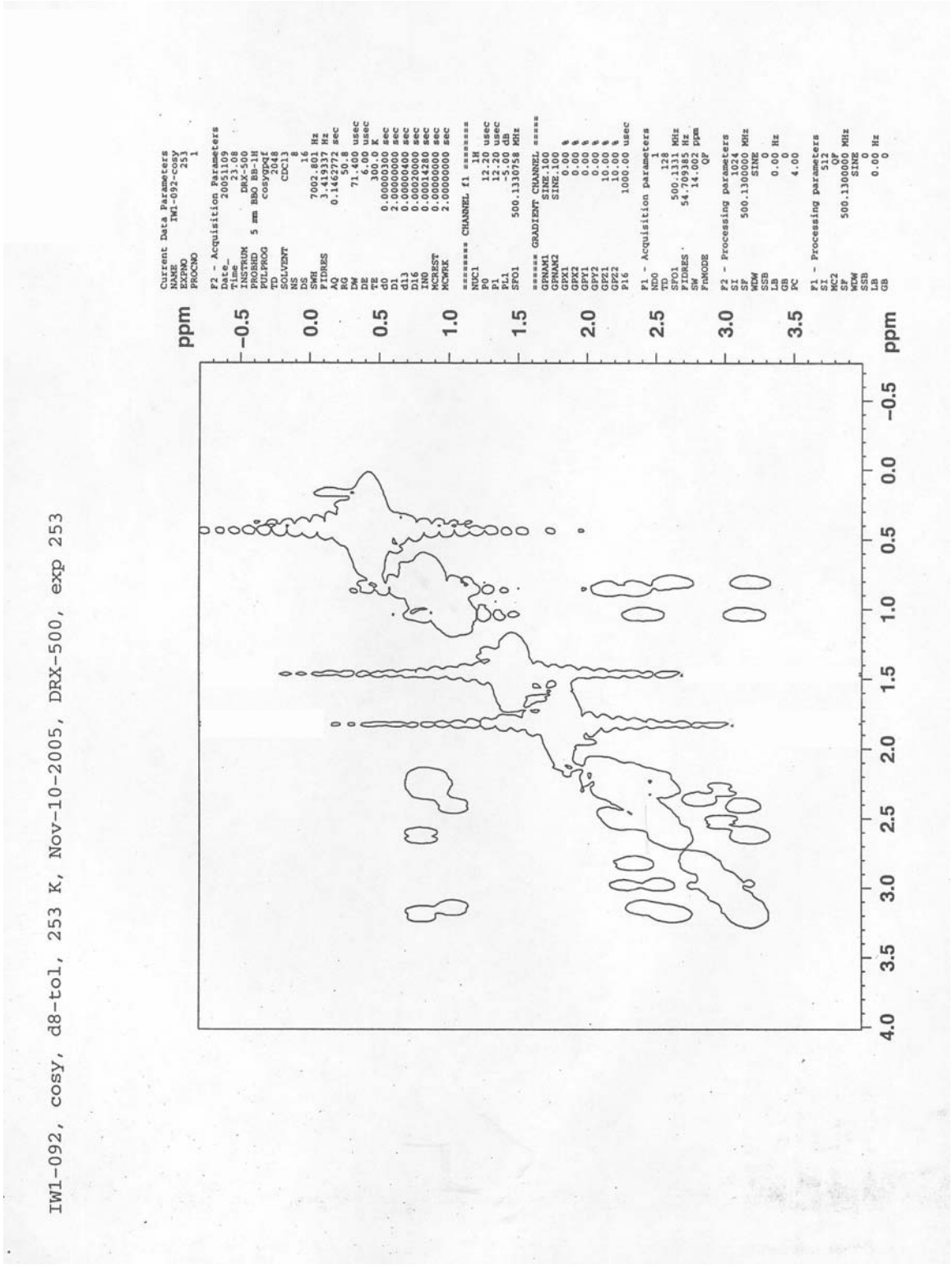

Figure 3. ^{1}H-^{1}H correlation spectra of 2 (500 MHz, d_8-toluene, 273 K).

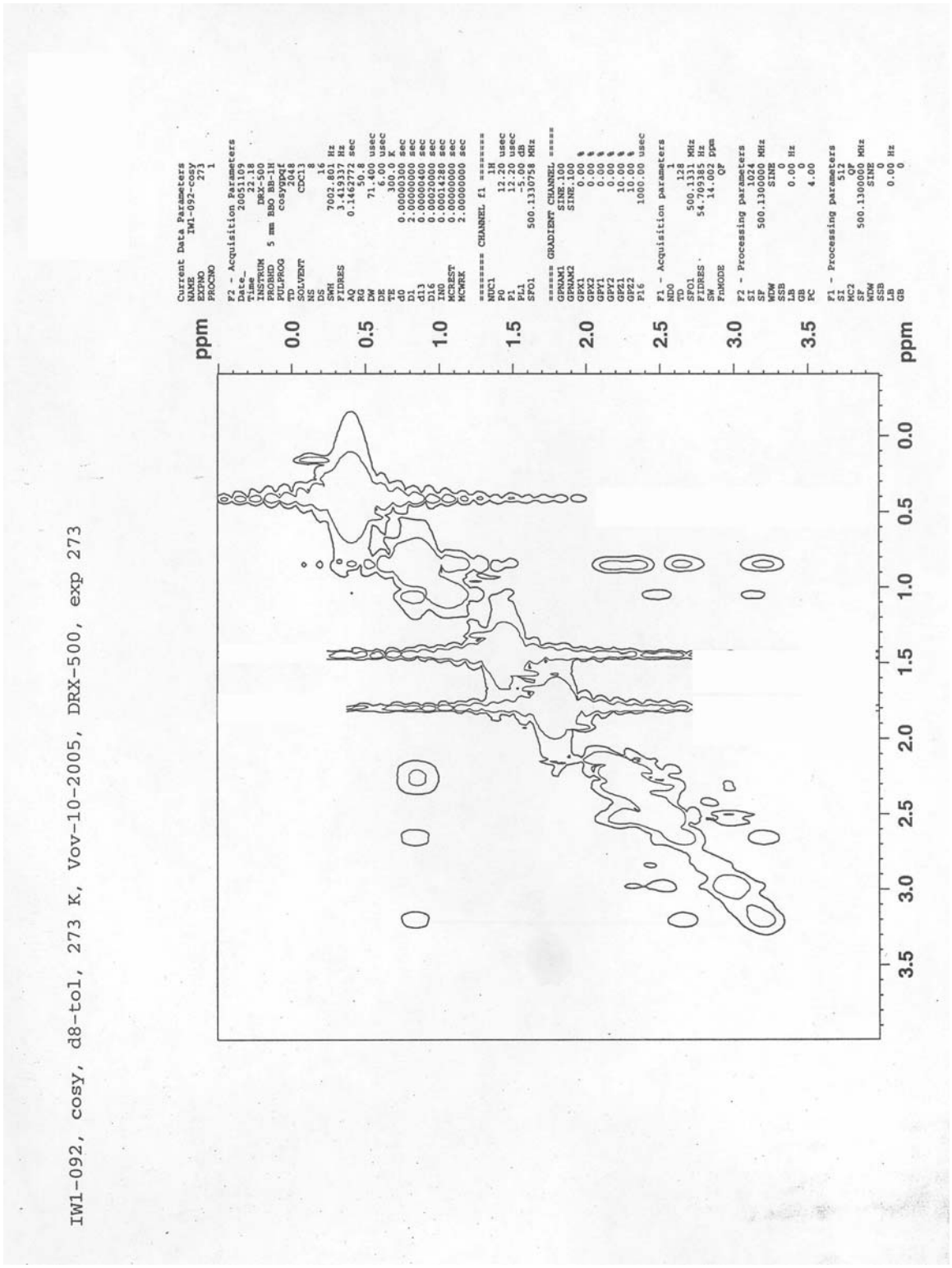

Figure 4. ^{1}H-^{1}H correlation spectra of 2 (500 MHz, d_8-toluene, 353 K).

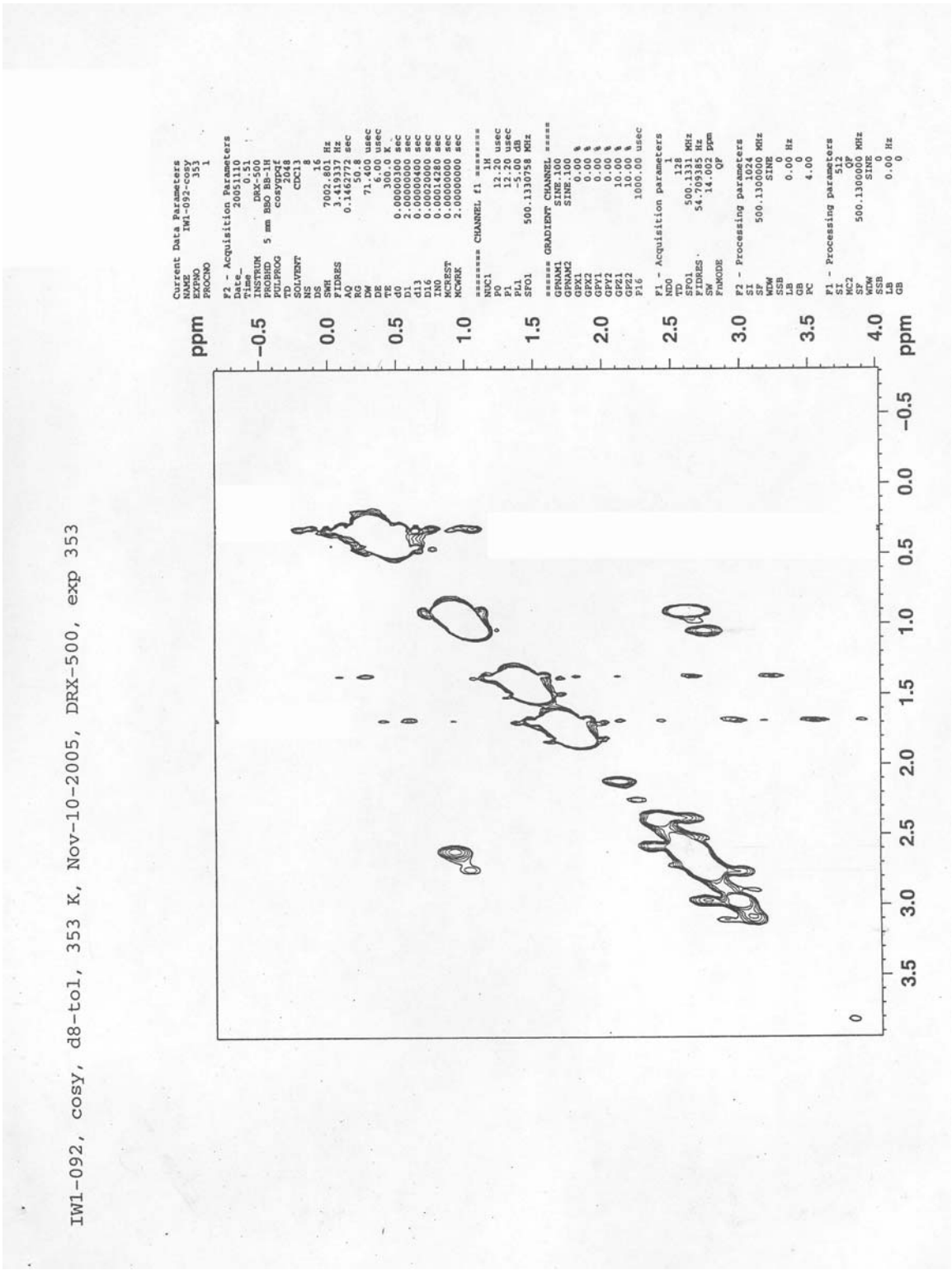

Figure 5. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 193 K).

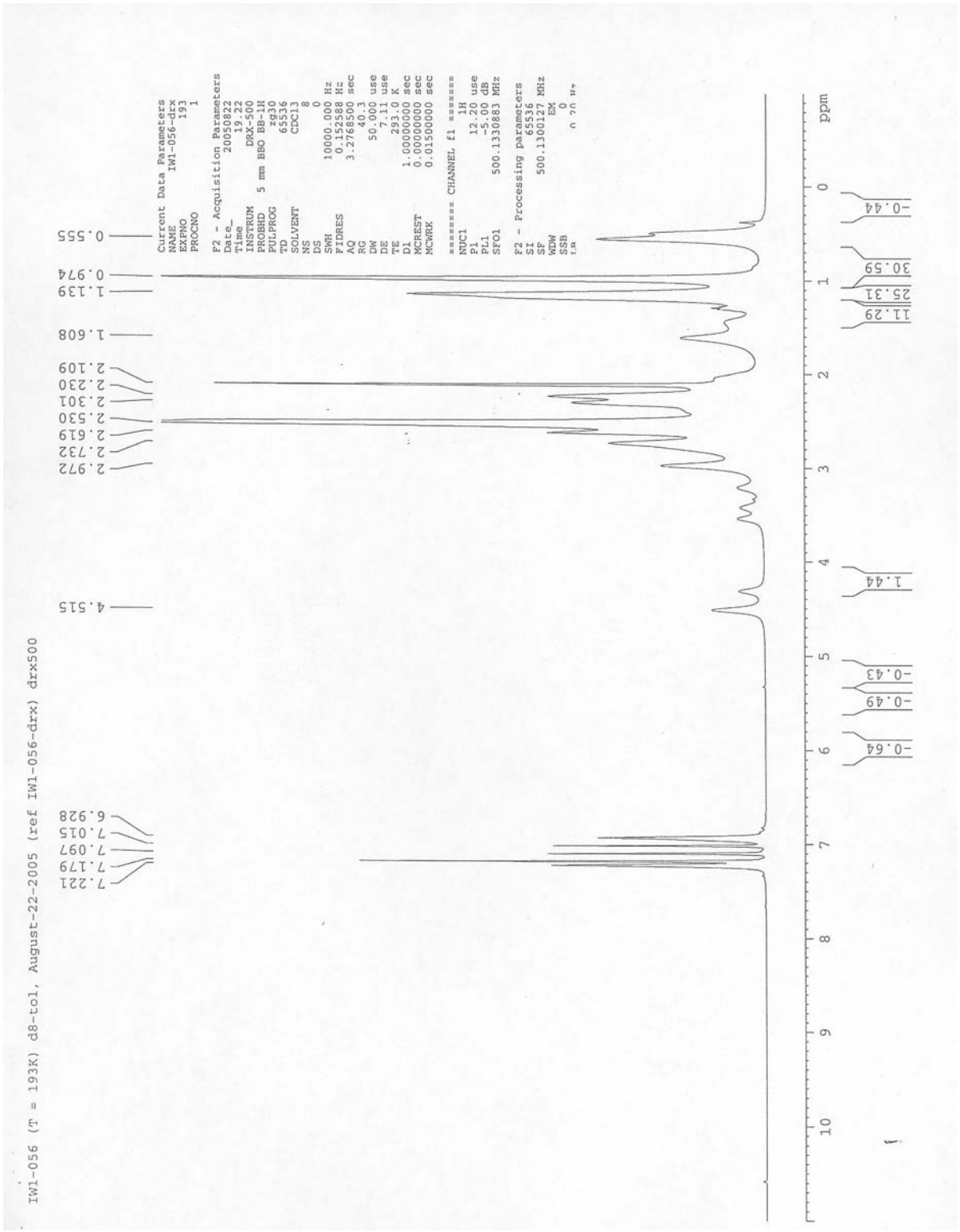

Figure 6. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 213 K).

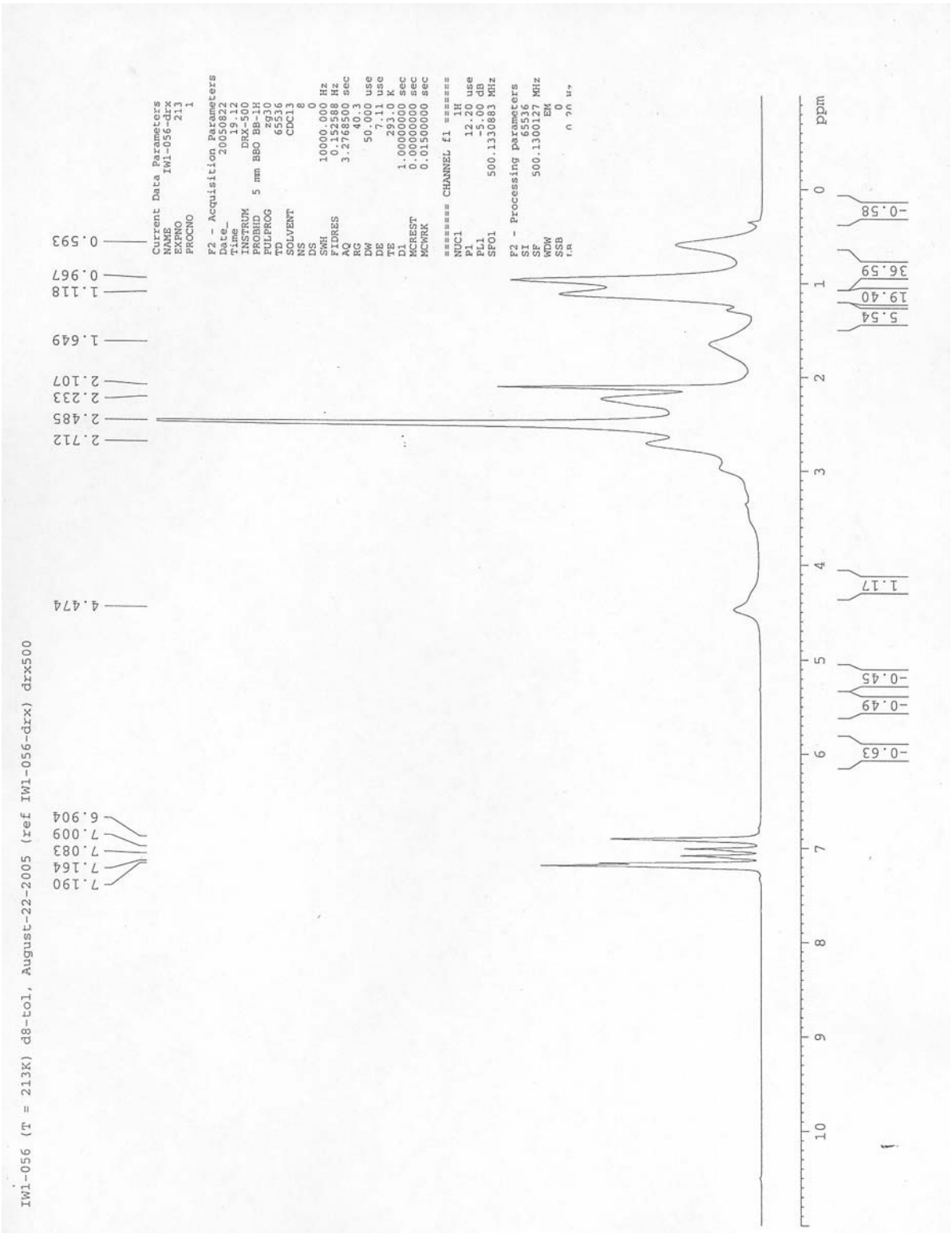

Figure 7. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 233 K).

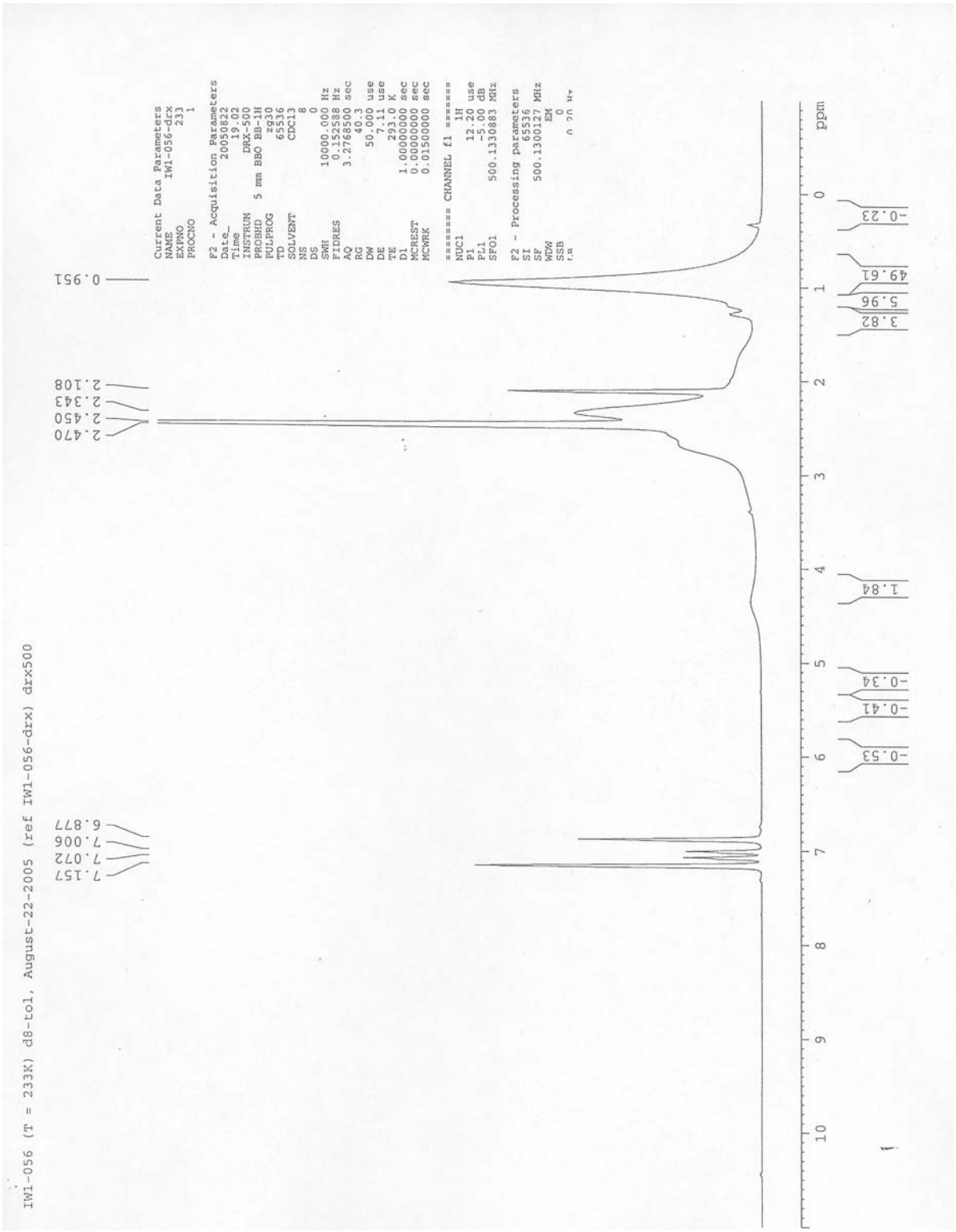

Figure 8. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 253 K).

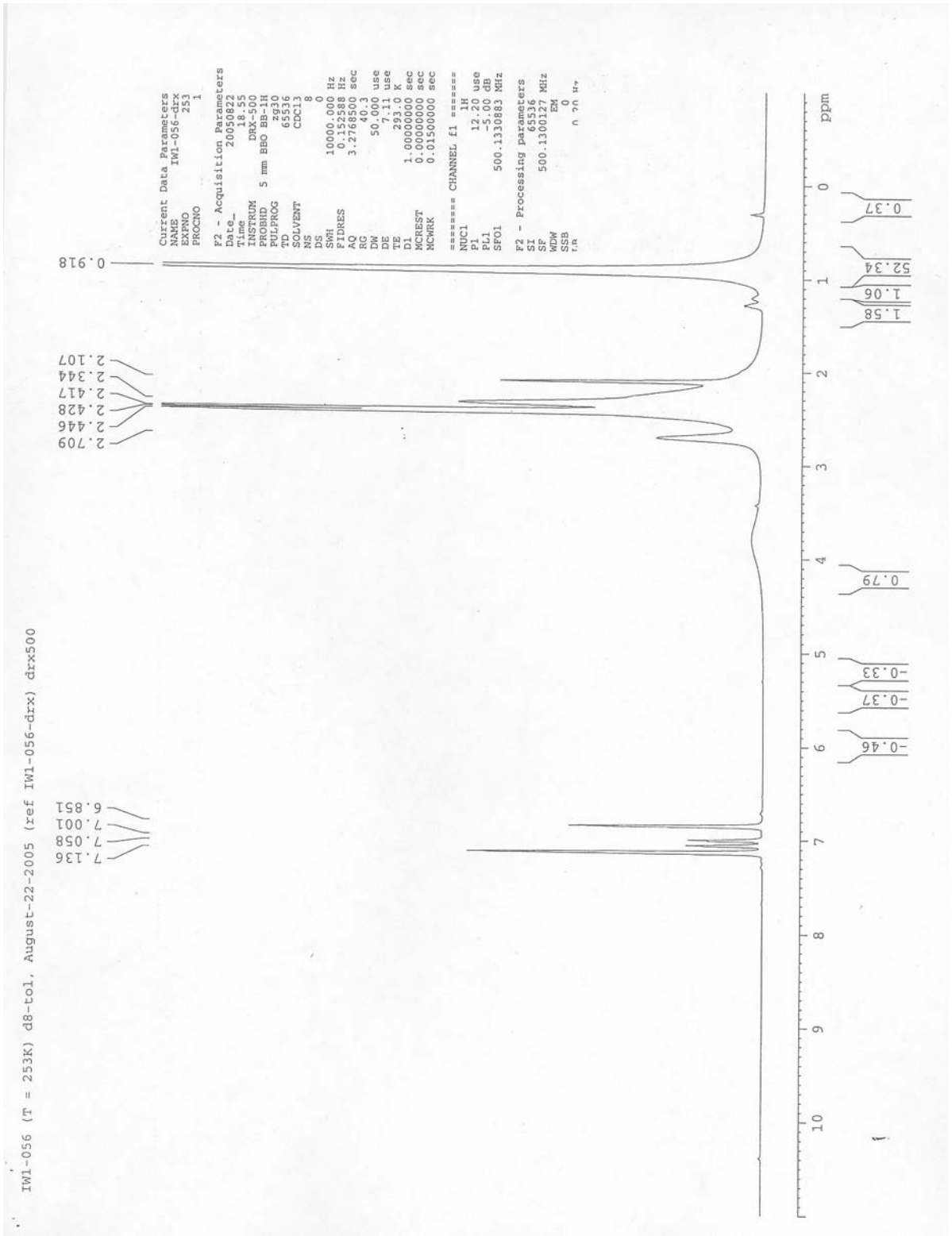

Figure 9. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 273 K).

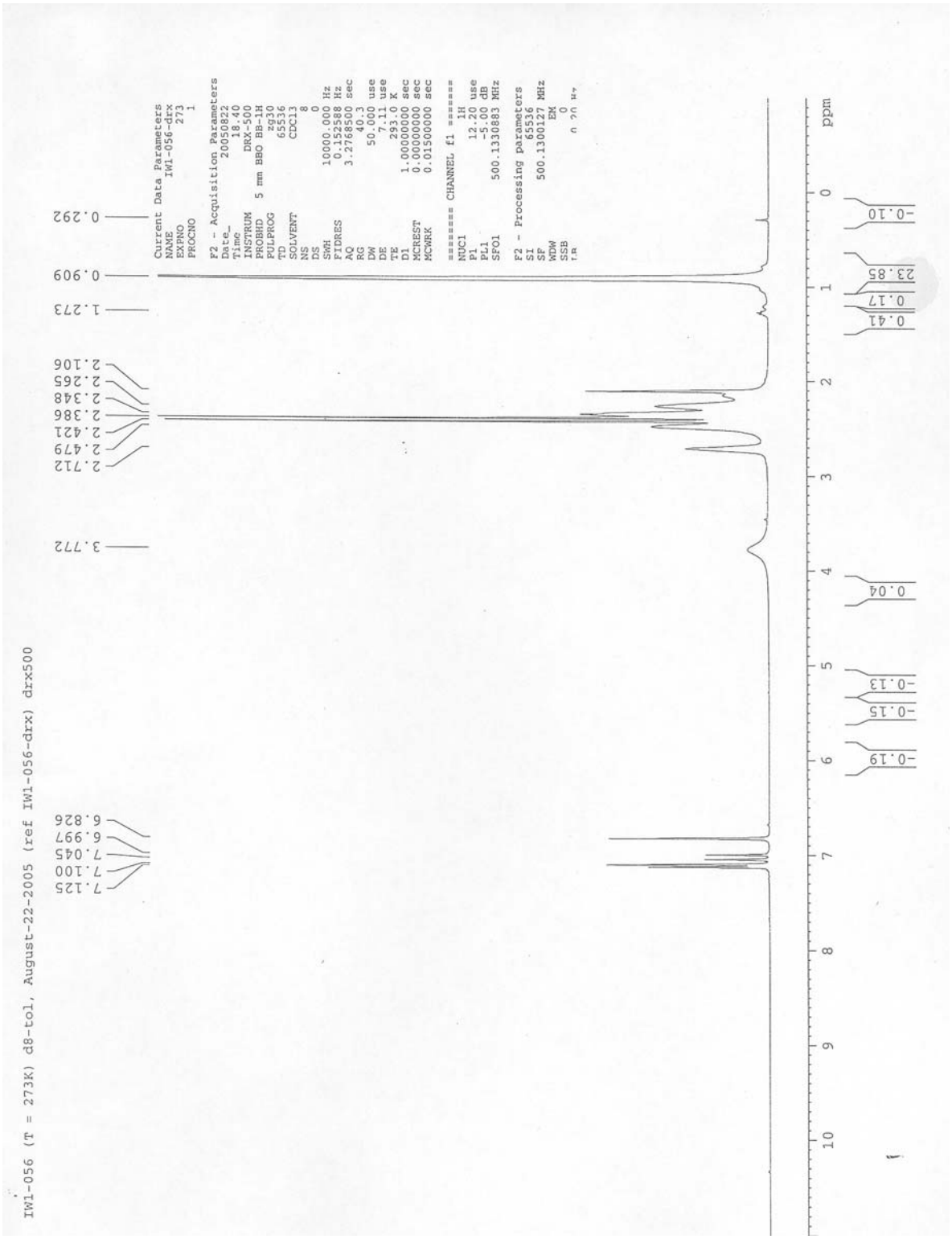

Figure 10. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 298 K).

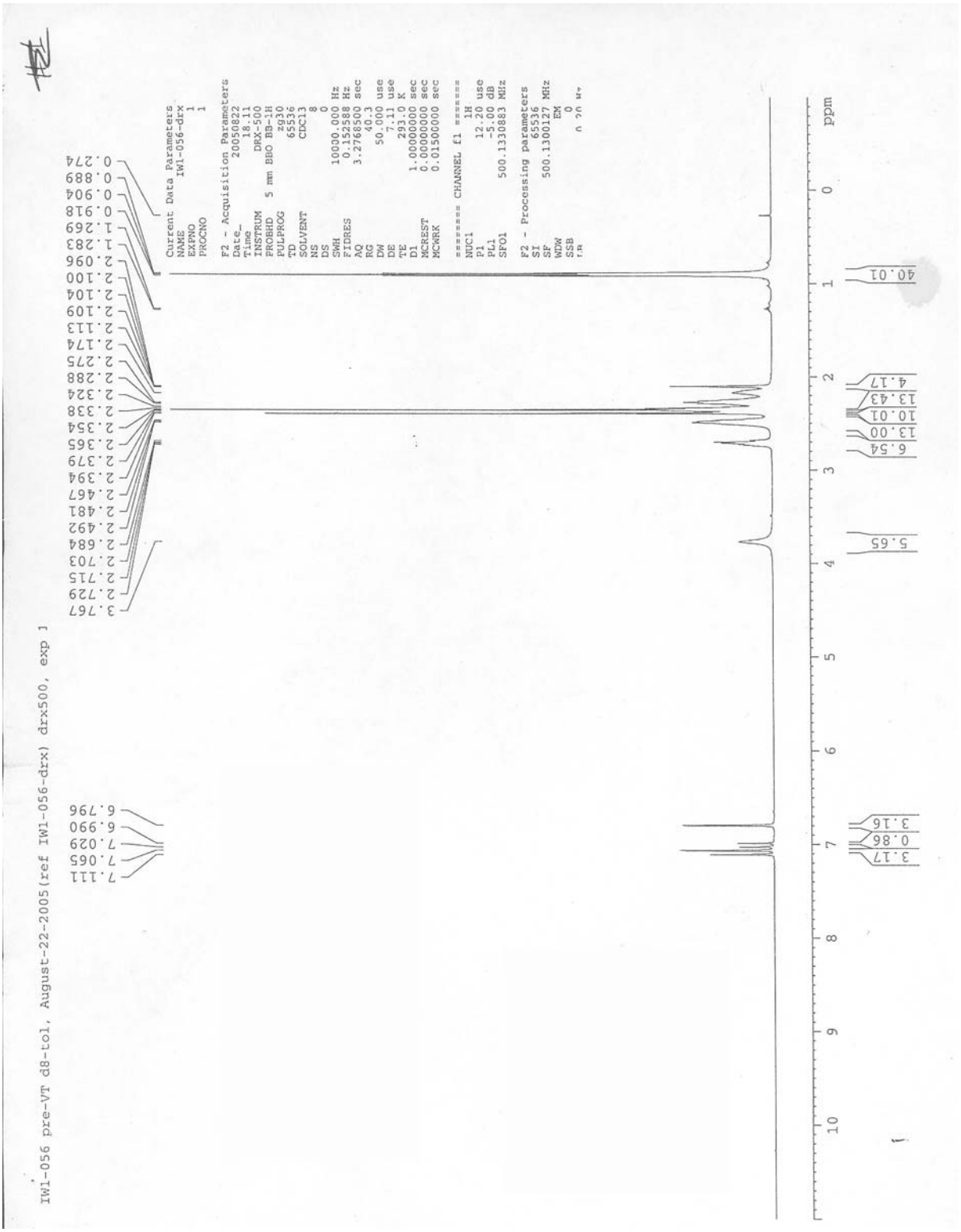

Figure 11. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 303 K).

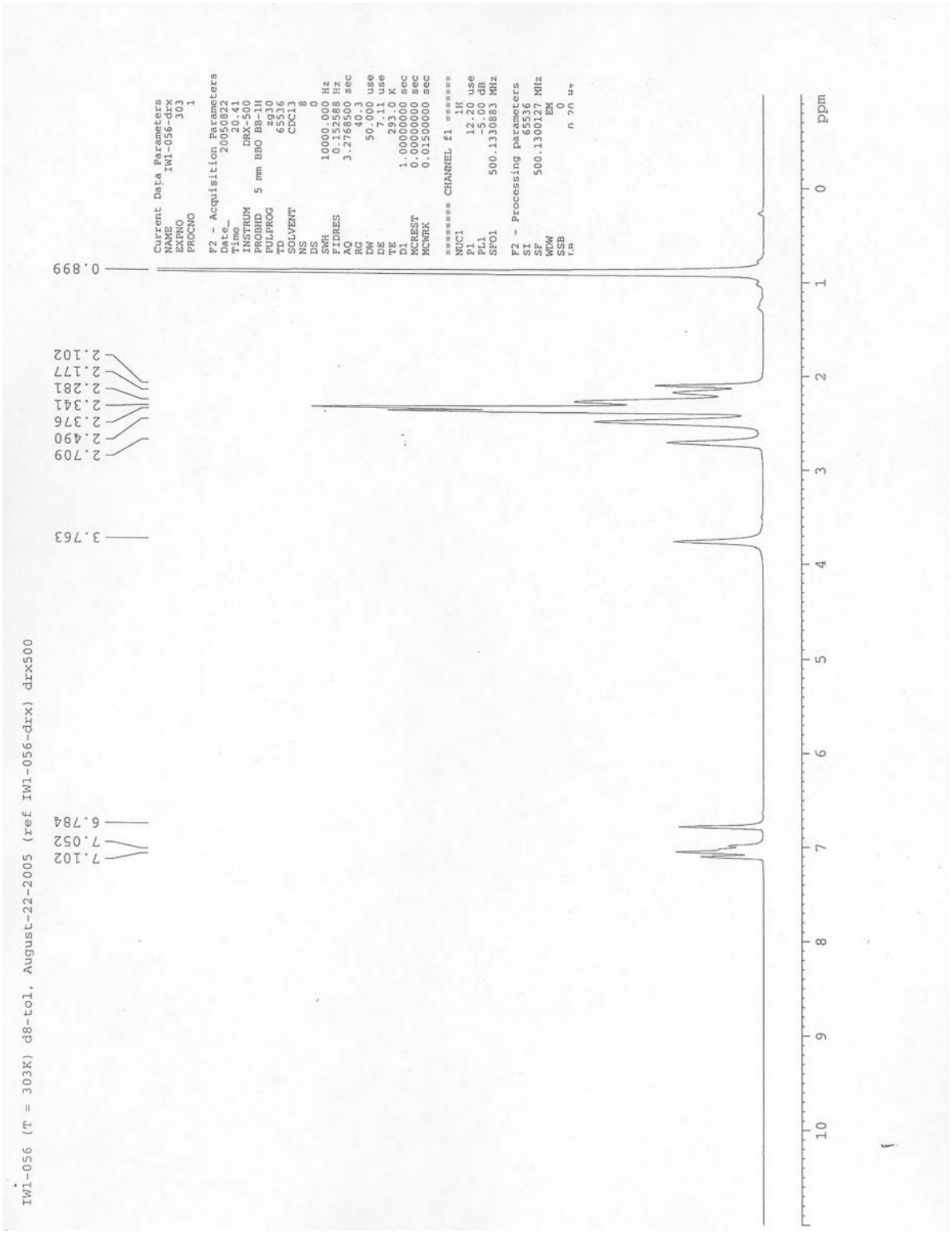

Figure 12. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 323 K).

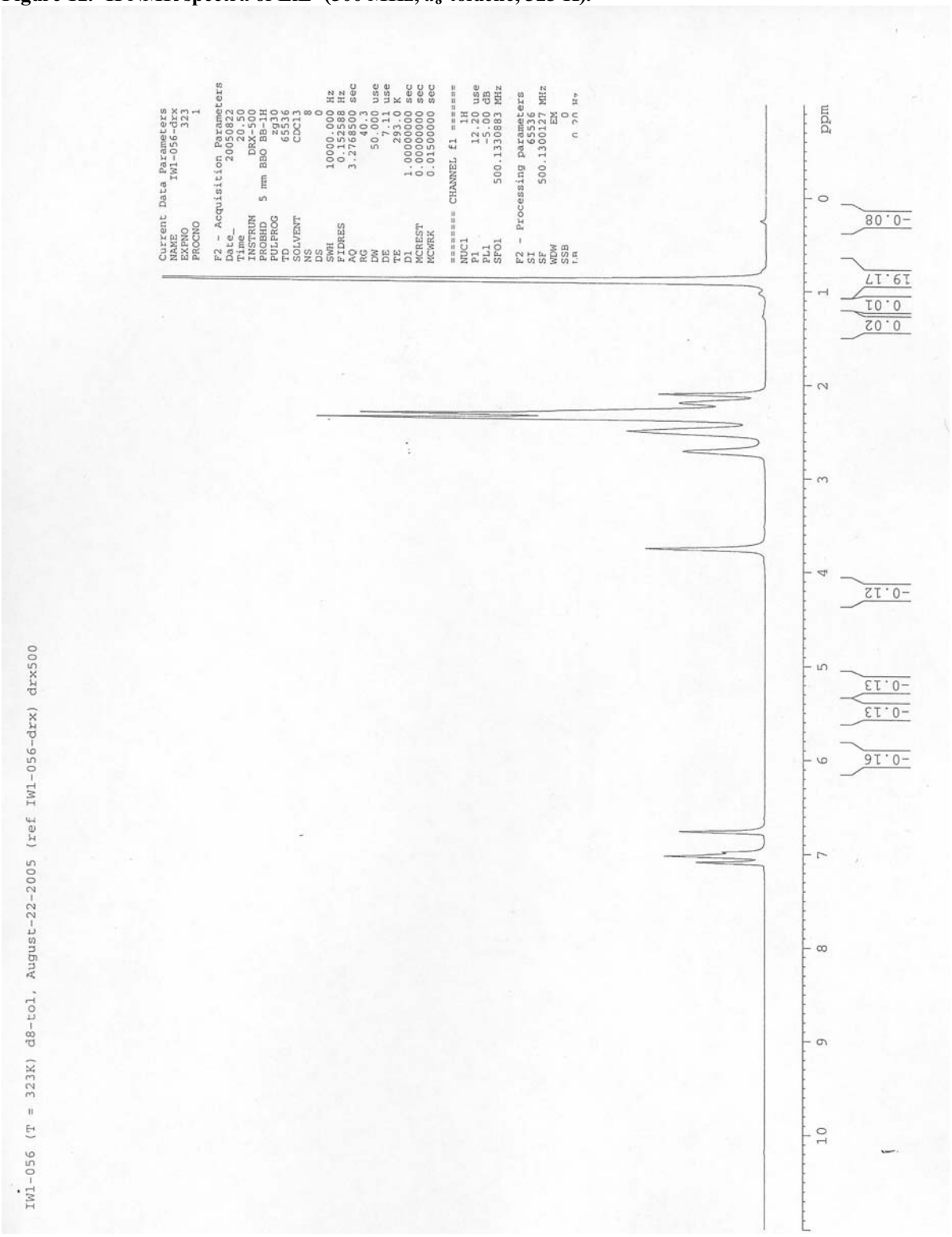

Figure 13. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 343 K).

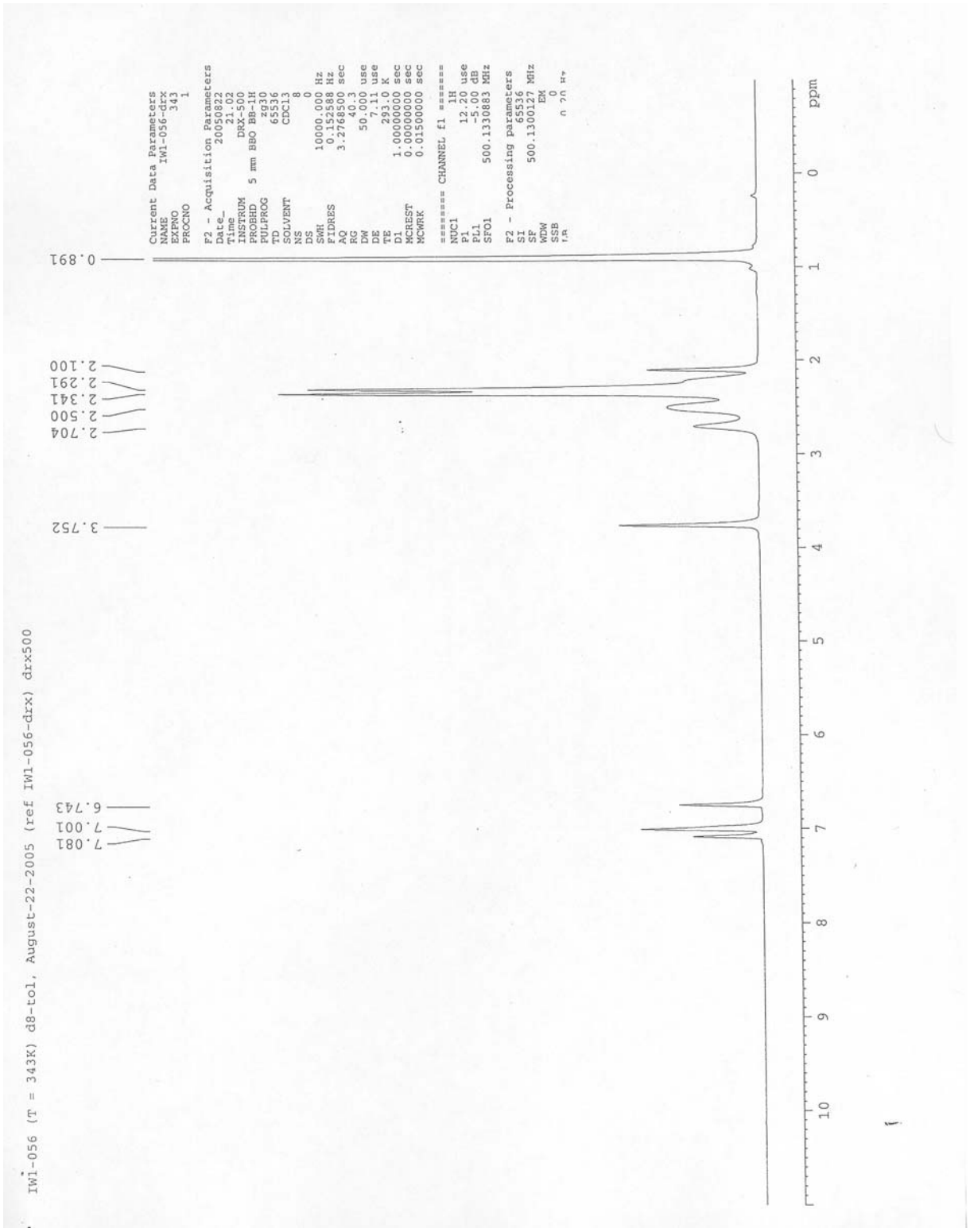

Figure 14. ^{1}H NMR spectra of LiL^{1} (500 MHz, d_8-toluene, 363 K).