Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

$Zn(OTf)_2$-Catalyzed Hydroamination of Ynamides with Aromatic Amines

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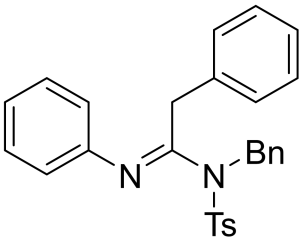
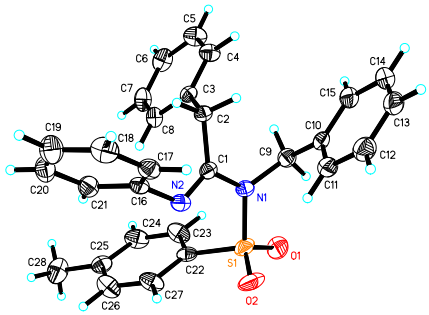
I. X-Ray Structure for compound 3 aa

ORTEP drawing of the X-ray crystallographic structure of 3aa





CCDC- 2052690. For detailed crystallographic data, please refer to the Cambridge Crystallographic Data Centre at http://ccdc.cam.ac.uk.

Table 1. Crystal data and structure refinement for **3aa**.

Identification code	**3aa**	
Empirical formula	C28 H26 N2 O2 S	
Formula weight	454.57	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.0012(8) Å	α = 90°.
	b = 22.074(2) Å	β = 90.349(3)°.
	c = 10.7284(10) Å	γ = 90°.
Volume	2368.4(4) $Å^3$	
Z	4	
Density (calculated)	1.275 Mg/m^3	
Absorption coefficient	0.165 mm^{-1}	
F(000)	960	
Crystal size	0.150 x 0.120 x 0.070 mm^3	

Theta range for data collection	2.748 to 25.497°.
Index ranges	-10<=h<=12, -26<=k<=26, -12<=l<=12
Reflections collected	22334
Independent reflections	4391 [R(int) = 0.0700]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6366
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4391 / 0 / 299
Goodness-of-fit on F^2	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0608, wR2 = 0.1143
R indices (all data)	R1 = 0.0994, wR2 = 0.1316
Extinction coefficient	n/a
Largest diff. peak and hole	0.203 and -0.405 e.Å^{-3}

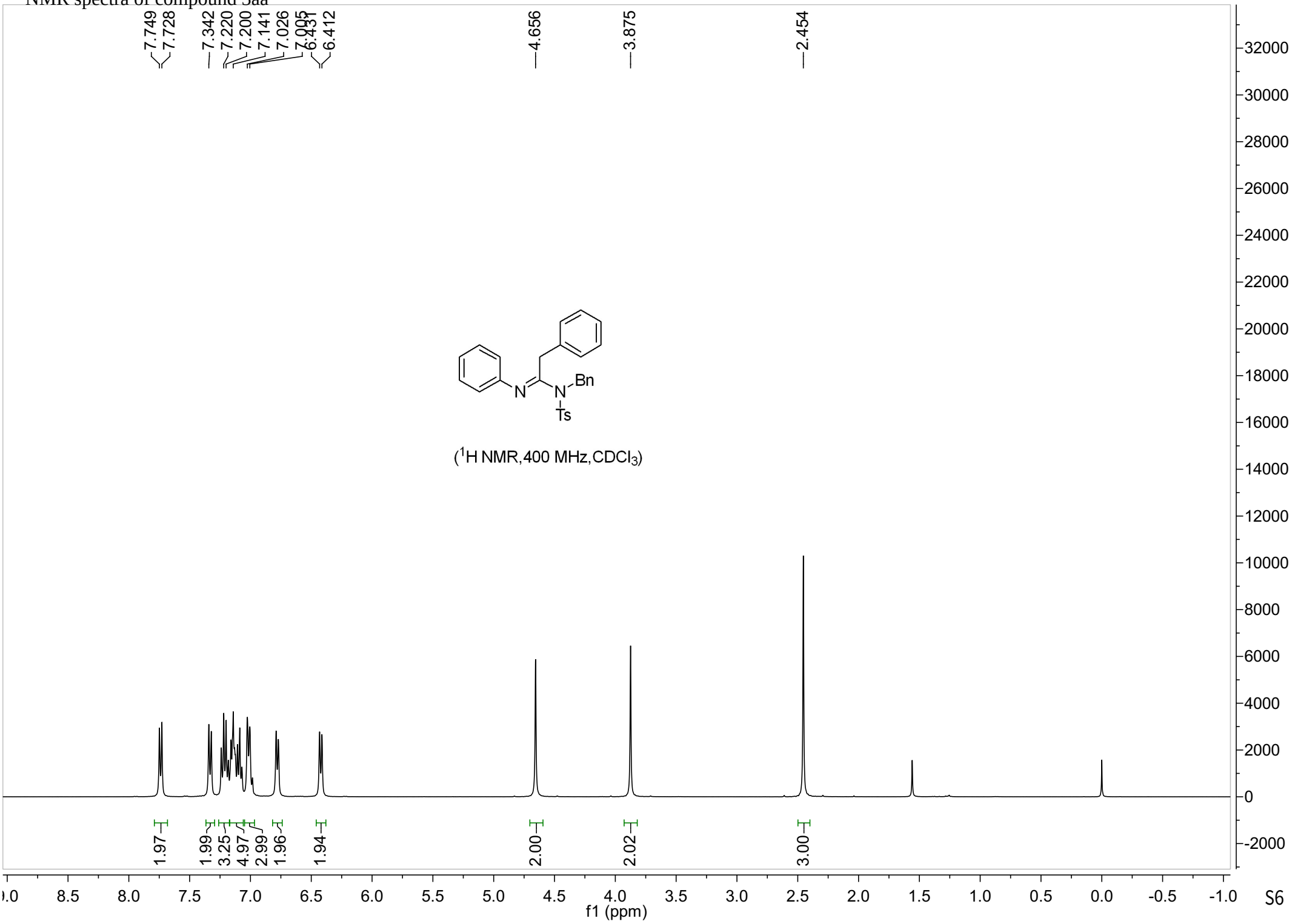
Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for mo_dd20113_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8100(1)	7058(1)	4279(1)	51(1)
O(1)	7489(3)	7597(1)	4769(2)	75(1)
O(2)	9393(2)	6888(1)	4727(2)	69(1)
N(1)	6984(2)	6508(1)	4528(2)	41(1)
N(2)	8289(2)	5804(1)	3514(2)	41(1)
C(1)	7160(3)	5931(1)	3982(3)	36(1)
C(2)	5928(3)	5537(1)	3962(3)	34(1)
C(3)	4779(3)	5804(1)	3208(3)	34(1)
C(4)	3478(3)	5761(1)	3637(3)	46(1)
C(5)	2421(3)	5975(2)	2925(3)	56(1)
C(6)	2666(3)	6248(2)	1797(3)	57(1)
C(7)	3950(4)	6308(2)	1373(3)	53(1)
C(8)	5003(3)	6081(1)	2069(3)	44(1)
C(9)	5931(3)	6607(1)	5469(3)	45(1)
C(10)	6063(3)	6215(1)	6608(3)	42(1)
C(11)	7270(3)	5974(1)	7001(3)	49(1)
C(12)	7334(4)	5626(2)	8076(3)	64(1)
C(13)	6196(4)	5511(2)	8747(3)	67(1)

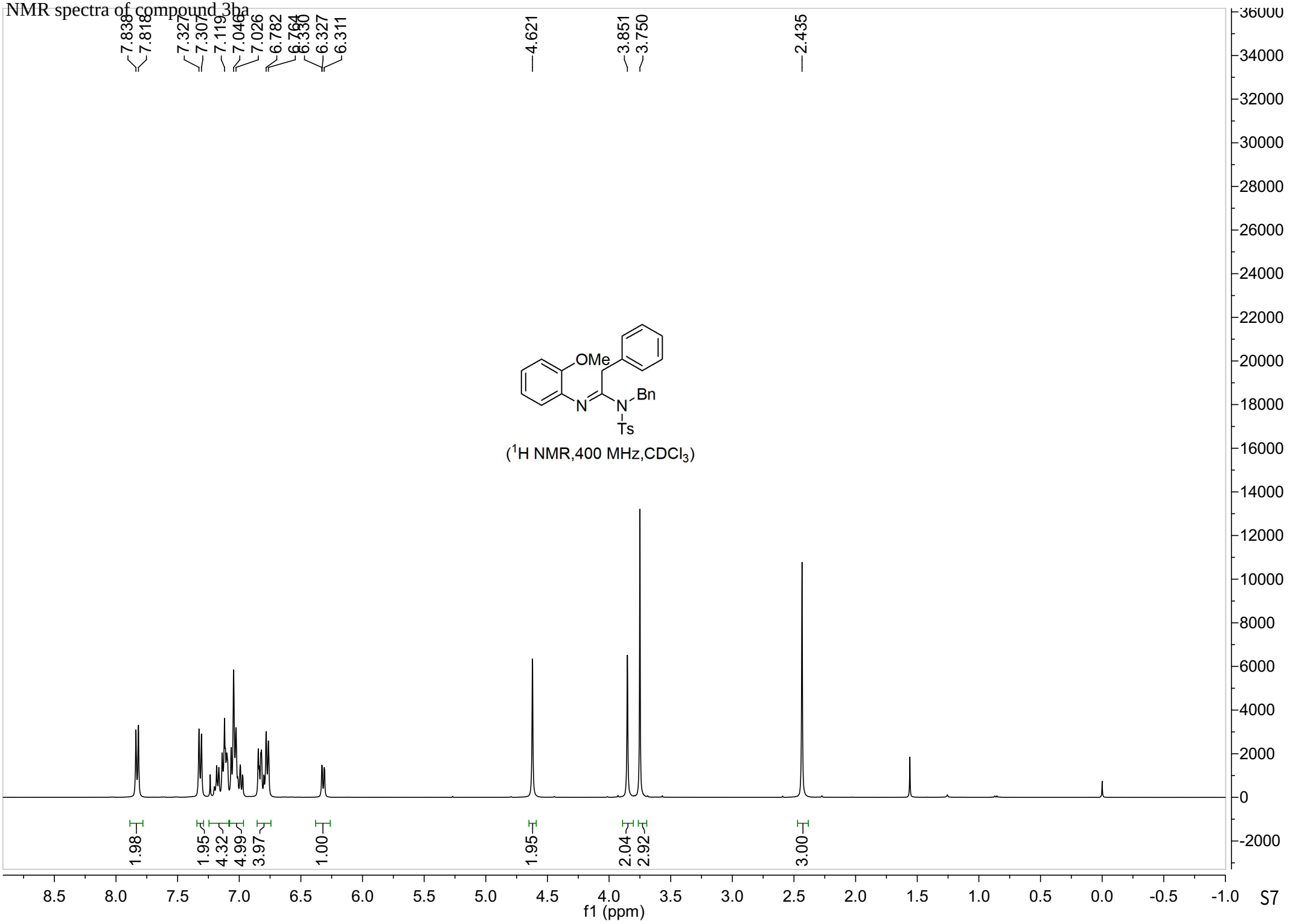
C(14)	4997(4)	5742(2)	8368(3)	68(1)
C(15)	4926(3)	6094(2)	7292(3)	55(1)
C(16)	8494(3)	5239(1)	2933(3)	37(1)
C(17)	8778(3)	4729(1)	3649(3)	45(1)
C(18)	8981(3)	4171(2)	3075(4)	60(1)
C(19)	8915(4)	4123(2)	1797(4)	70(1)
C(20)	8689(3)	4631(2)	1088(3)	62(1)
C(21)	8482(3)	5189(2)	1651(3)	49(1)
C(22)	8149(3)	7123(1)	2654(3)	40(1)
C(23)	7080(3)	7395(2)	2048(4)	59(1)
C(24)	7116(3)	7457(2)	769(4)	61(1)
C(25)	8175(3)	7256(1)	82(3)	49(1)
C(26)	9226(3)	6993(2)	716(4)	60(1)
C(27)	9223(3)	6922(1)	1991(3)	54(1)
C(28)	8213(4)	7340(2)	-1317(3)	75(1)

II. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectrum

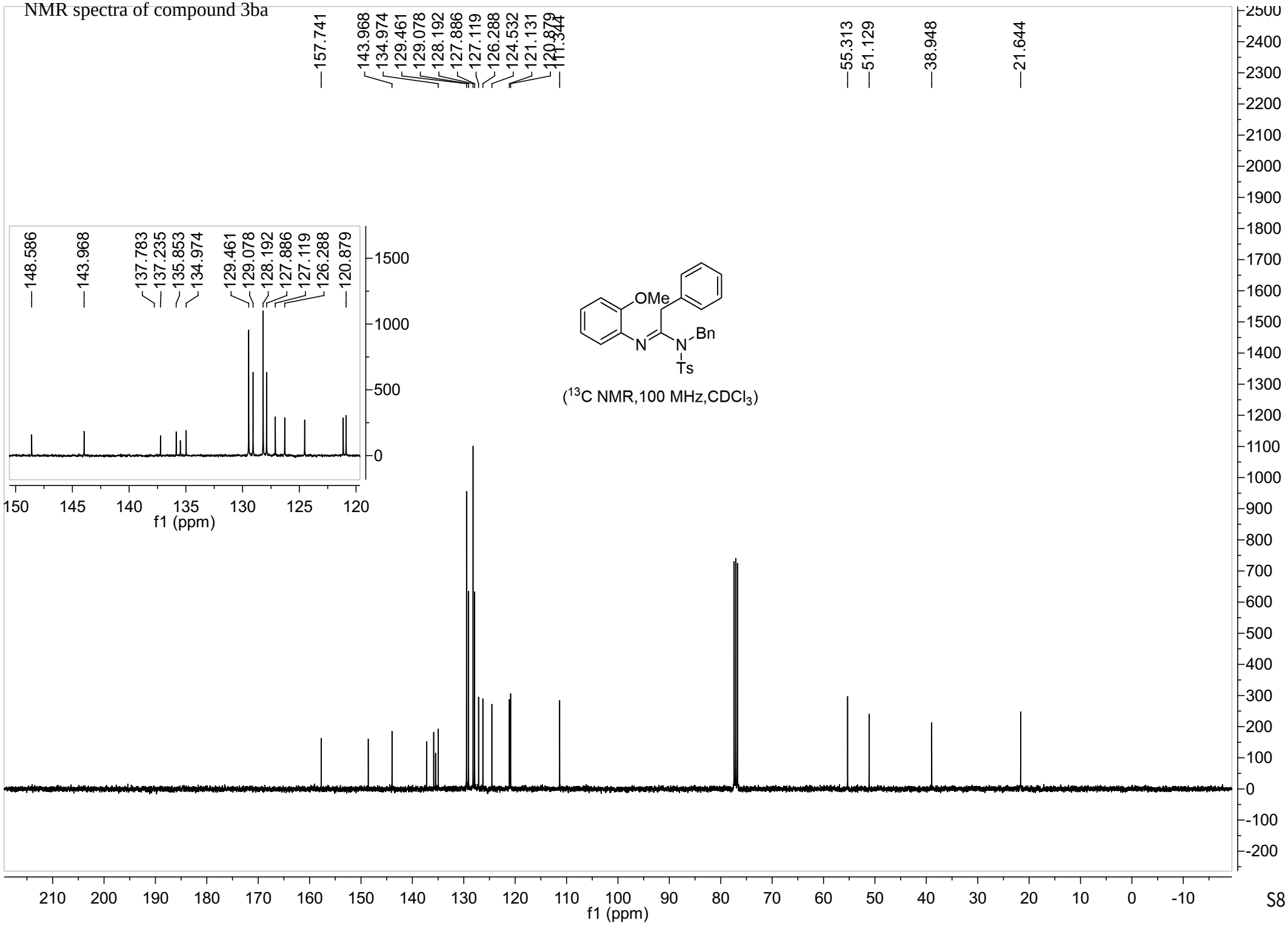
NMR spectra of compound 3aa



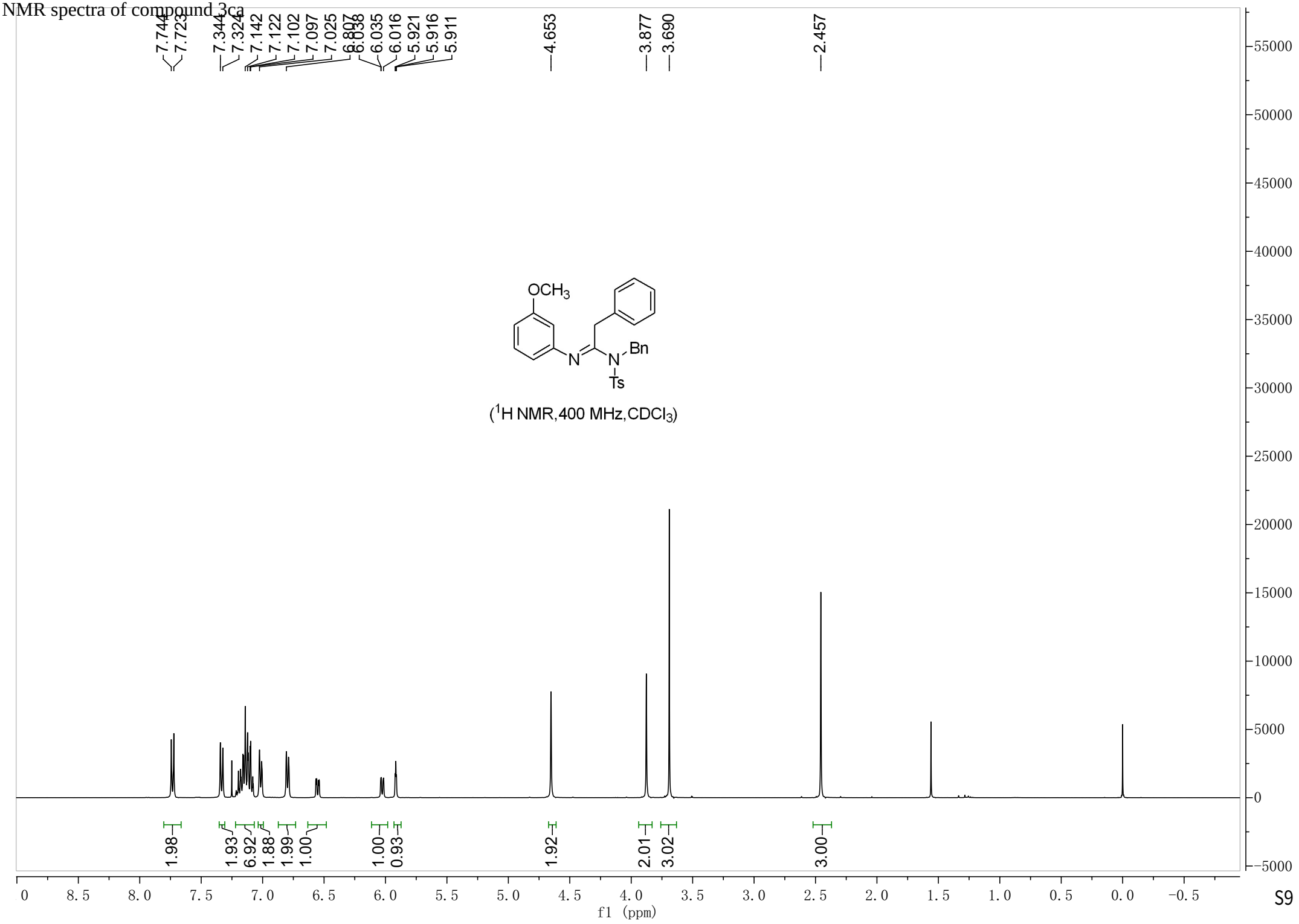
NMR spectra of compound 3ba



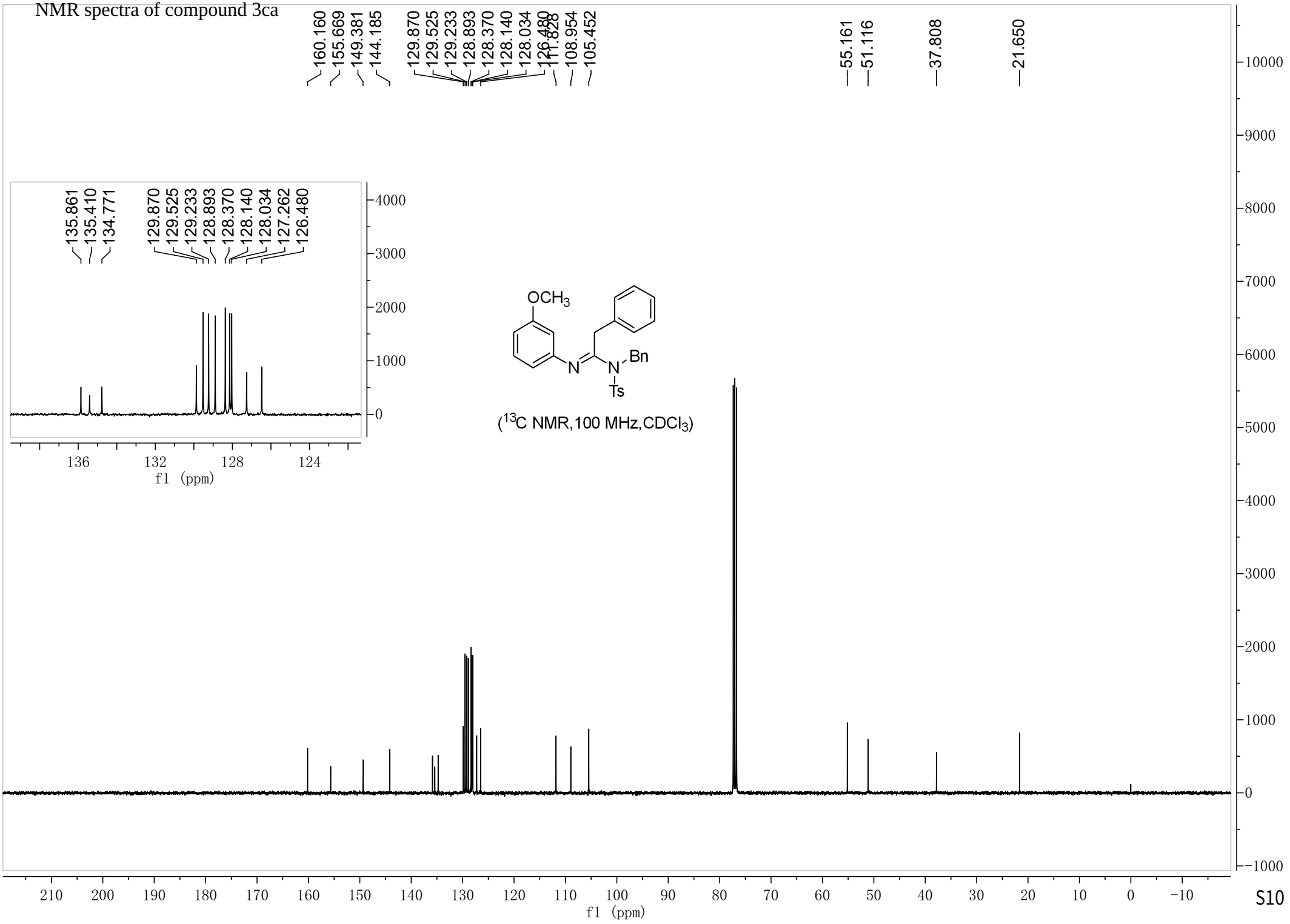
NMR spectra of compound 3ba



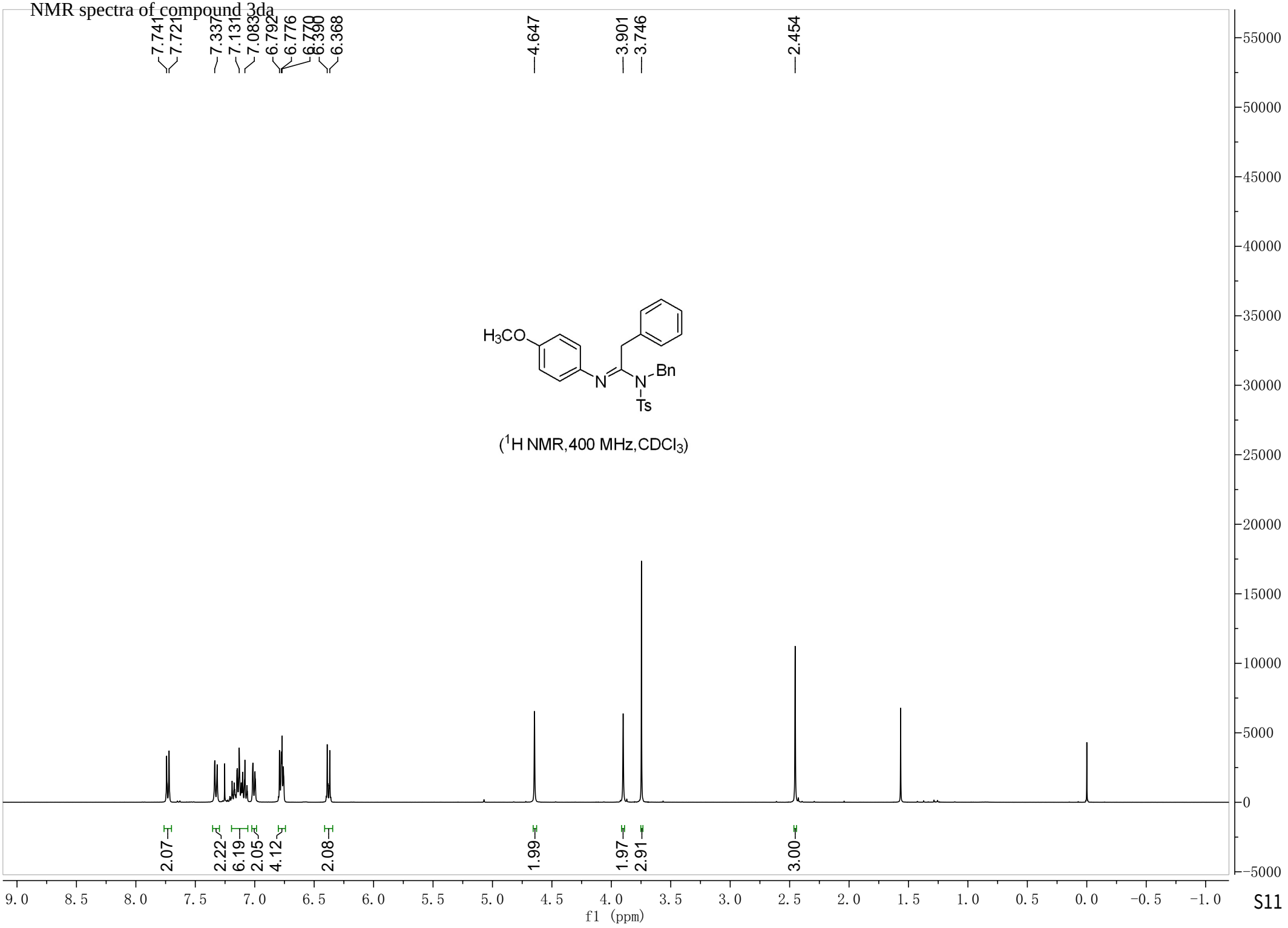
NMR spectra of compound 3ca



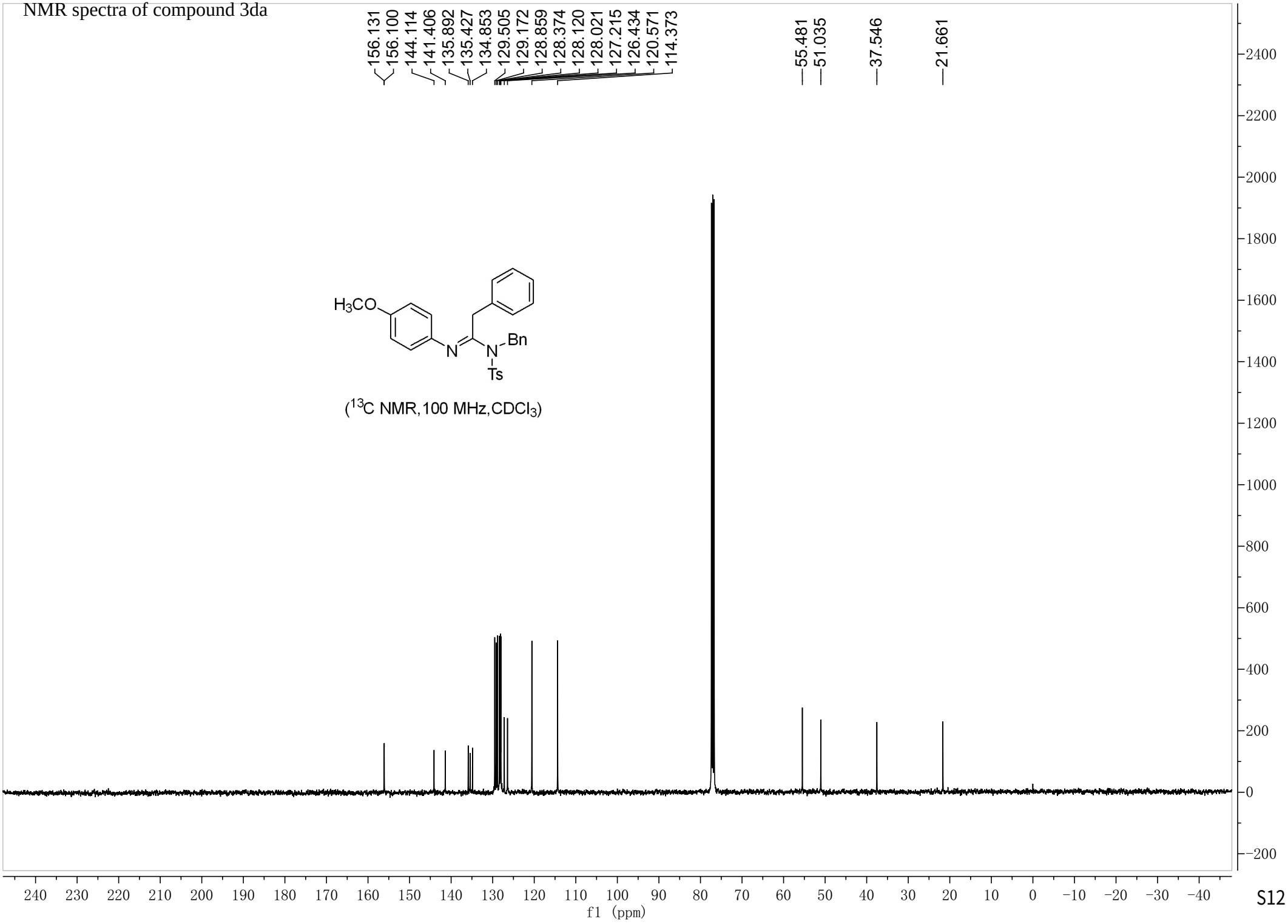
NMR spectra of compound 3ca



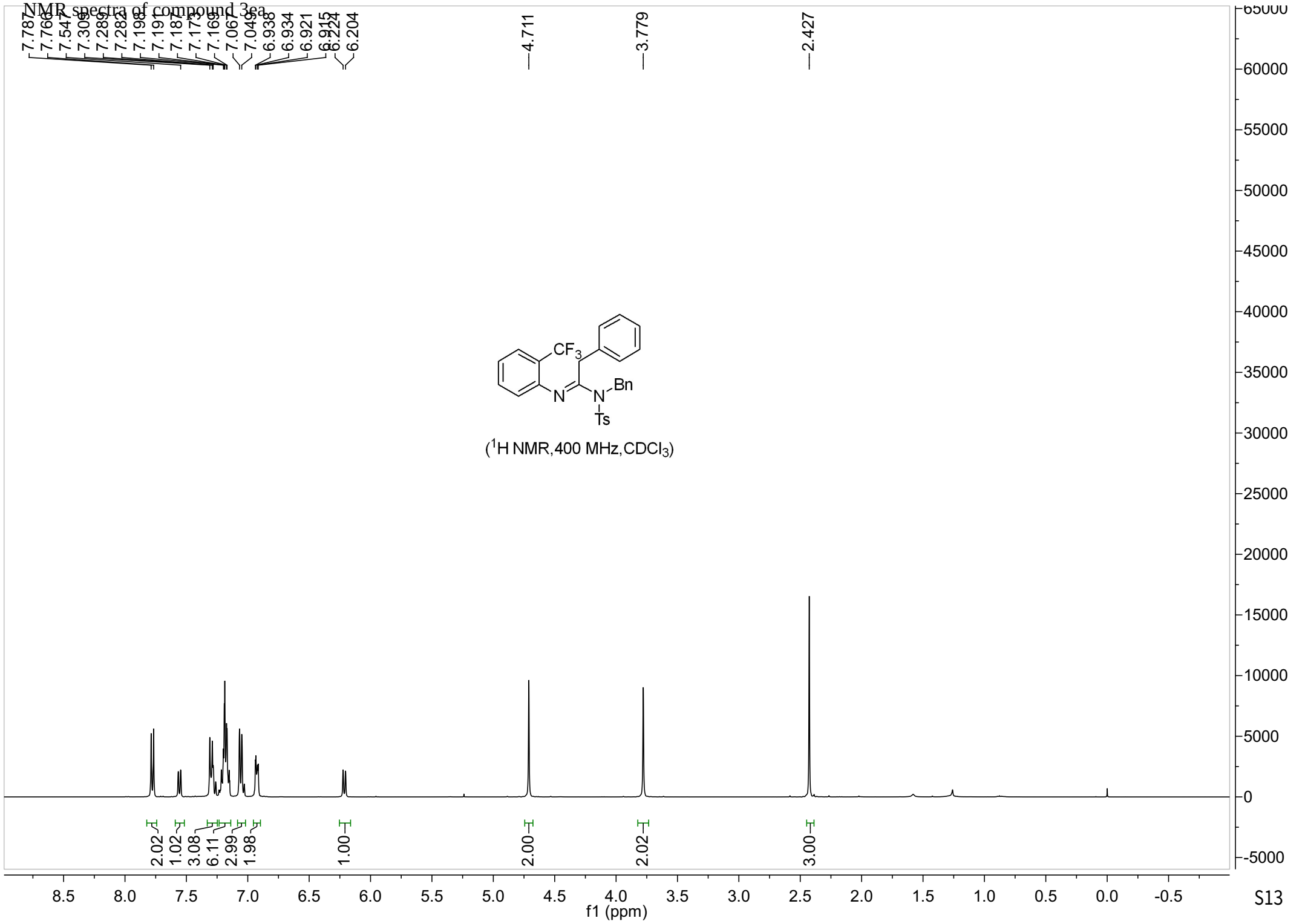
NMR spectra of compound 3da



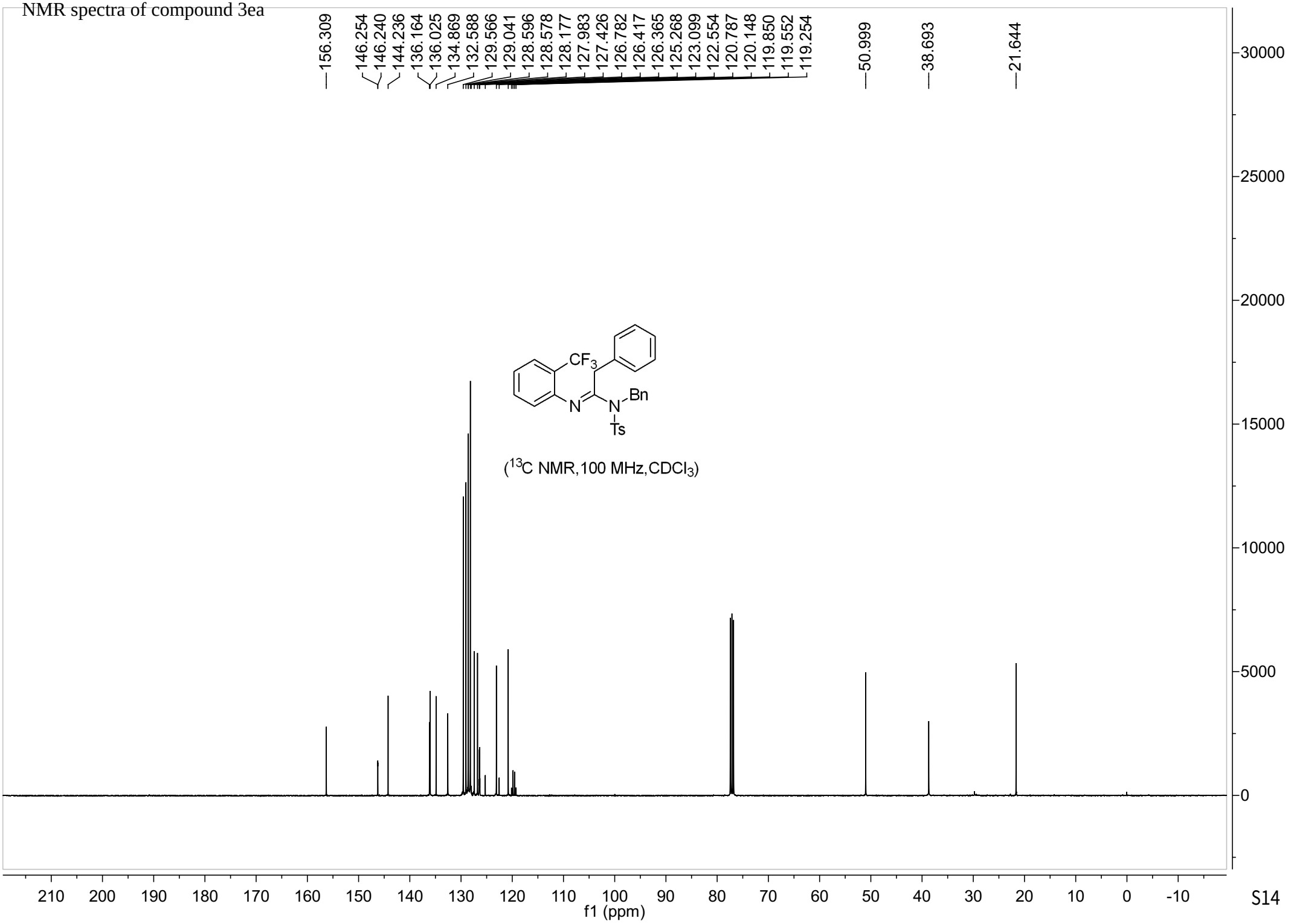
NMR spectra of compound 3da



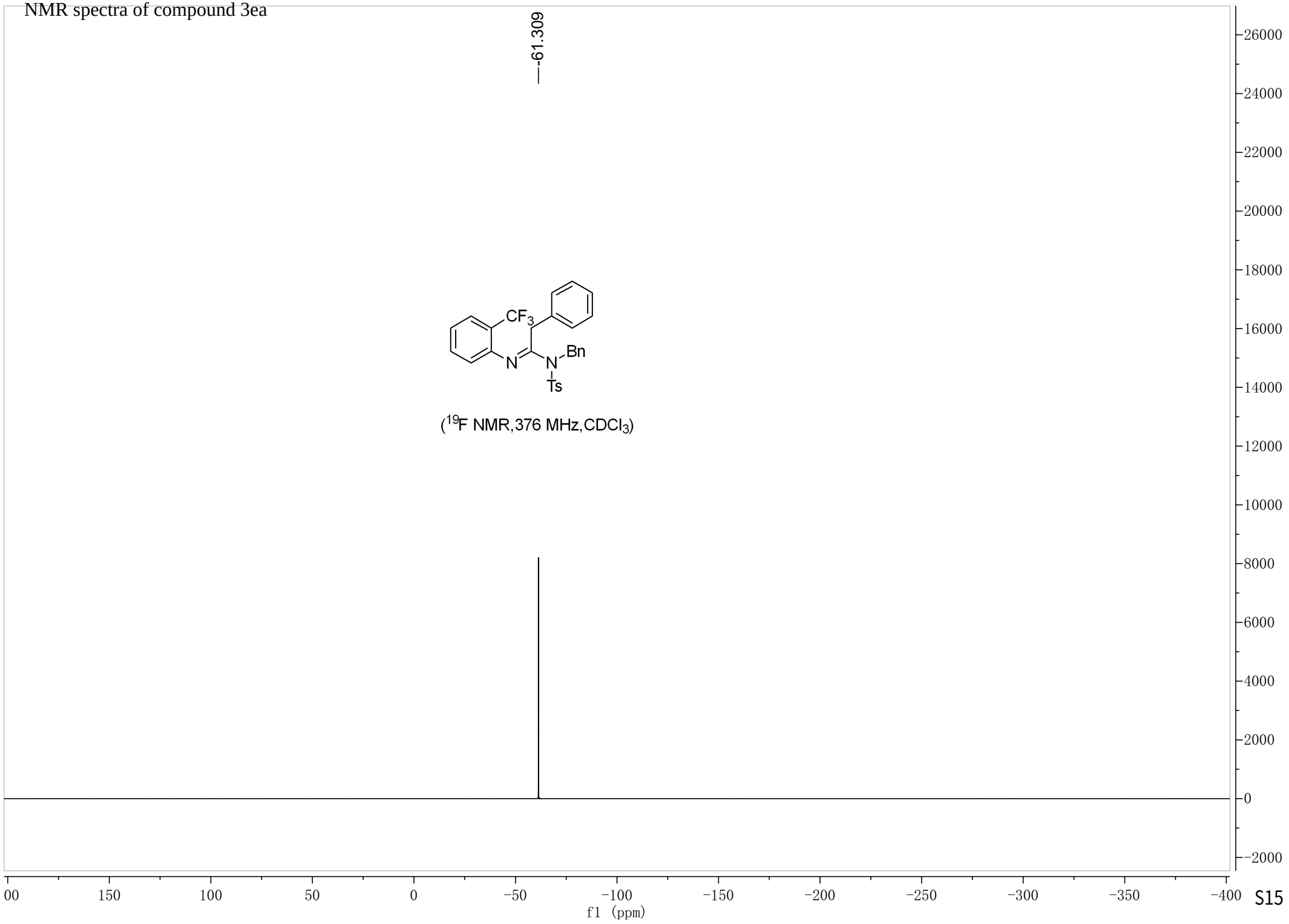
NMR spectra of compound 3ea



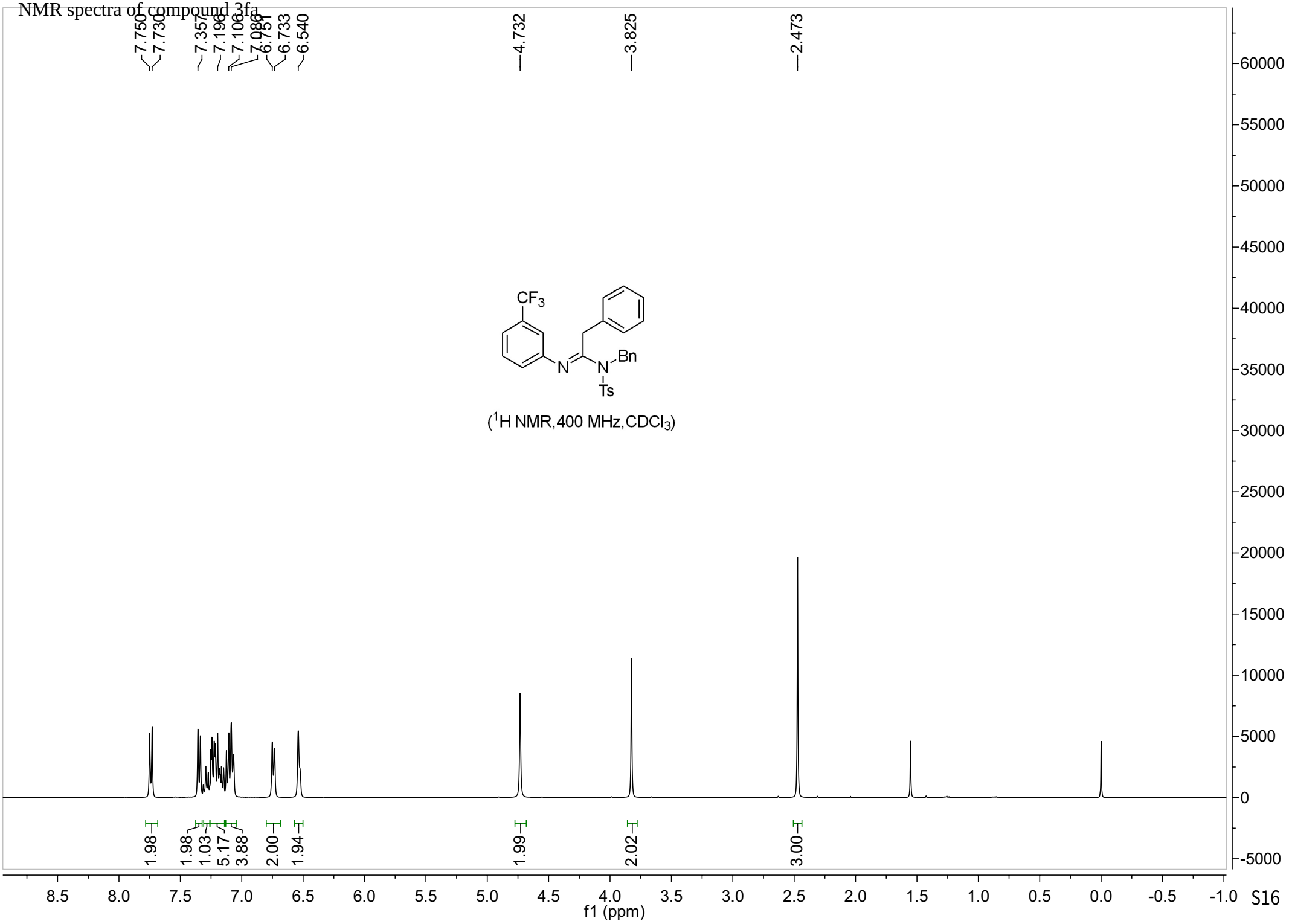
NMR spectra of compound 3ea



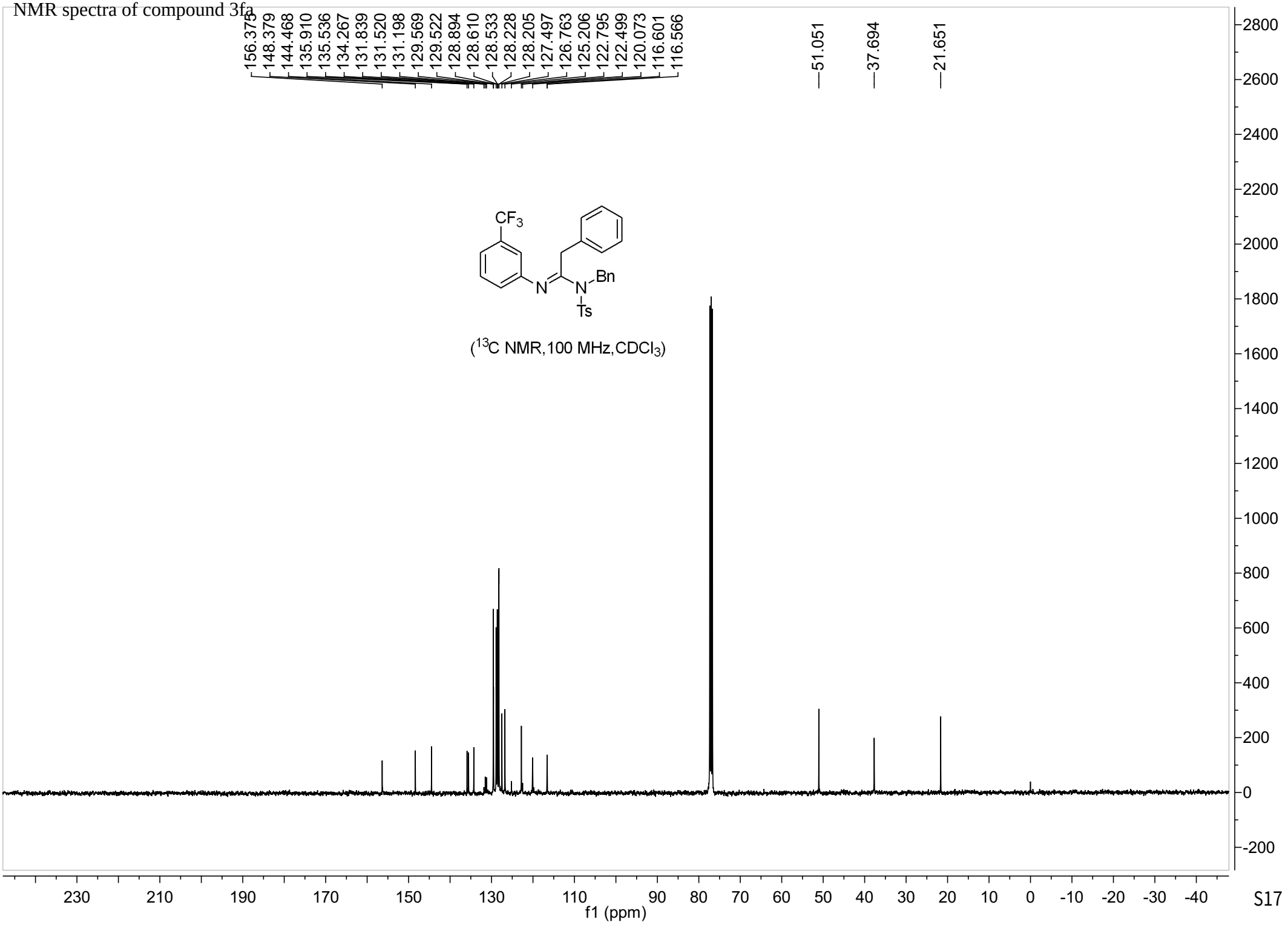
NMR spectra of compound 3ea



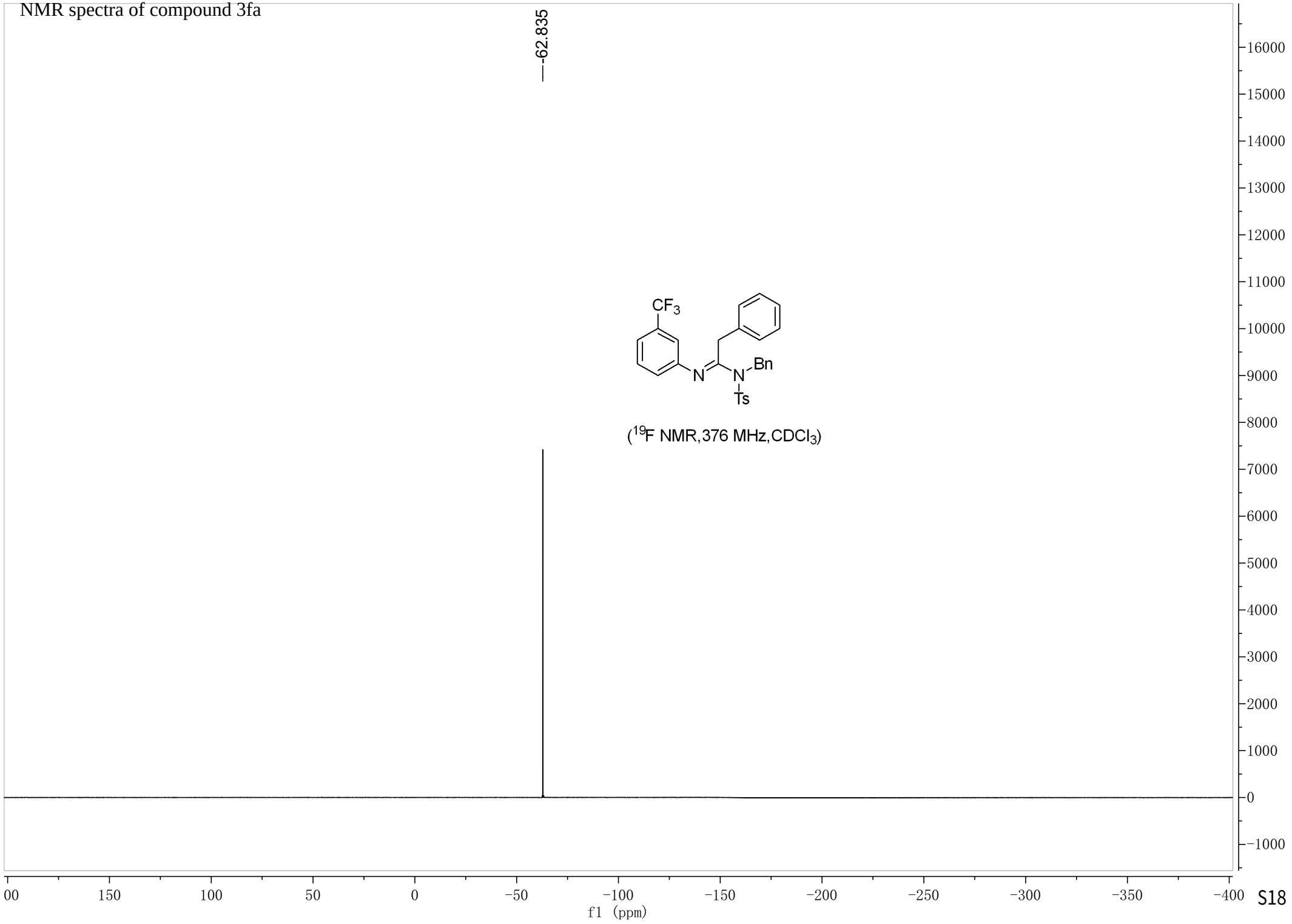
NMR spectra of compound 3fa



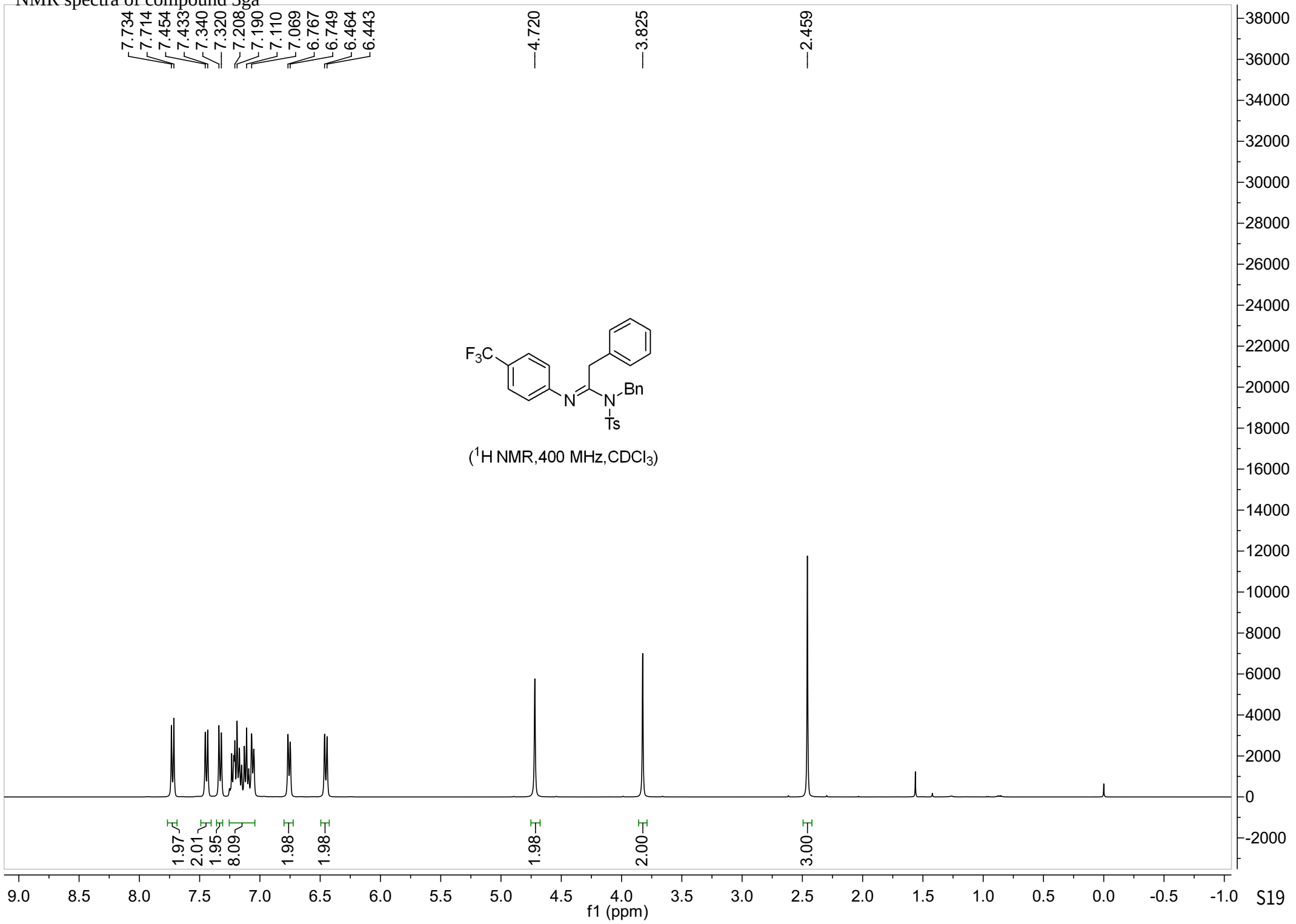
NMR spectra of compound 3fa



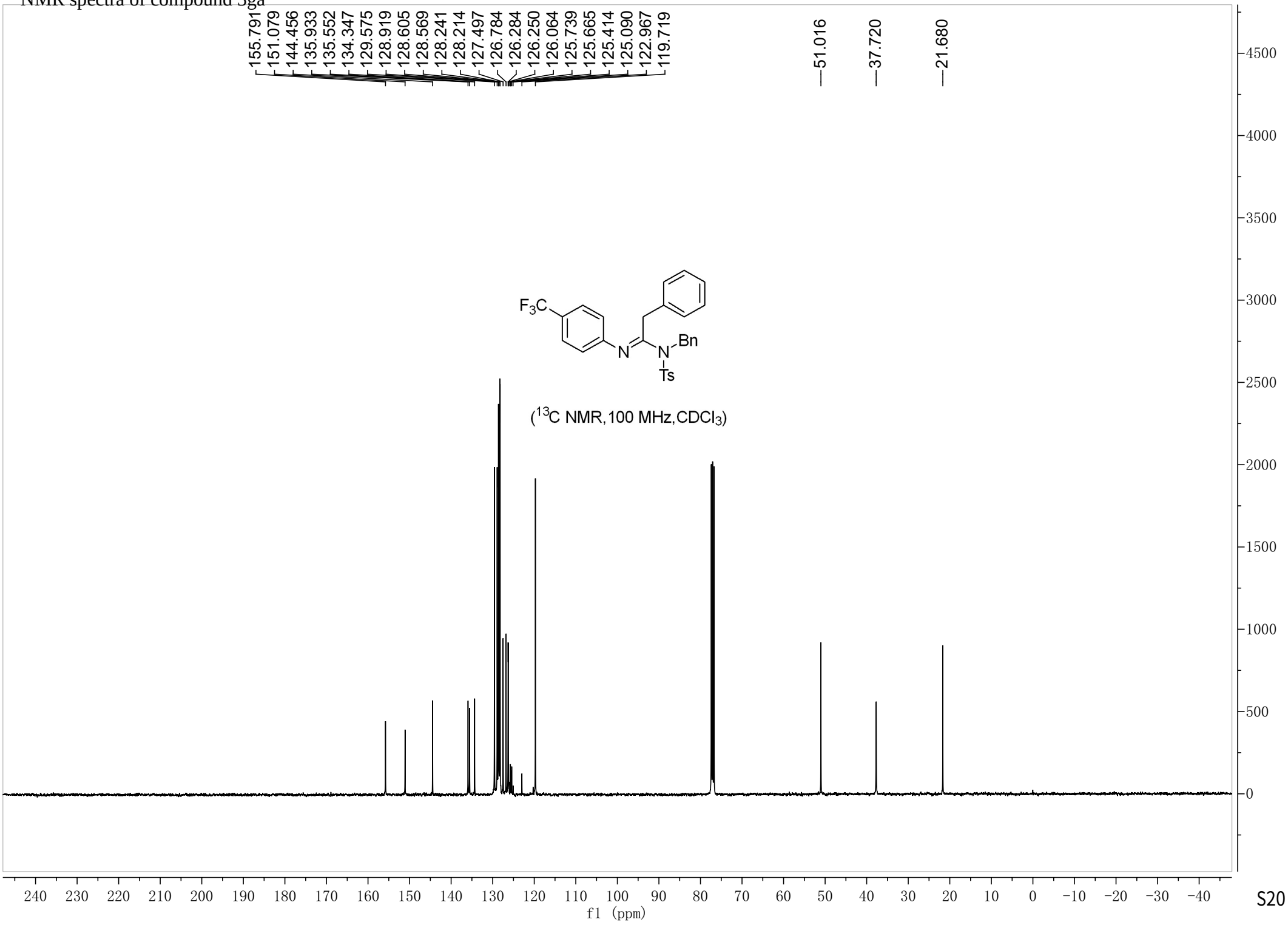
NMR spectra of compound 3fa



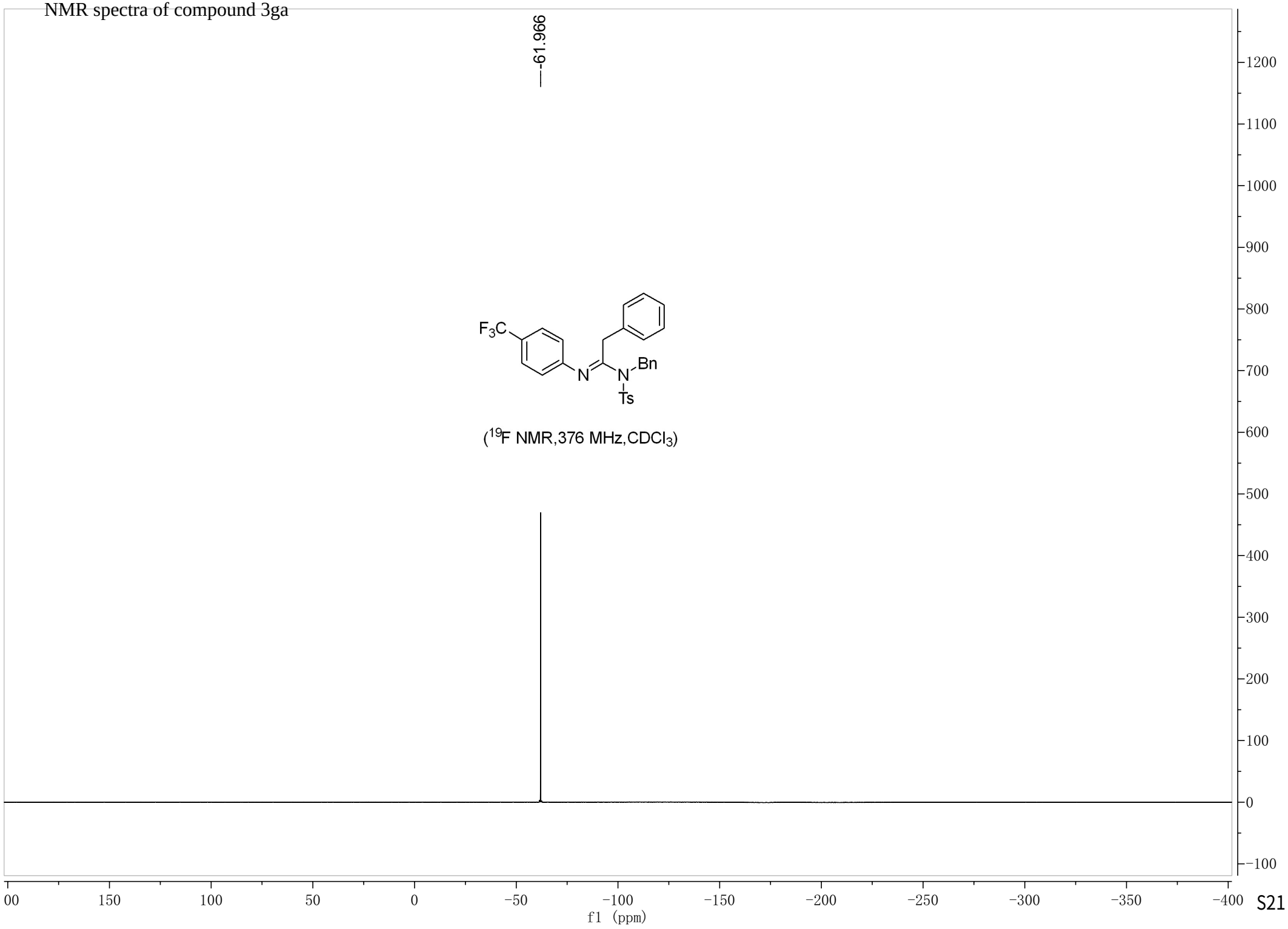
NMR spectra of compound 3ga



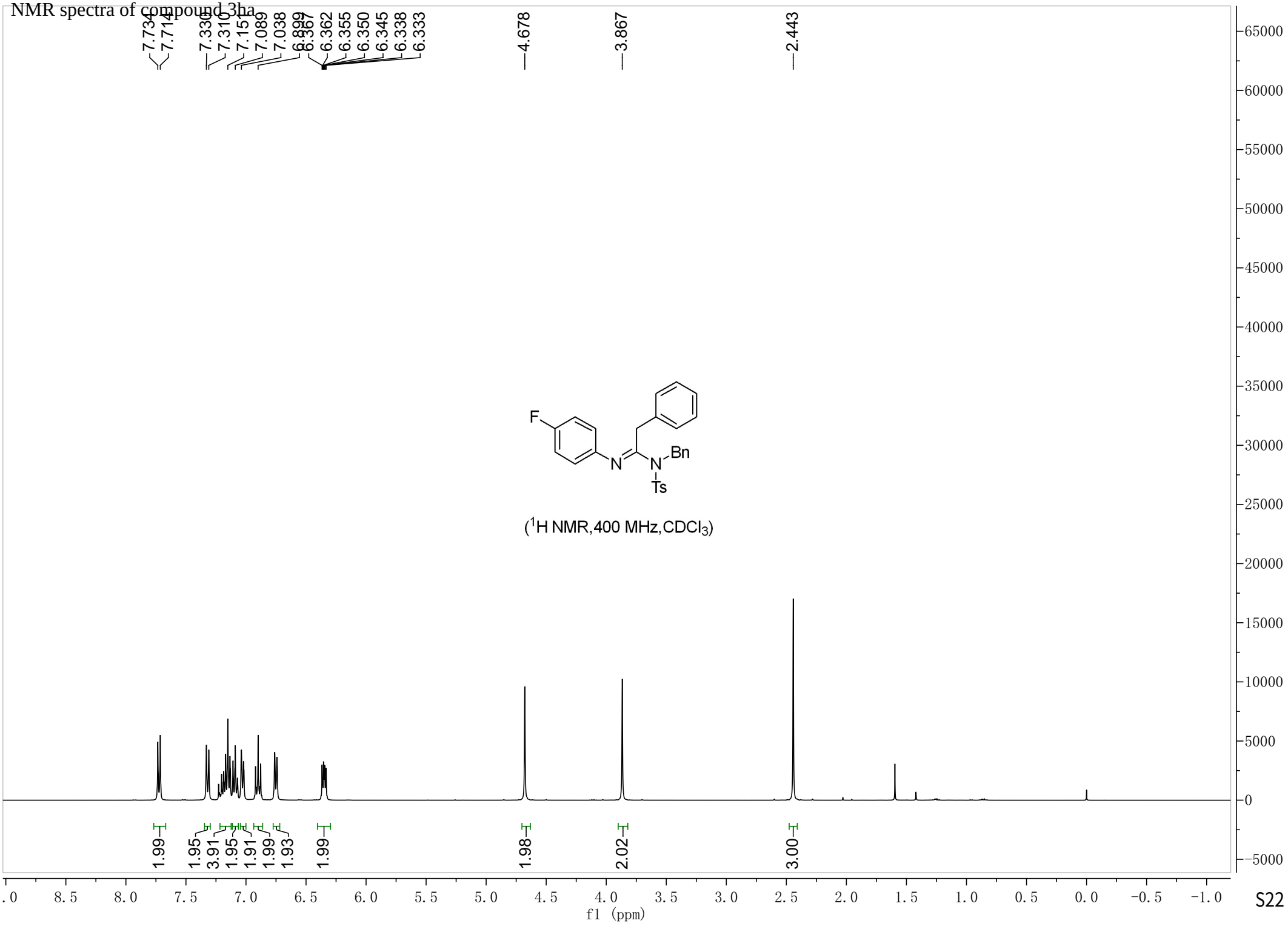
NMR spectra of compound 3ga



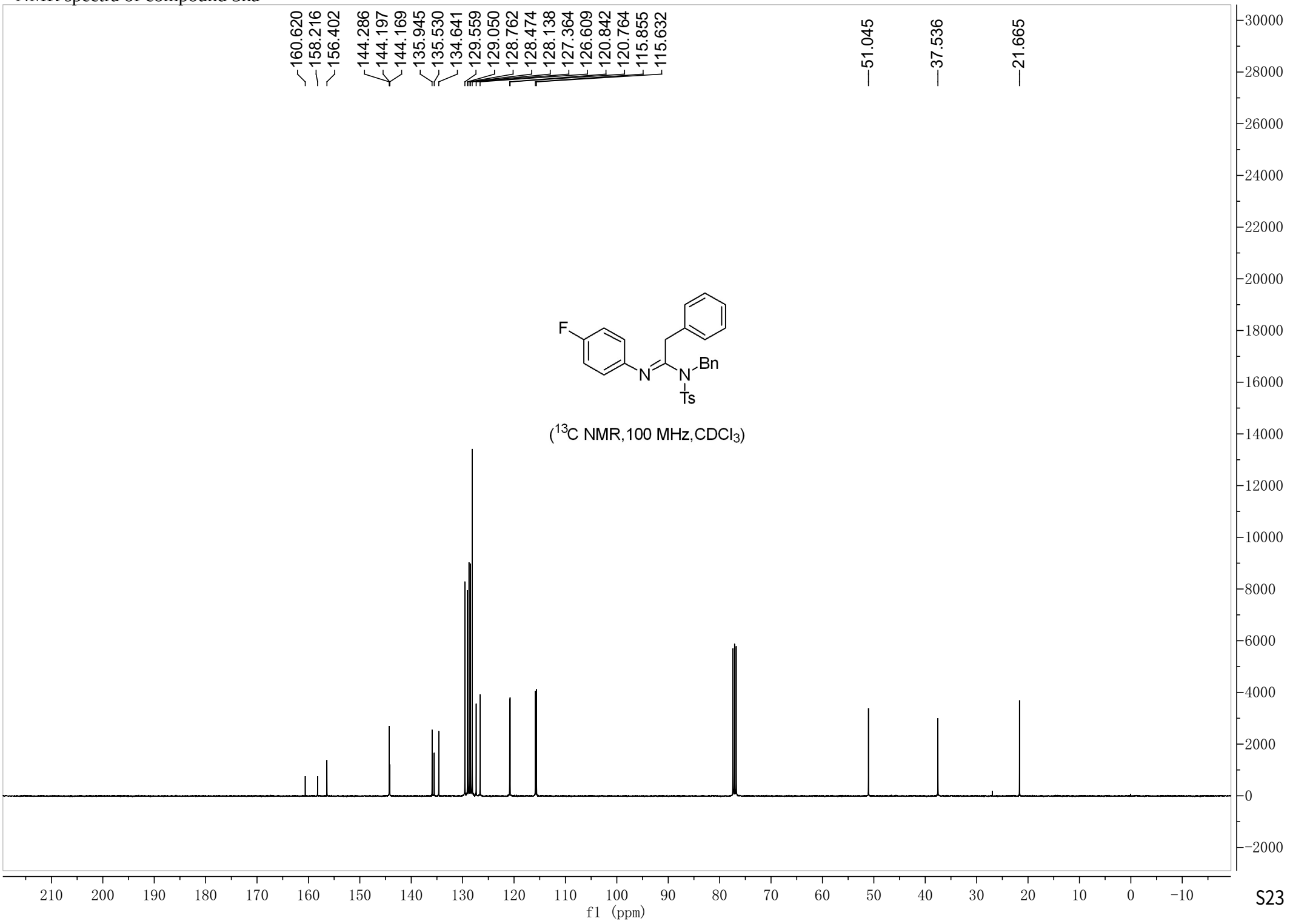
NMR spectra of compound 3ga



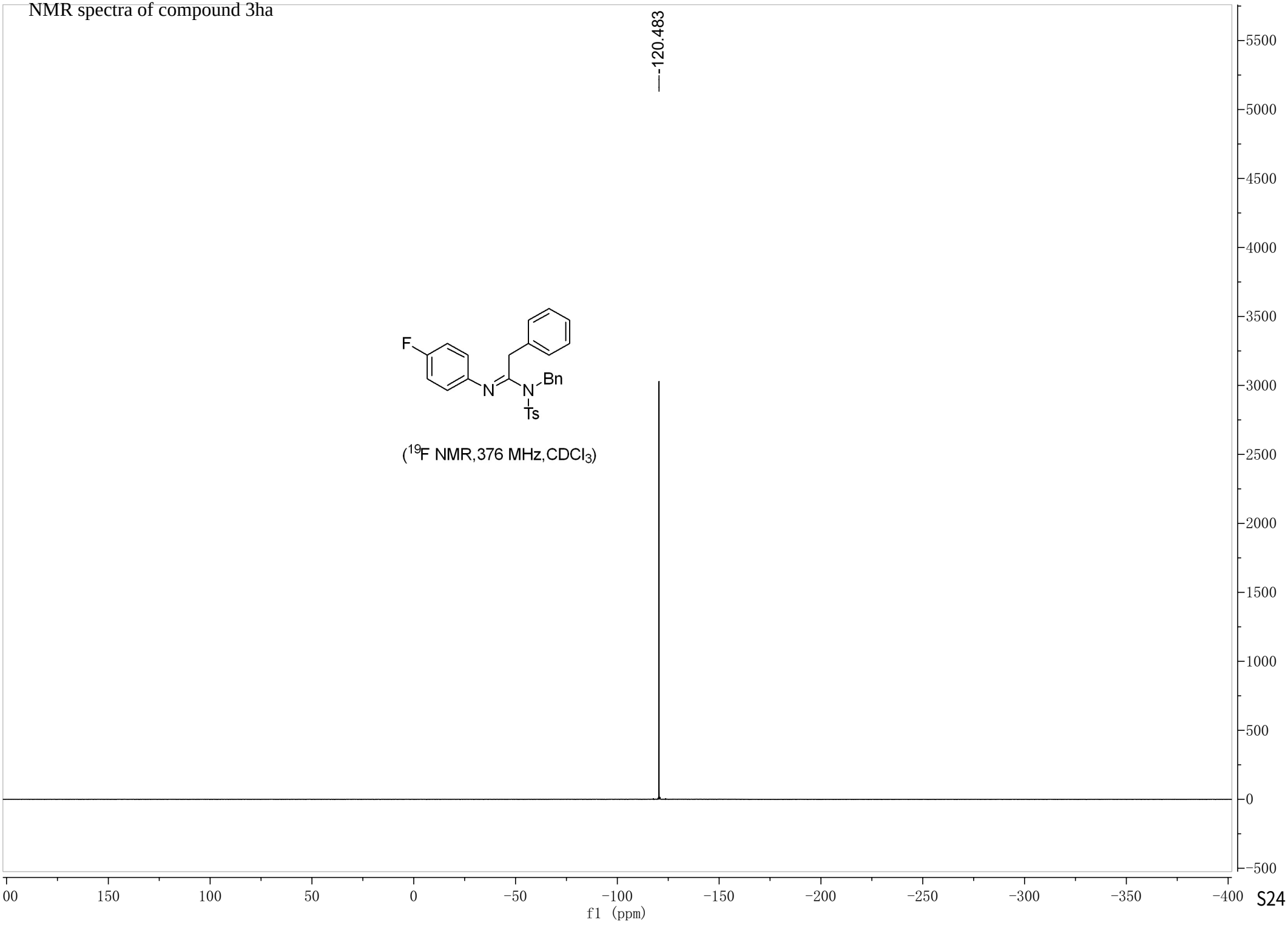
NMR spectra of compound 3ha



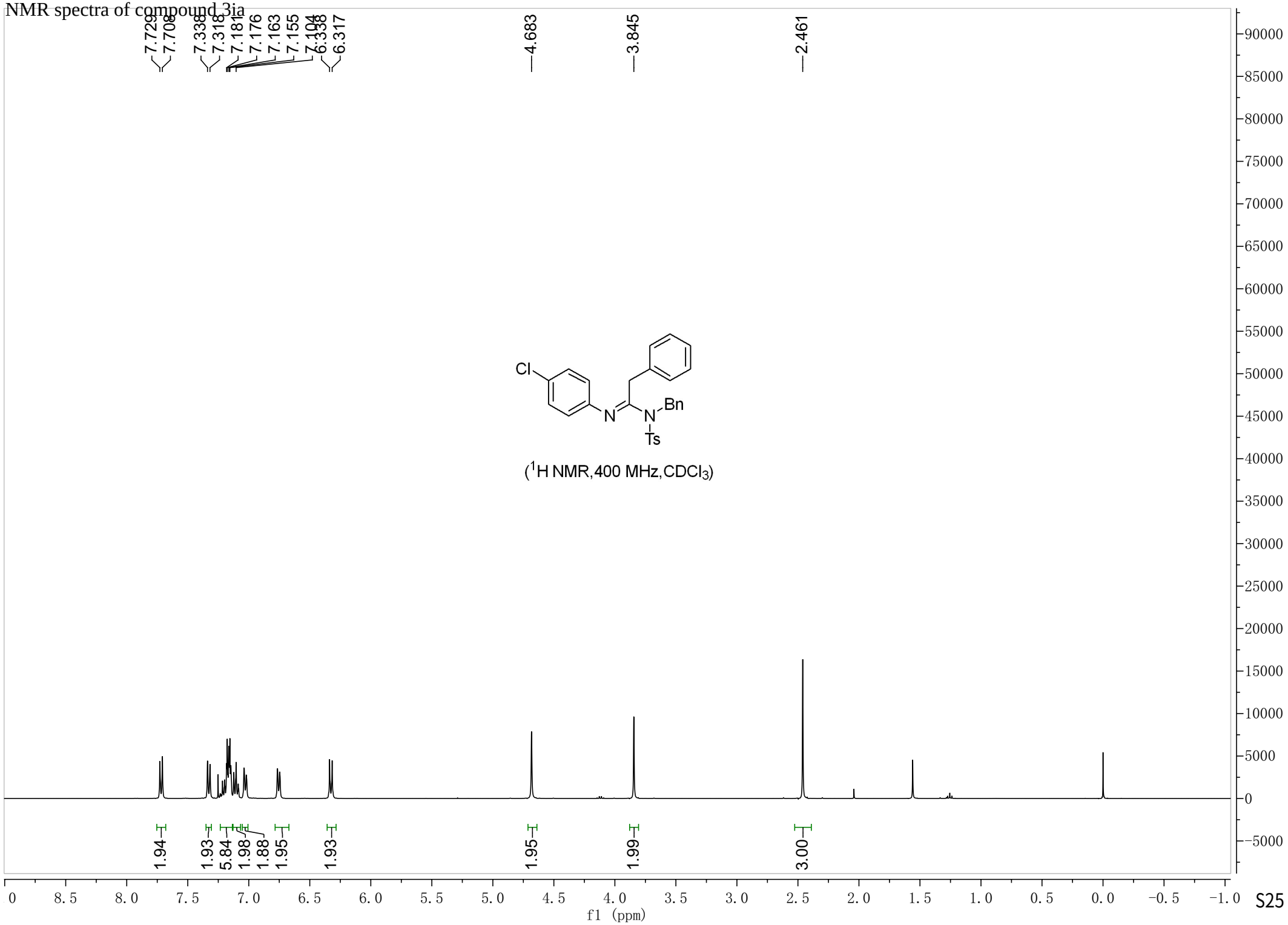
NMR spectra of compound 3ha



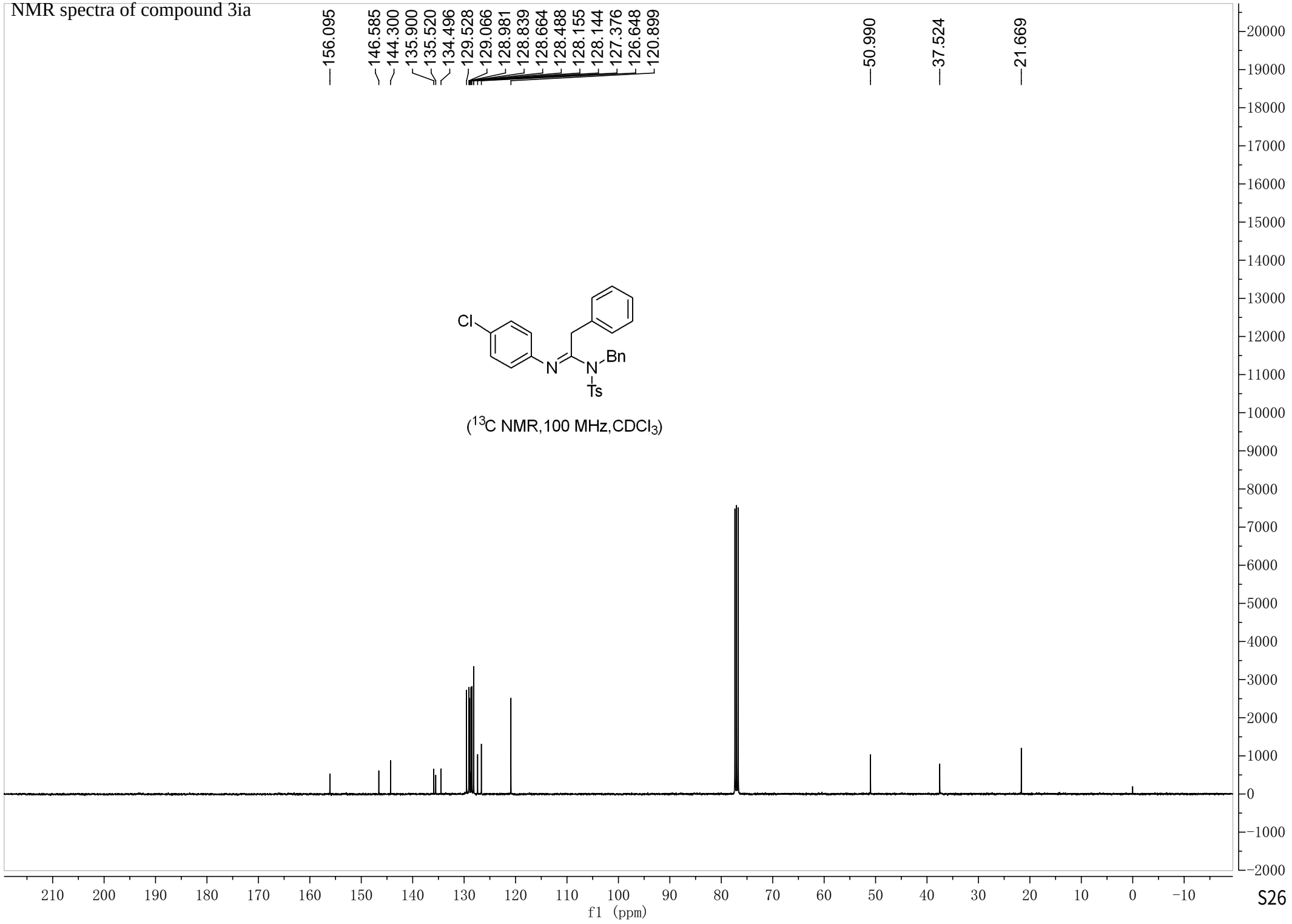
NMR spectra of compound 3ha



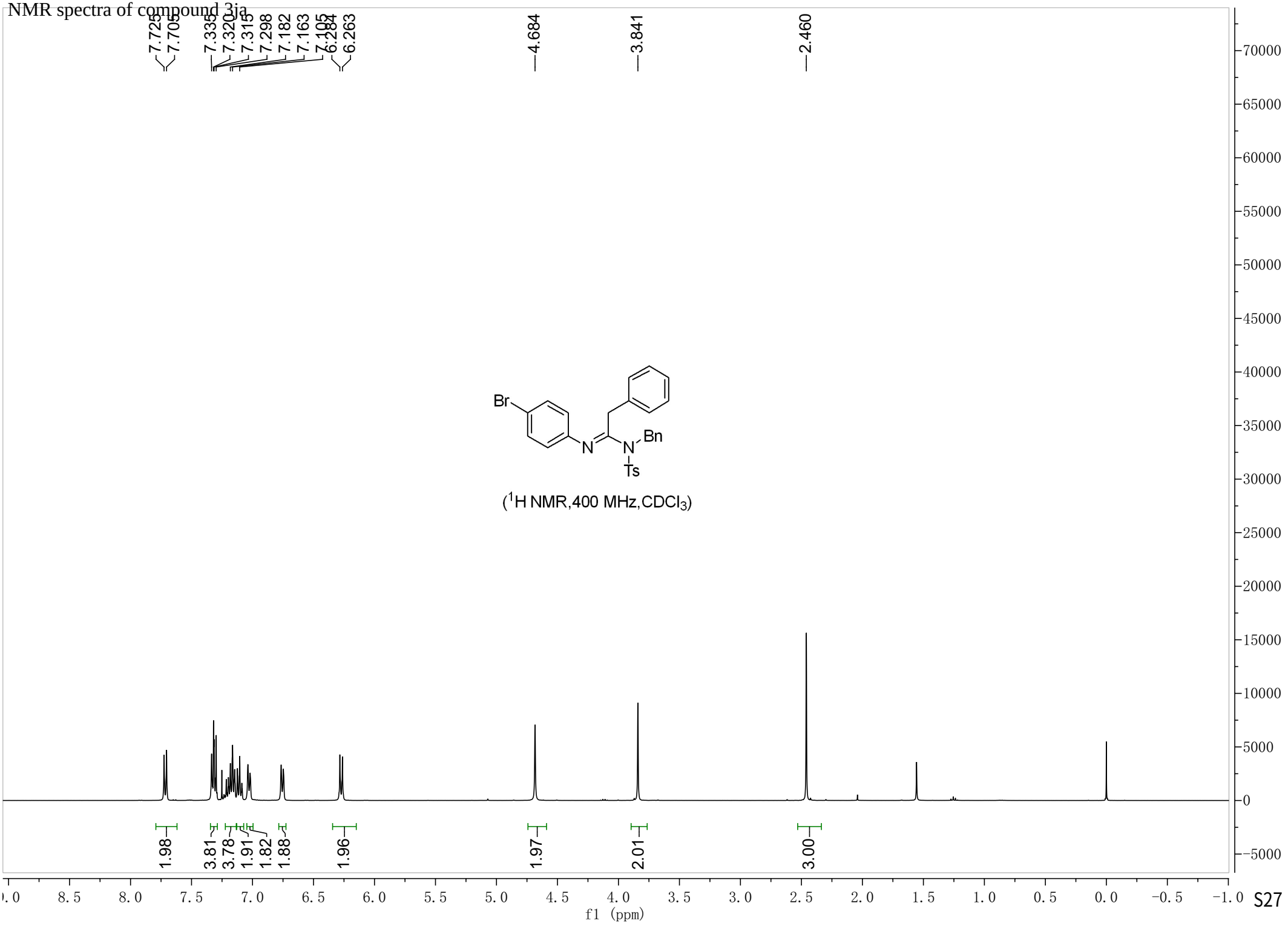
NMR spectra of compound 3ia



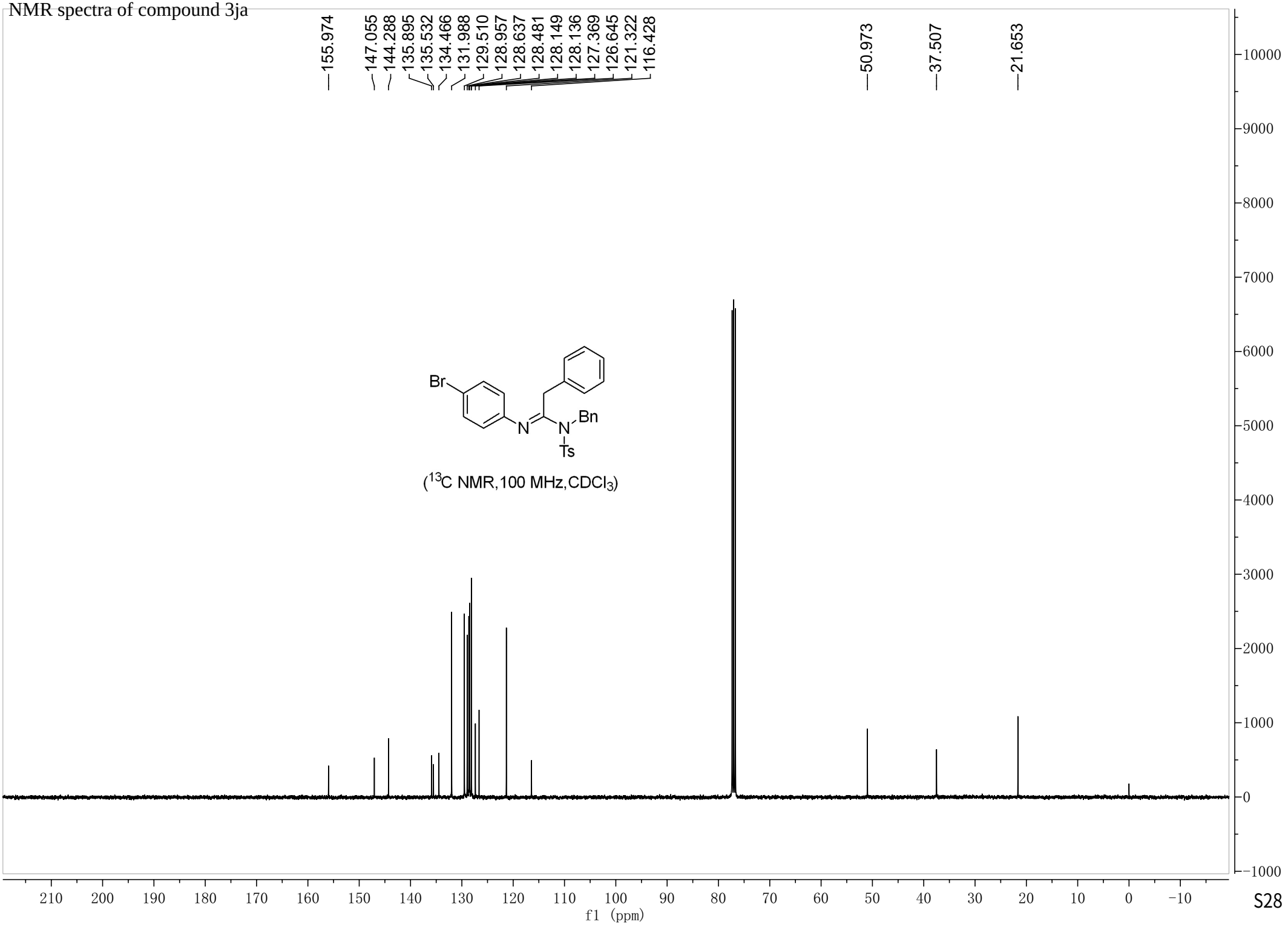
NMR spectra of compound 3ia



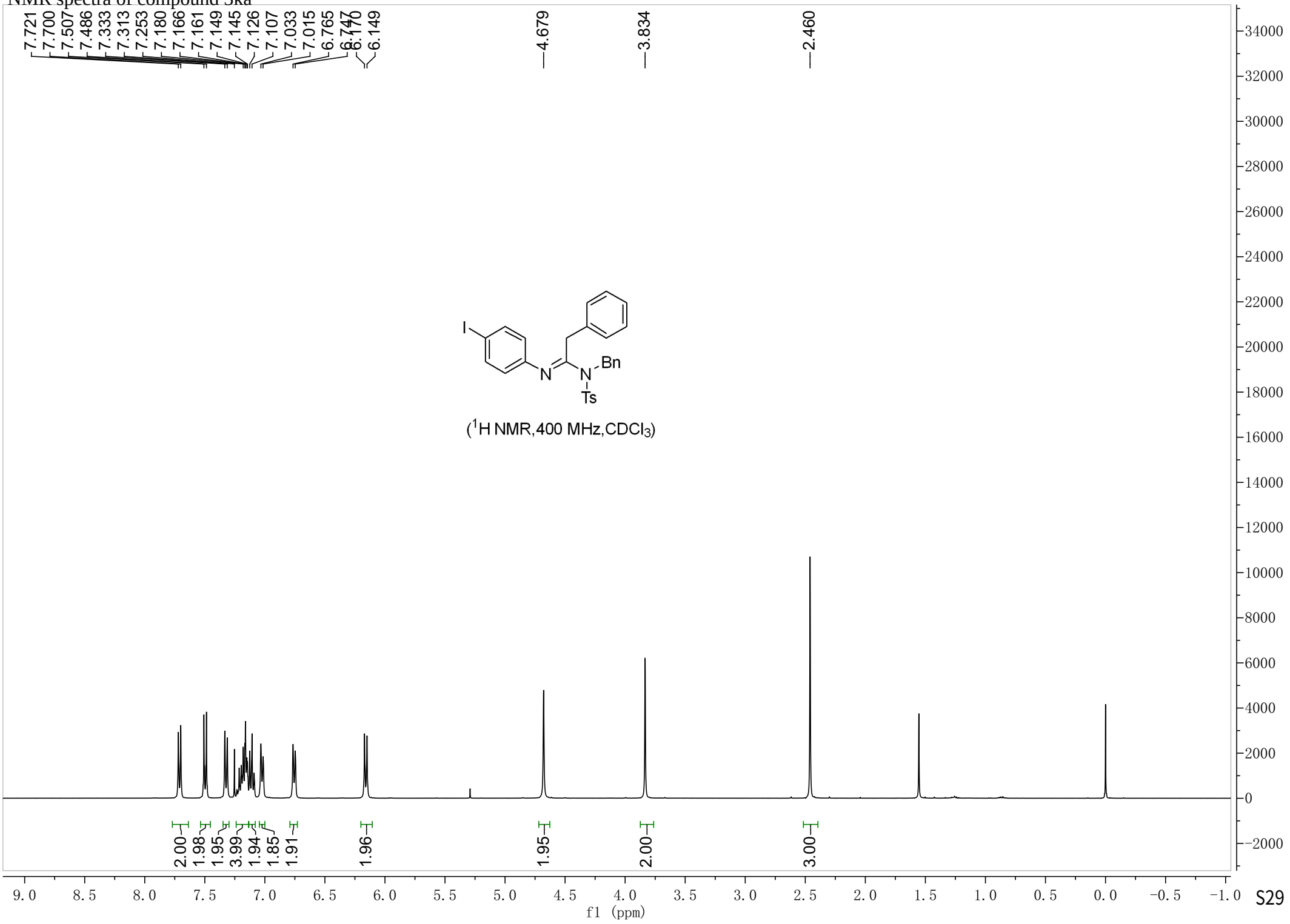
NMR spectra of compound 3ja



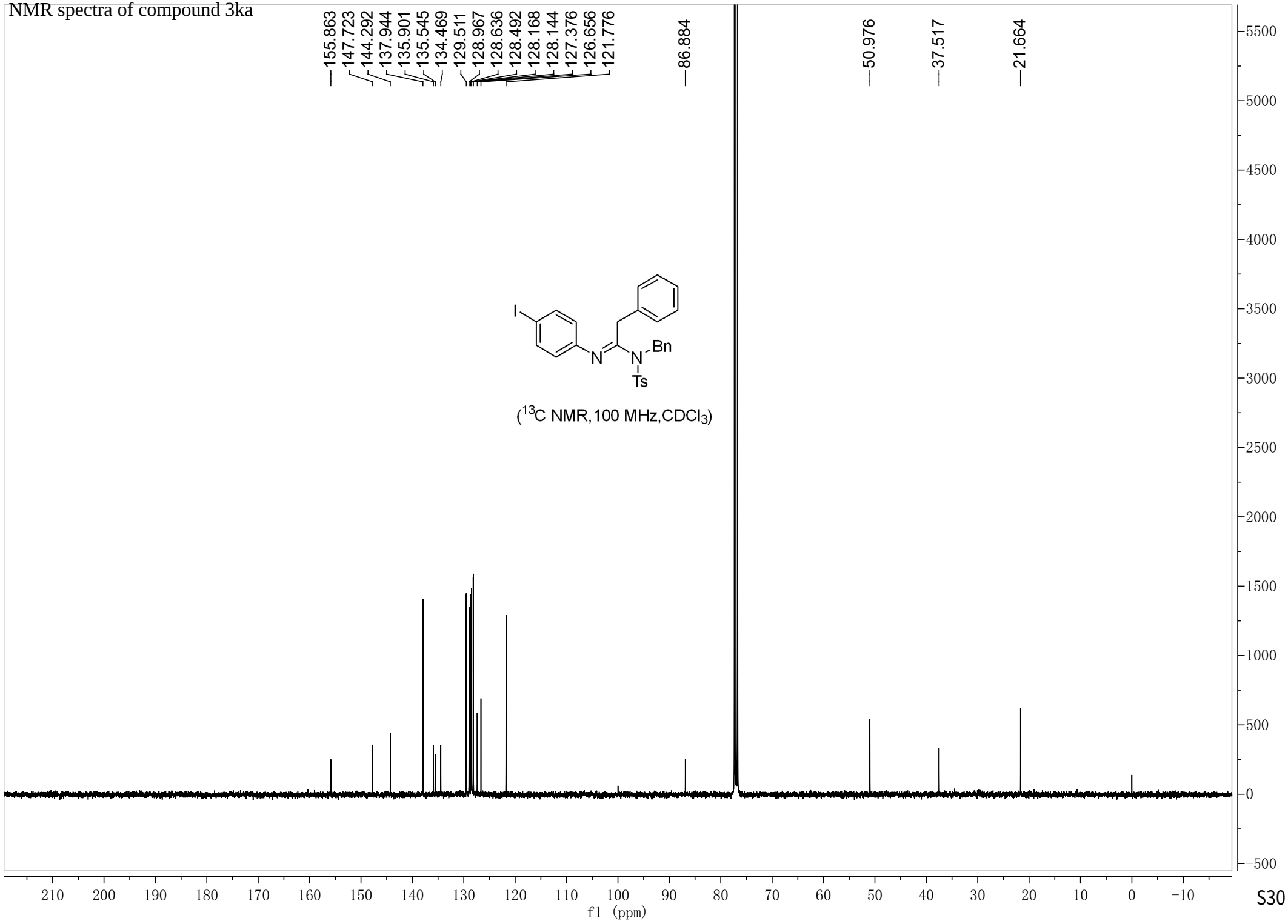
NMR spectra of compound 3ja



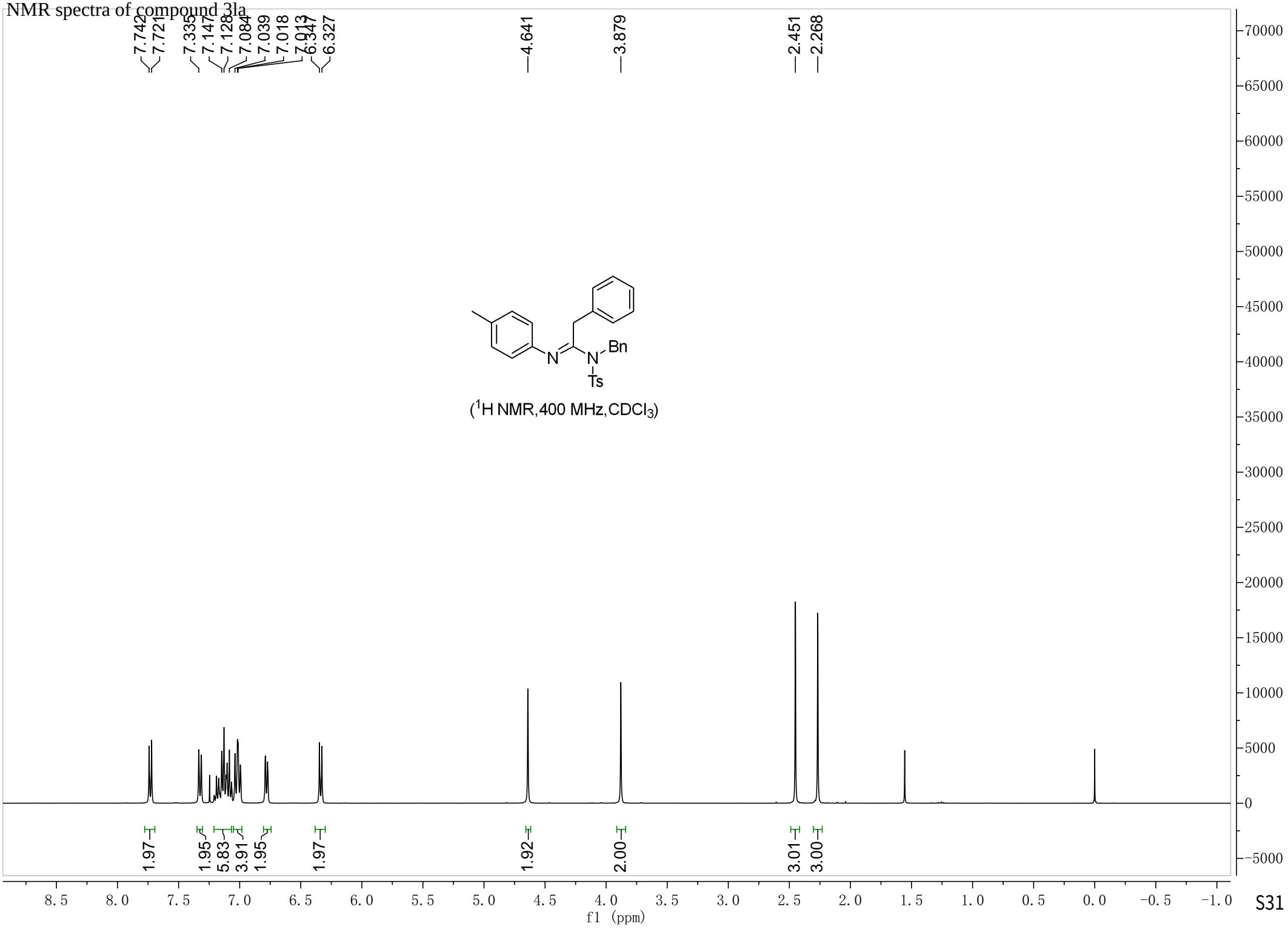
NMR spectra of compound 3ka



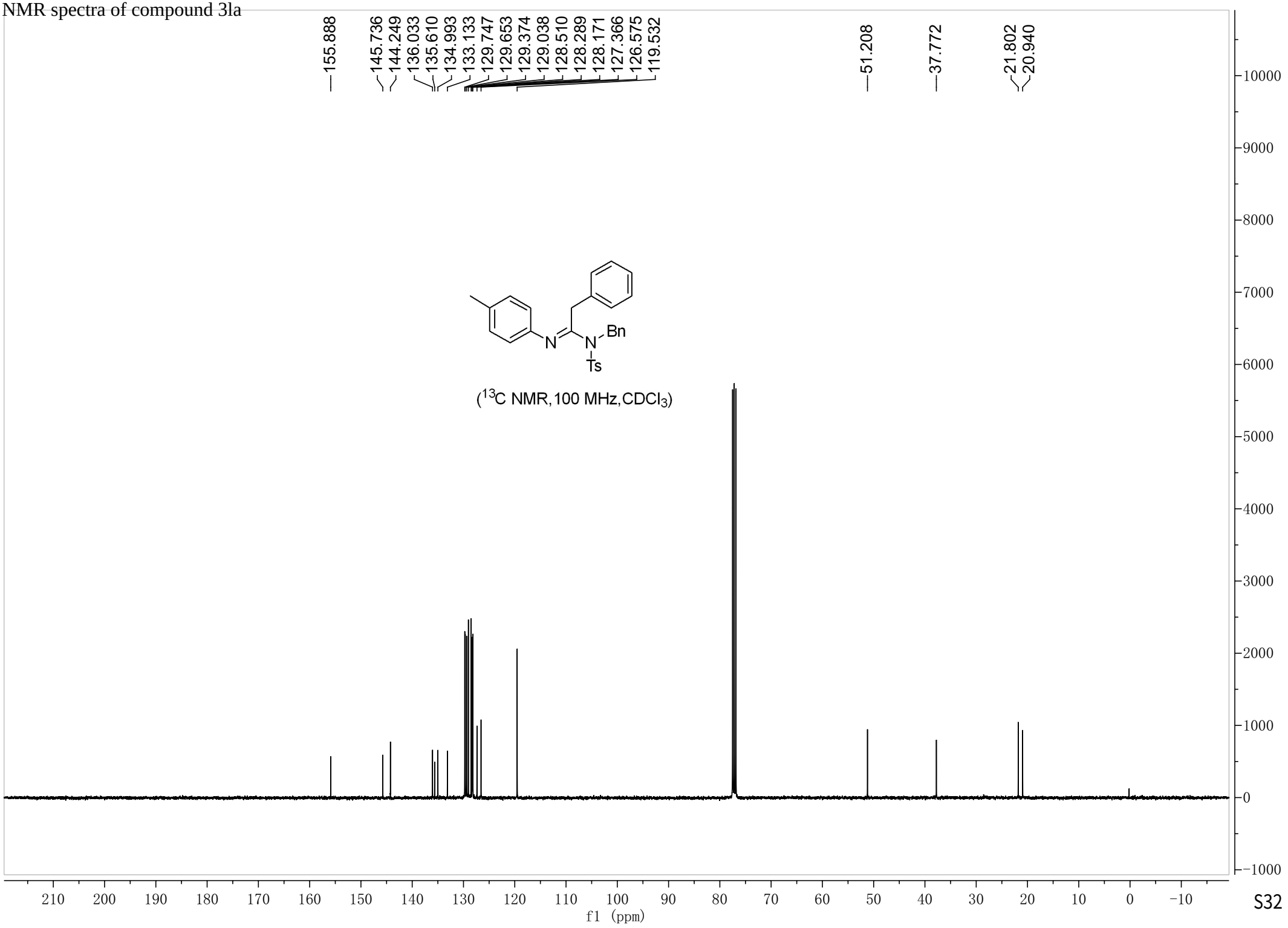
NMR spectra of compound 3ka



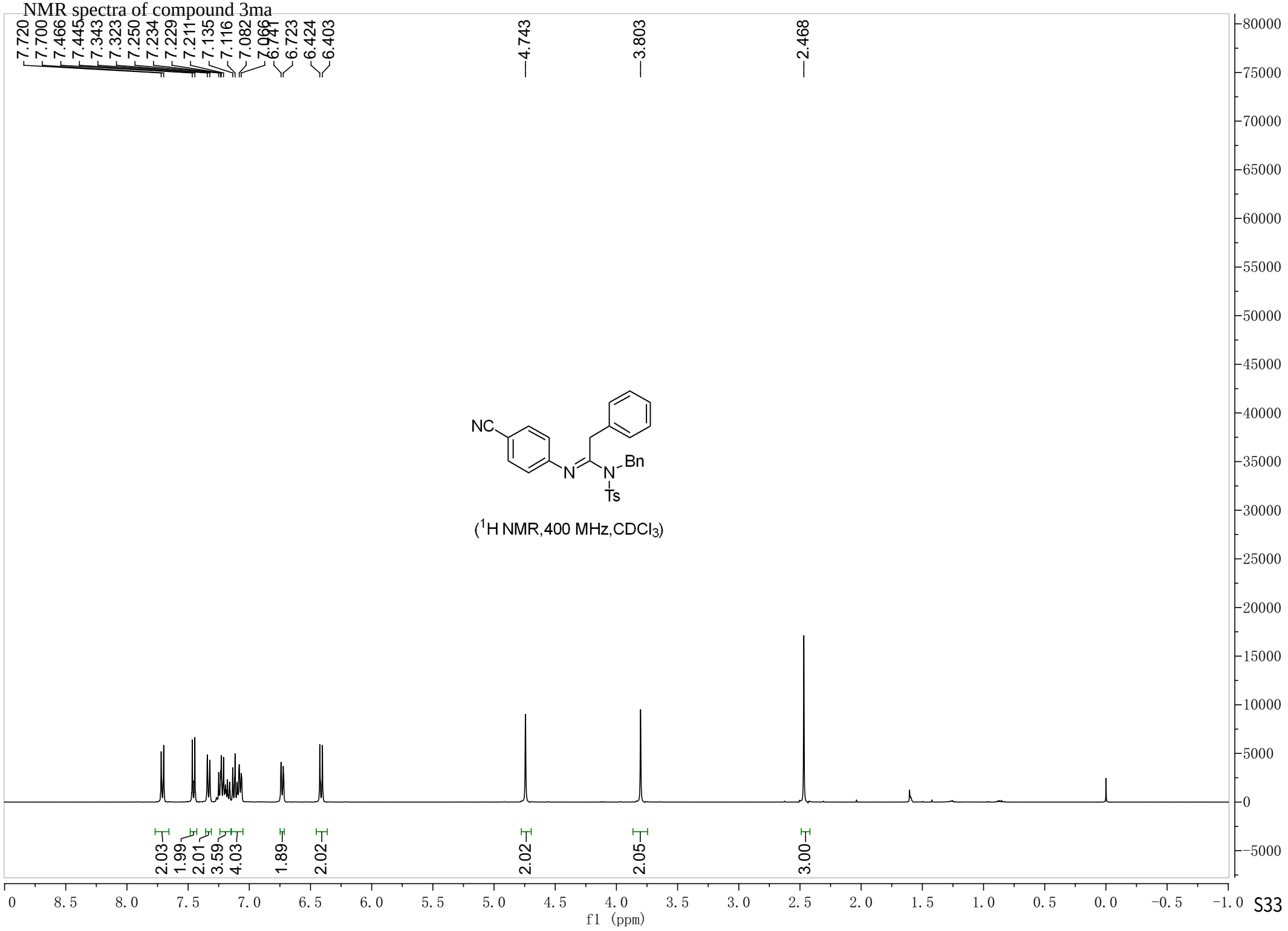
NMR spectra of compound 3la



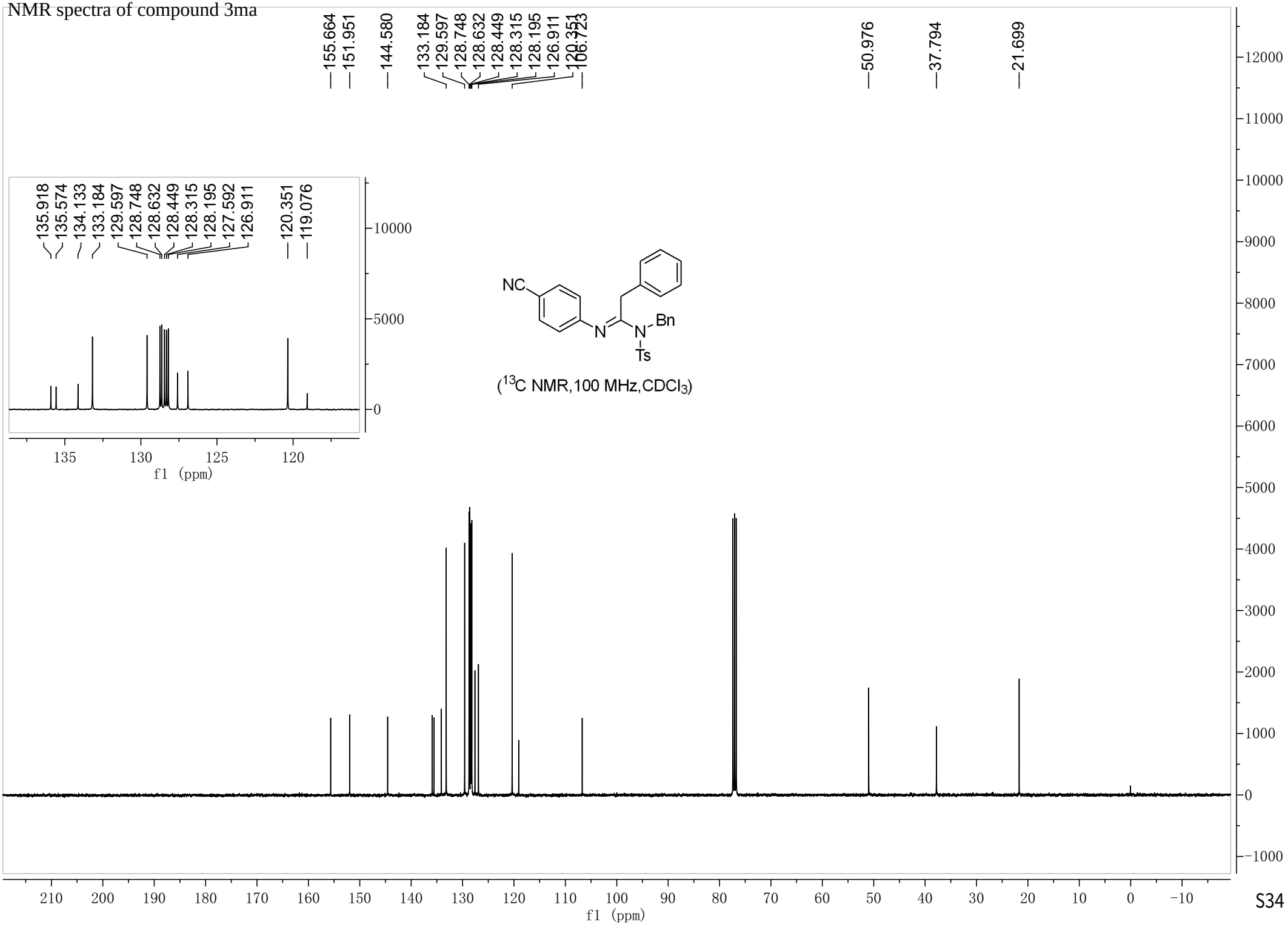
NMR spectra of compound 3la



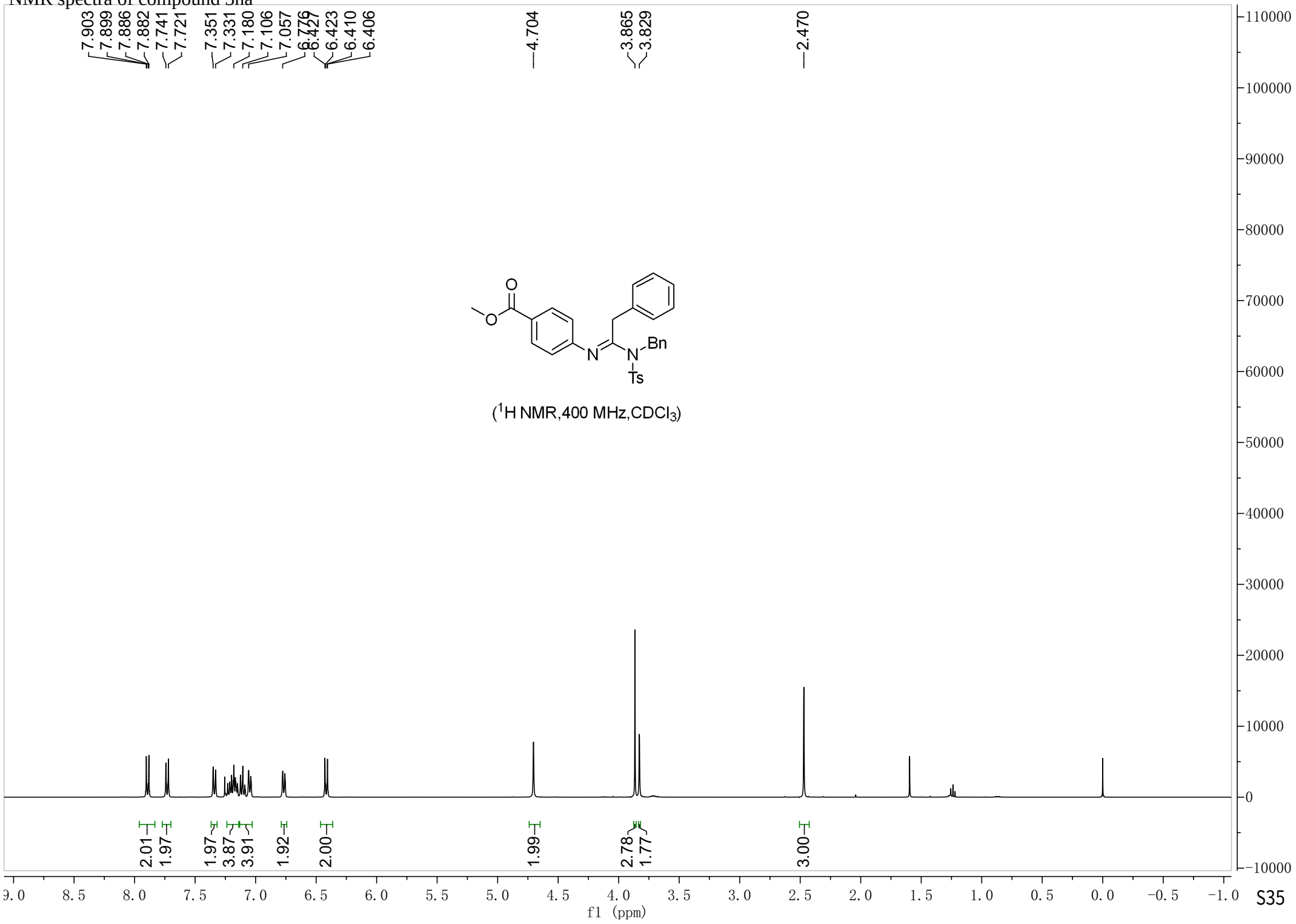
NMR spectra of compound 3ma



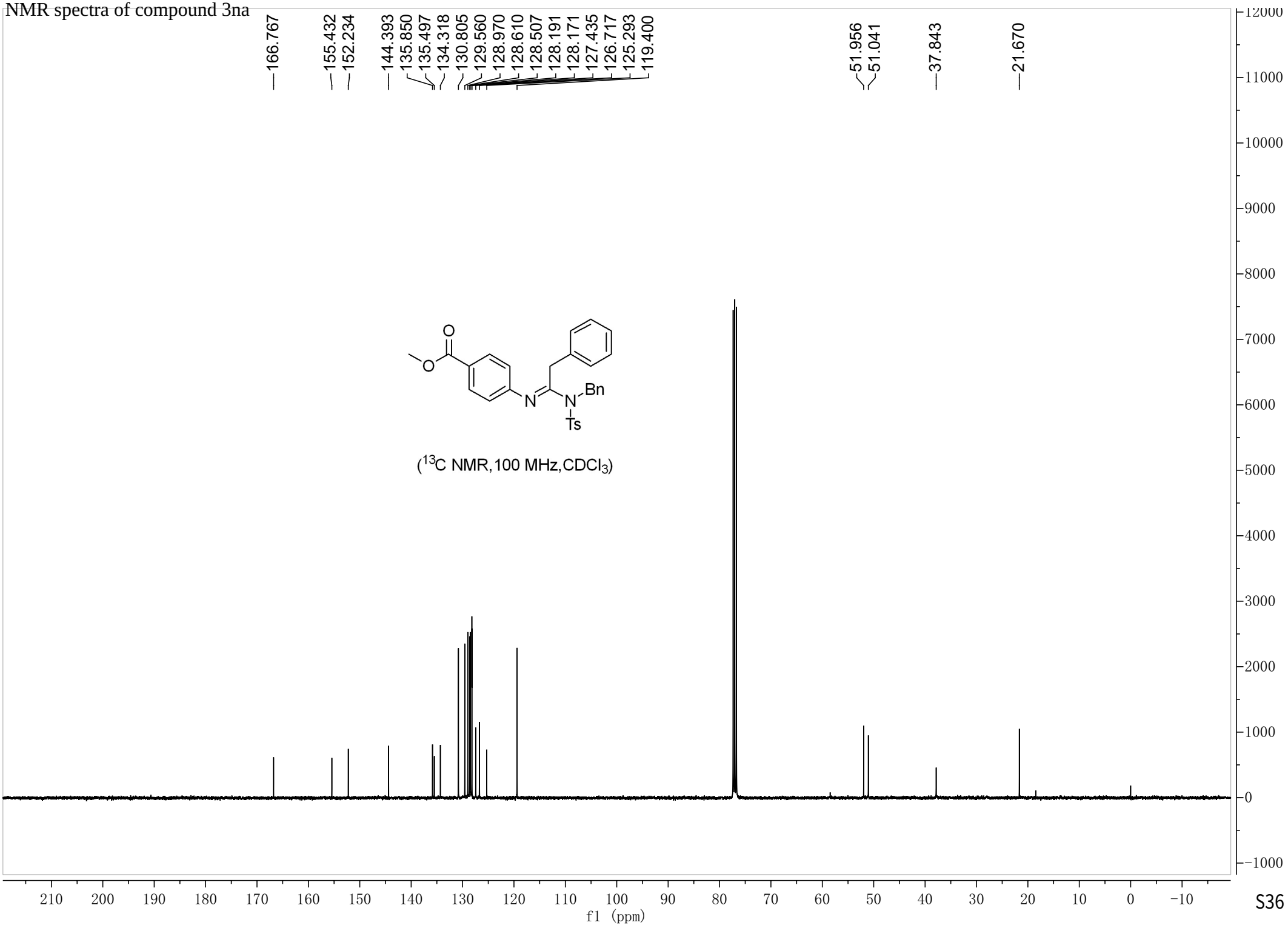
NMR spectra of compound 3ma



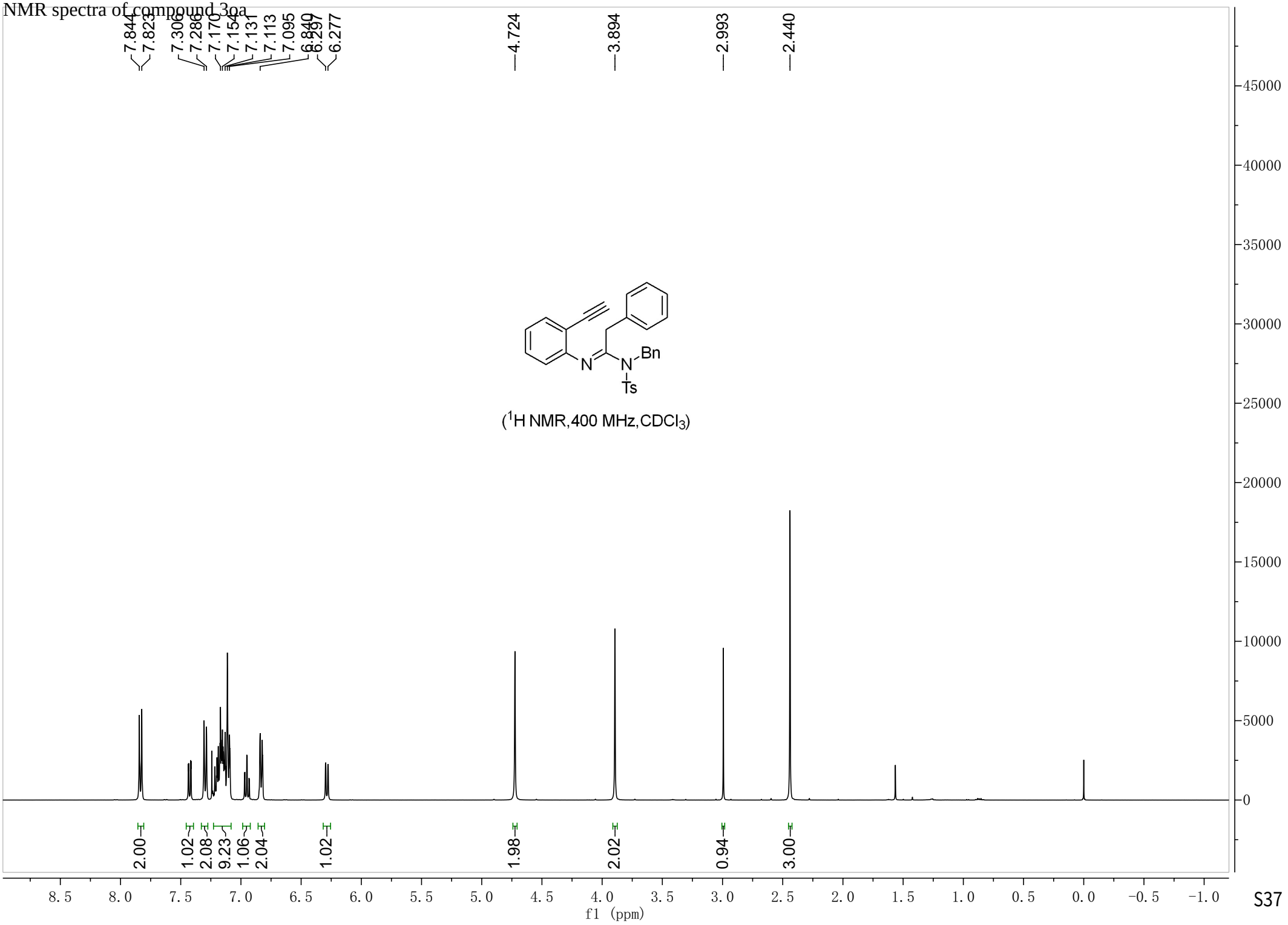
NMR spectra of compound 3na



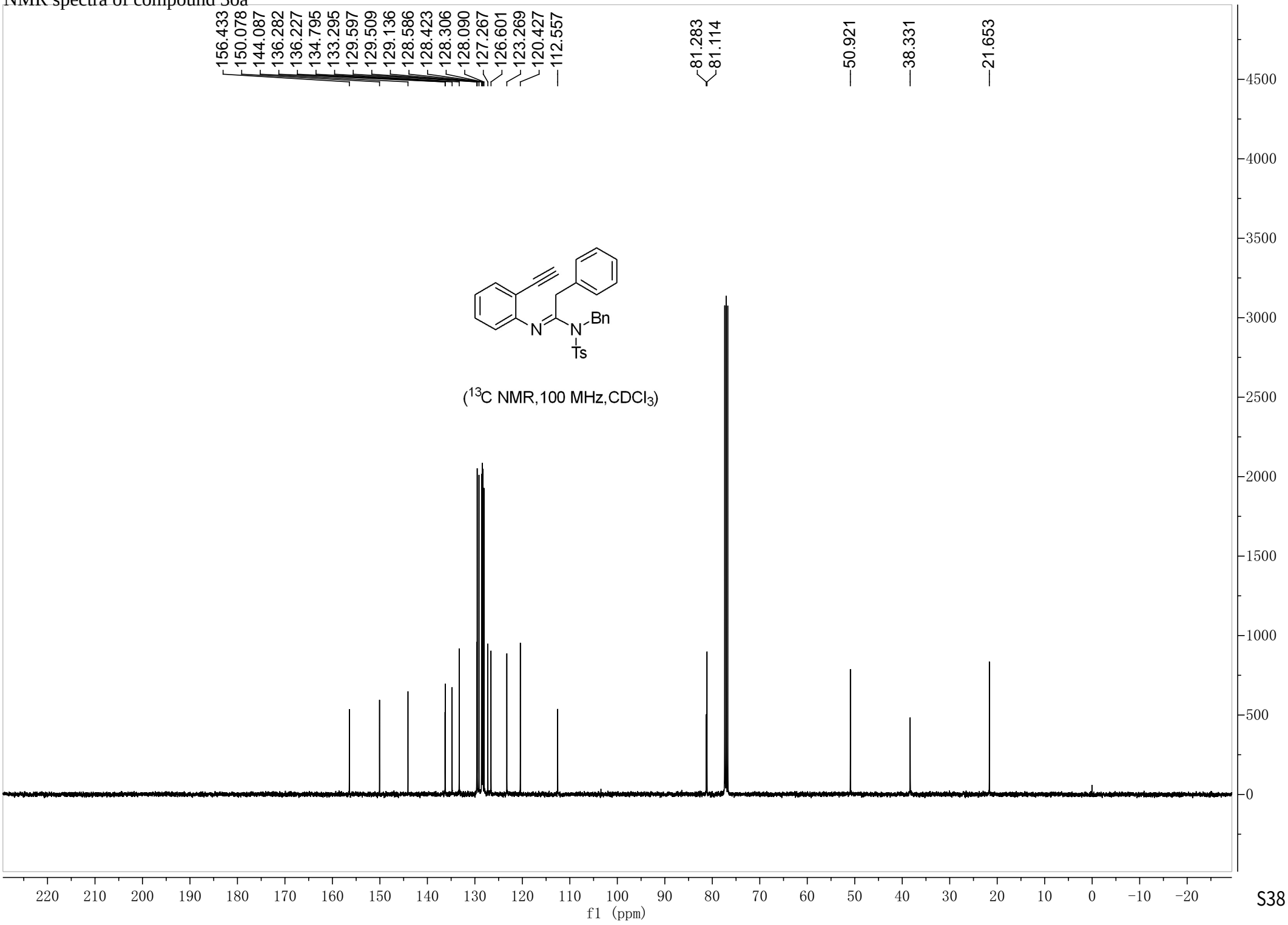
NMR spectra of compound 3na



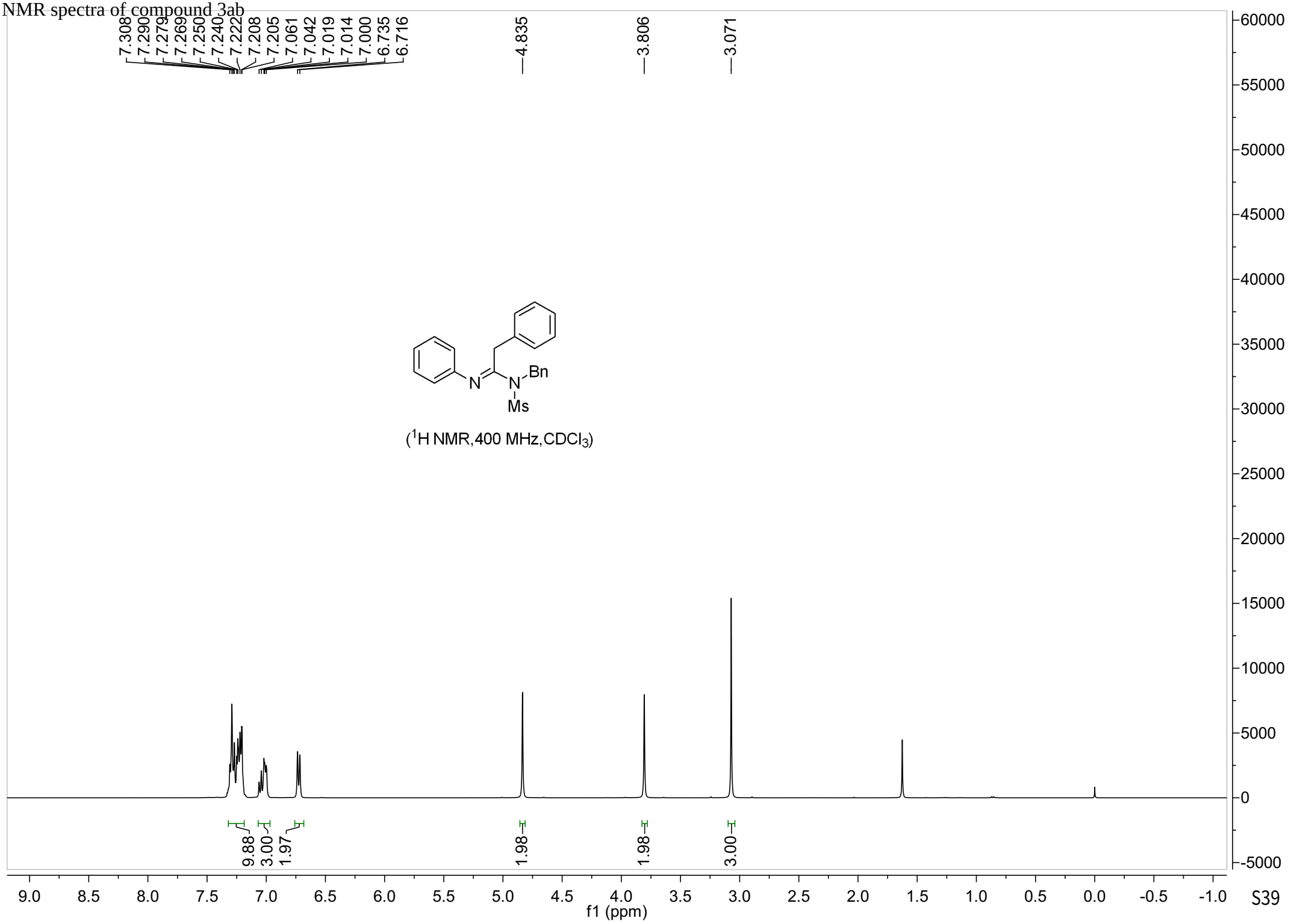
NMR spectra of compound 3oa



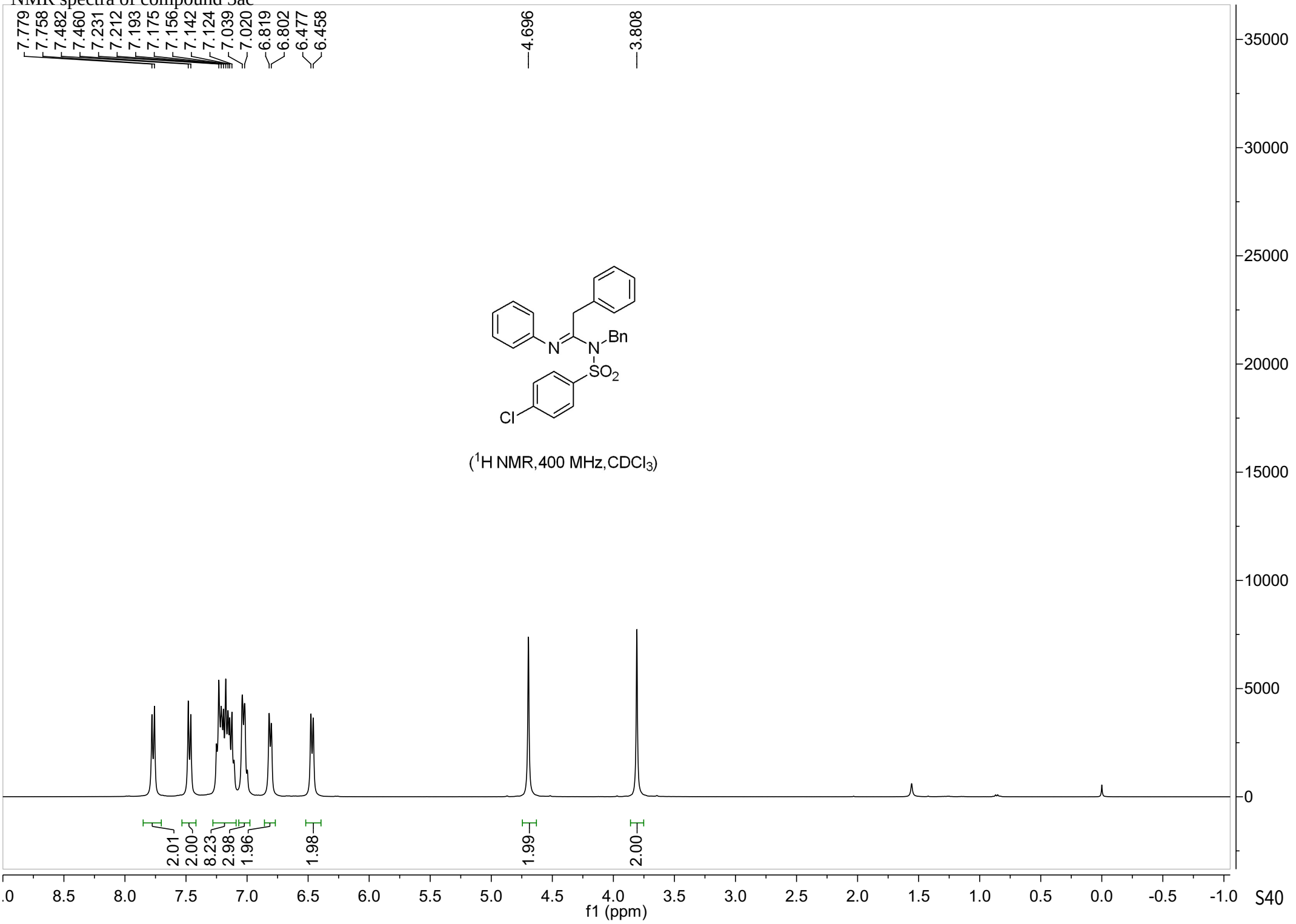
NMR spectra of compound 3oa



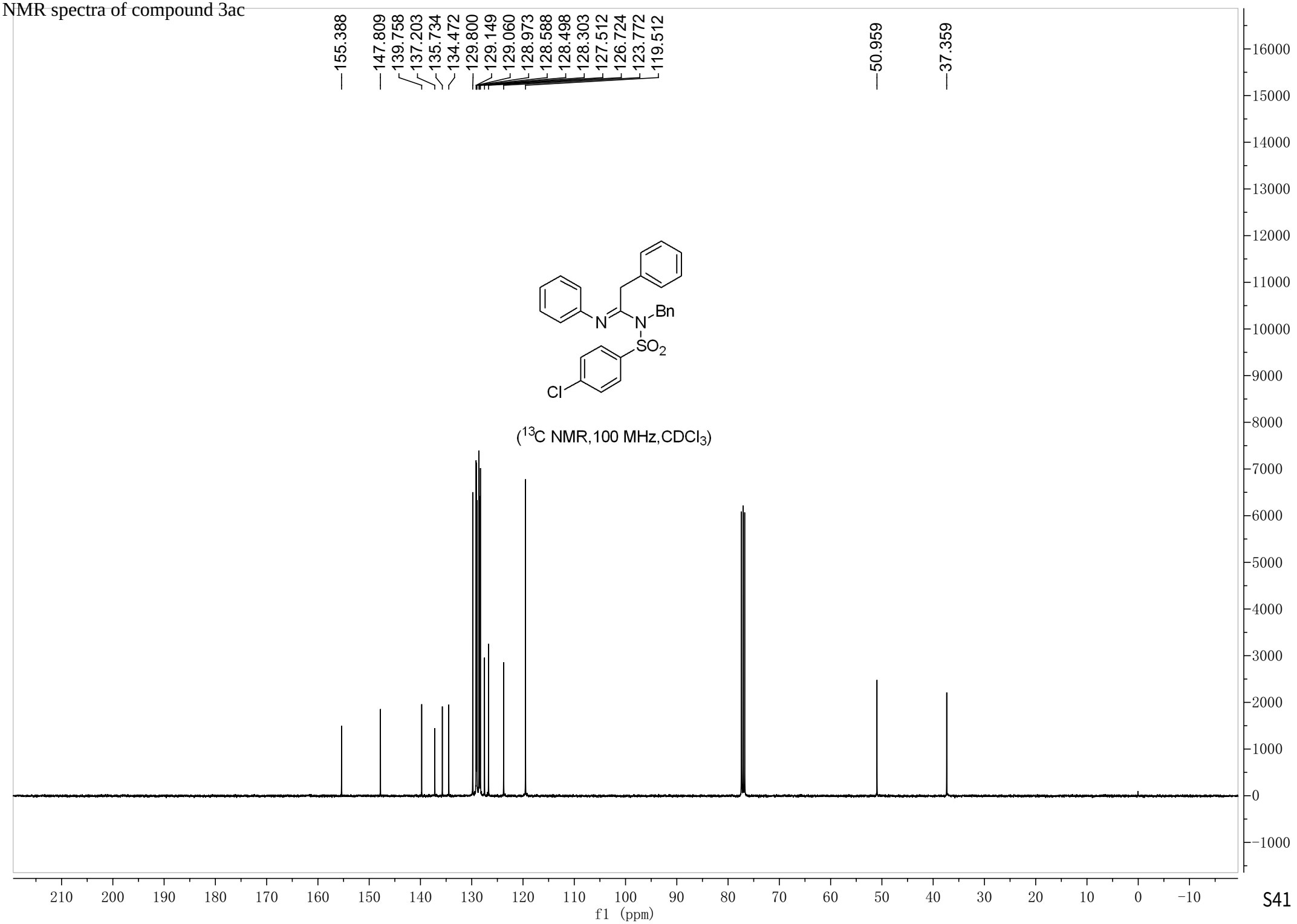
NMR spectra of compound 3ab



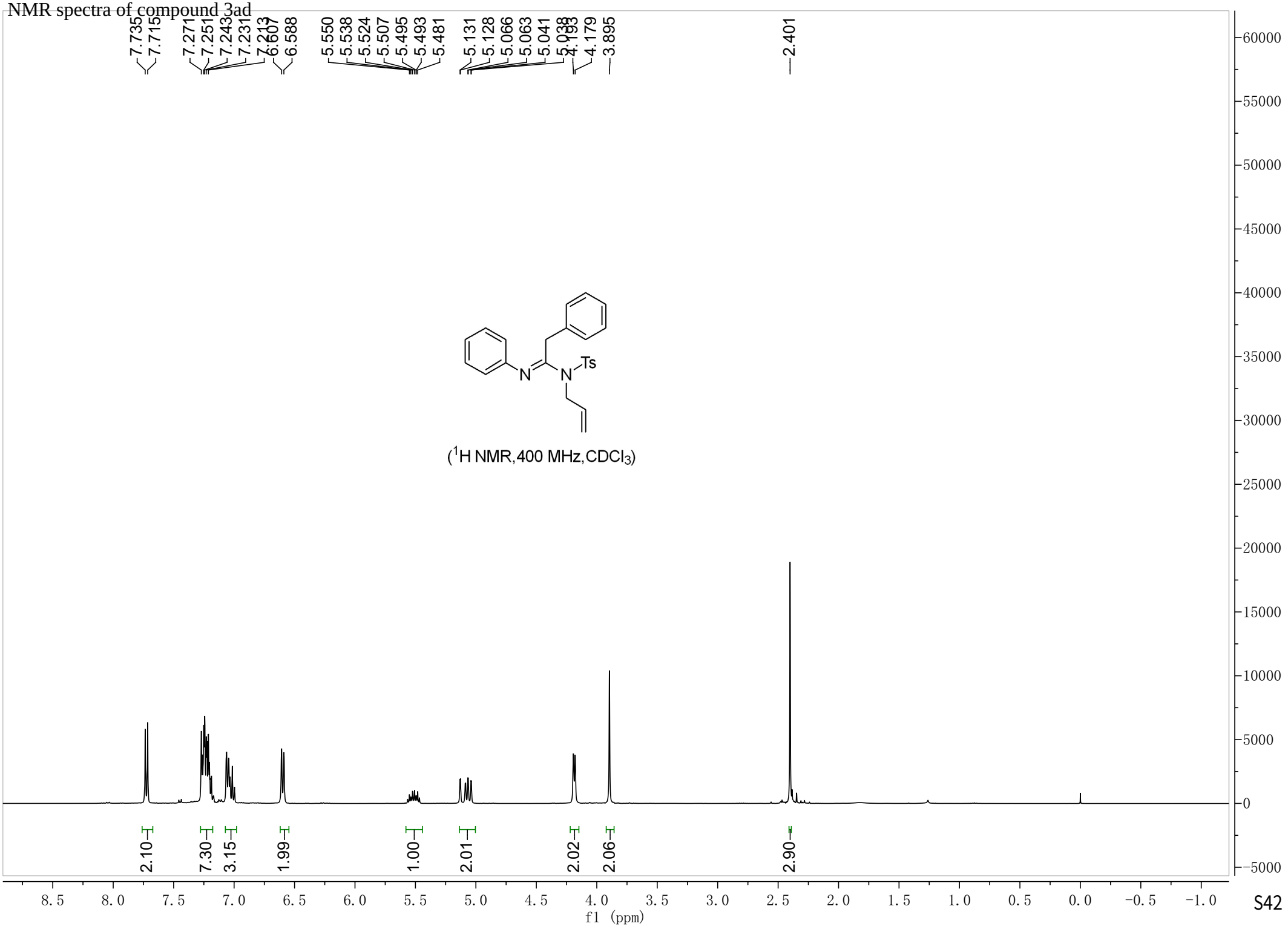
NMR spectra of compound 3ac



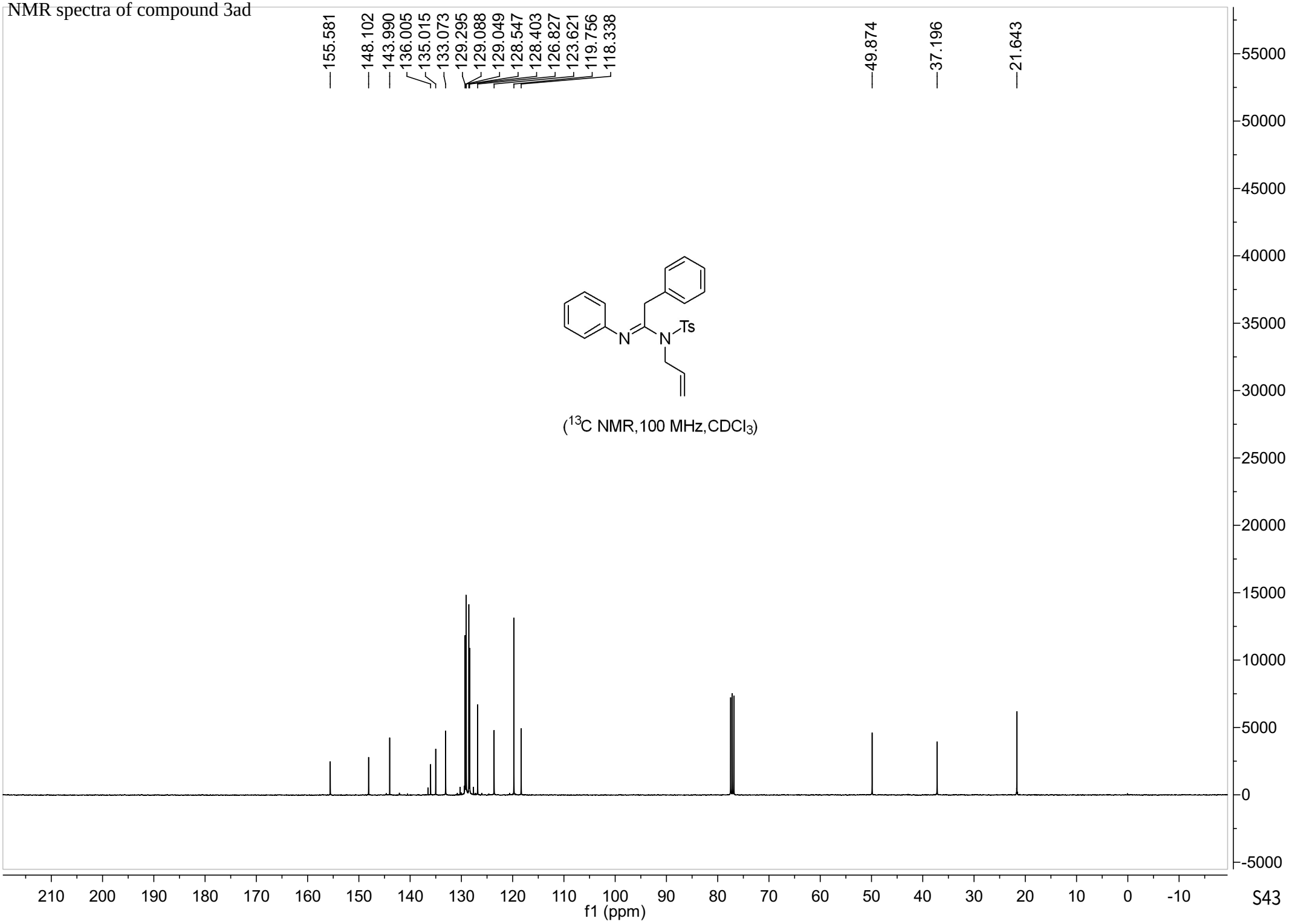
NMR spectra of compound 3ac



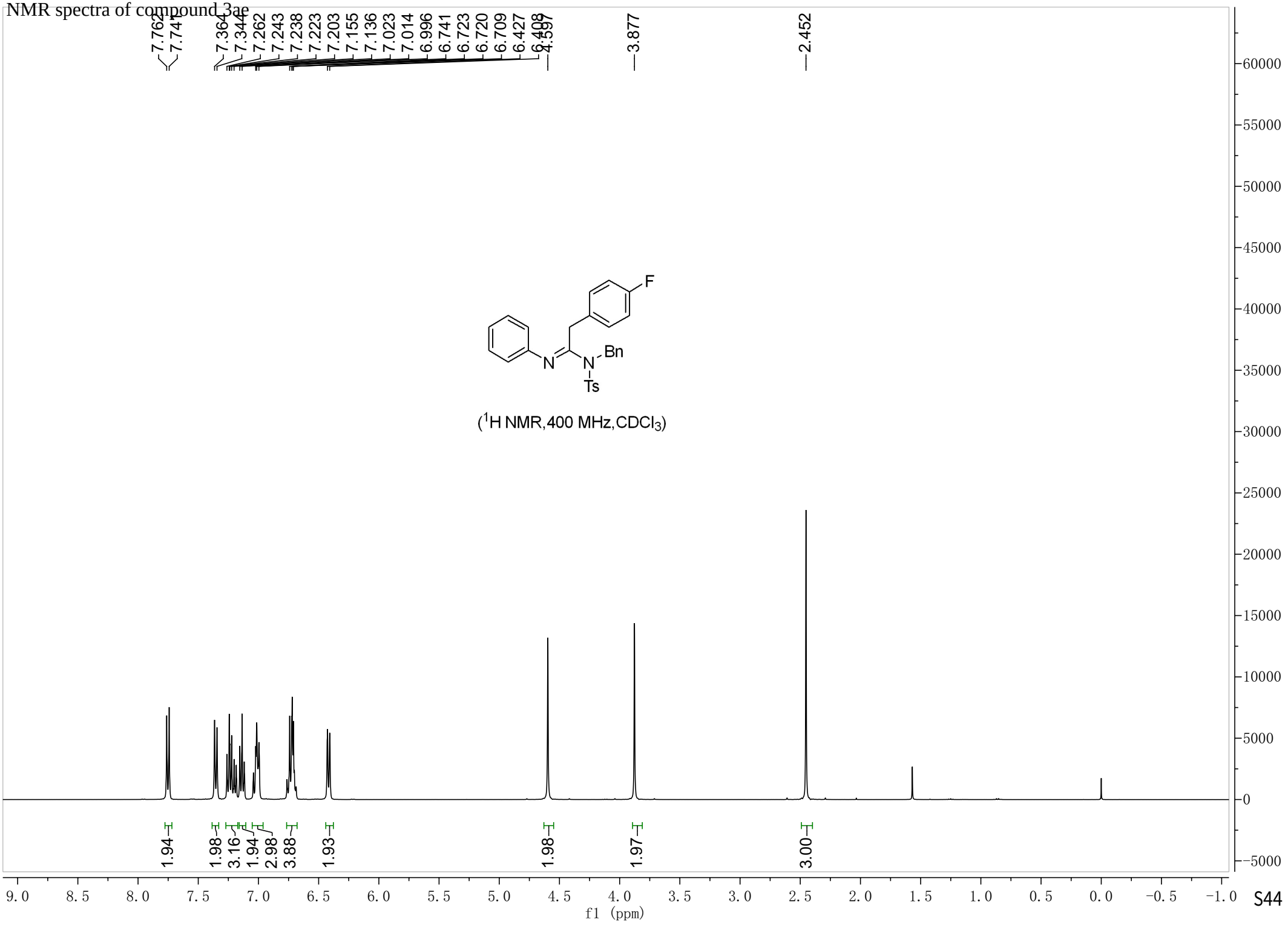
NMR spectra of compound 3ad



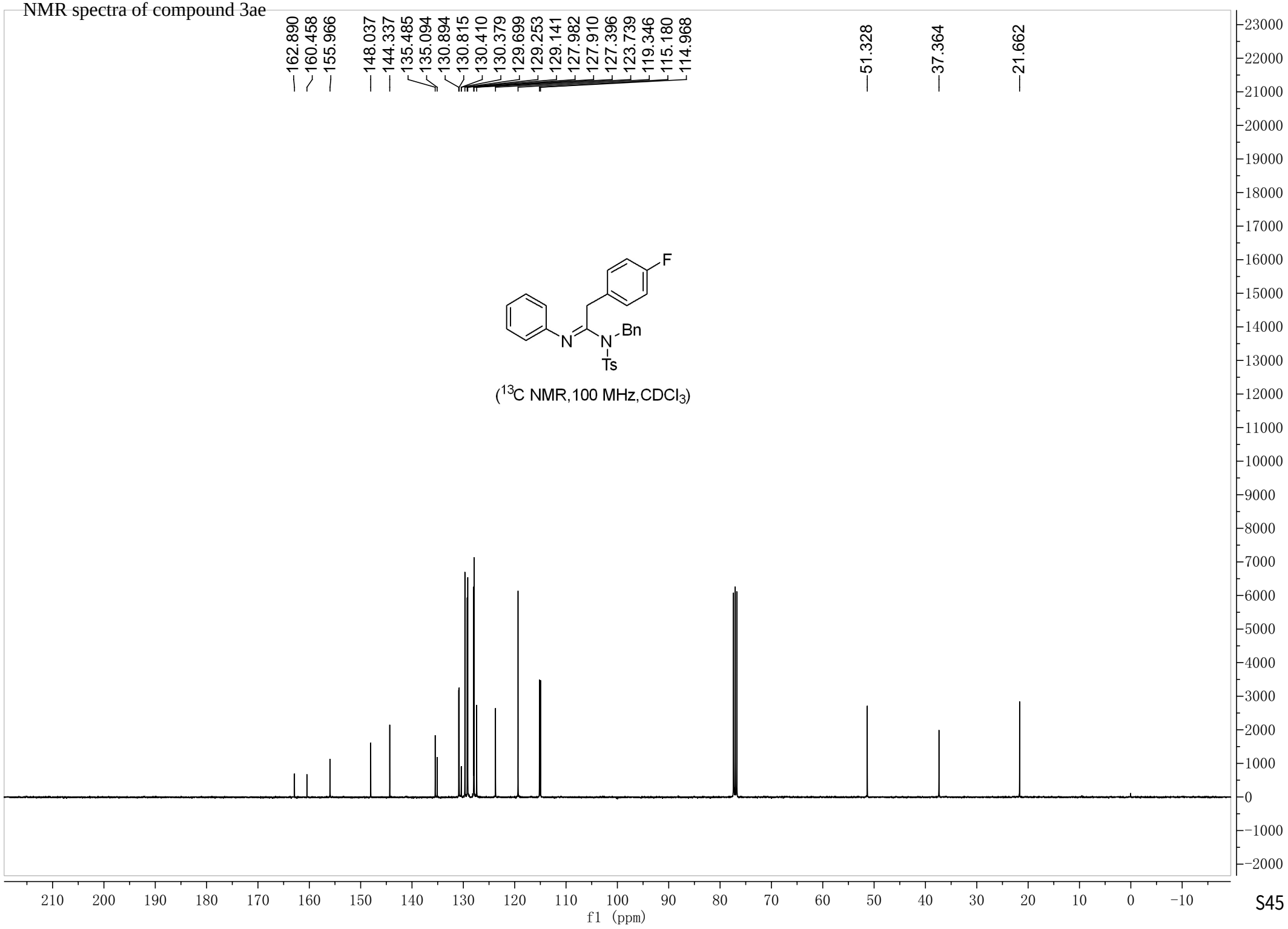
NMR spectra of compound 3ad



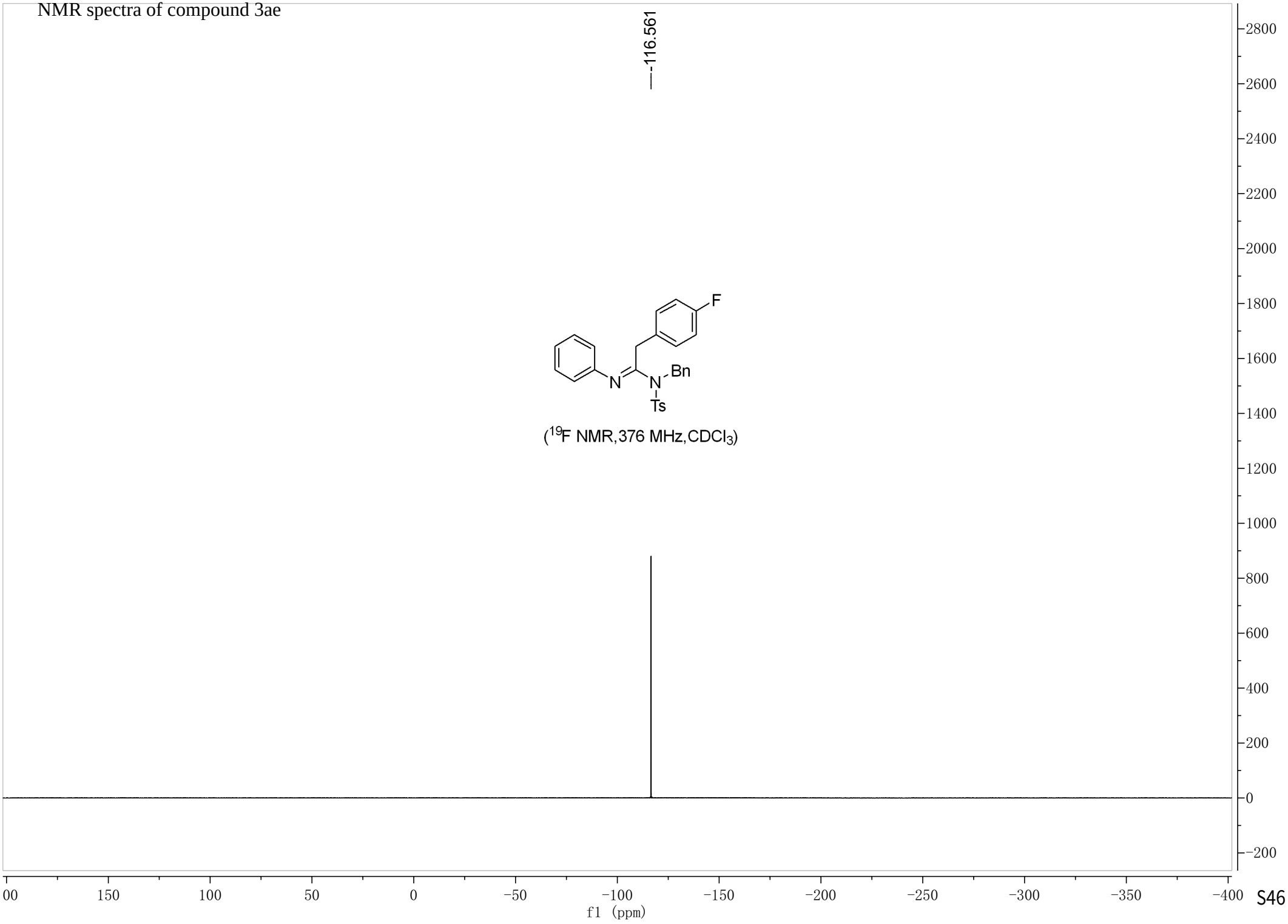
NMR spectra of compound 3ae



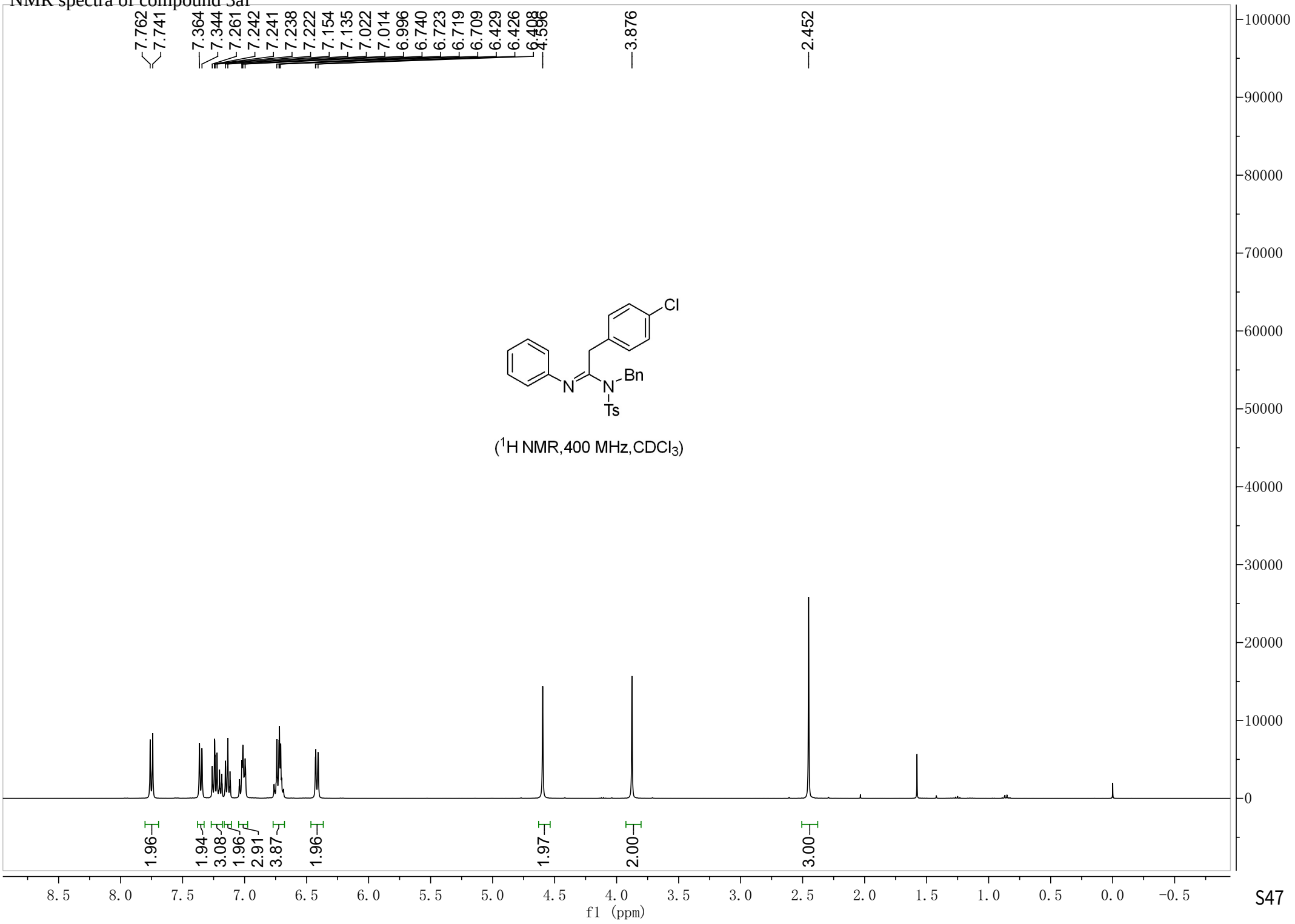
NMR spectra of compound 3ae



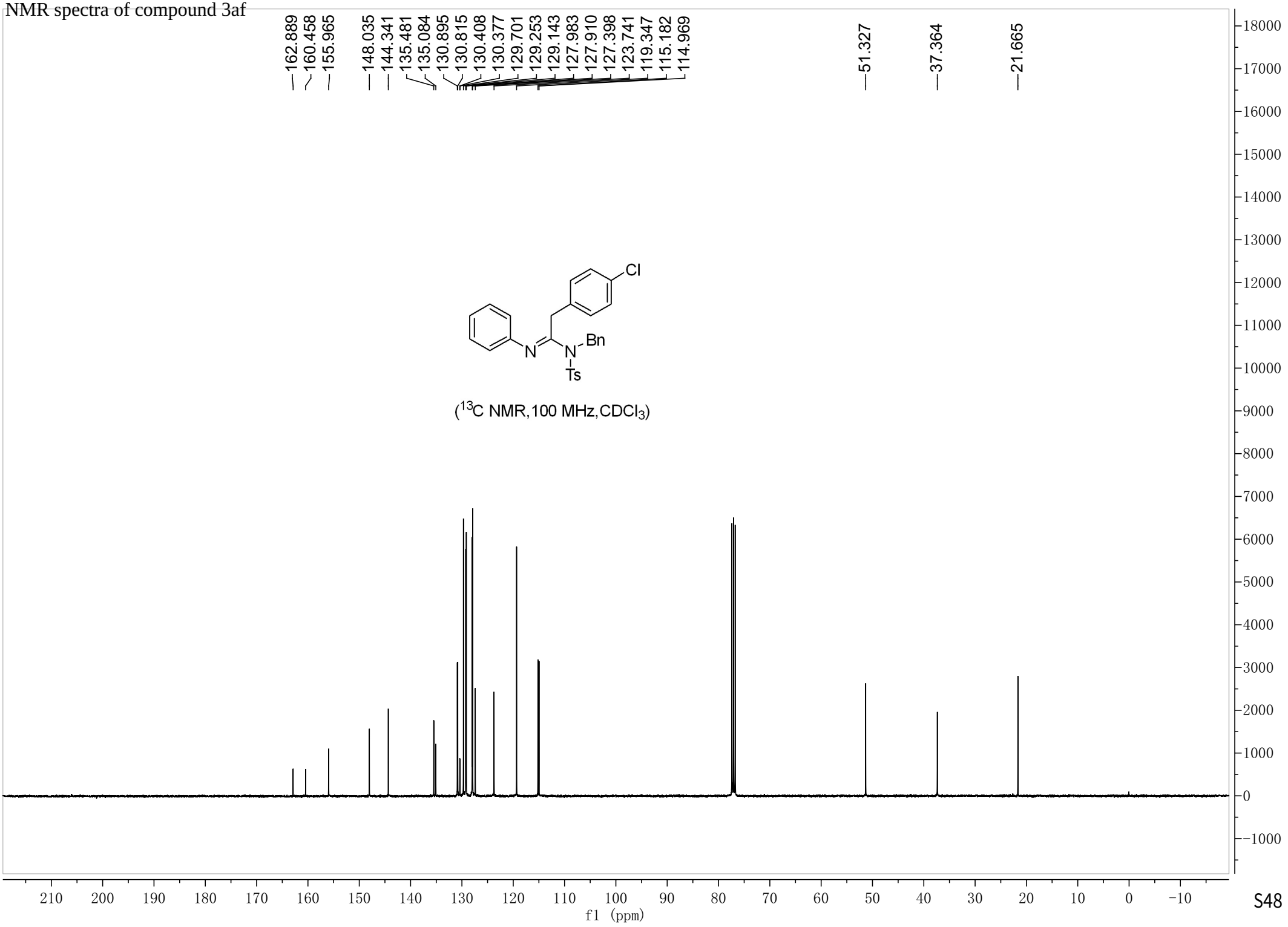
NMR spectra of compound 3ae



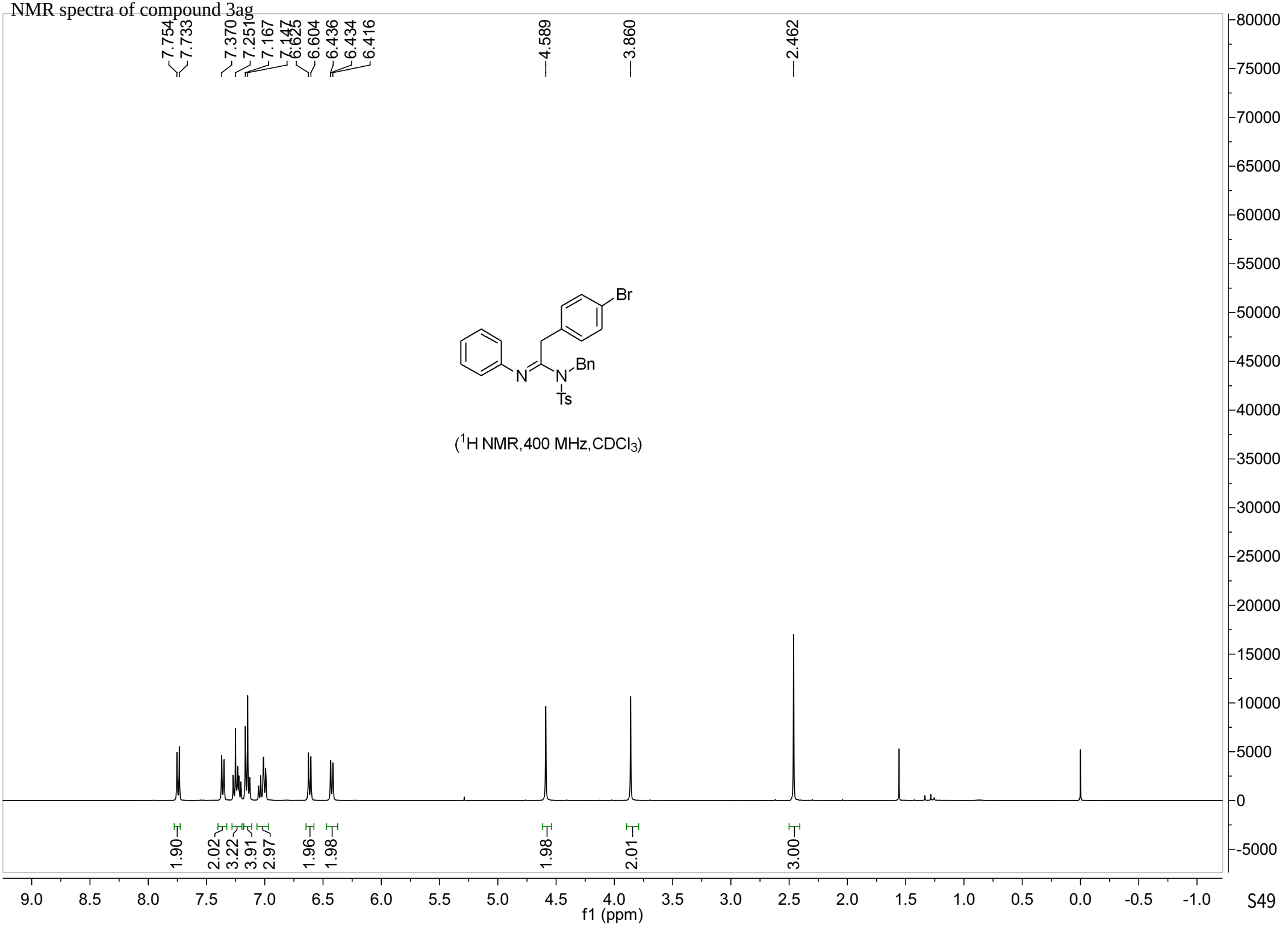
NMR spectra of compound 3af



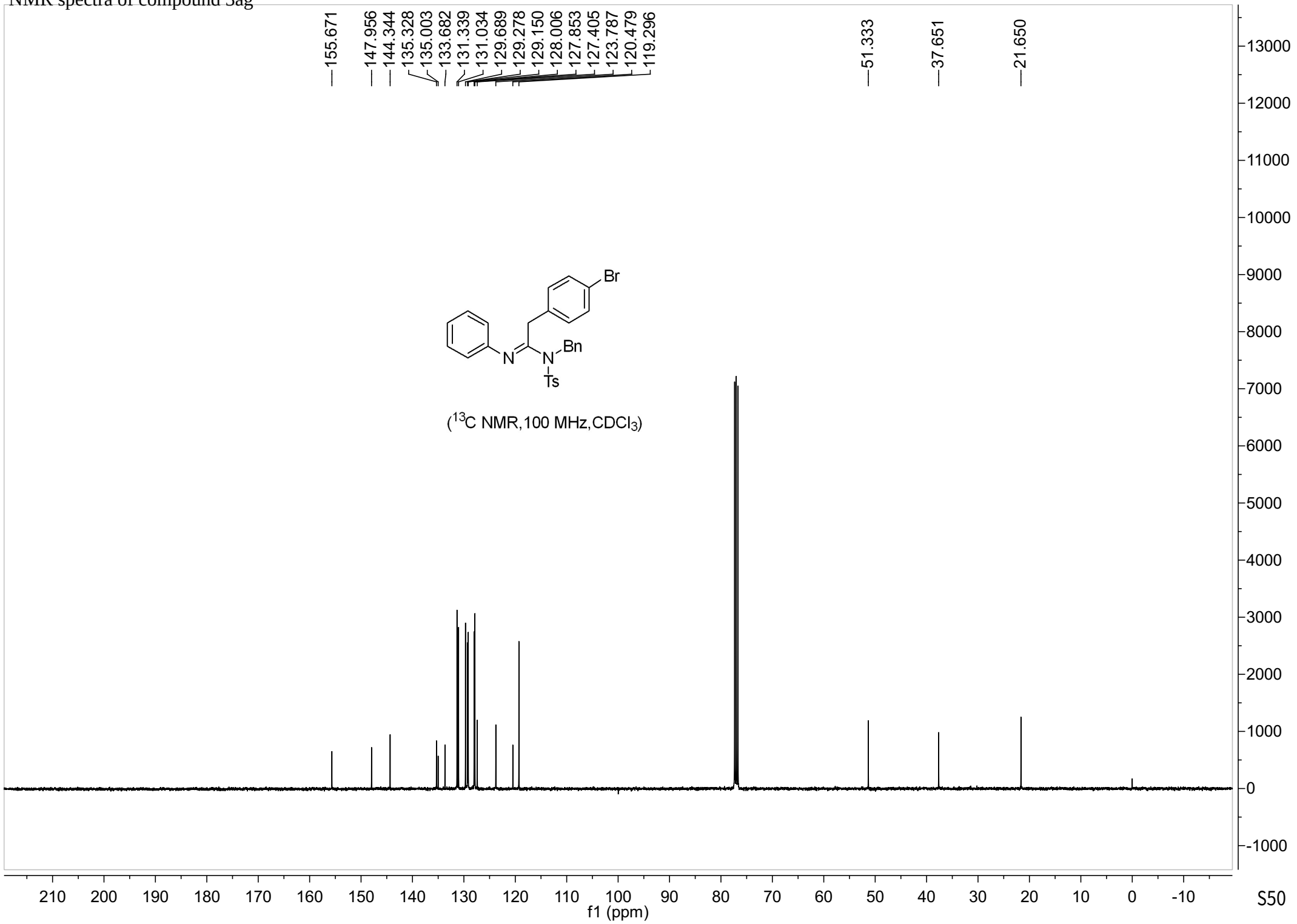
NMR spectra of compound 3af



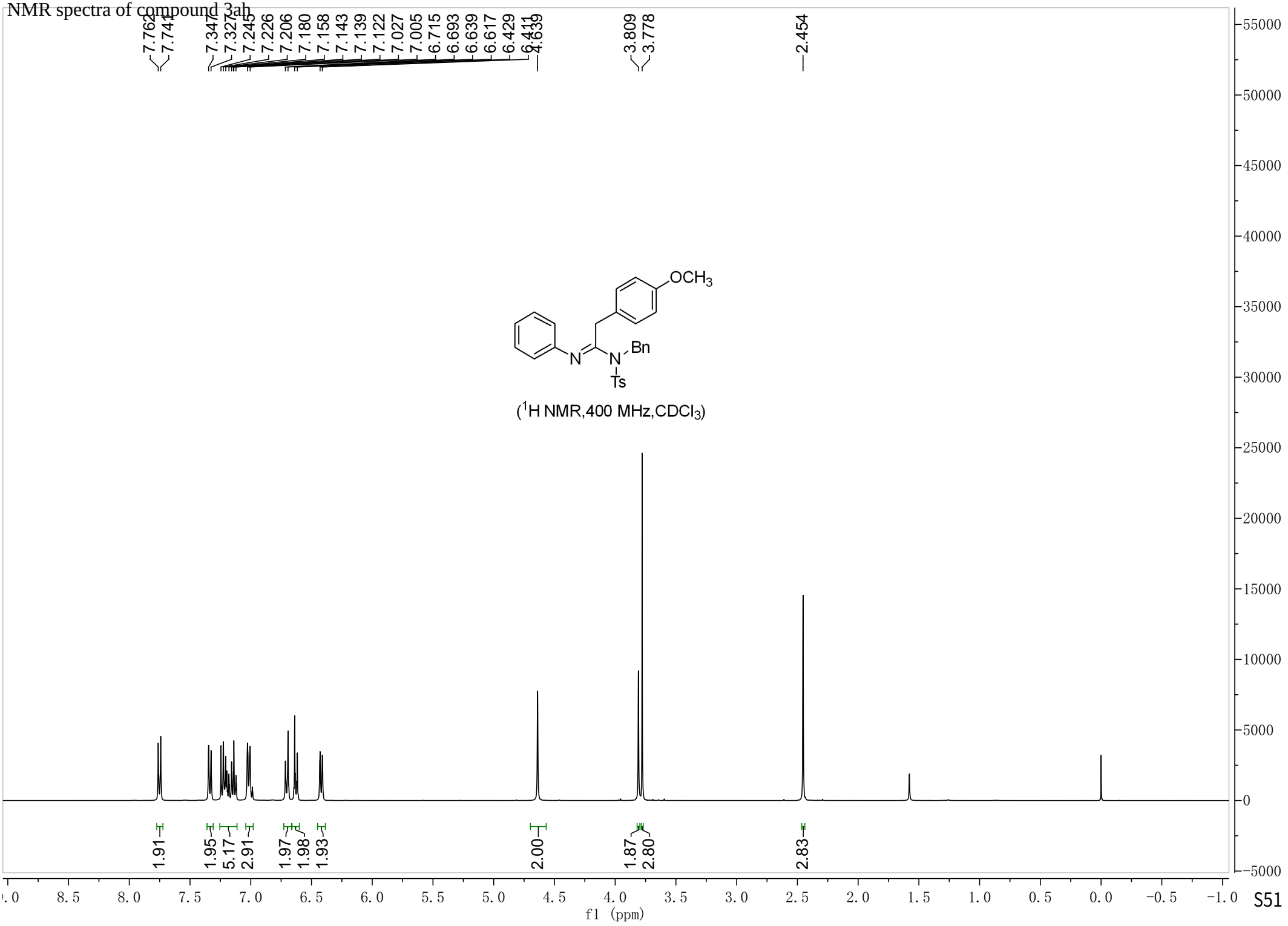
NMR spectra of compound 3ag



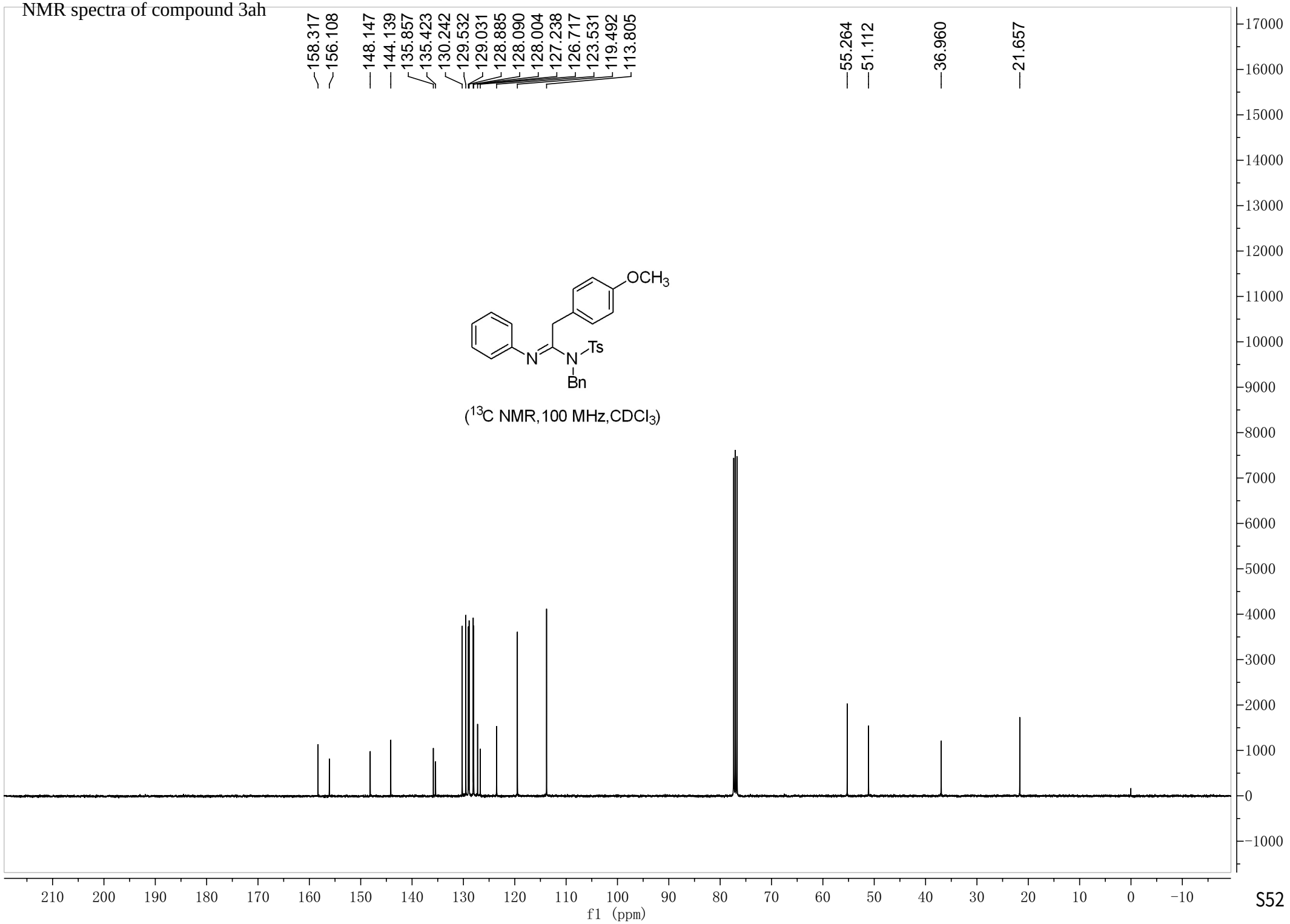
NMR spectra of compound 3ag



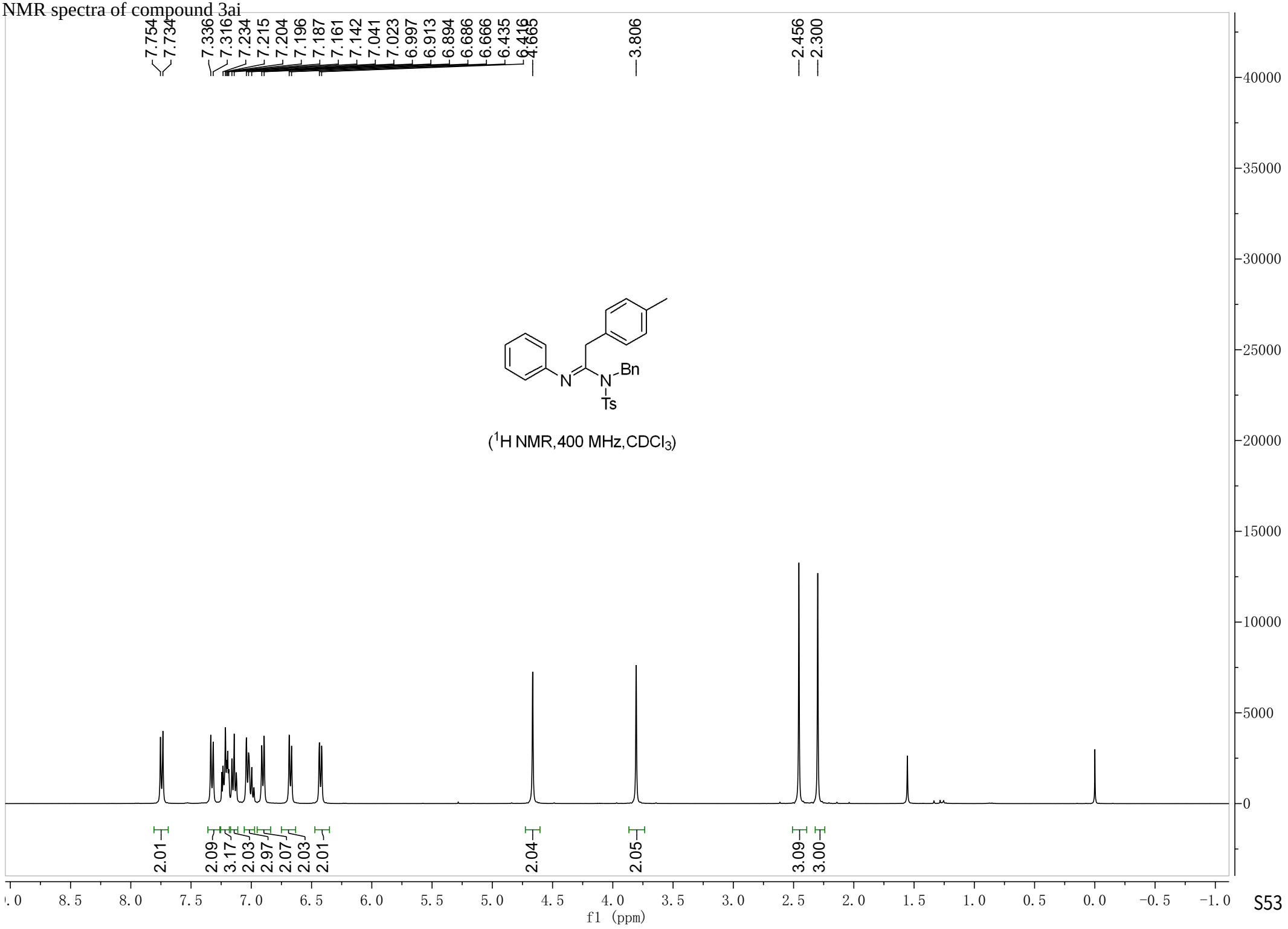
NMR spectra of compound 3ah



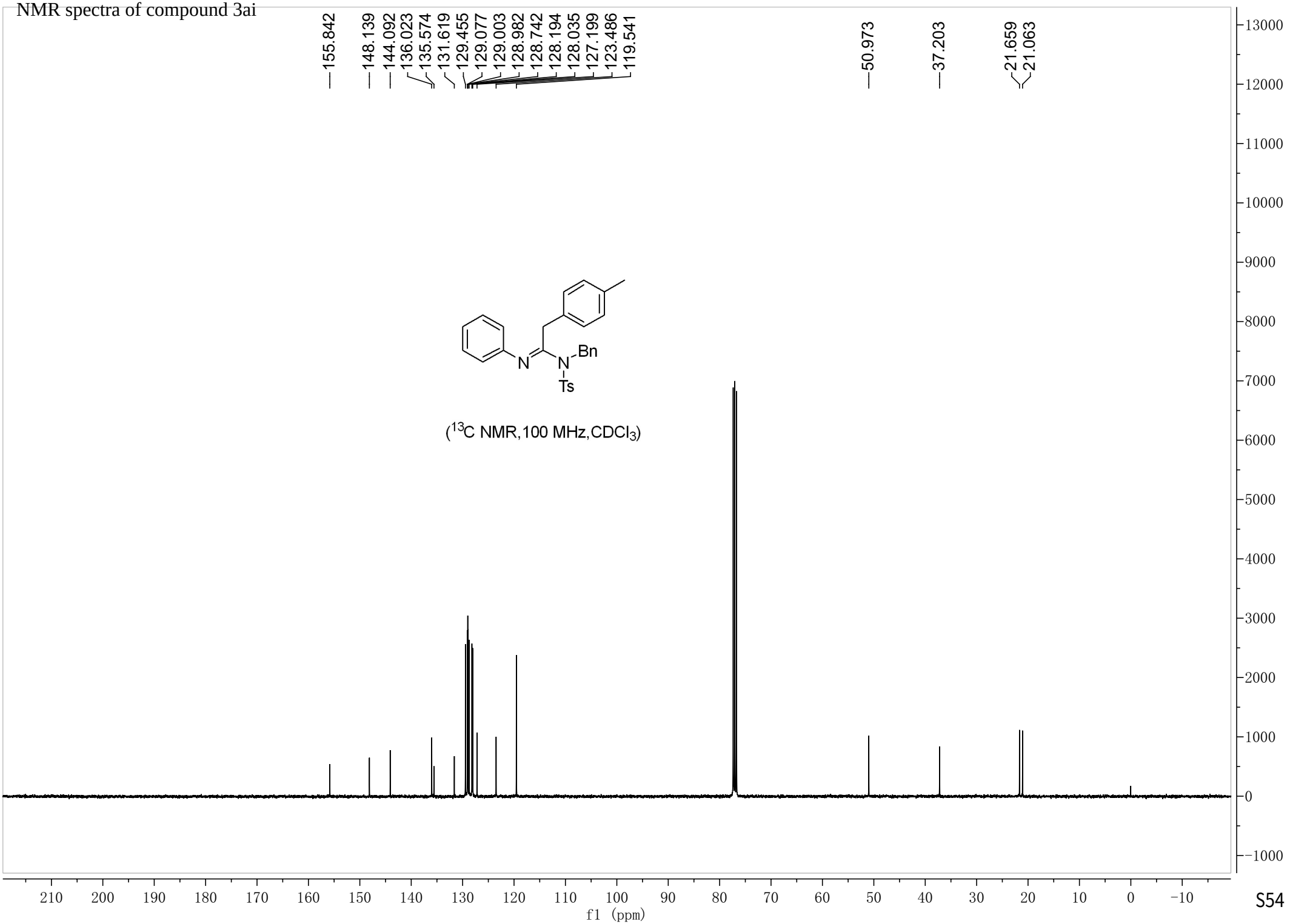
NMR spectra of compound 3ah



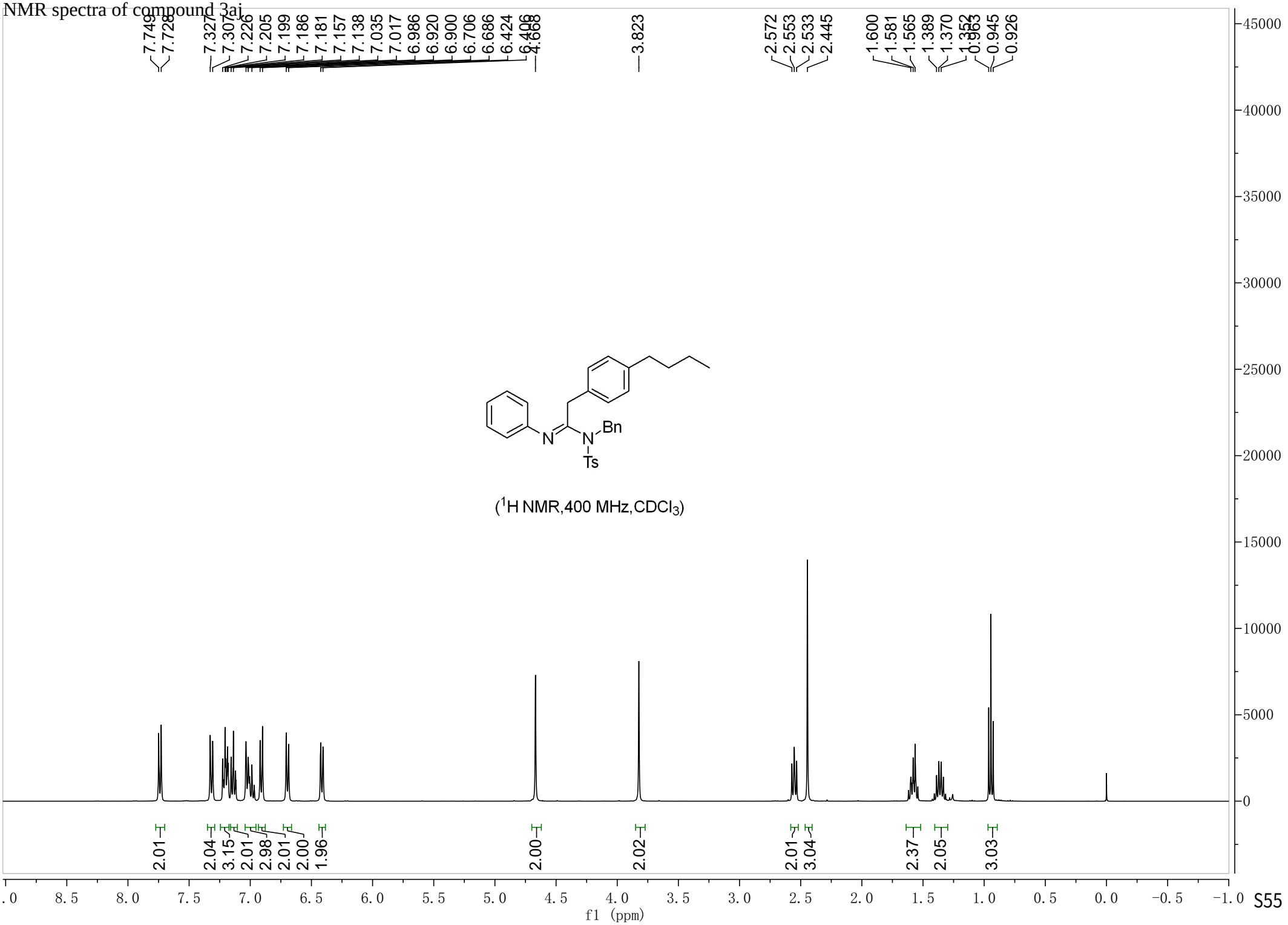
NMR spectra of compound 3ai



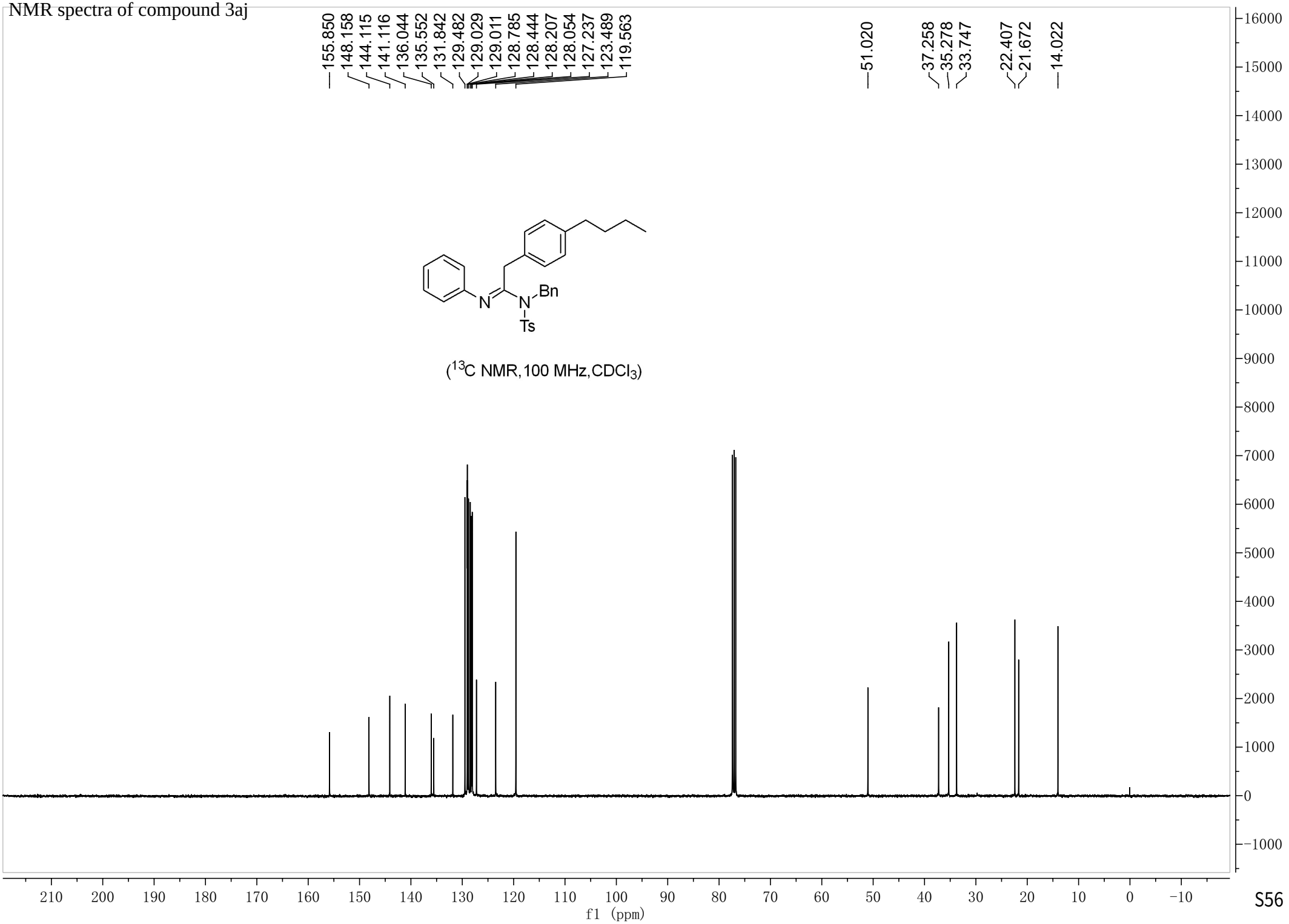
NMR spectra of compound 3ai



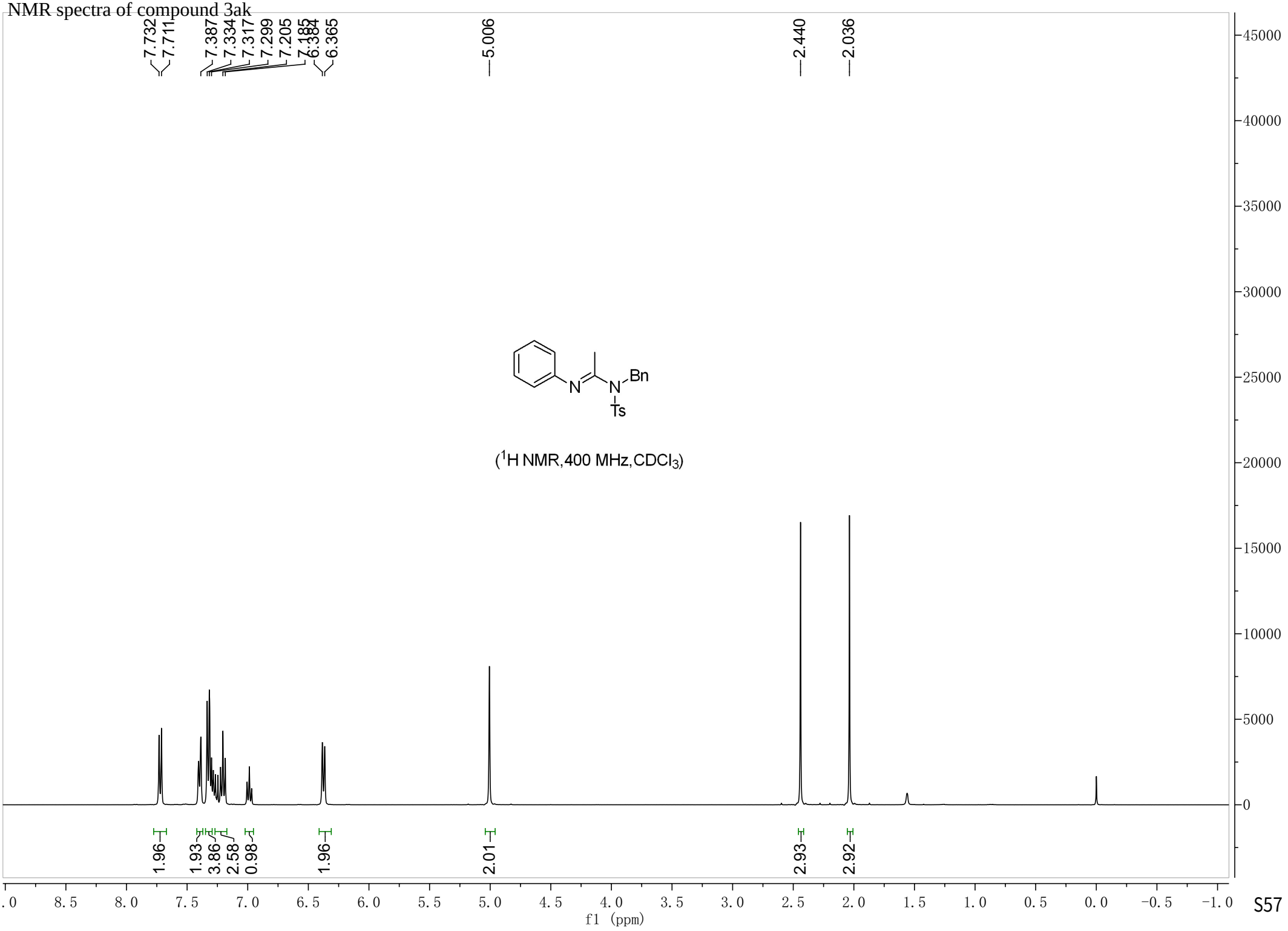
NMR spectra of compound 3aj



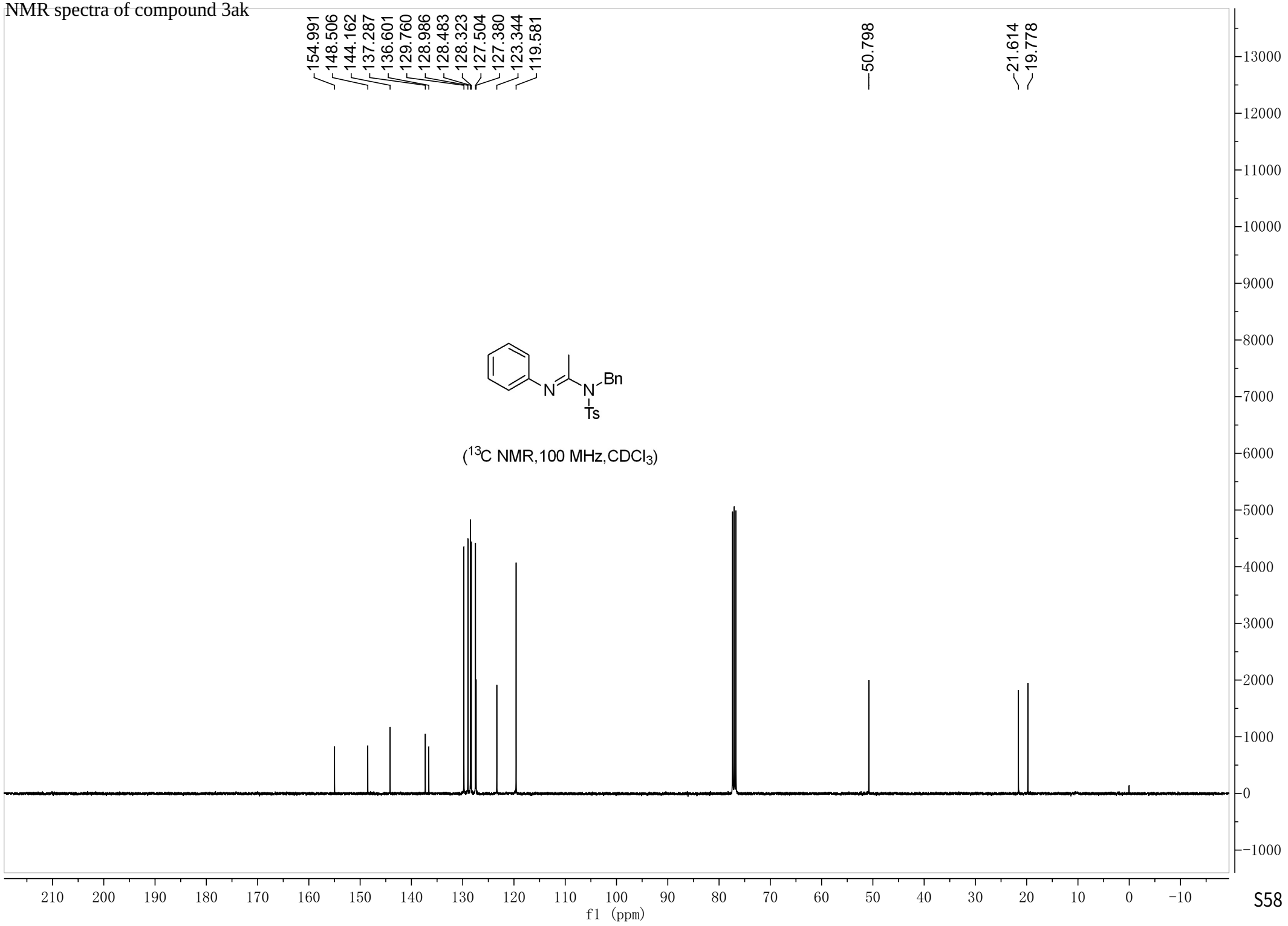
NMR spectra of compound 3aj



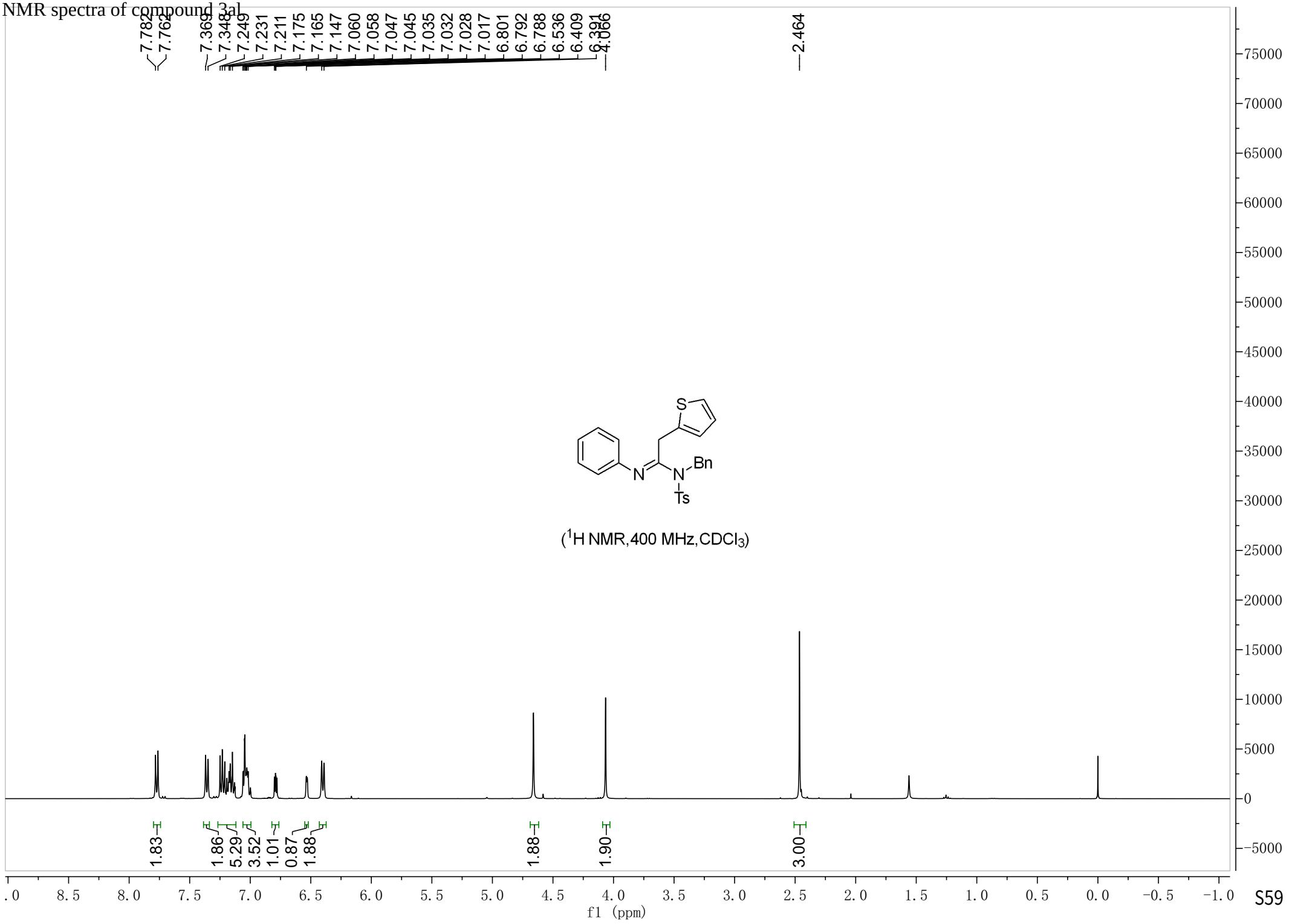
NMR spectra of compound 3ak



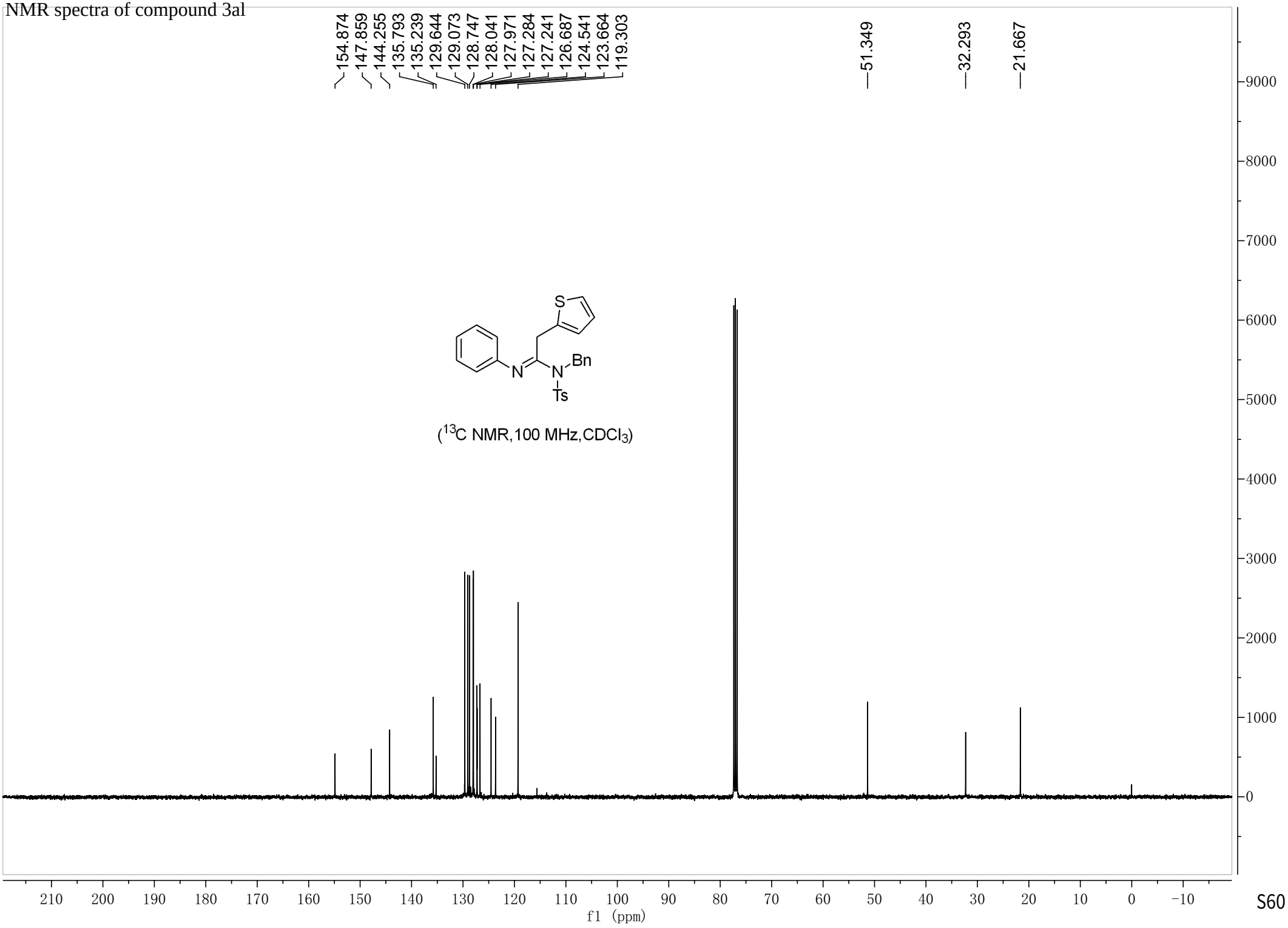
NMR spectra of compound 3ak



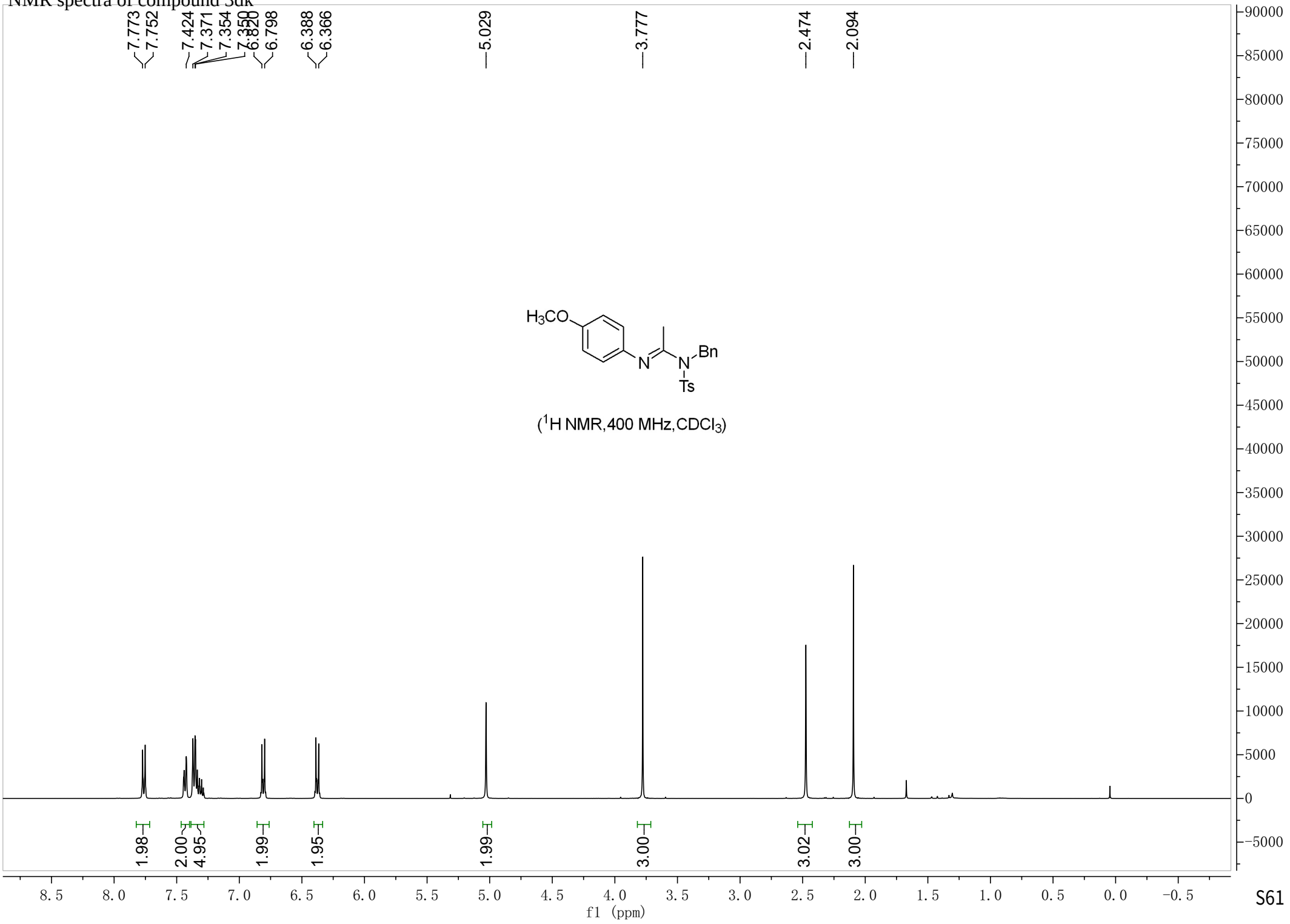
NMR spectra of compound 3al



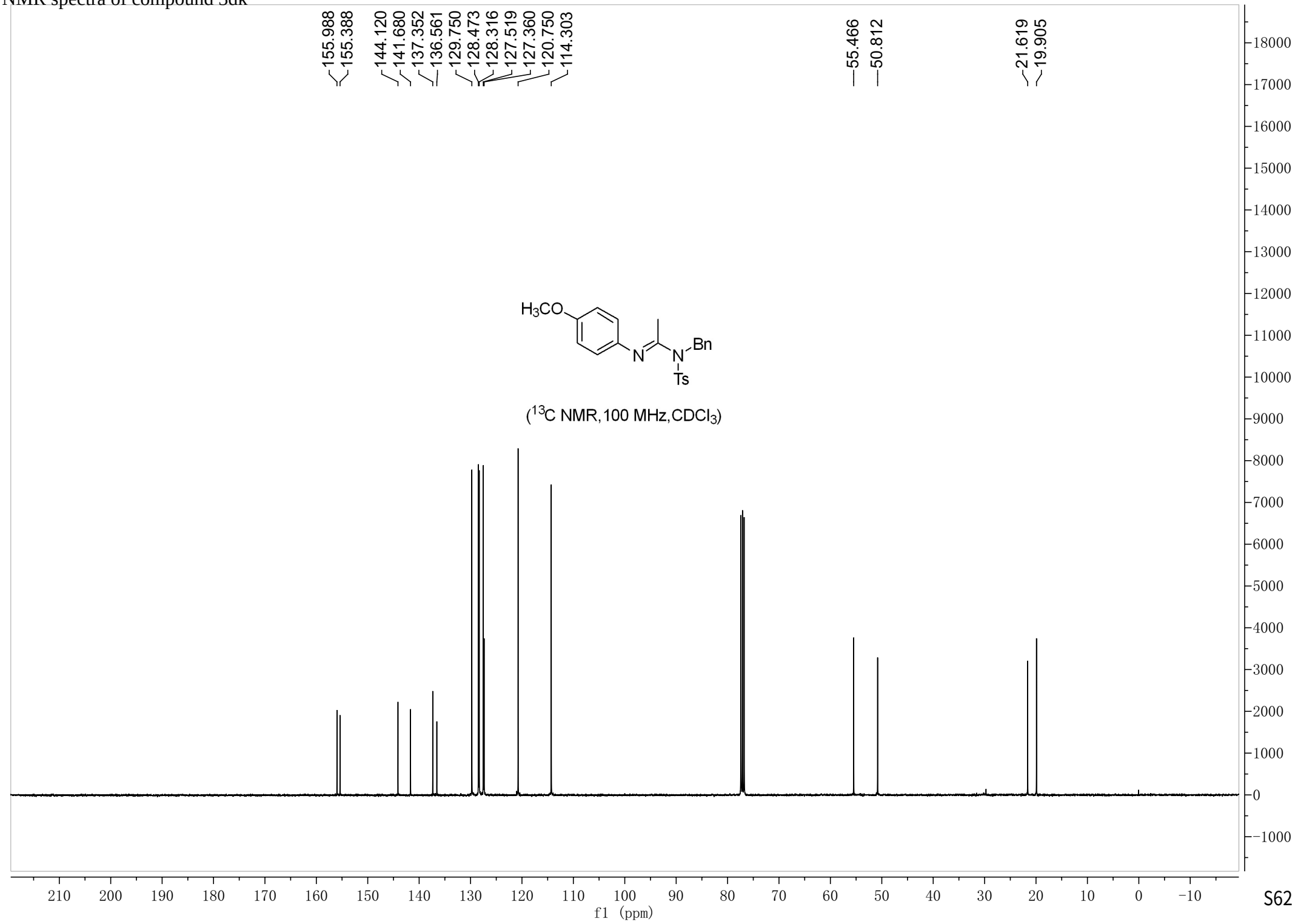
NMR spectra of compound 3al



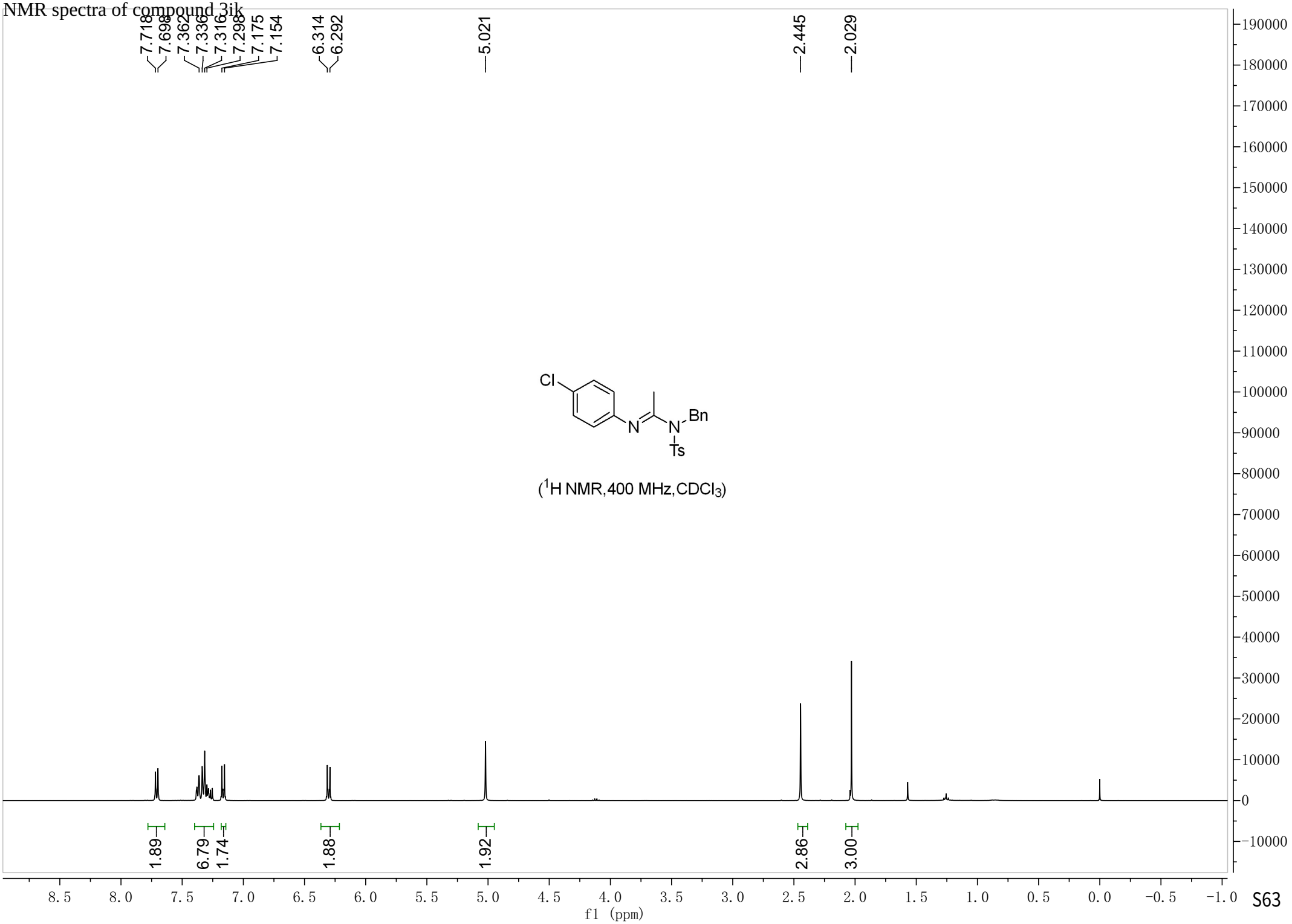
NMR spectra of compound 3dk



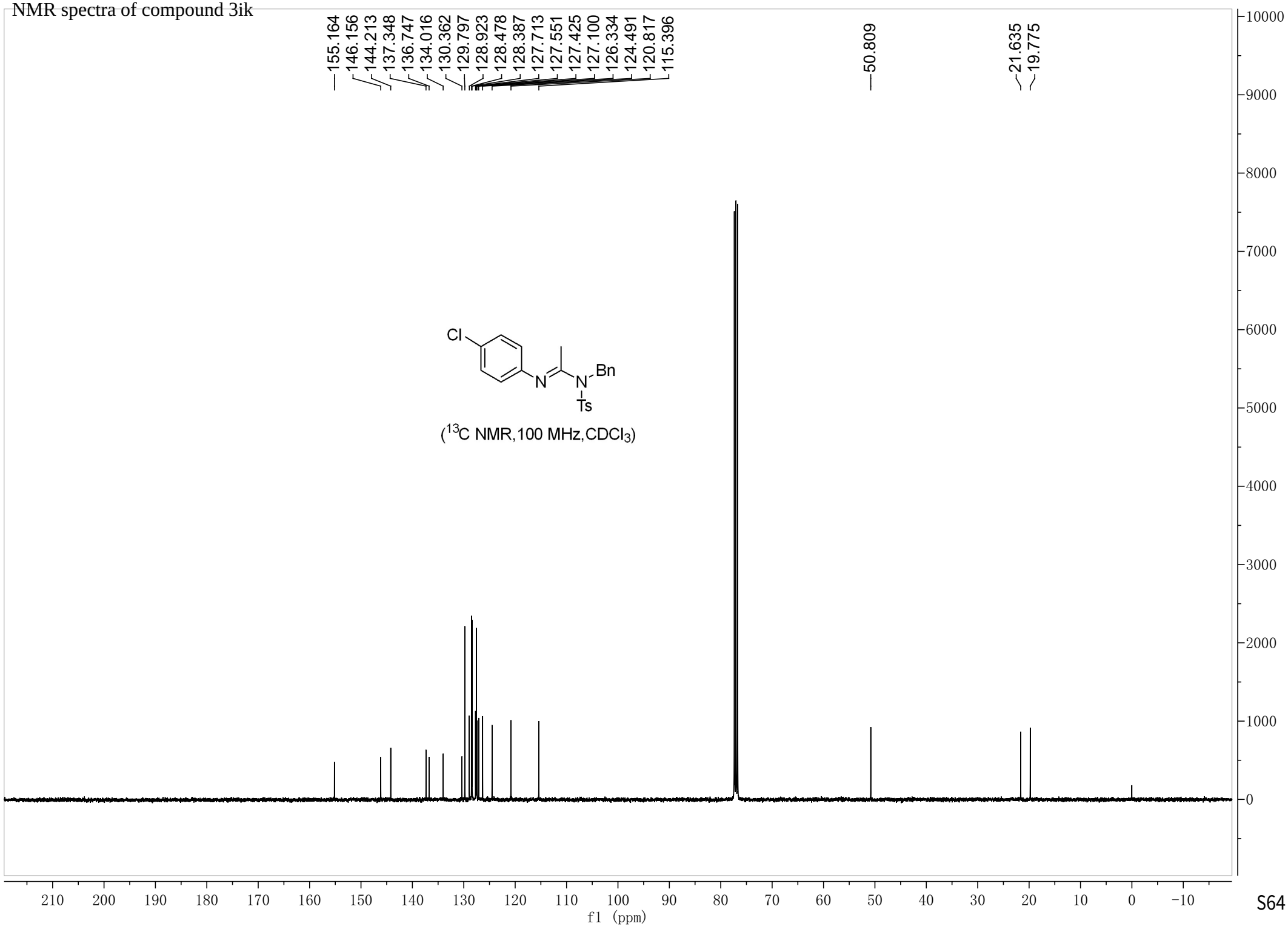
NMR spectra of compound 3dk



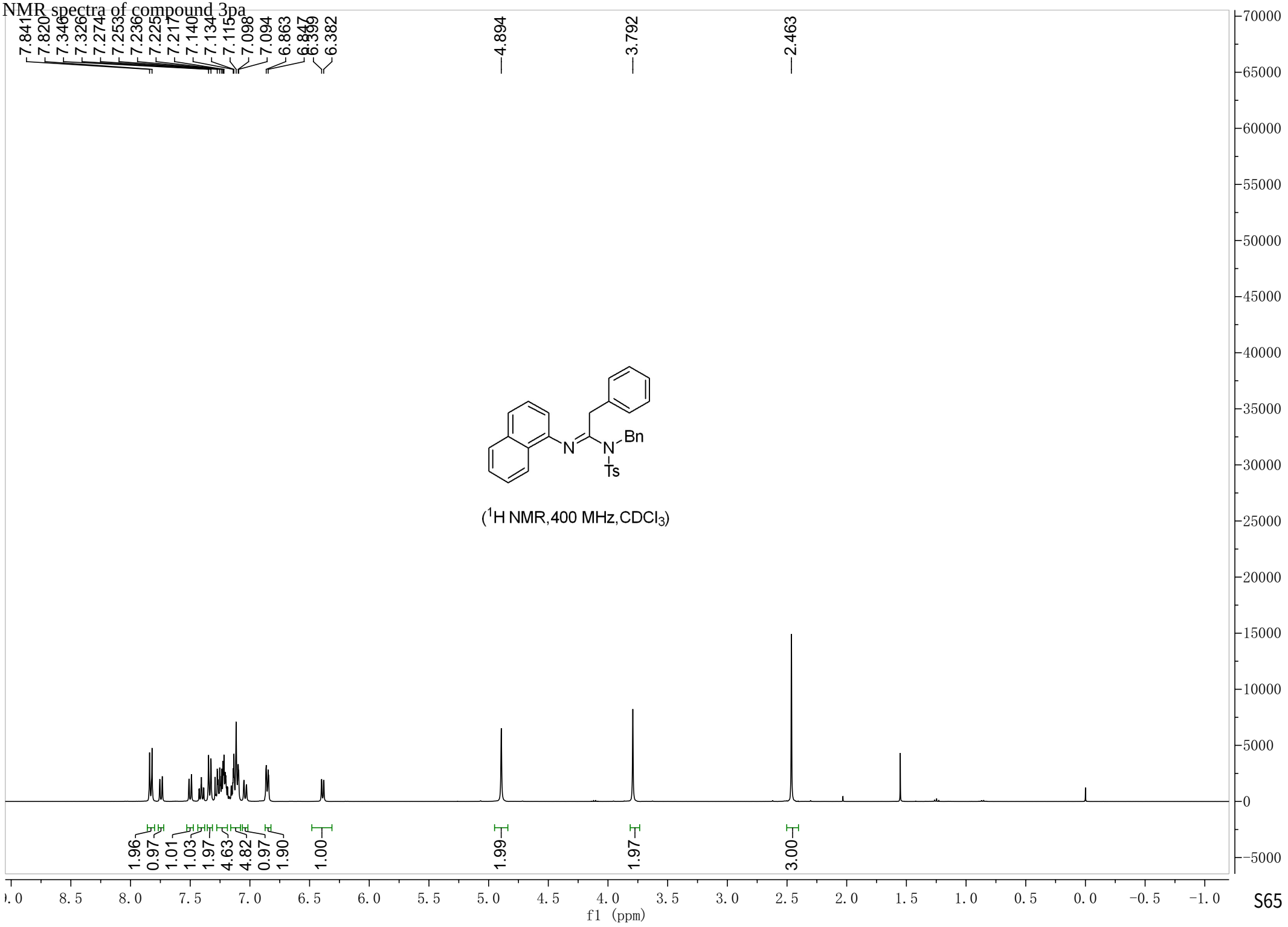
NMR spectra of compound 3ik



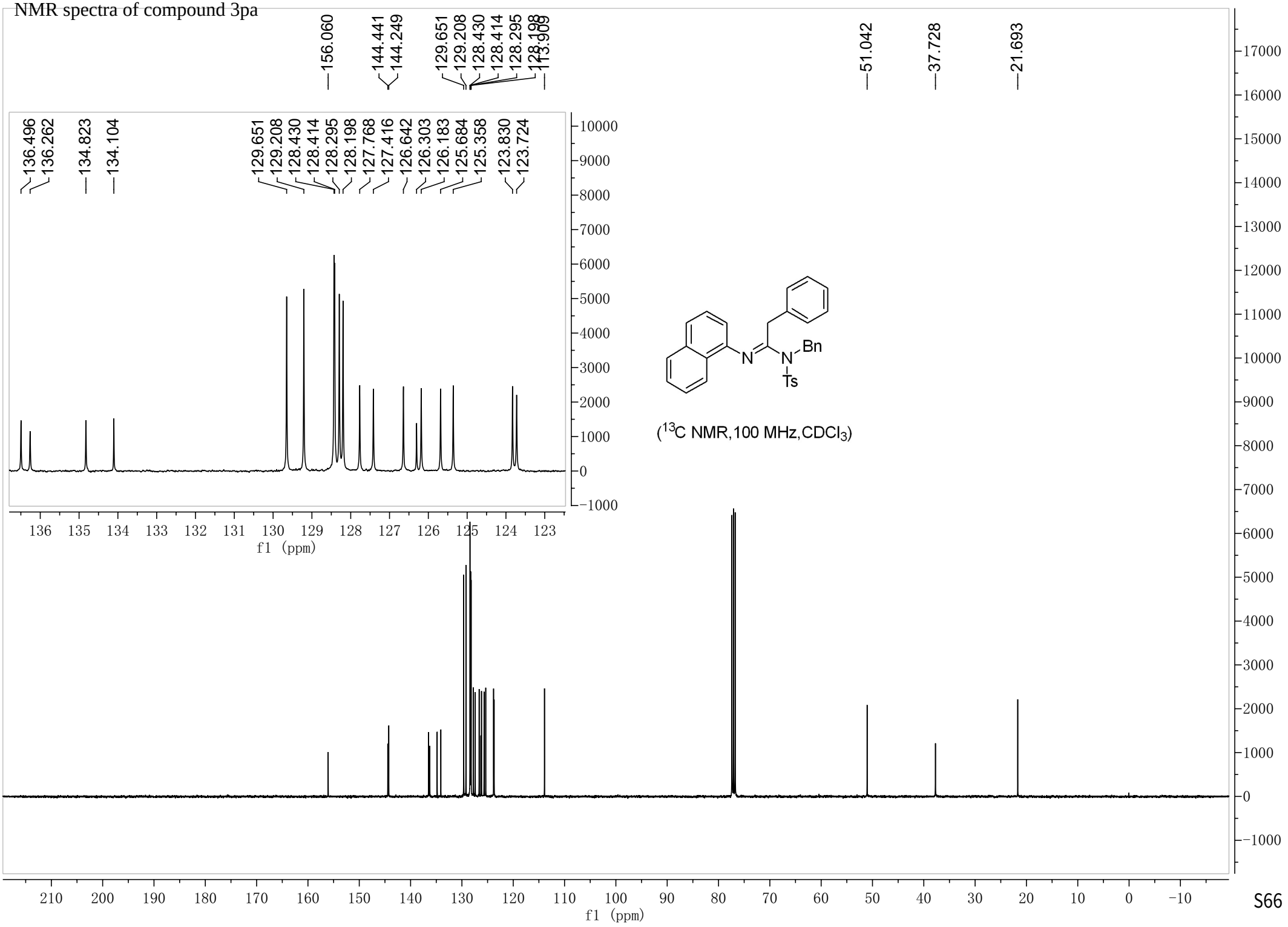
NMR spectra of compound 3ik



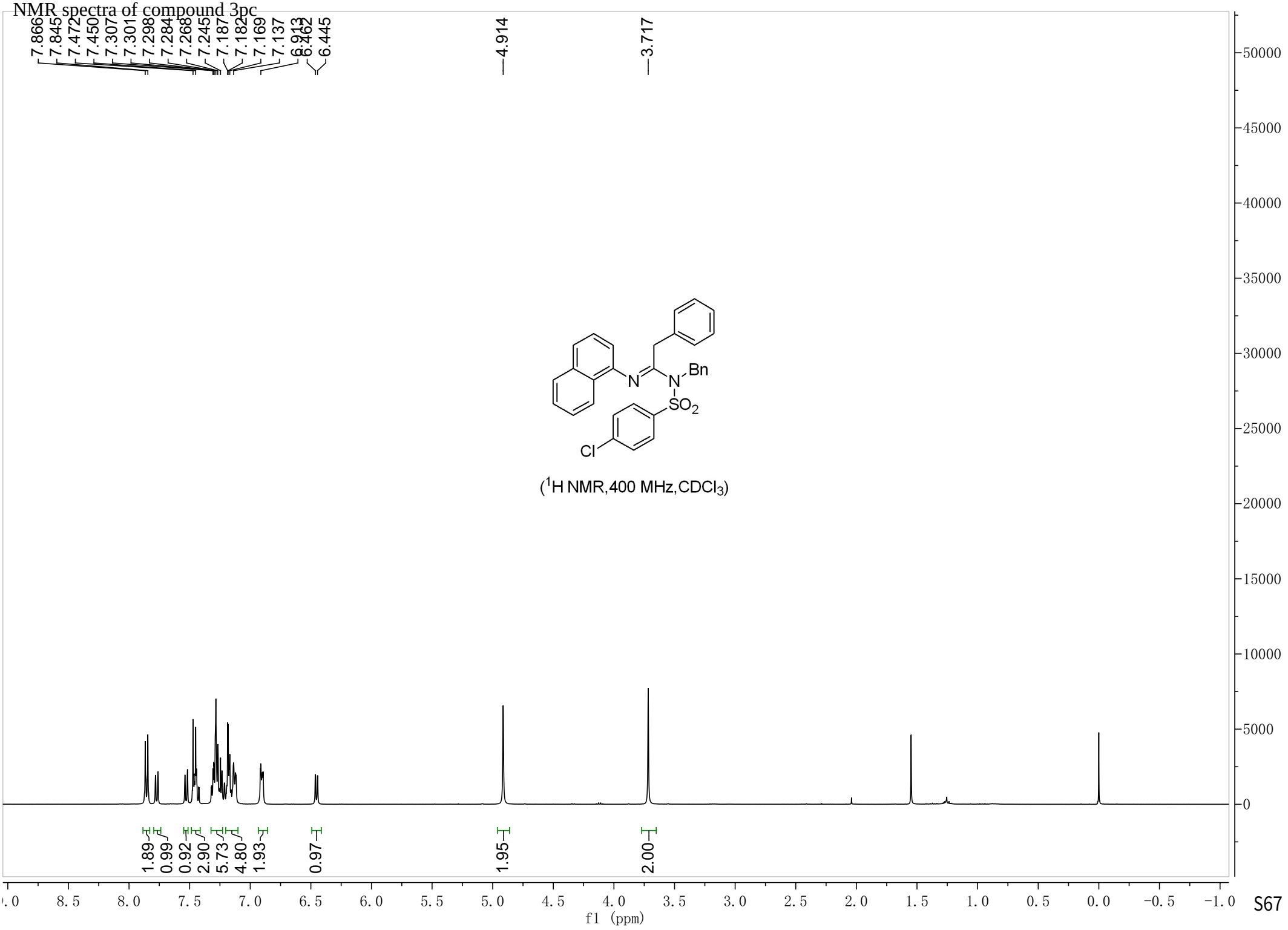
NMR spectra of compound 3pa



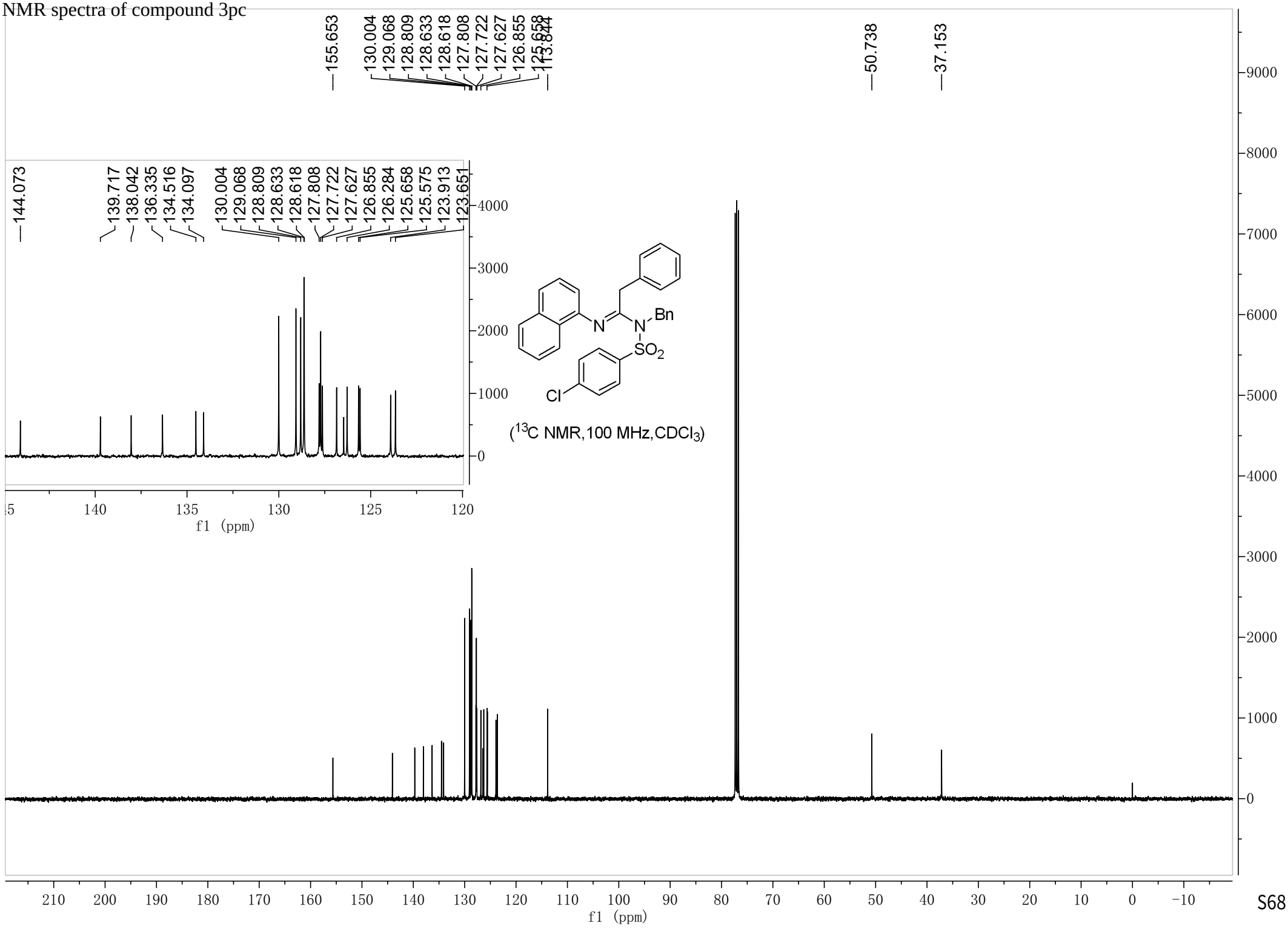
NMR spectra of compound 3pa



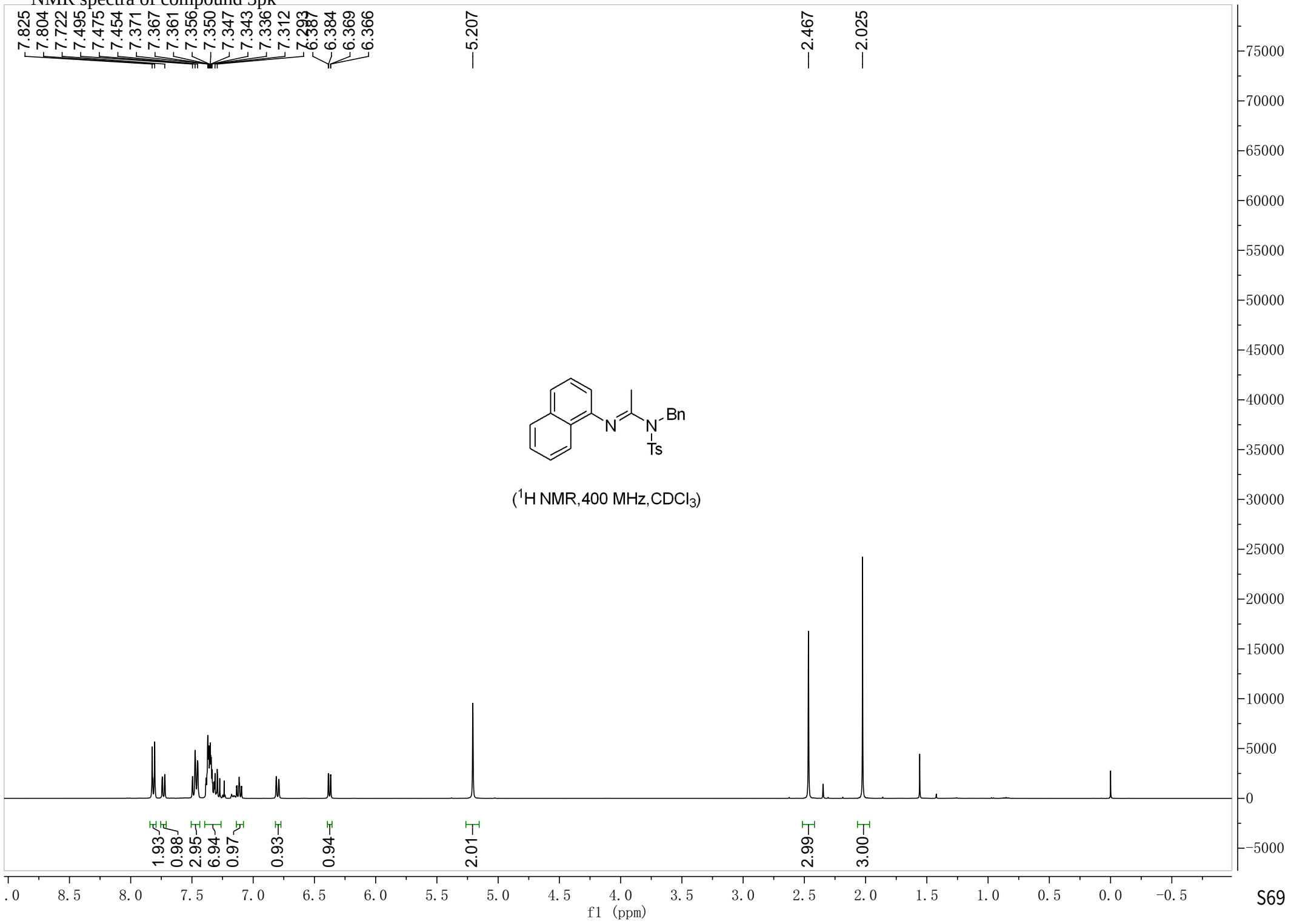
NMR spectra of compound 3pc



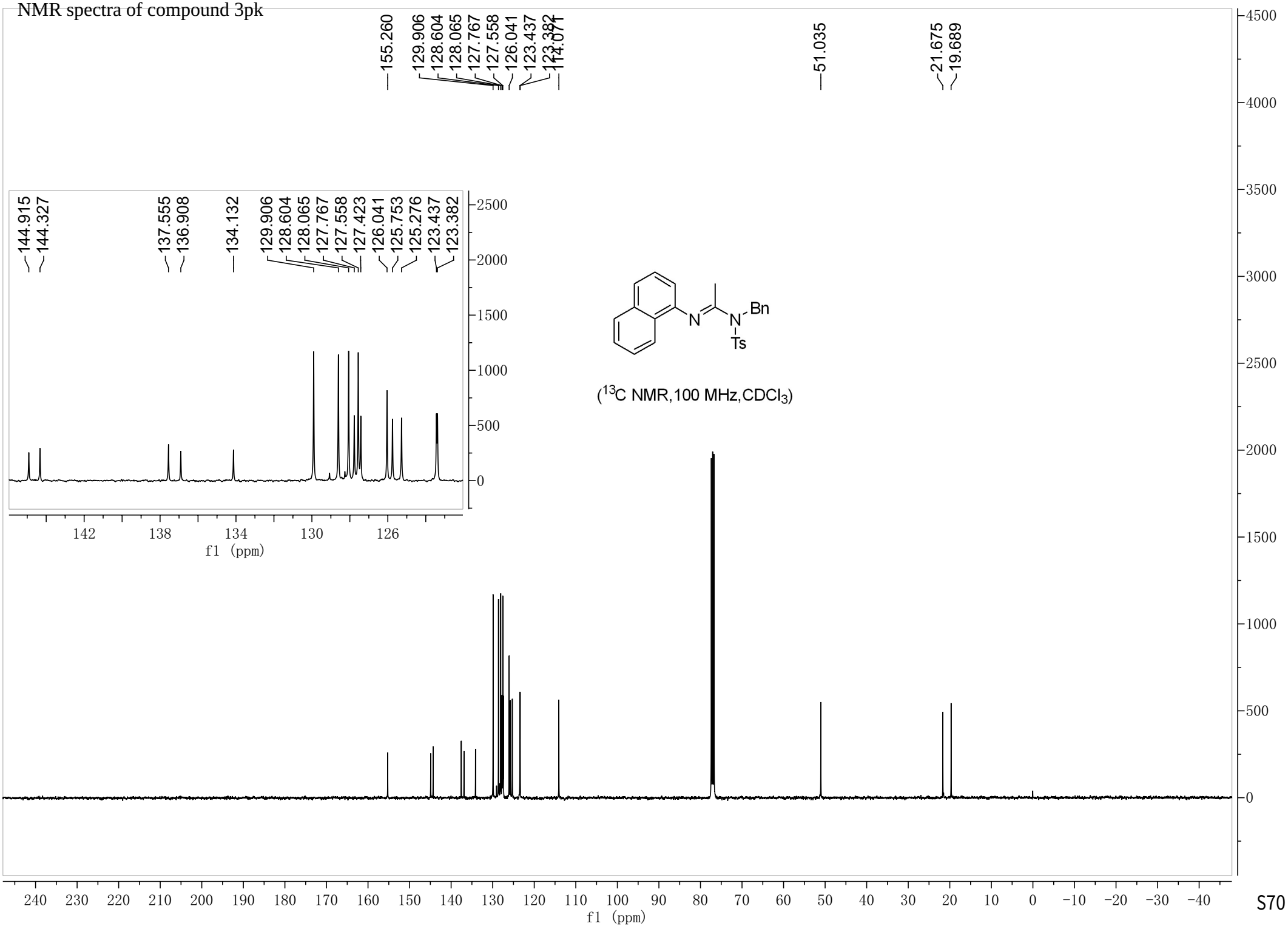
NMR spectra of compound 3pc



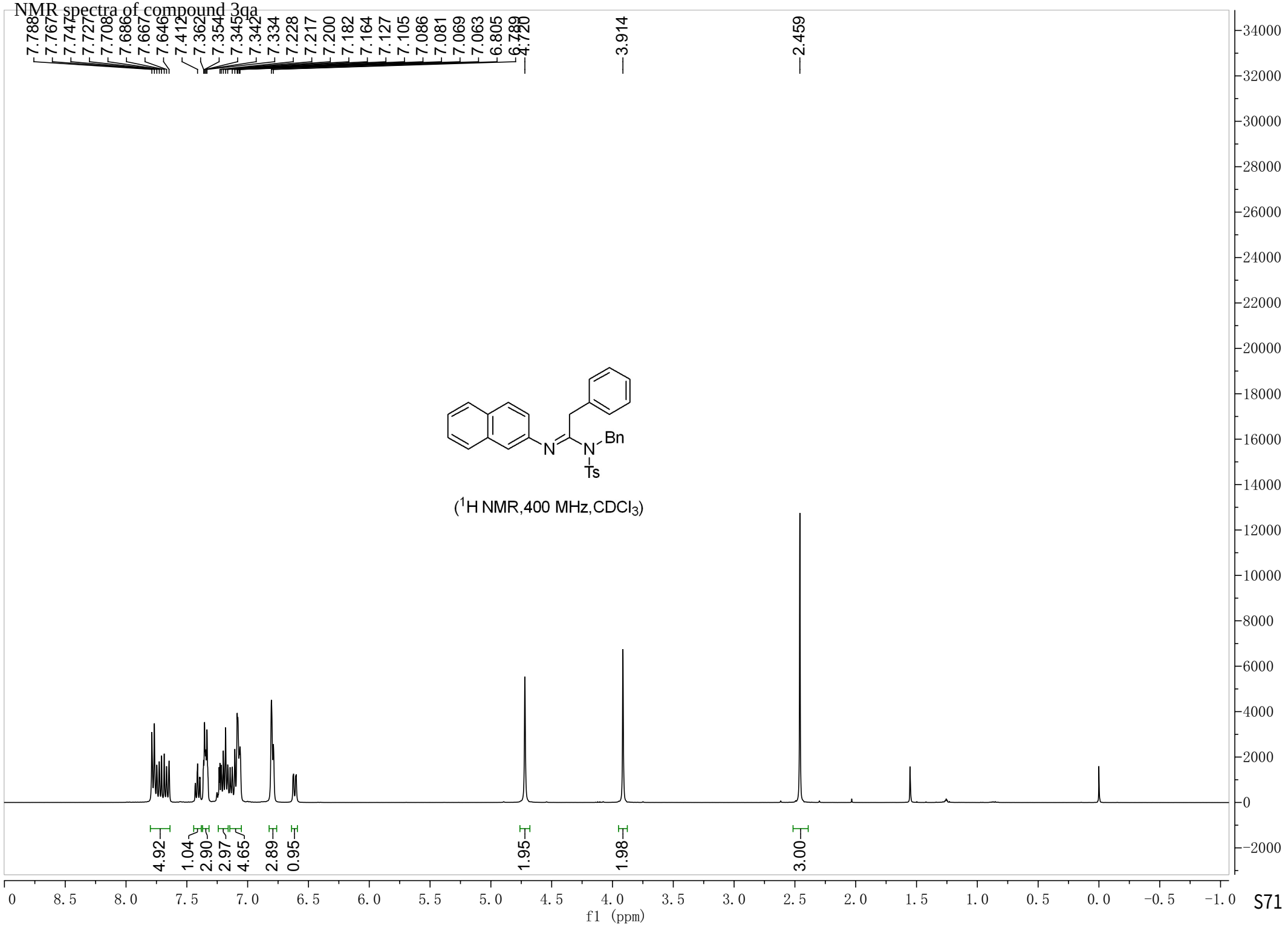
NMR spectra of compound 3pk



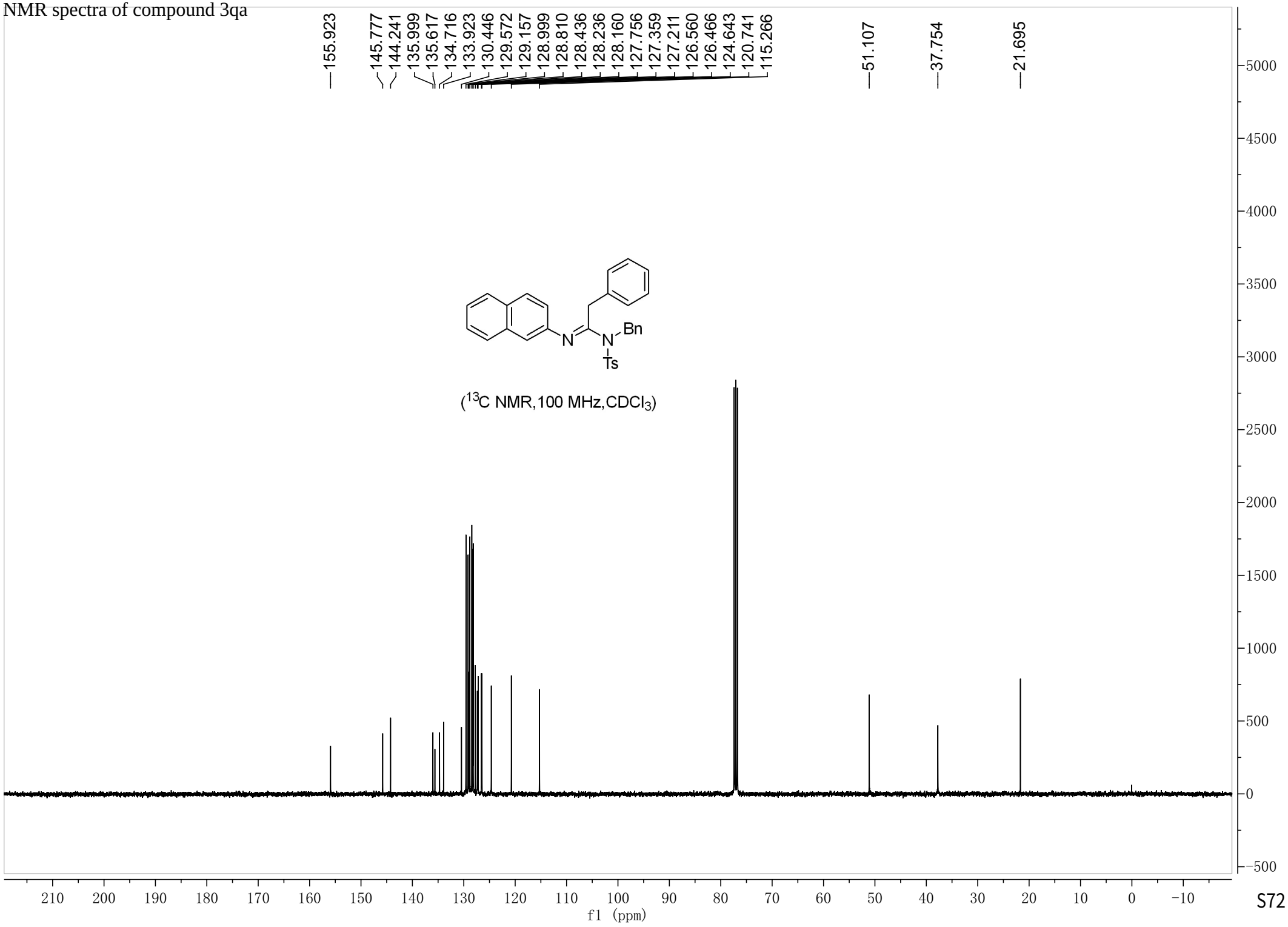
NMR spectra of compound 3pk



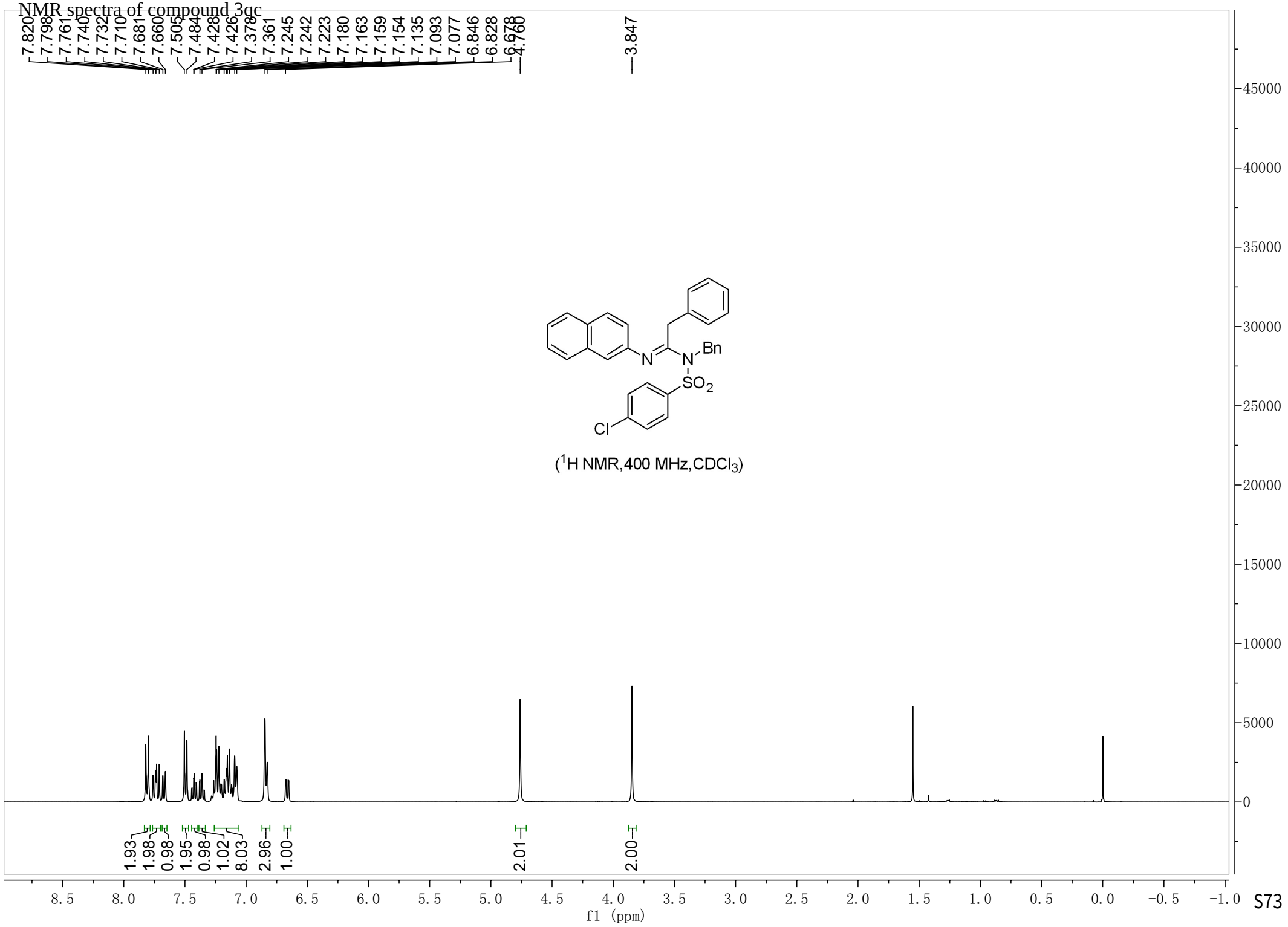
NMR spectra of compound 3qa



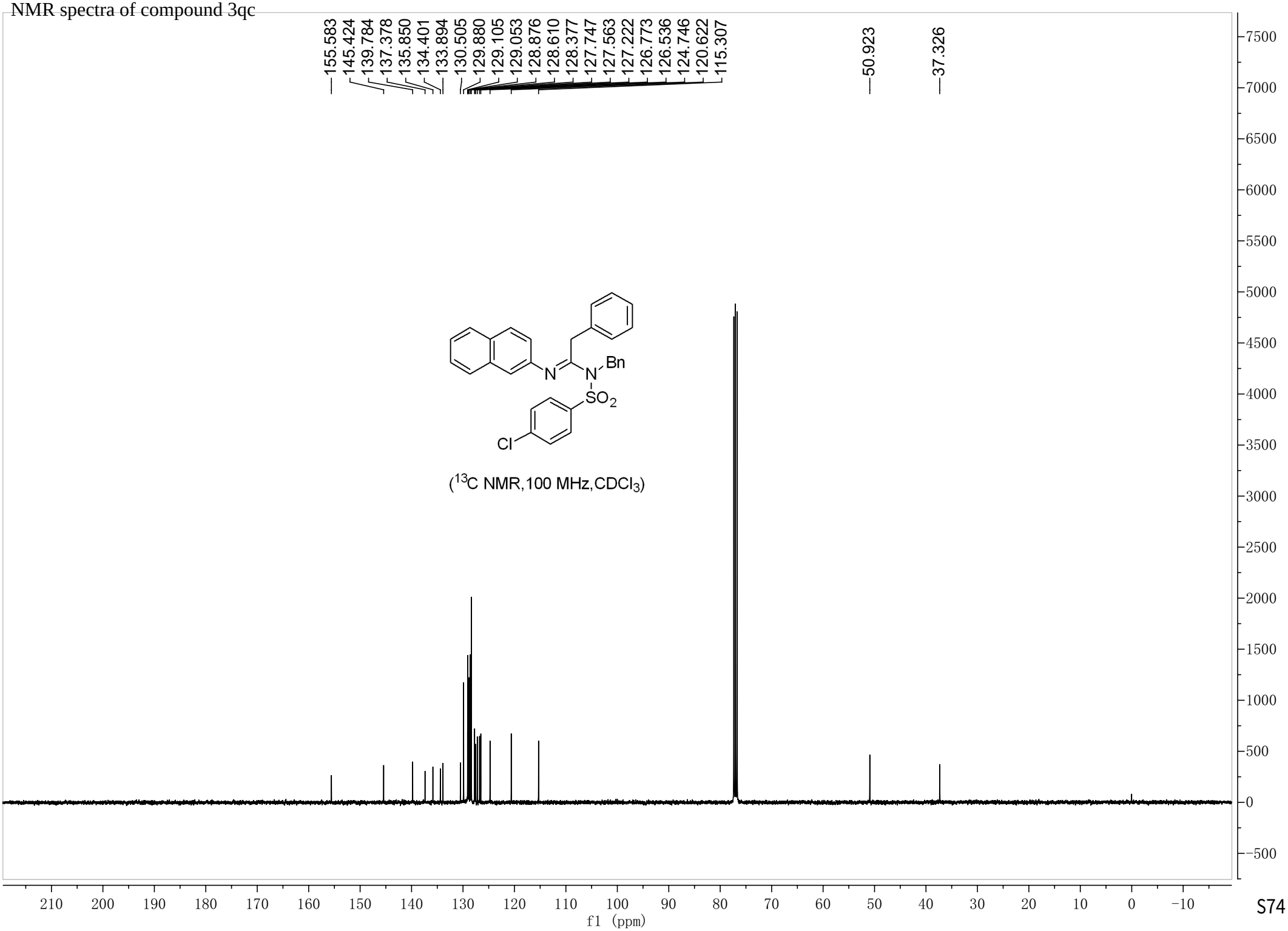
NMR spectra of compound 3qa



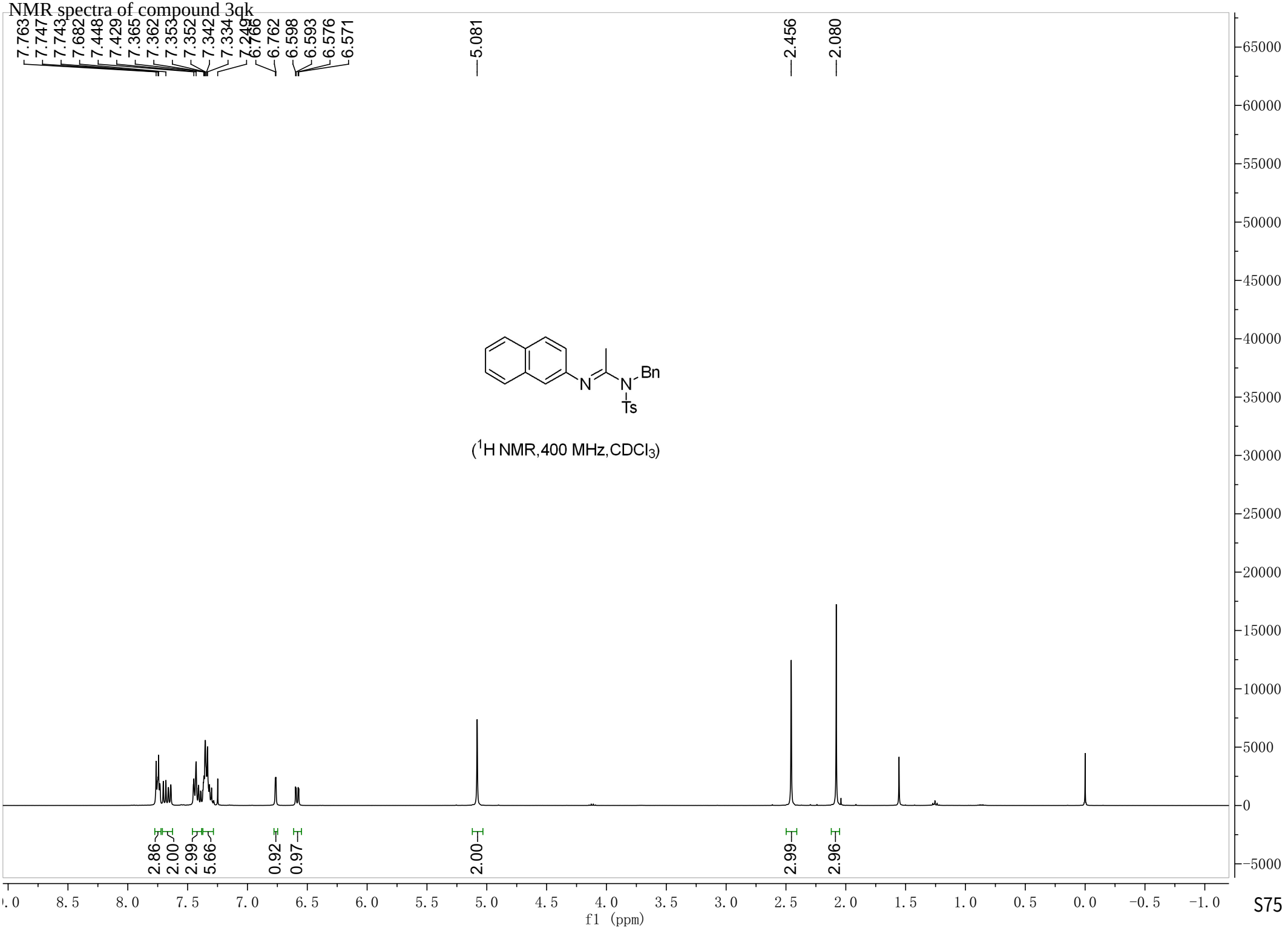
NMR spectra of compound 3qc



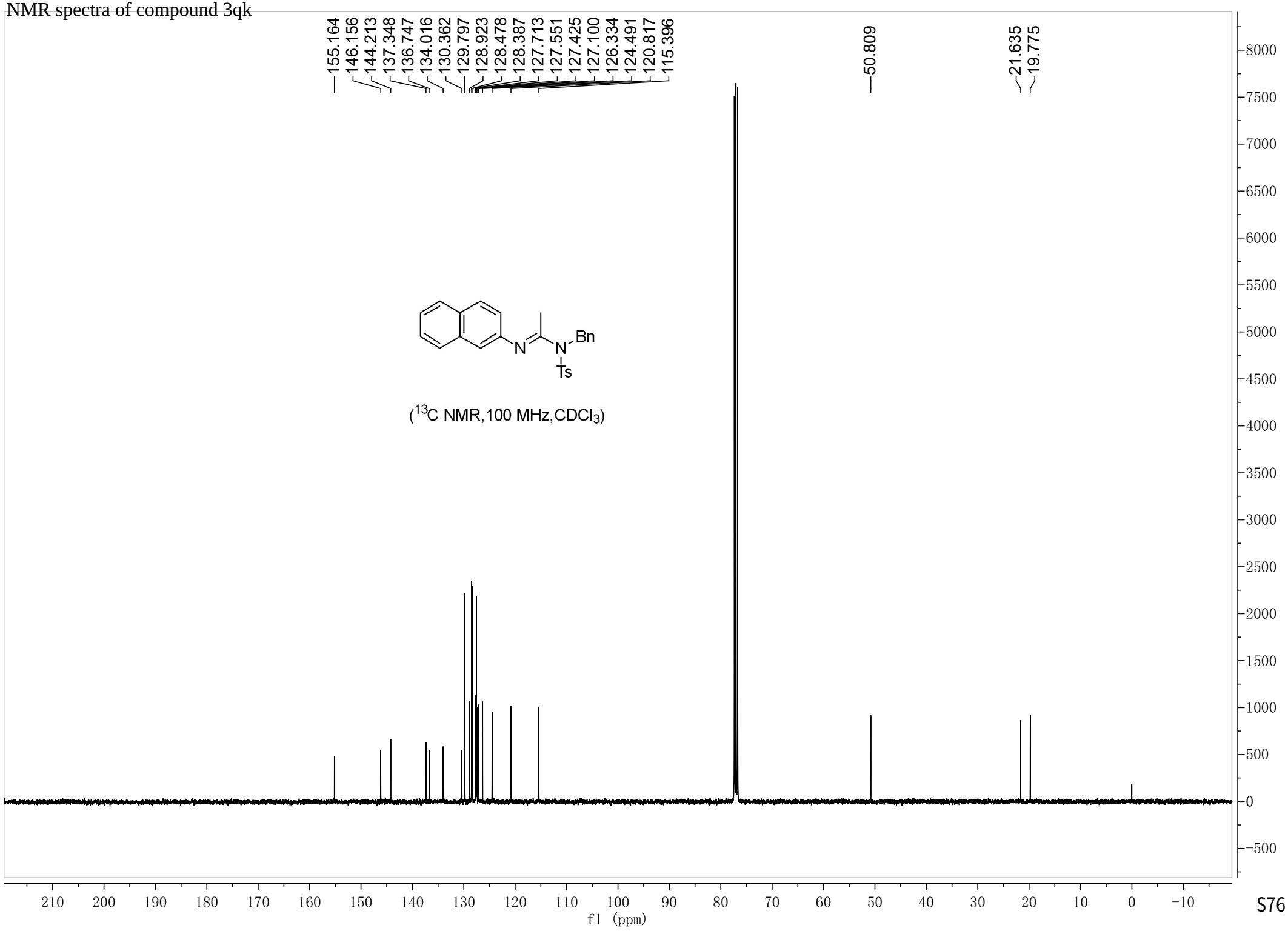
NMR spectra of compound 3qc



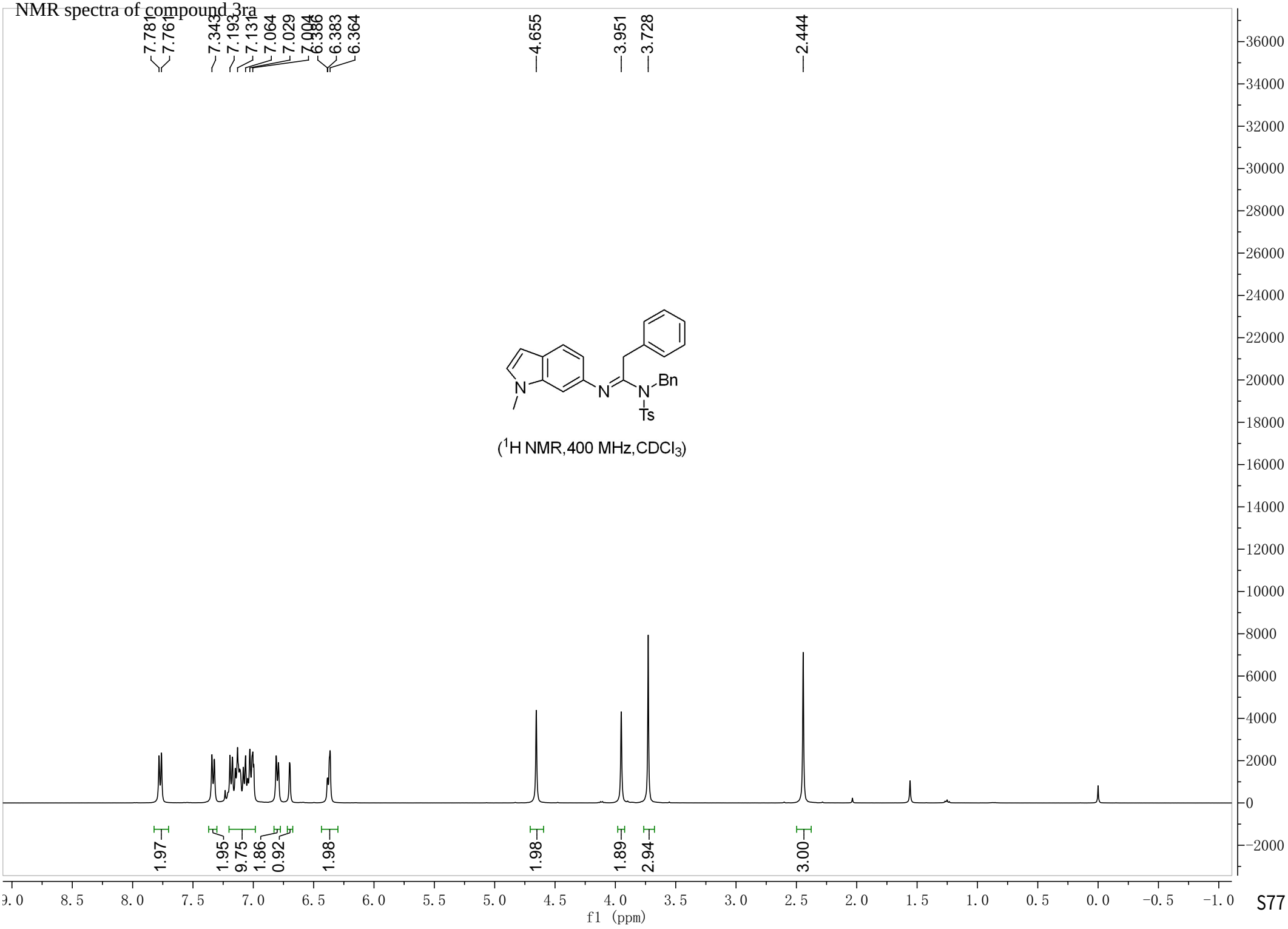
NMR spectra of compound 3qk



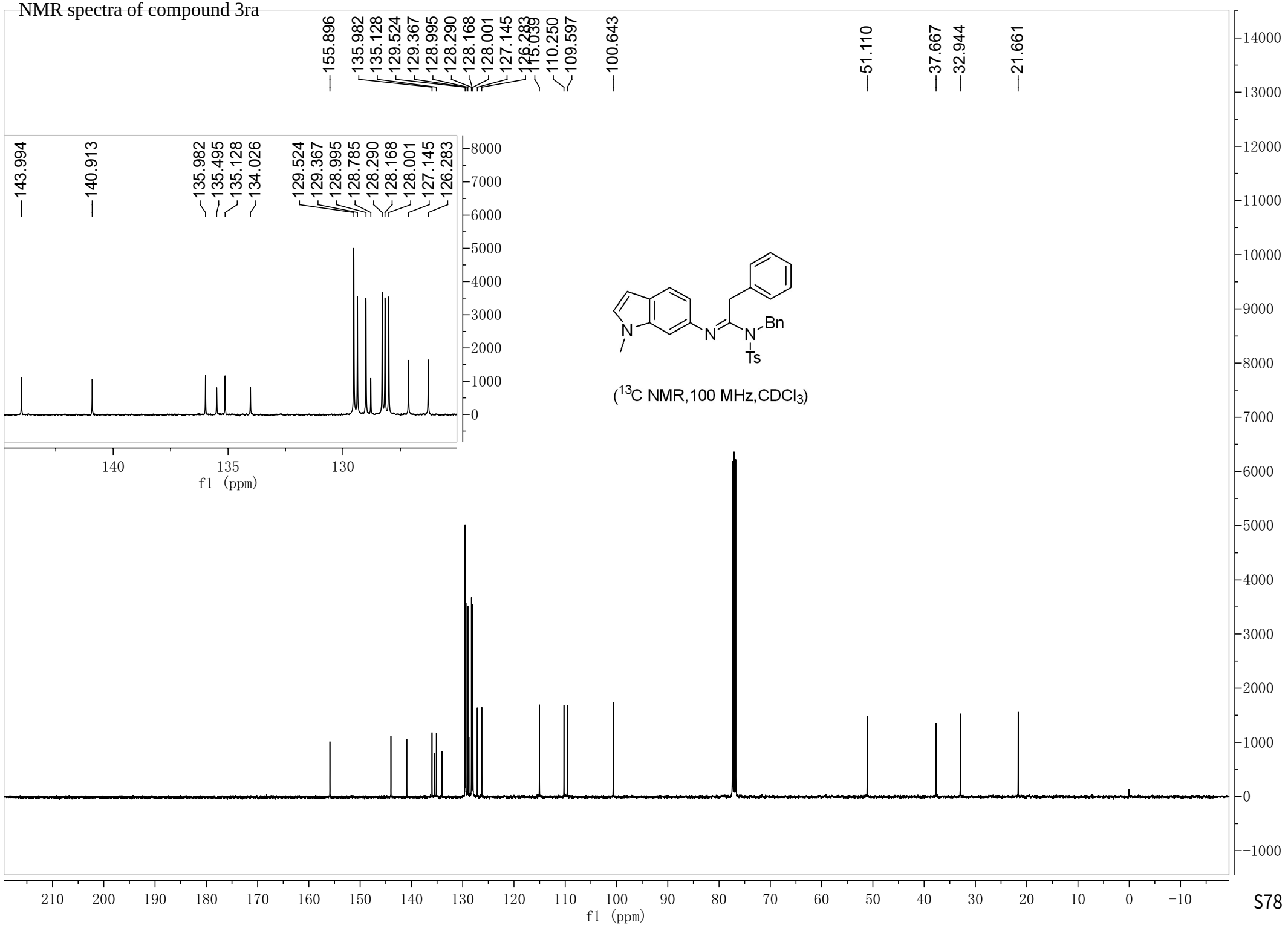
NMR spectra of compound 3qk



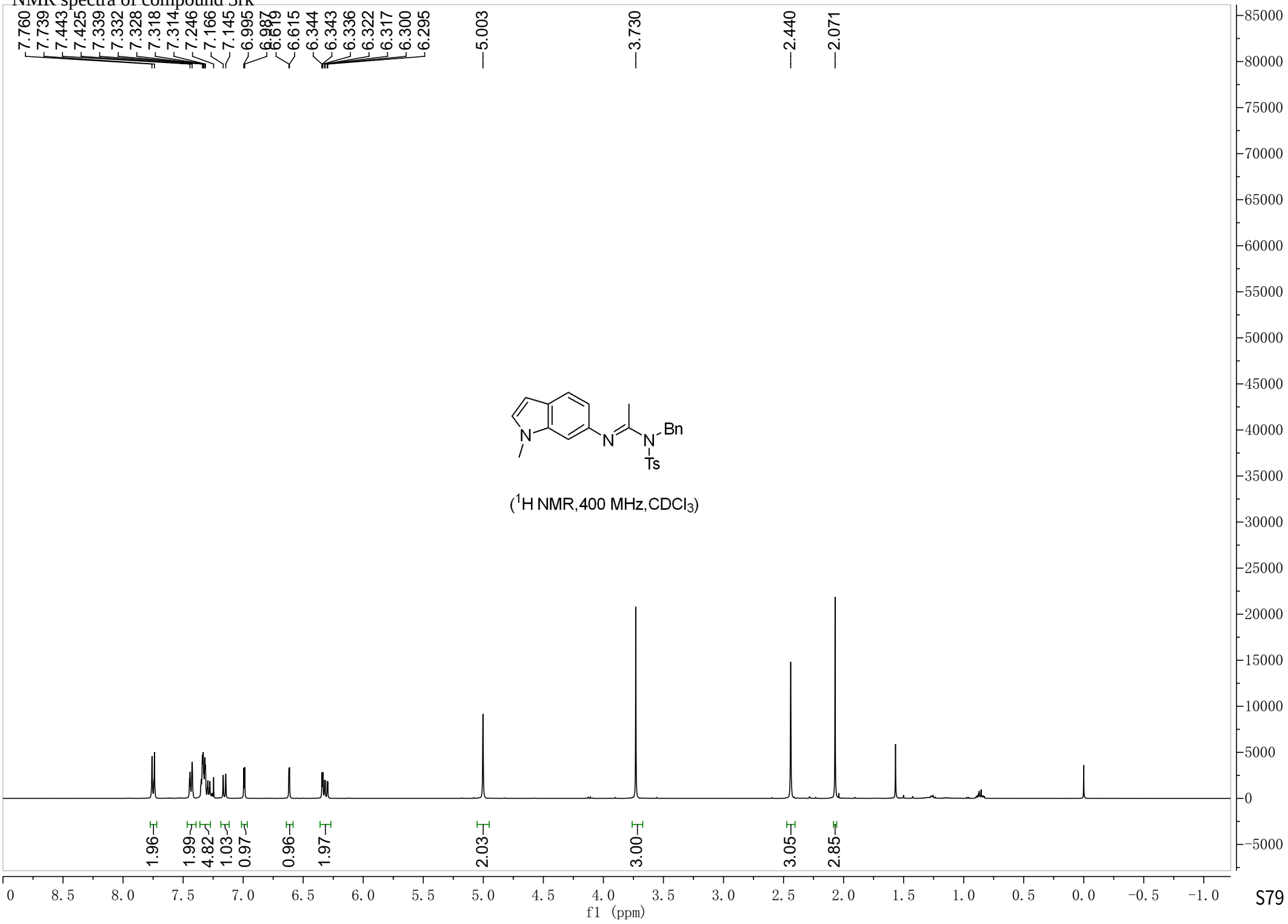
NMR spectra of compound 3ra



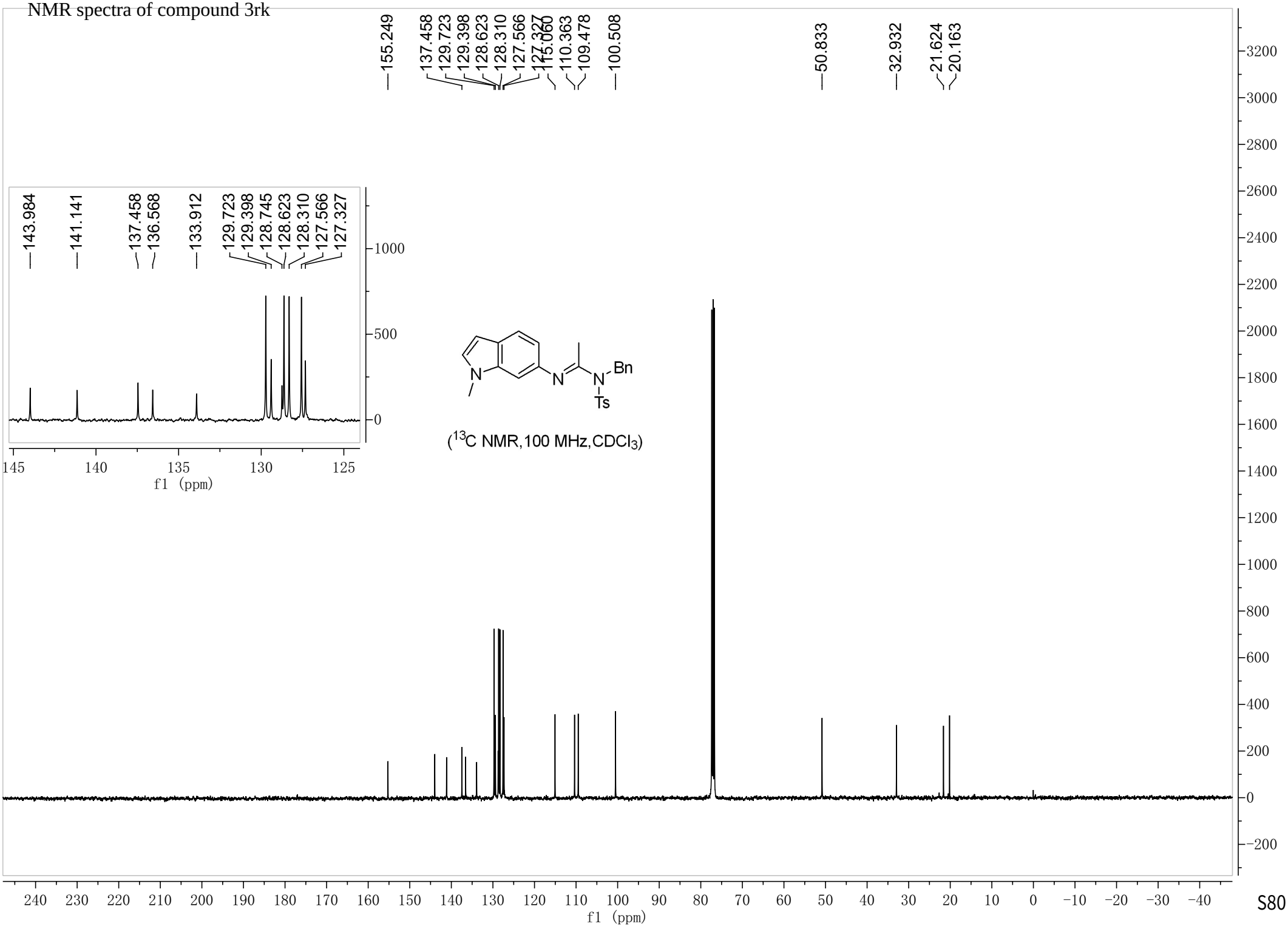
NMR spectra of compound 3ra



NMR spectra of compound 3rk



NMR spectra of compound 3rk



NMR spectra of compound 4