Supporting Information

New Journal of Chemistry

Electrochemical Synthesis of 1-*N*-phenyl-4-(arylsulfonyl)benzene-1,2-diamine Derivatives. A Mild and Regioselective Protocol

Mahnaz Sharafi-Kolkeshvandi,[a] Davood Nematollahi,*[b] Farzad Nikpour,[a] and Eslam Salahifar[b]

[a]Department of Chemistry, Faculty of Sciences, University of Kurdistan, P.O. Box 66315-416, Sanandaj, Iran.

[b]Faculty of Chemistry, Bu-Ali-Sina University, Hamedan 65174, Iran.

nemat@basu.ac.ir.

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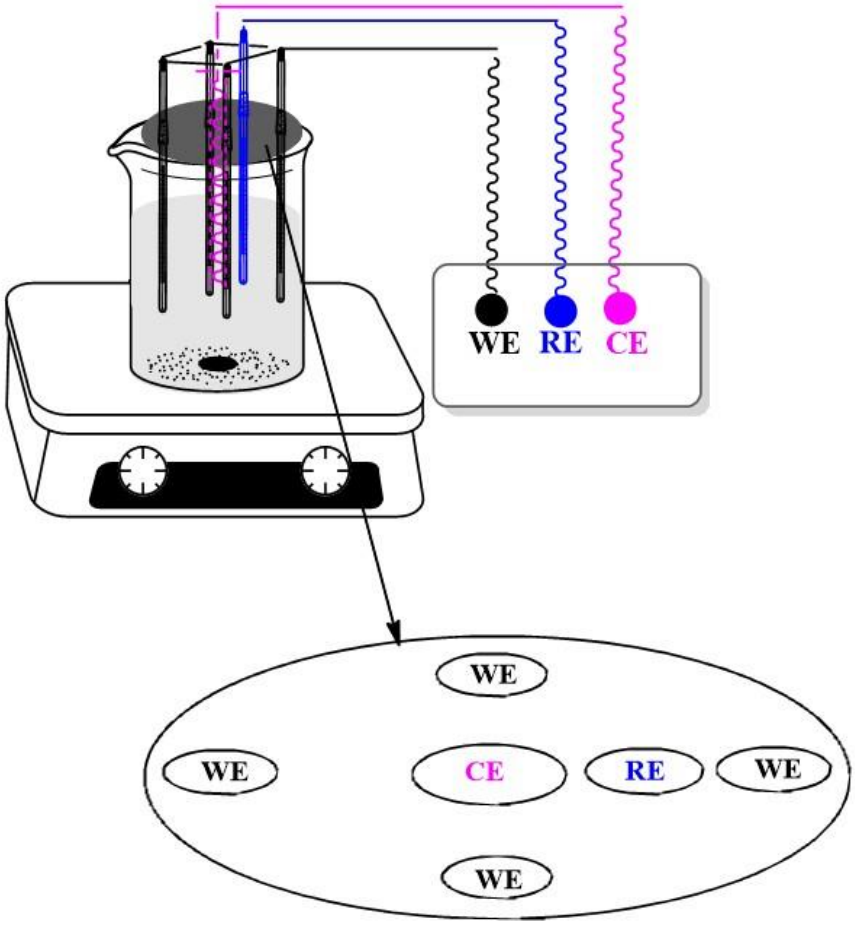
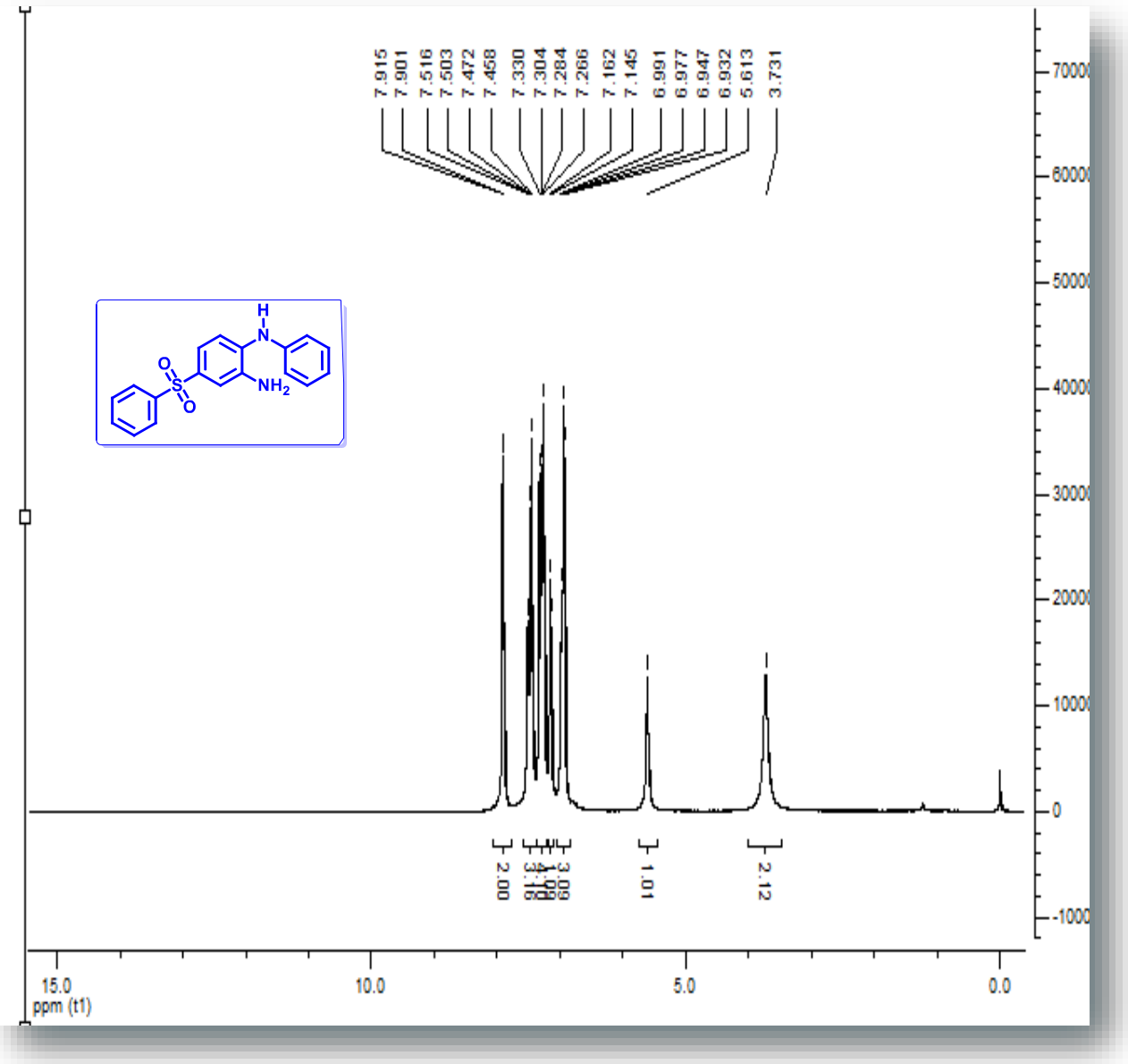
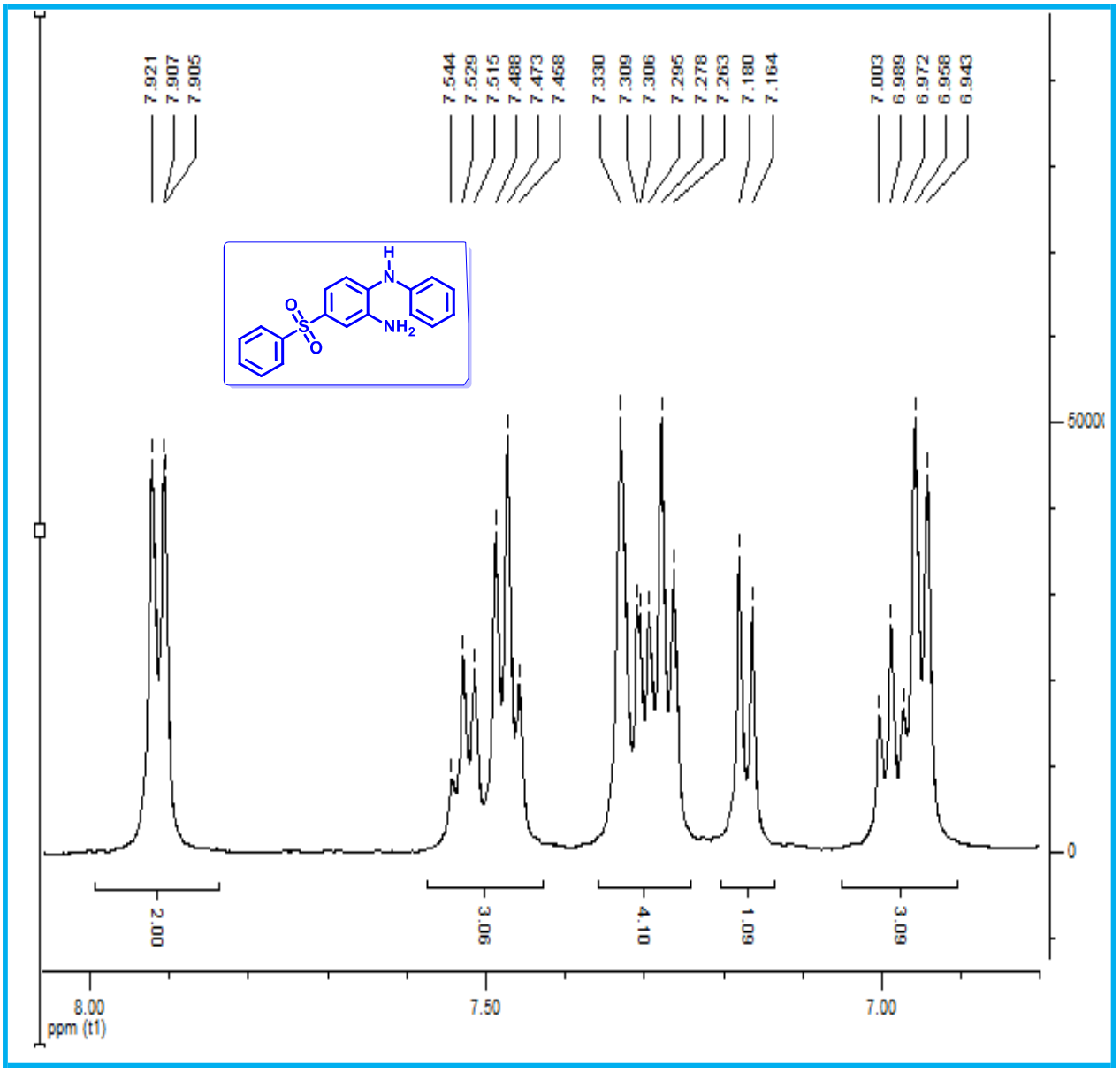


Arrangement of the electrodes and cell

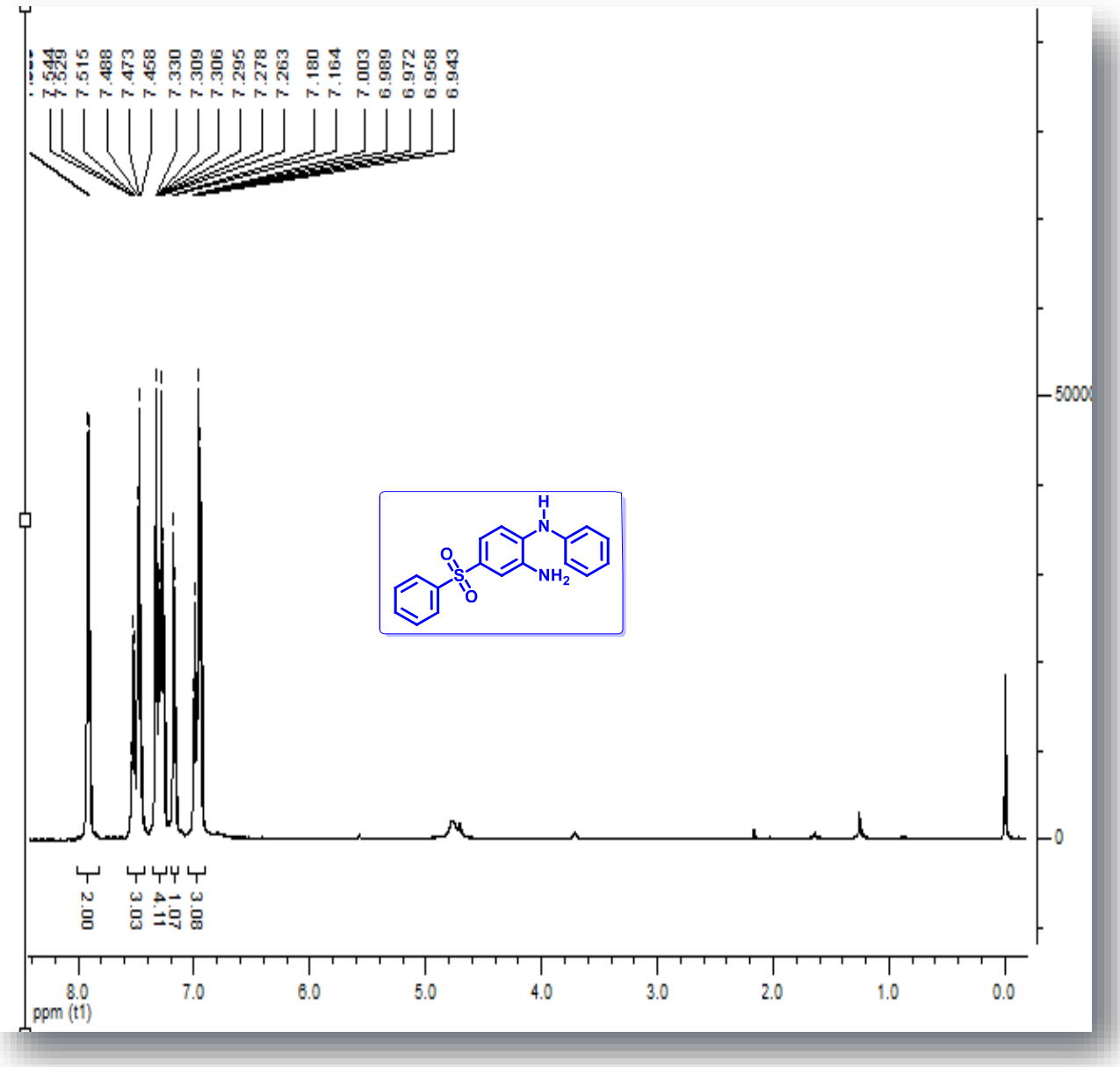
^{1}H NMR spectrum of 3a



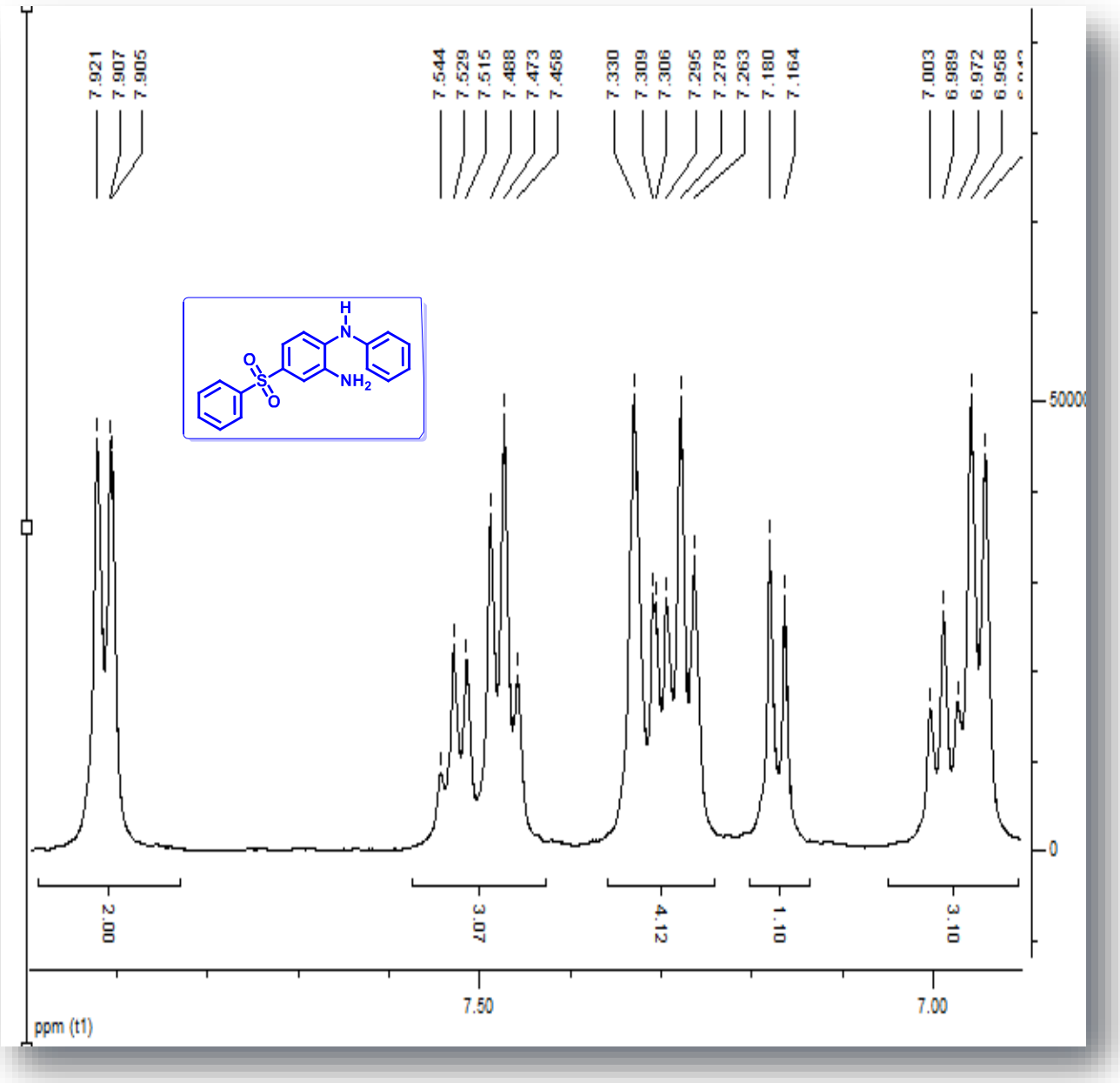
Expanded ^{1}H NMR spectrum of 3a



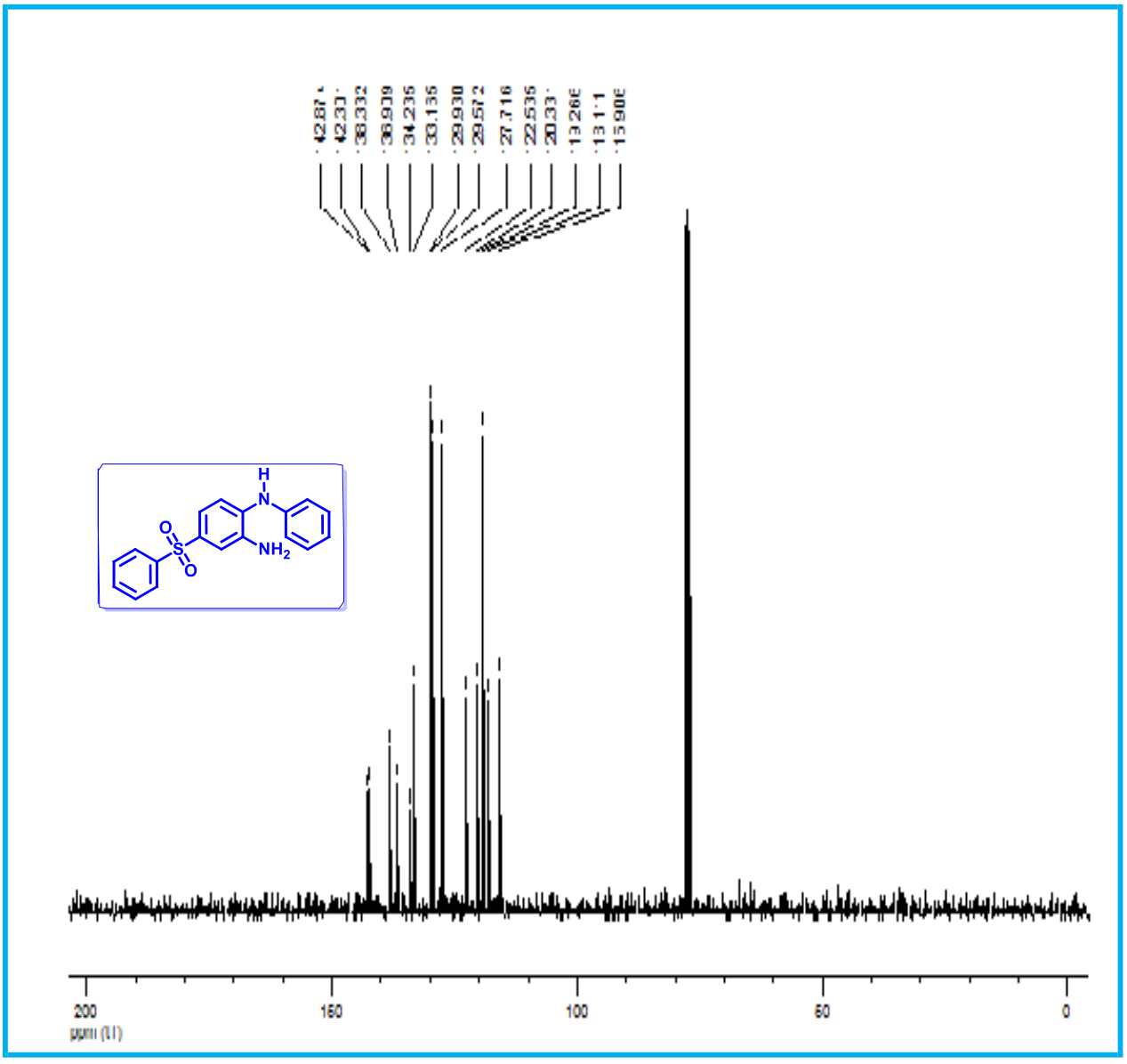
^{1}H NMR spectrum of 3a (with D_2O)



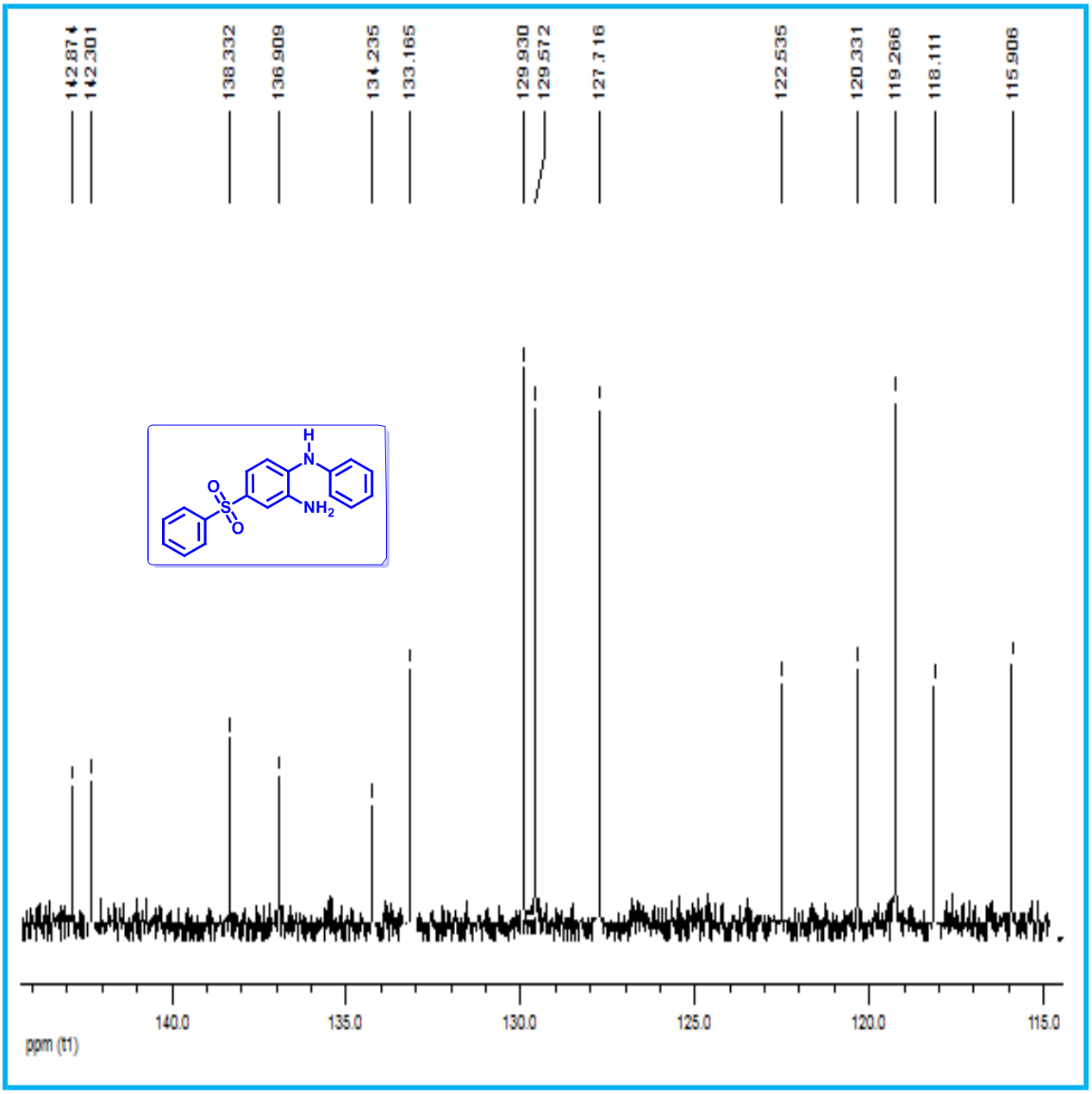
Expanded ^{1}H NMR spectrum of 3a with D_2O



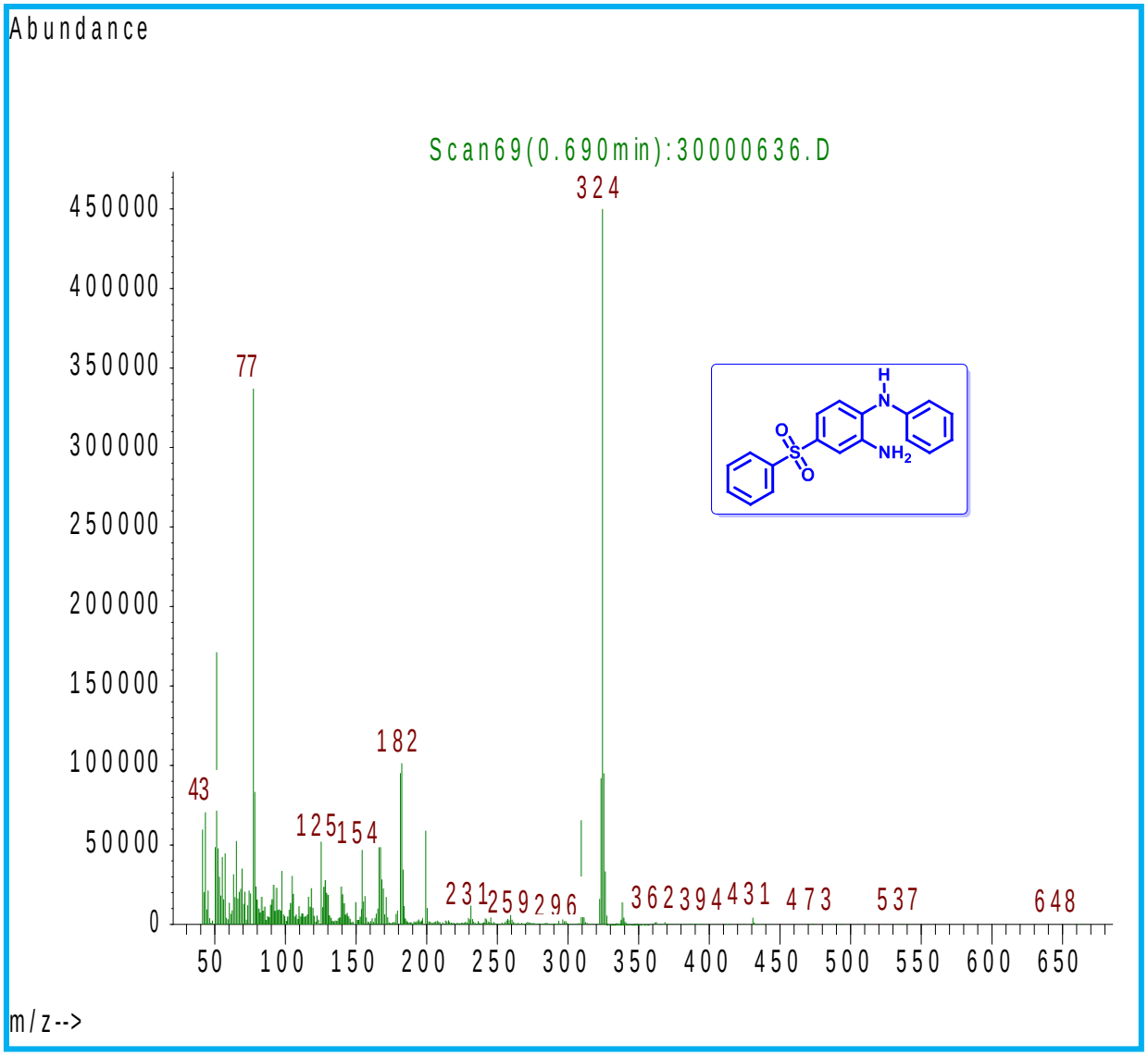
^{13}C NMR spectrum of 3a



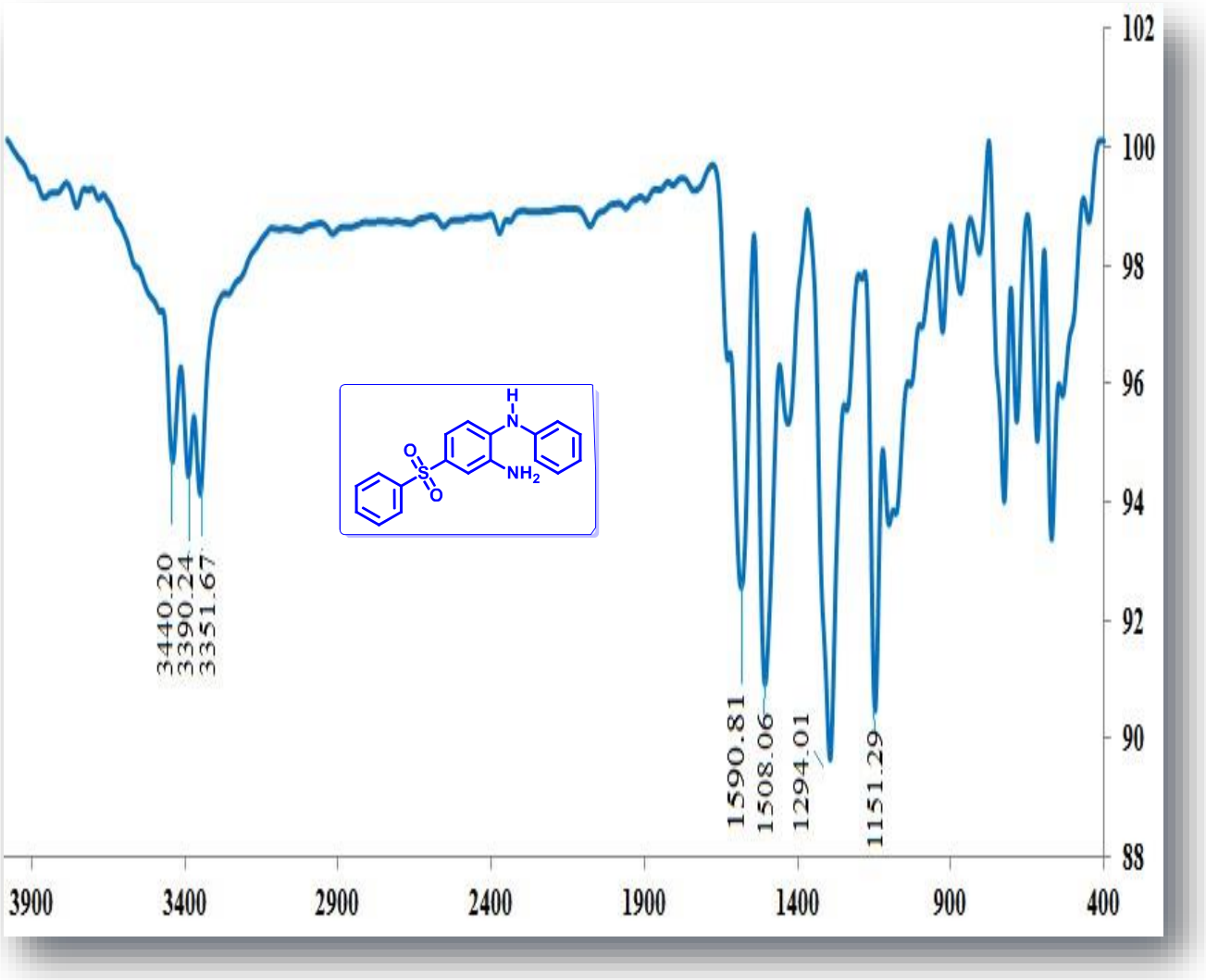
Expanded^{13}C NMR spectrum of 3a



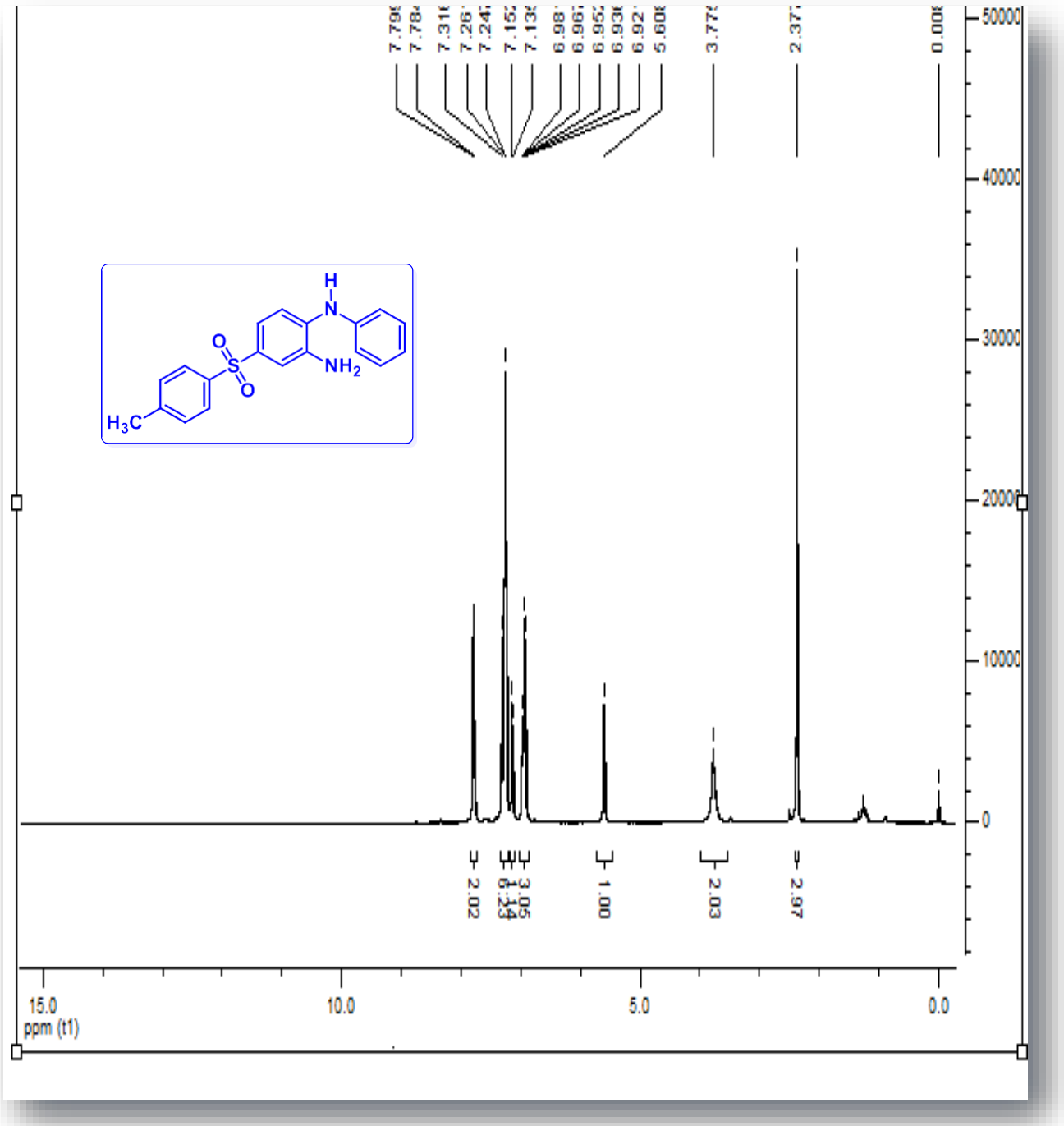
MS spectrum of 3a



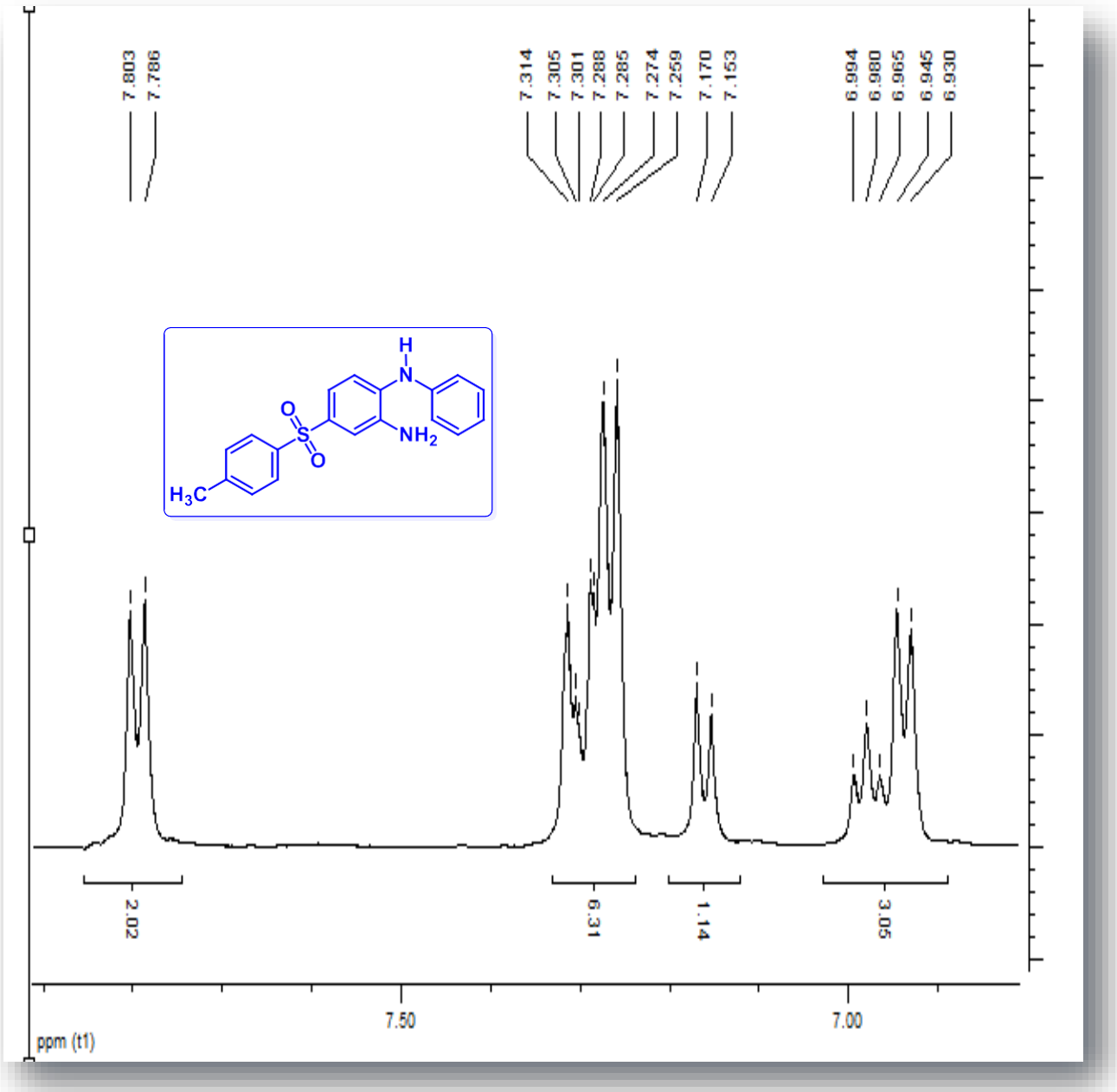
FT-IR spectrum of 3a



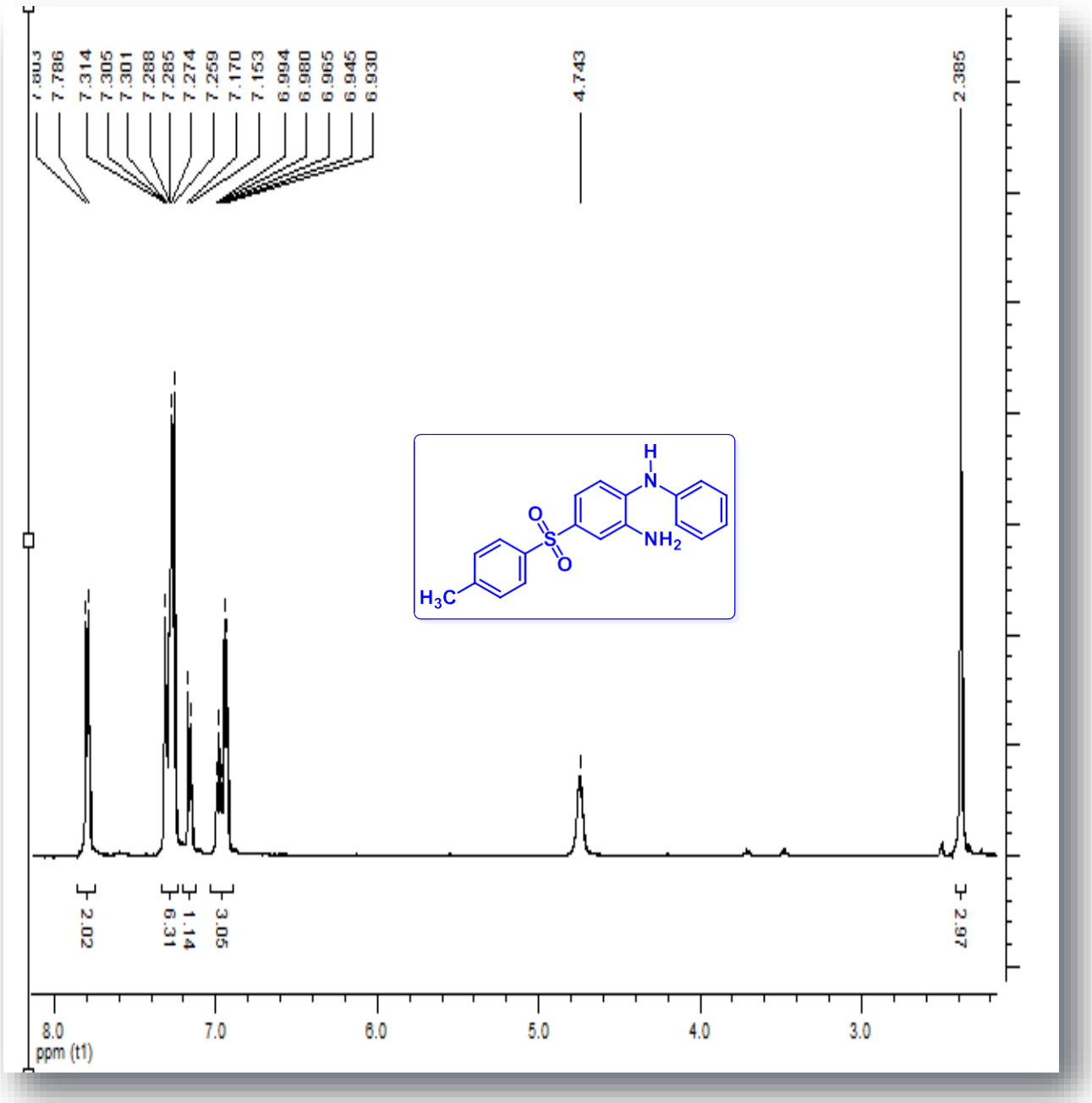
^{1}H NMR spectrum of 3b



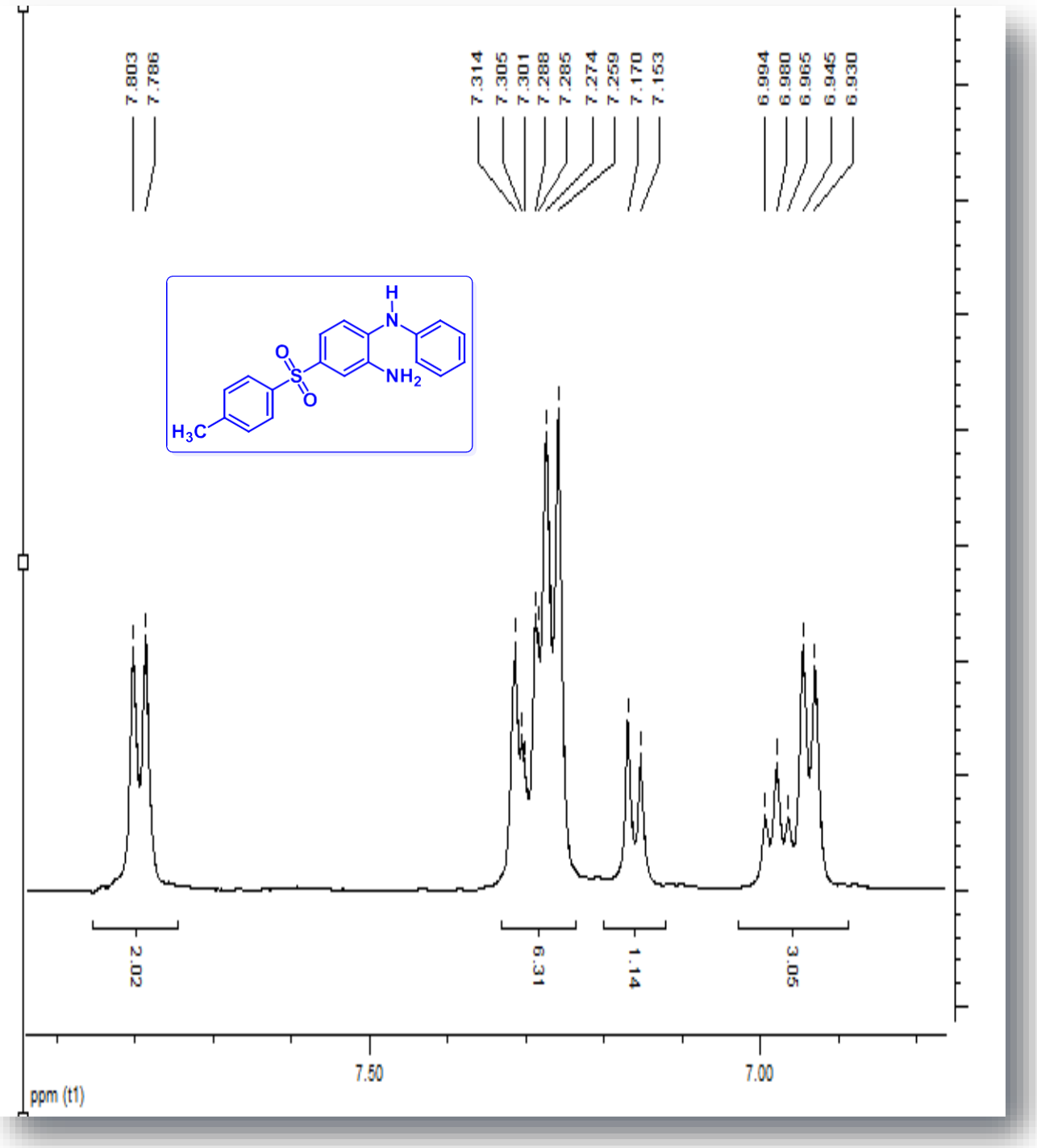
Expanded ^{1}H NMR spectrum of 3b



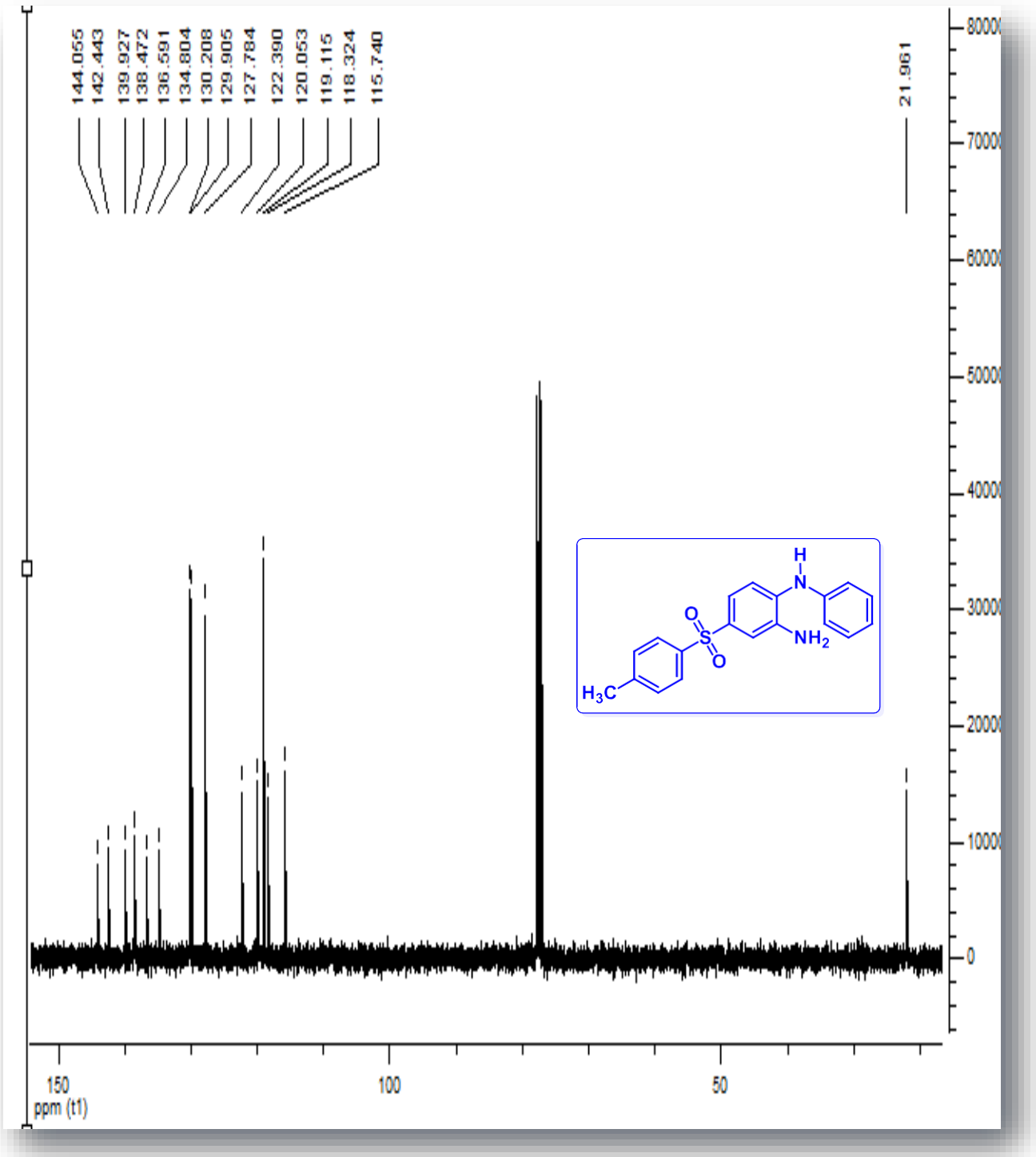
^{1}H NMR spectrum of 3b (with D_2O)



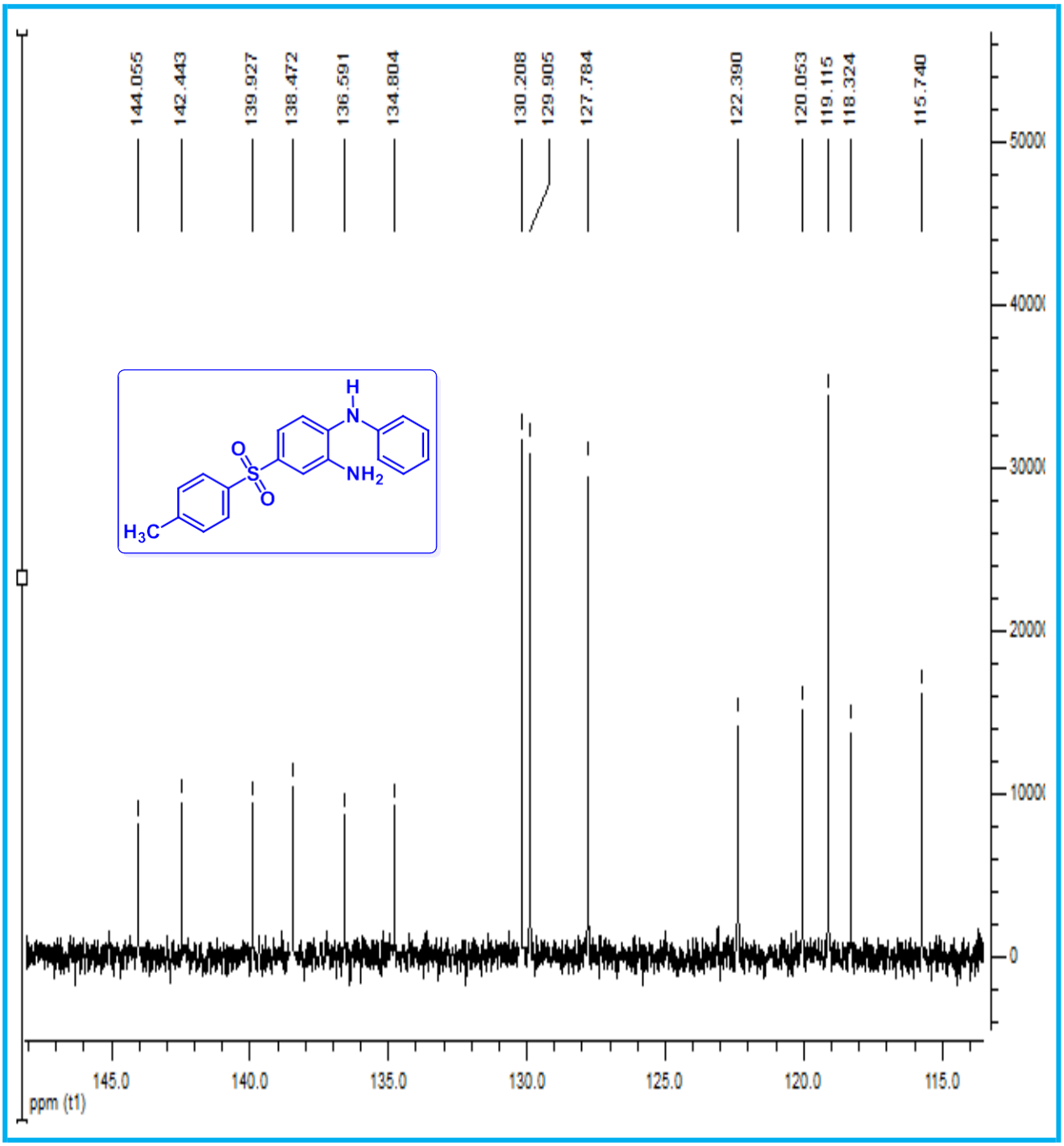
Expanded ^{1}H NMR spectrum of 3b with D_2O



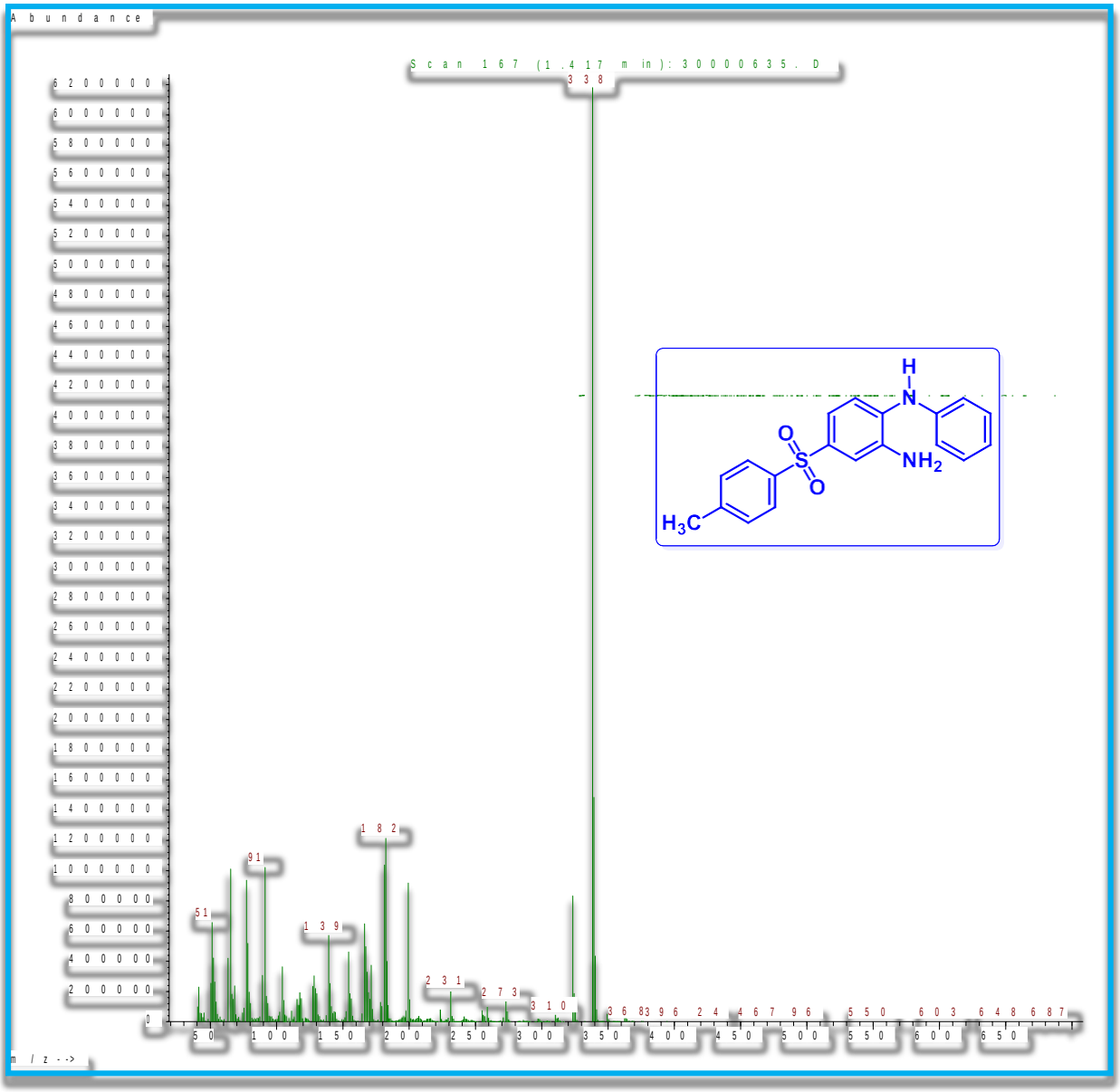
^{13}C NMR spectrum of 3b



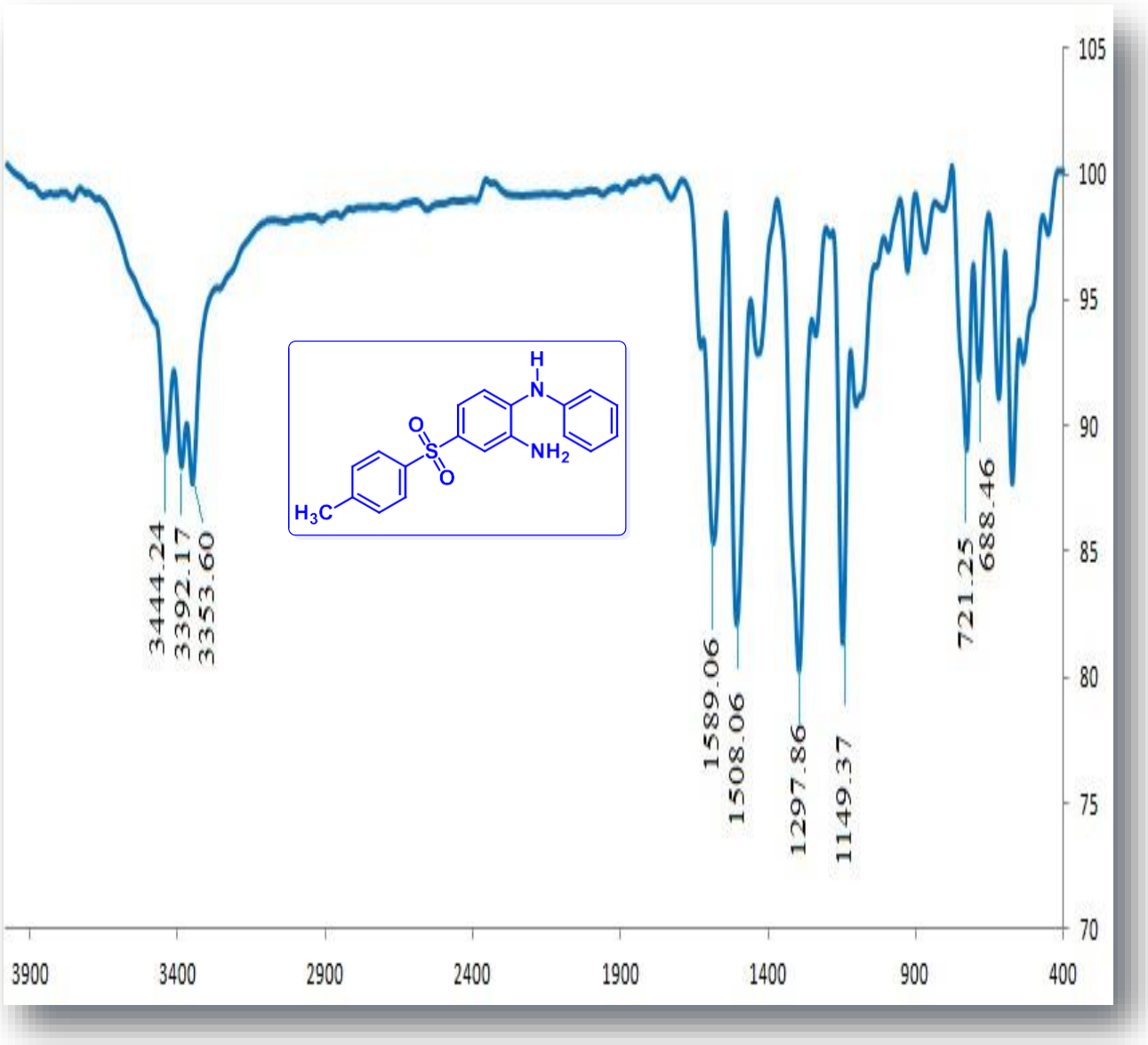
Expanded ^{13}C NMR spectrum of 3b



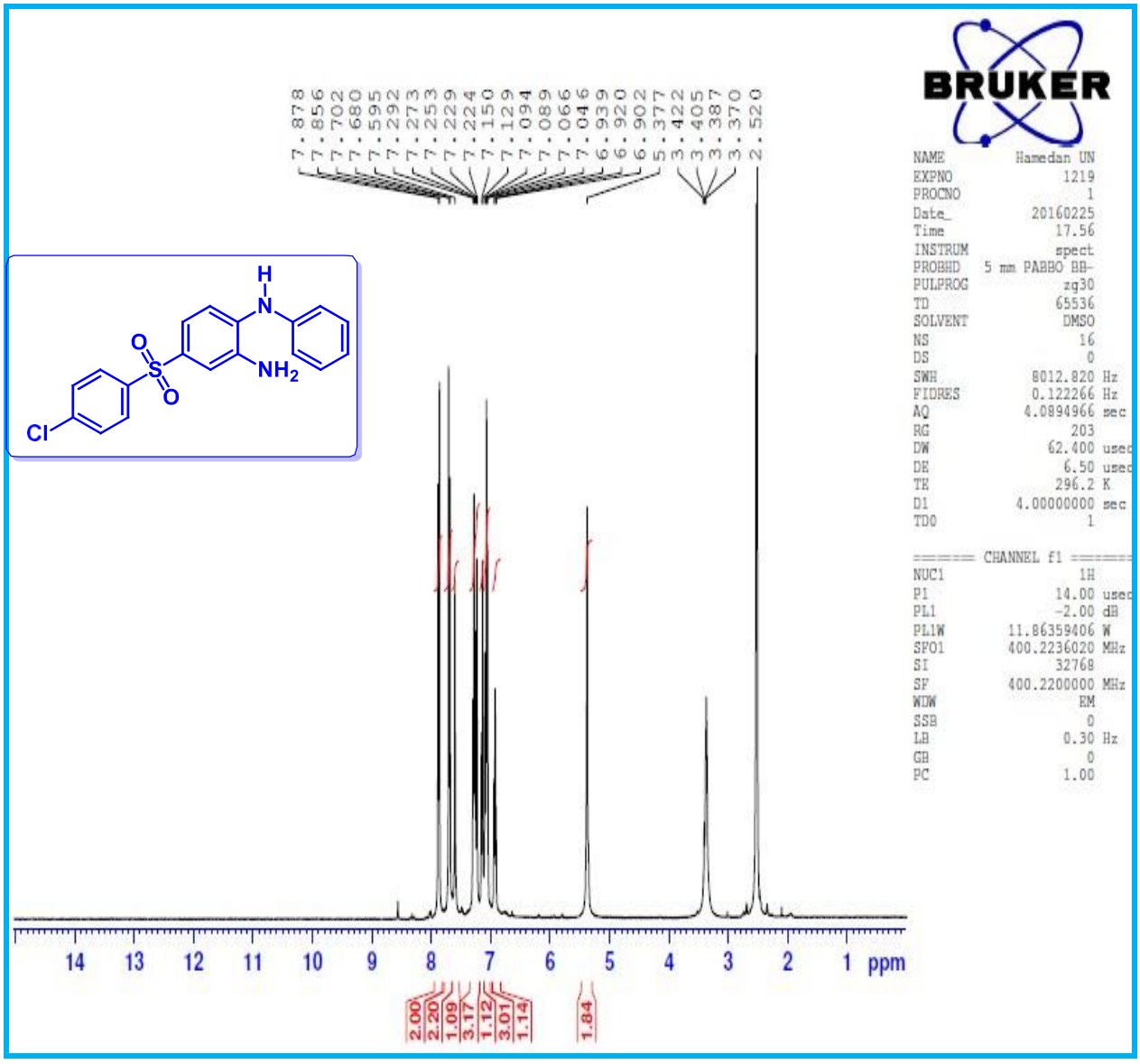
MS spectrum of 3b



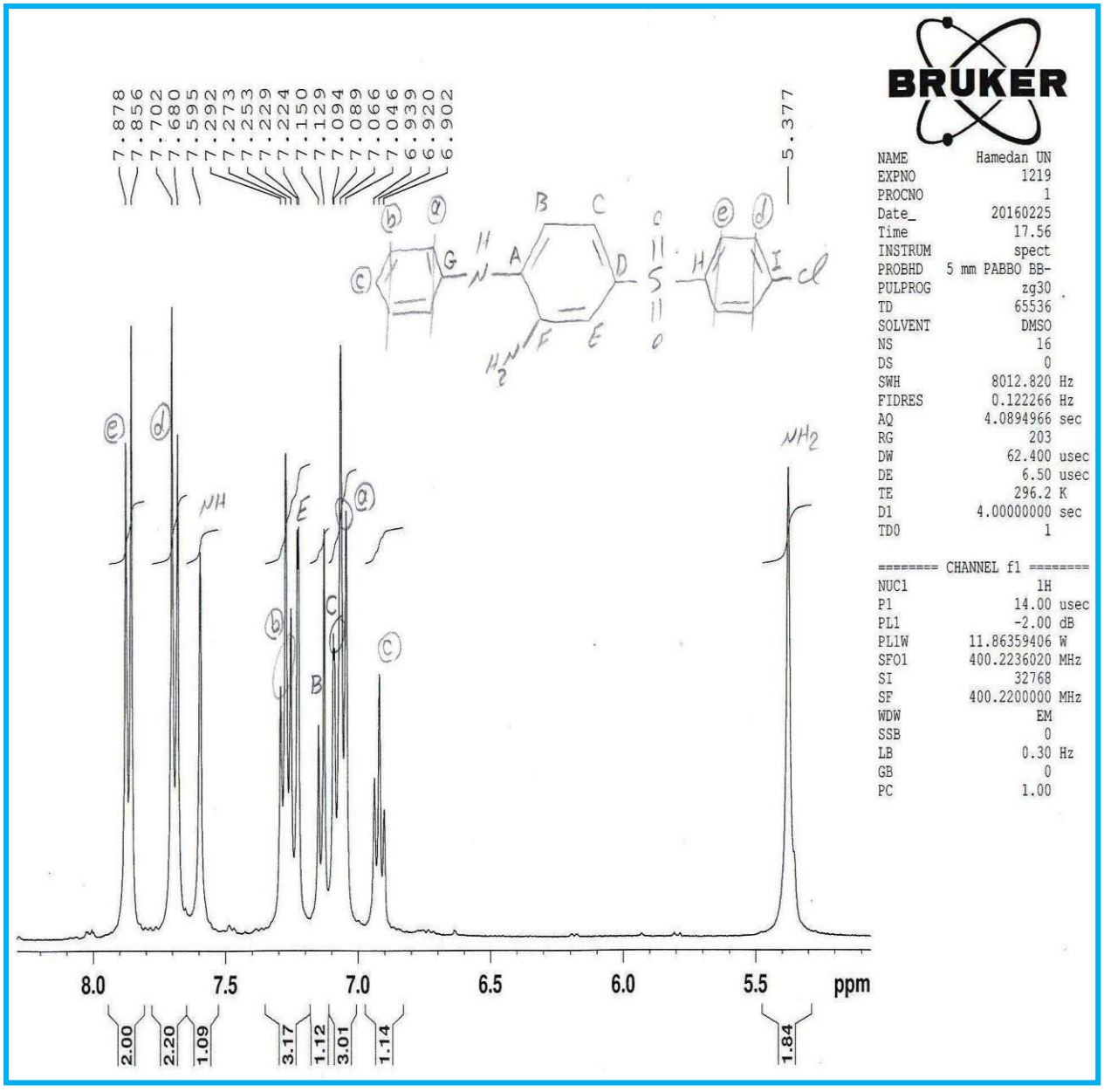
FT-IR spectrum of 3b



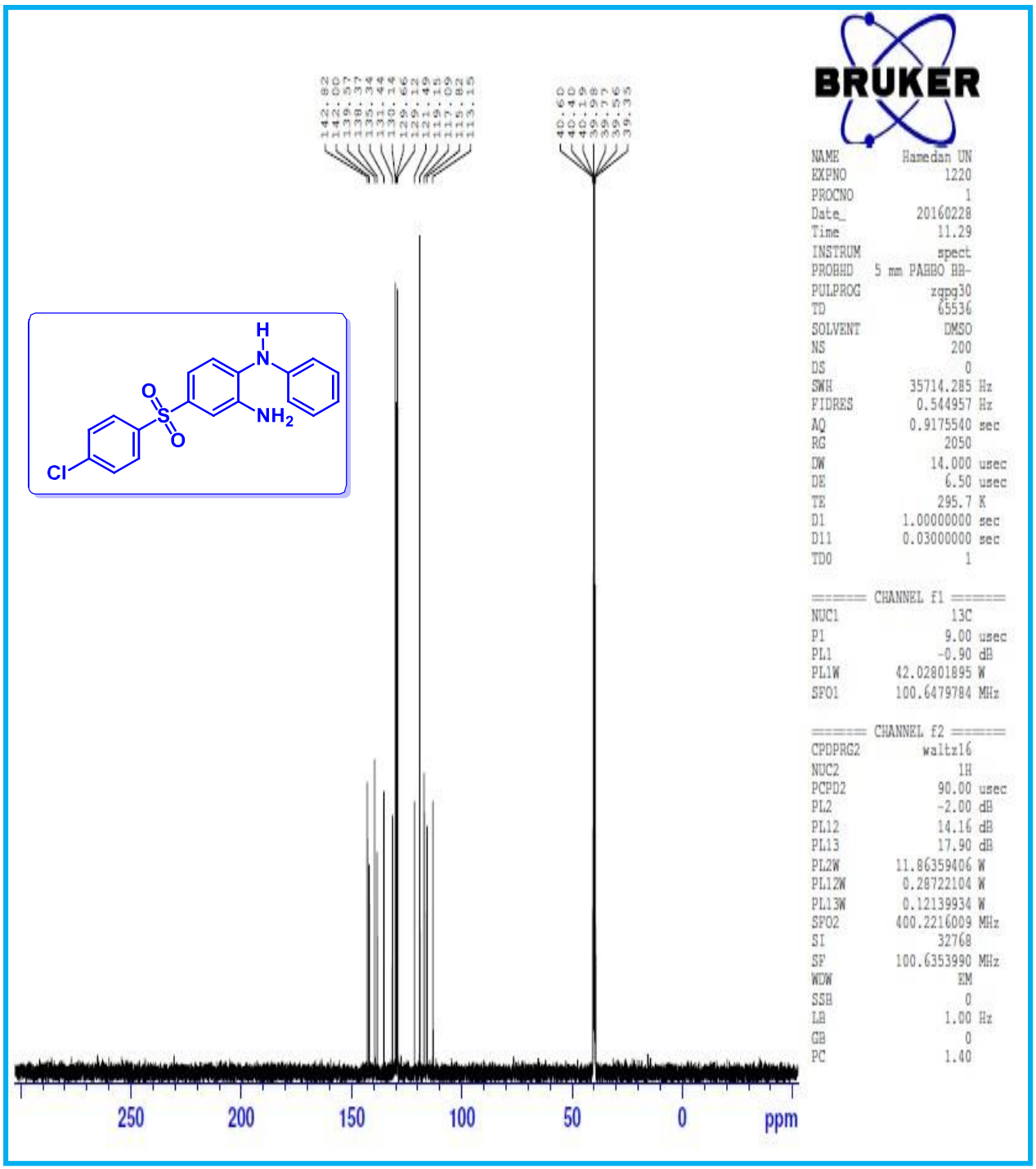
^{1}H NMR spectrum of 3c



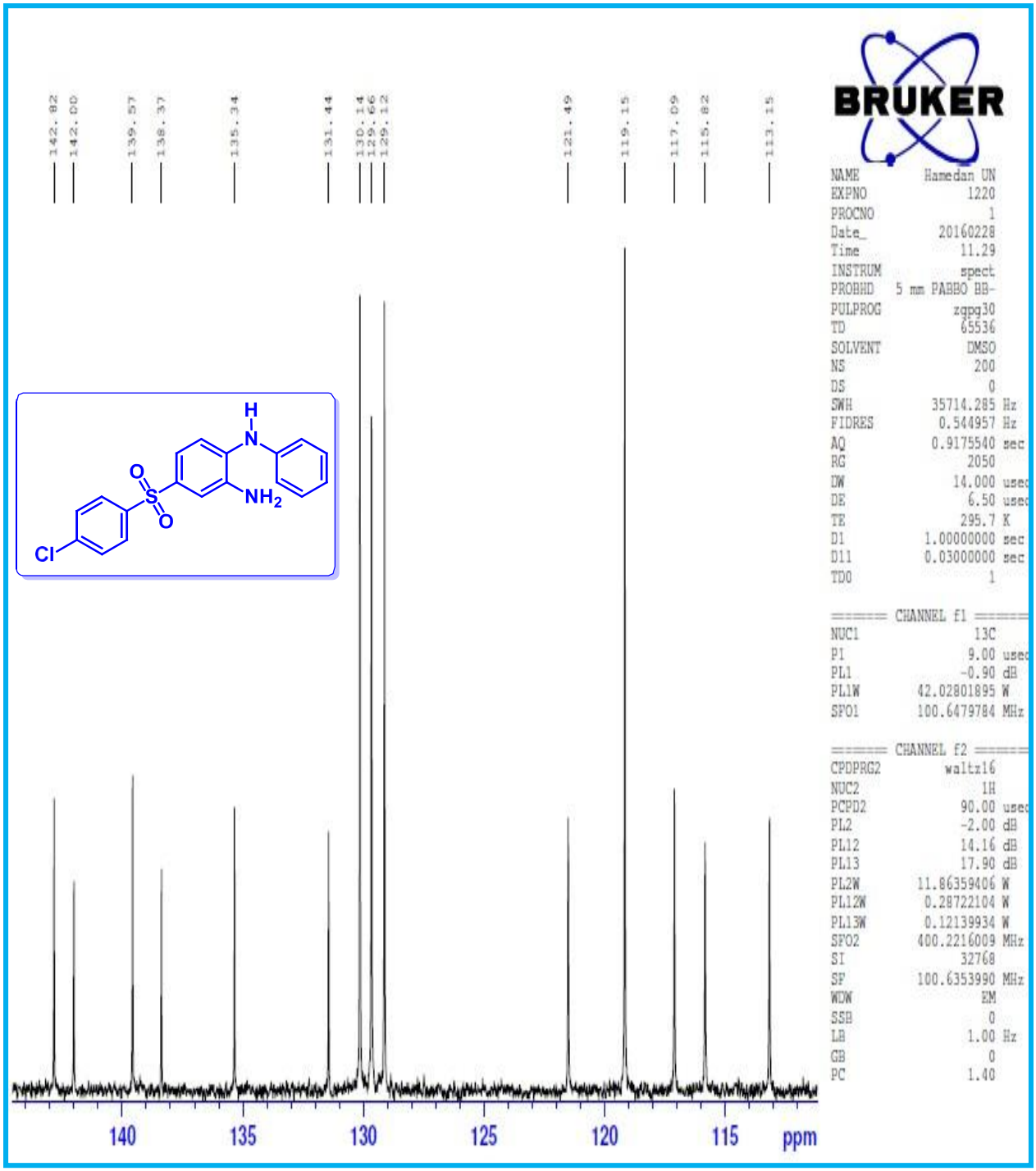
Expanded^{1}H NMR spectrum of 3c



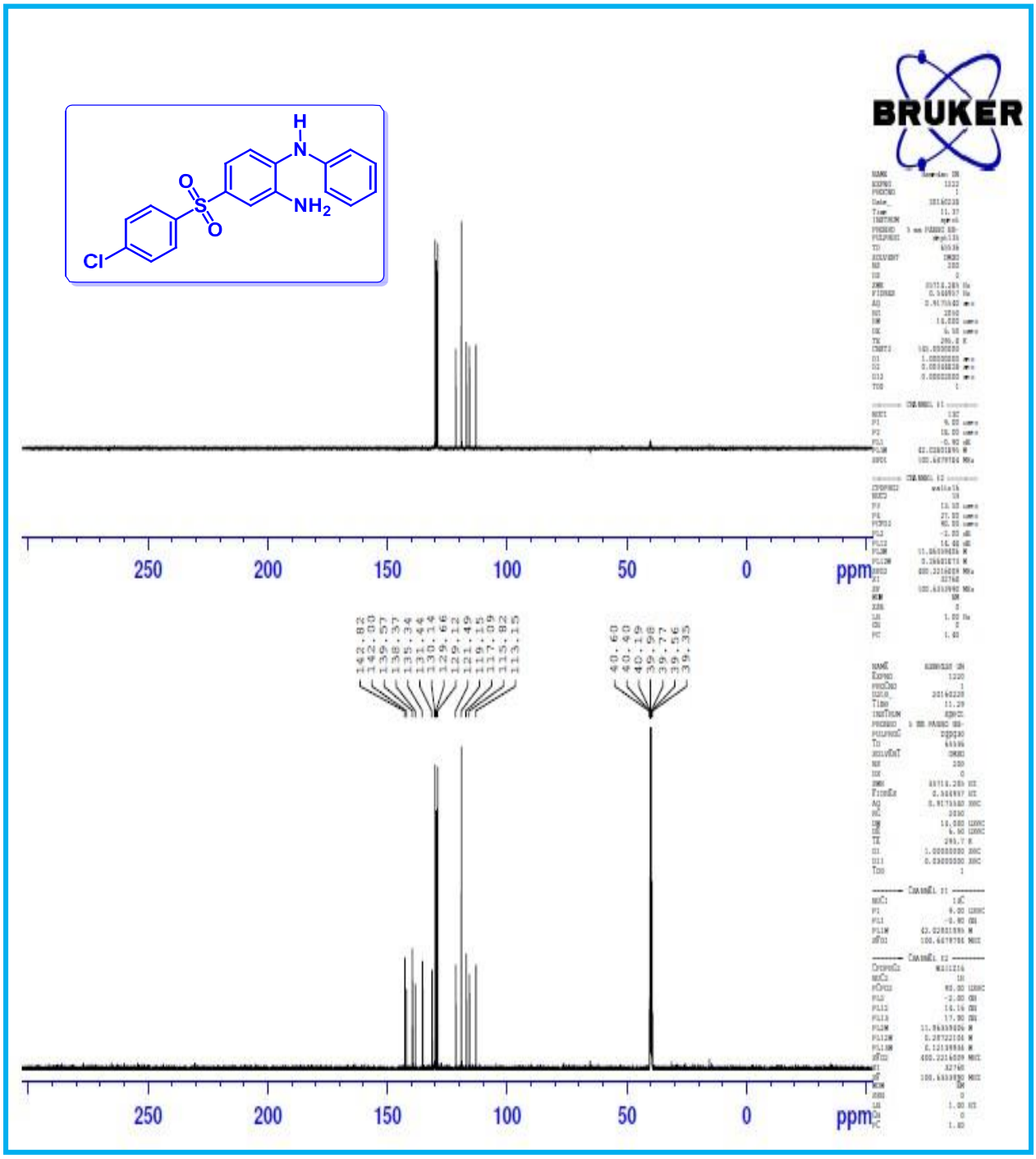
^{13}C NMR spectrum of 3c



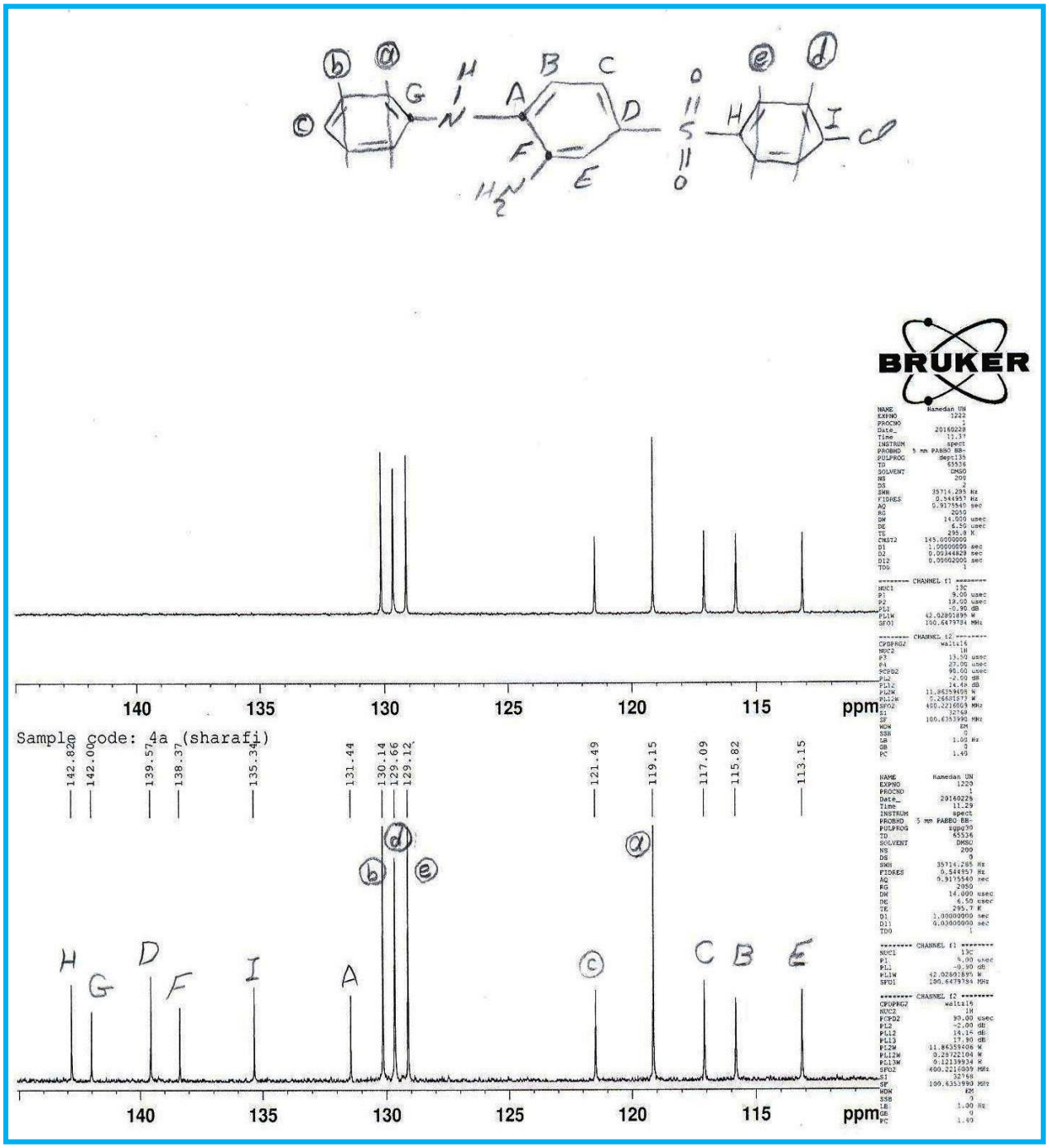
Expanded ^{13}C NMR spectrum of 3c



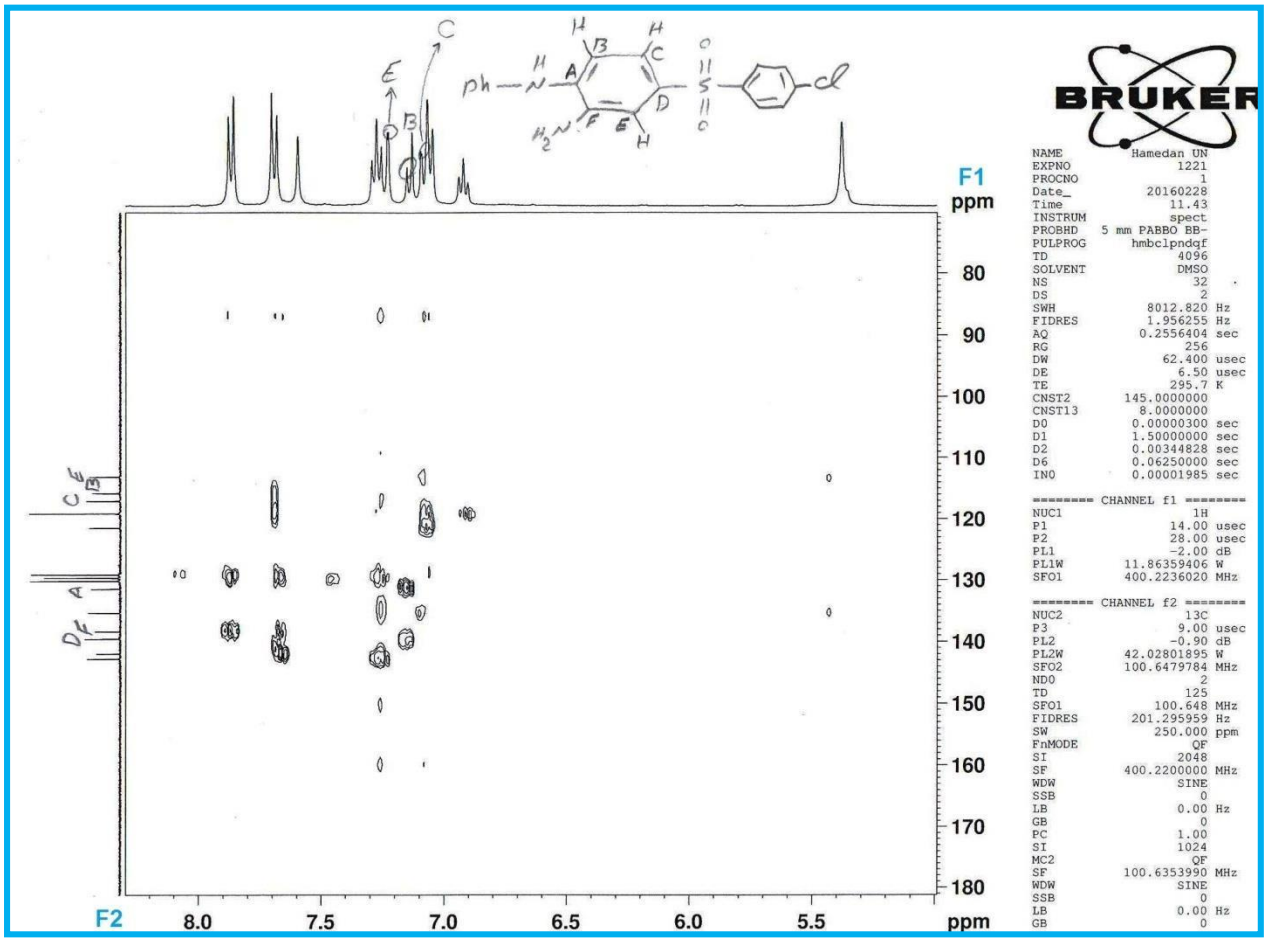
^{13}C-DEPT-135 spectrum of 3c



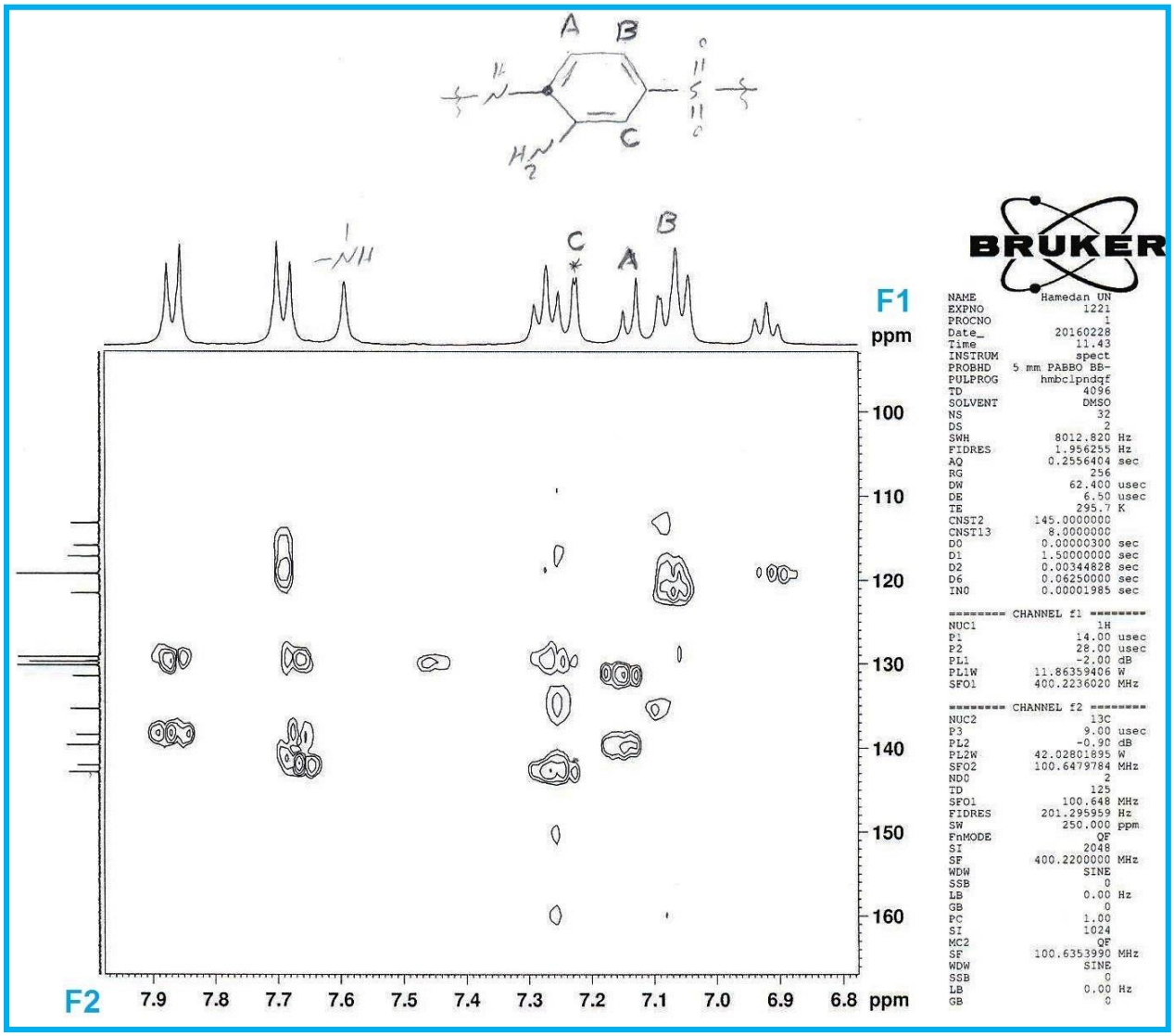
^{13}C –DEPT-135 expanded spectrum of 3c



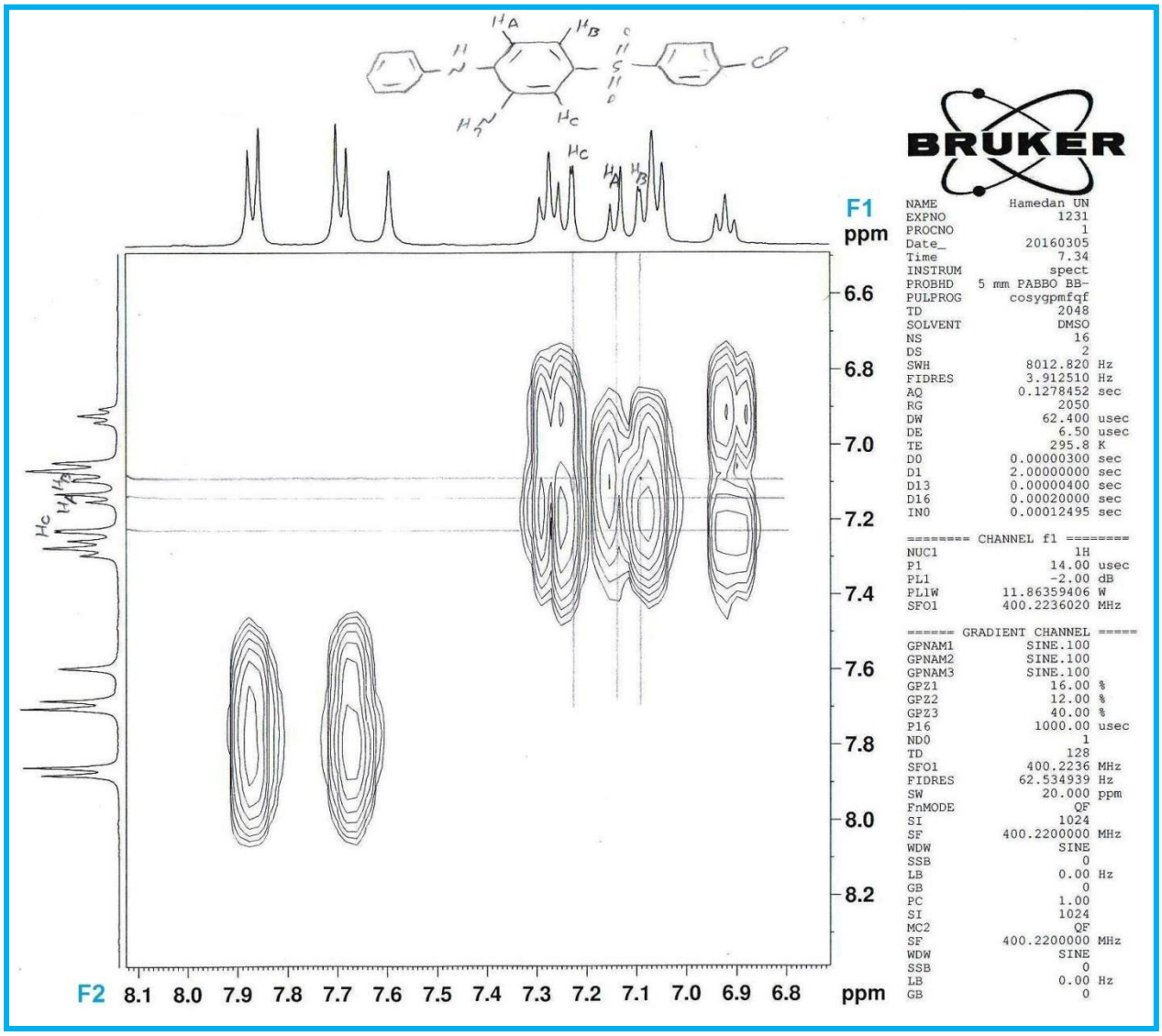
2D HMBC (F1 : ^{13}C, F2 : ^{1}H) spectrum of 3c



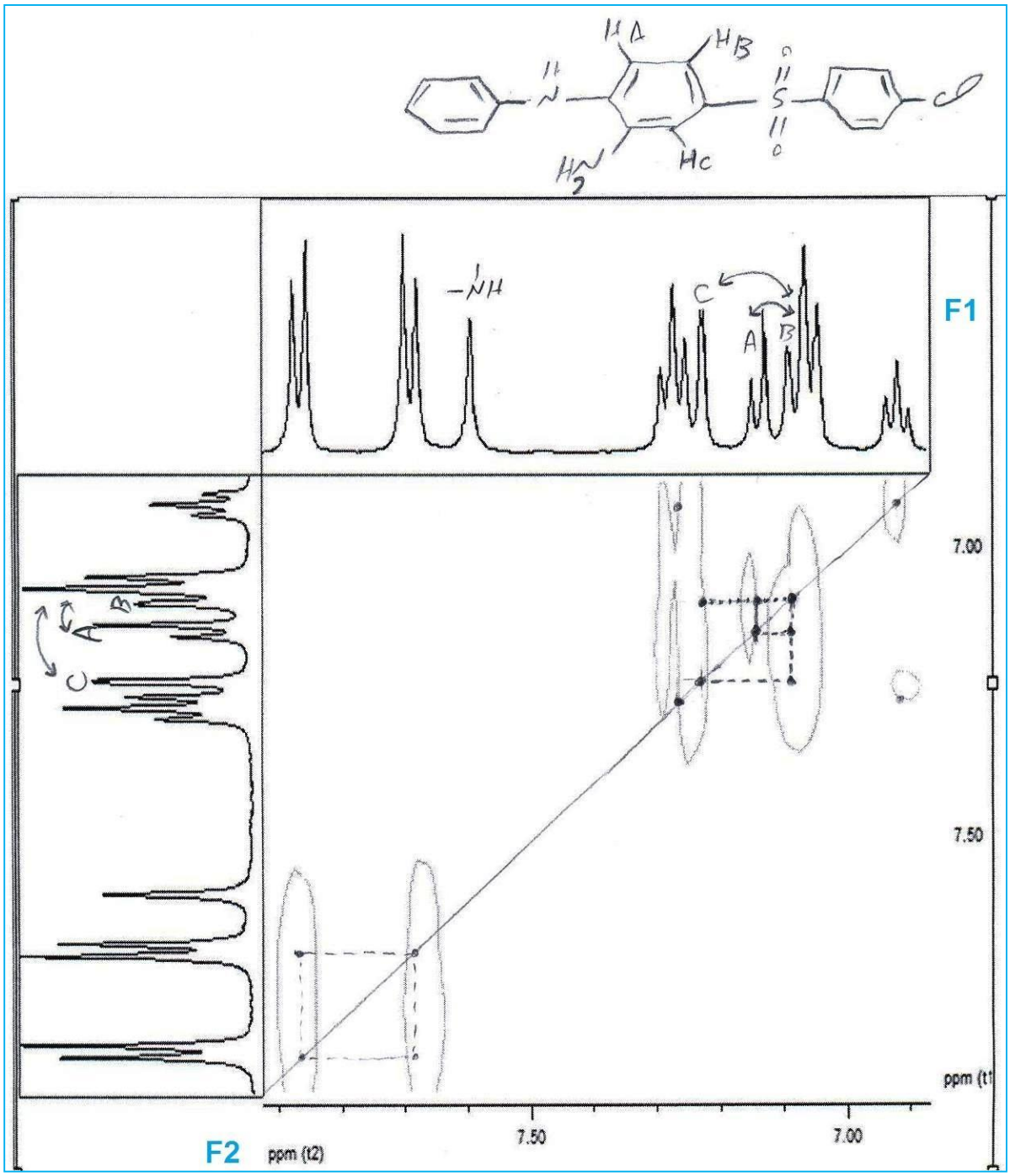
2D HMBC (F1 : ^{13}C, F2 : ^{1}H) expanded spectrum of 3c



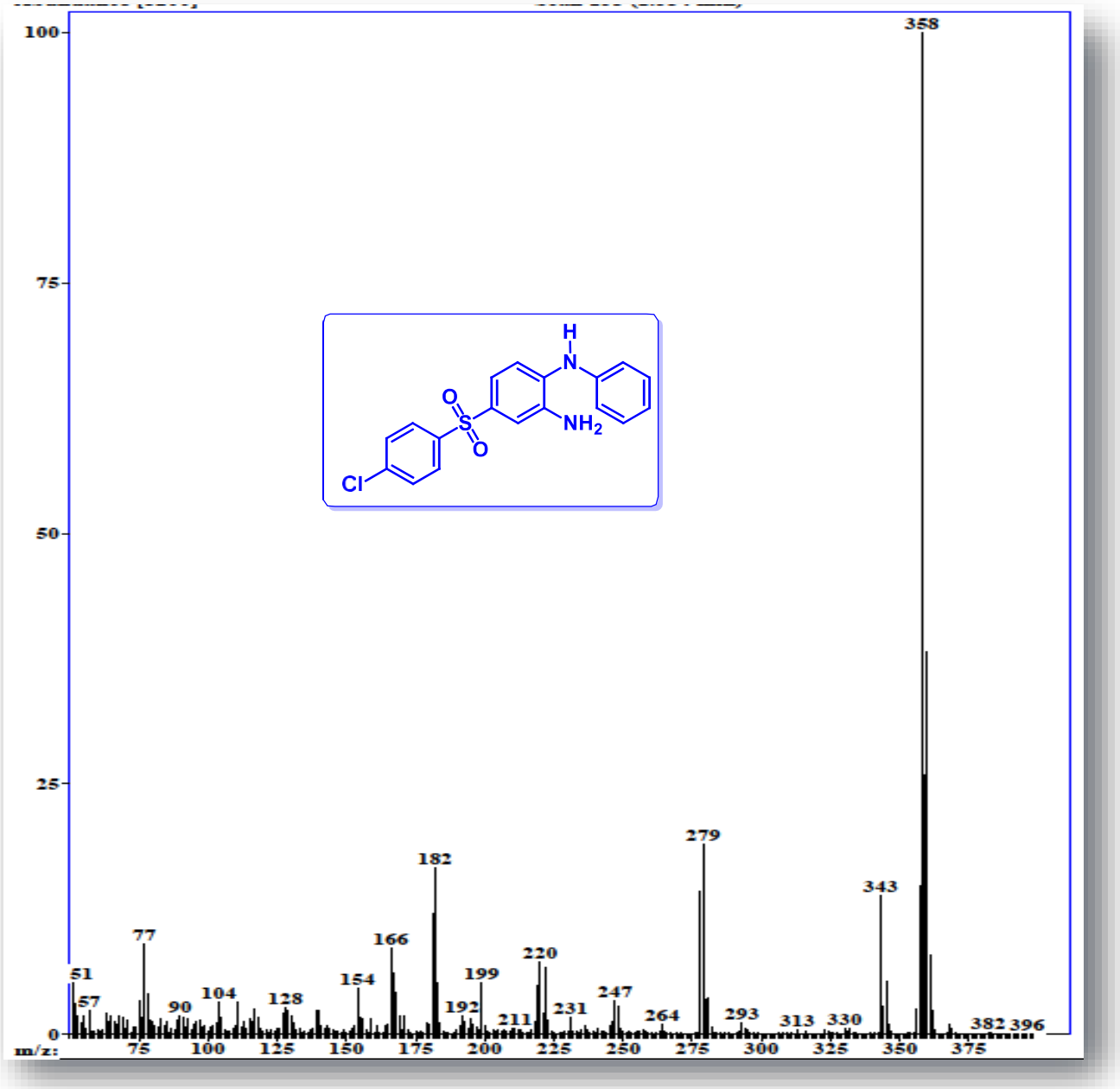
2D ^{1}HSQC(F1 : ^{1}H, F2 : ^{1}H) spectrum of 3c



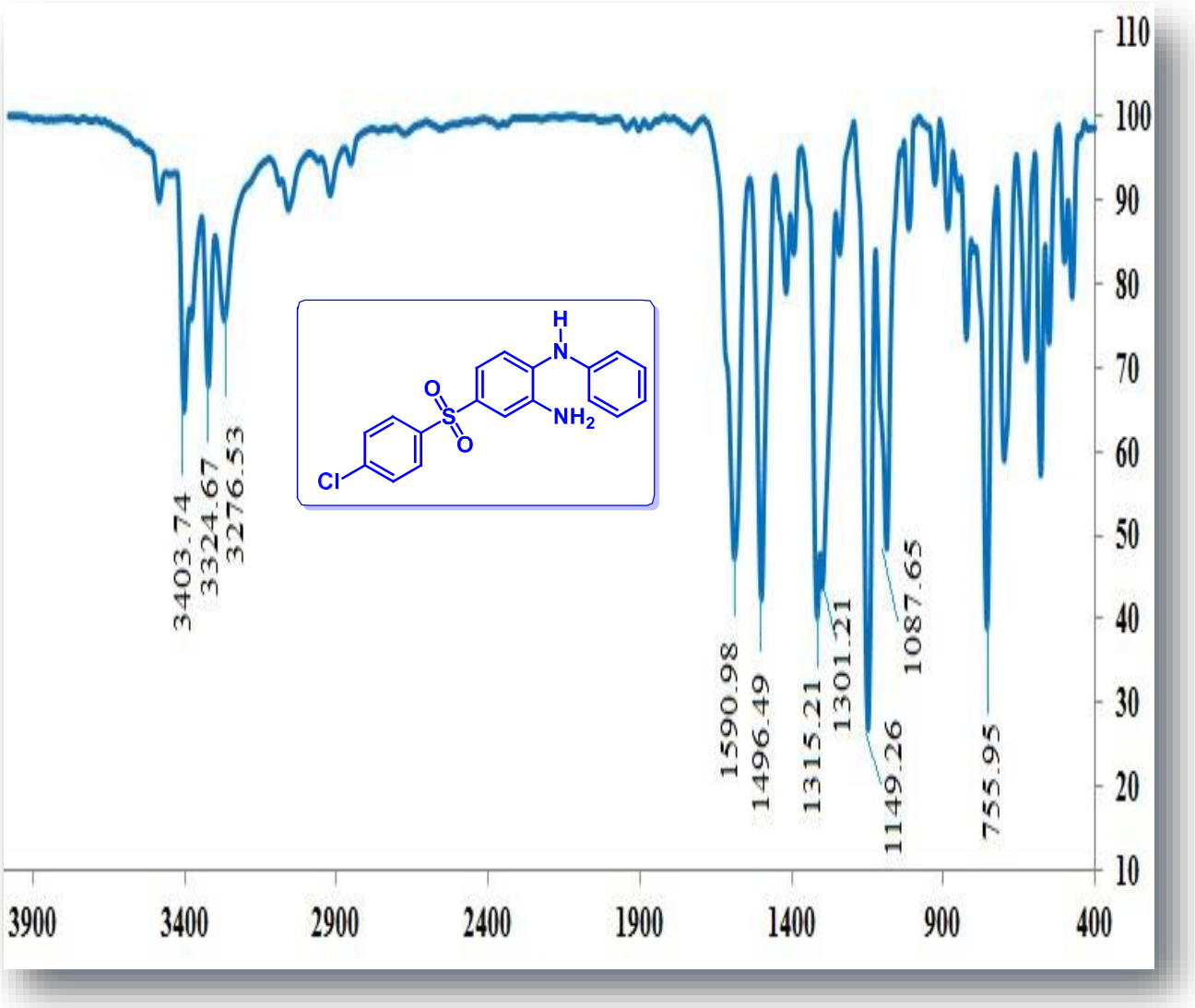
2D HSQC(F1 : ^{1}H, F2 : ^{1}H)expanded spectrum of 3c



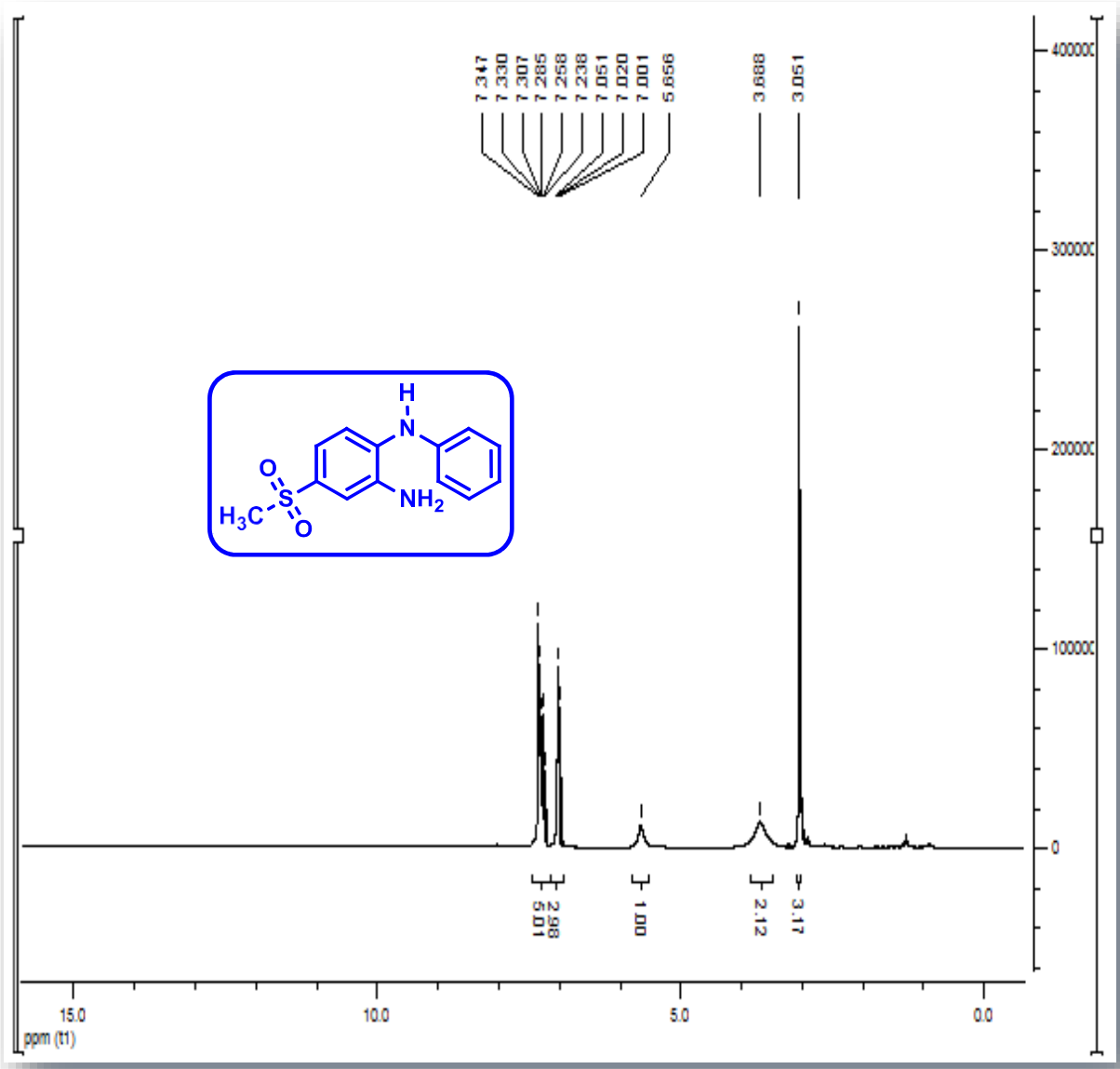
MS spectrum of 3c



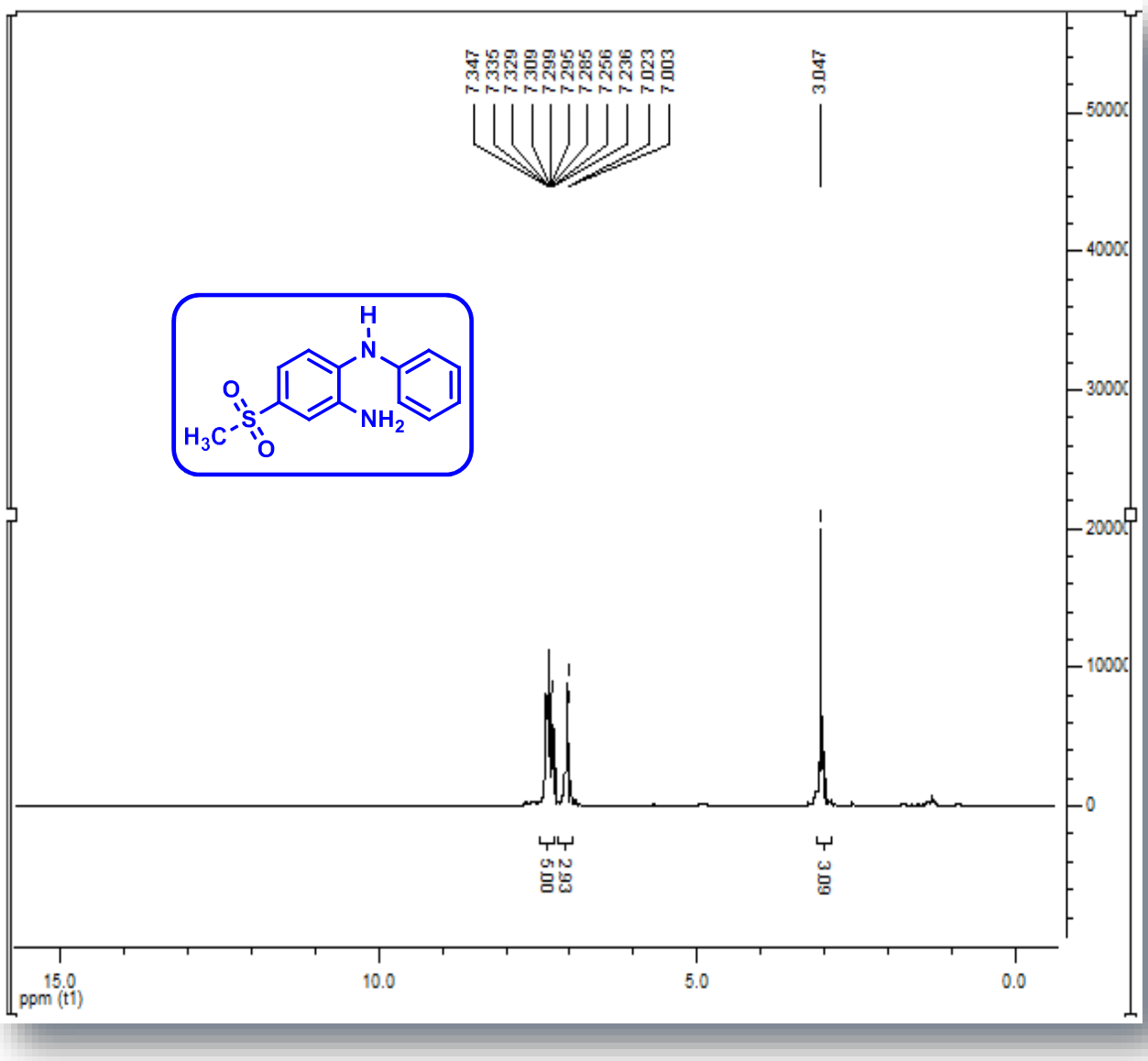
FT-IR spectrum of 3c



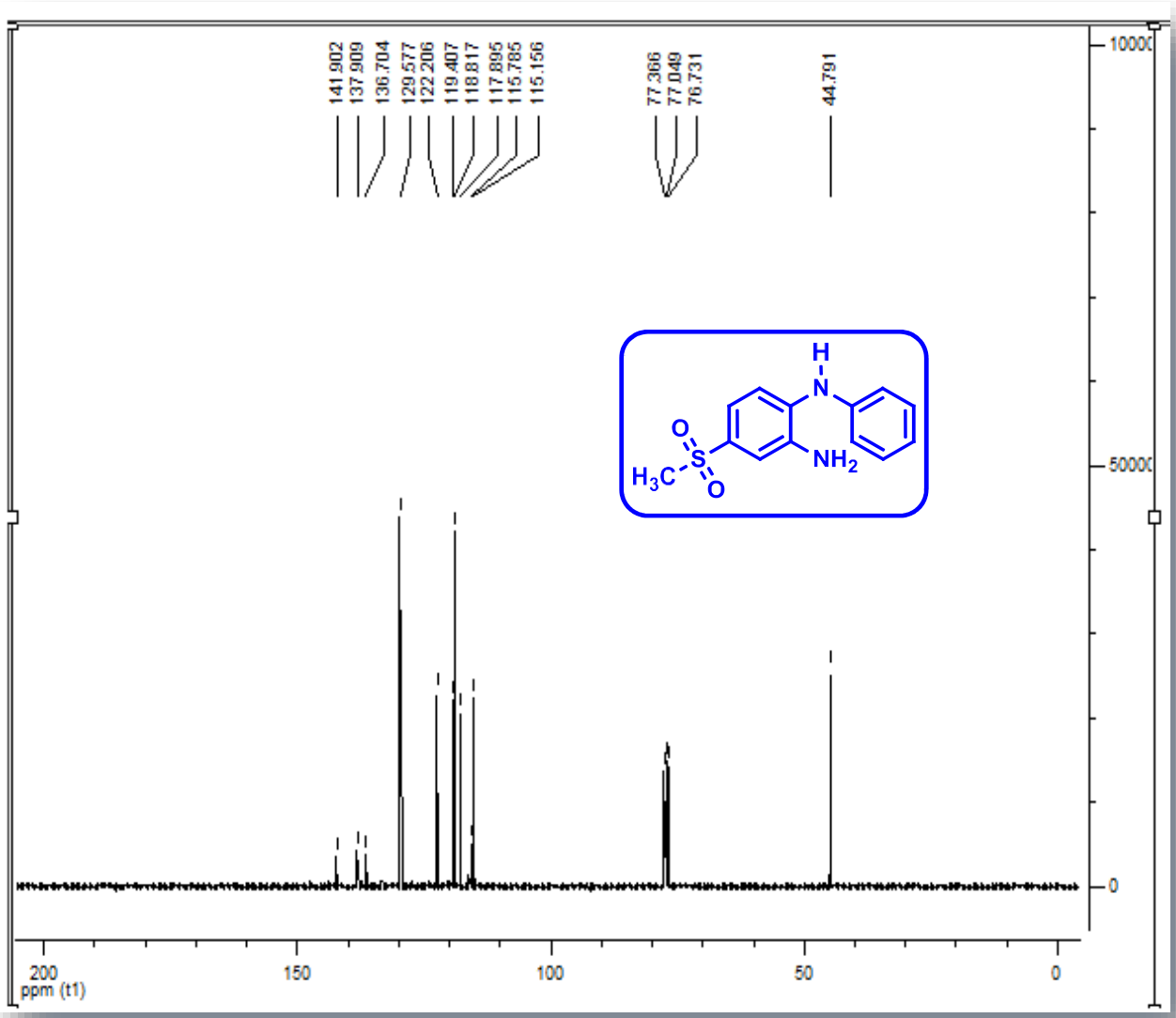
^{1}H NMR spectrum of 3d



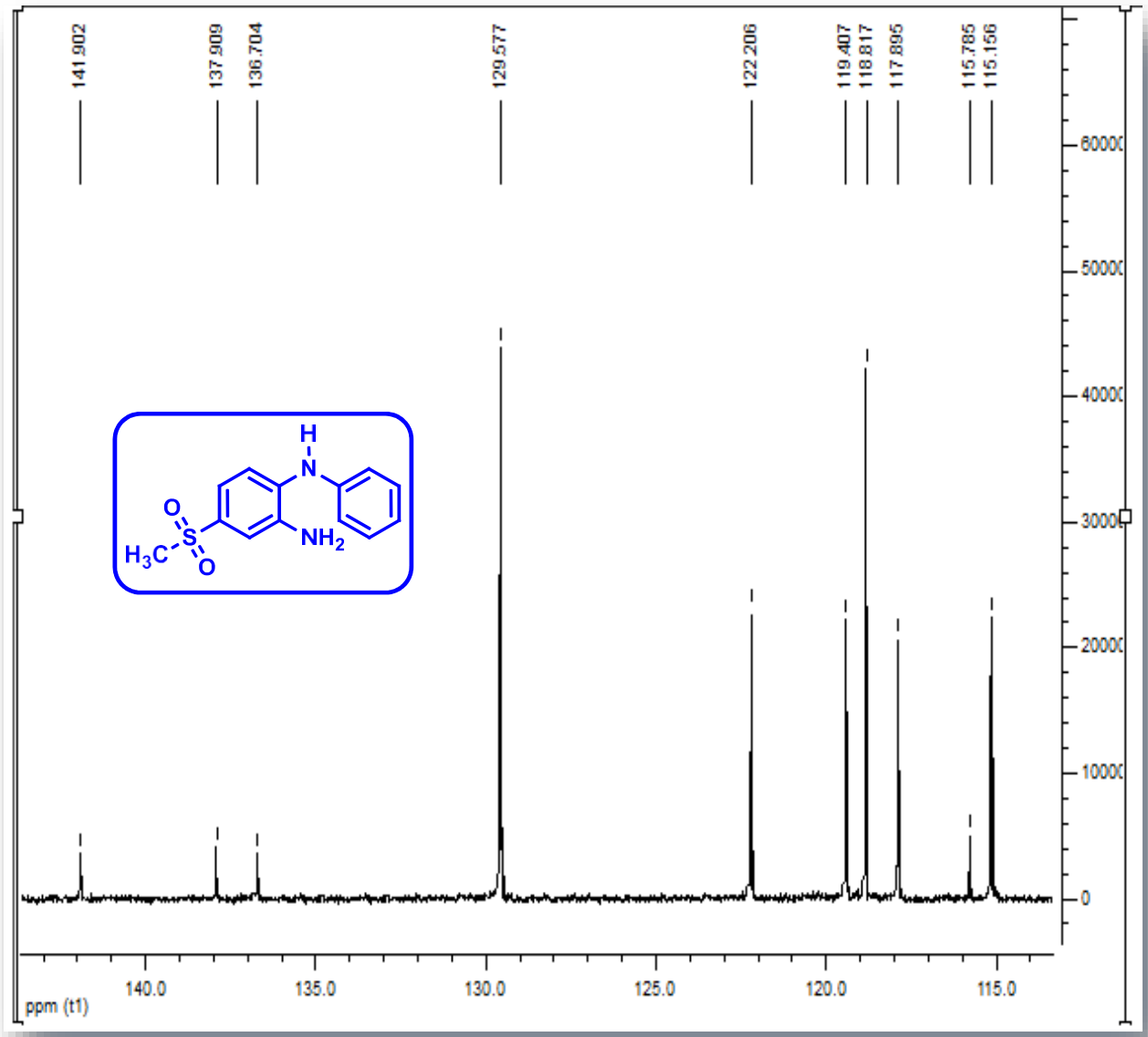
^{1}H NMR spectrum in D_2O of 3d



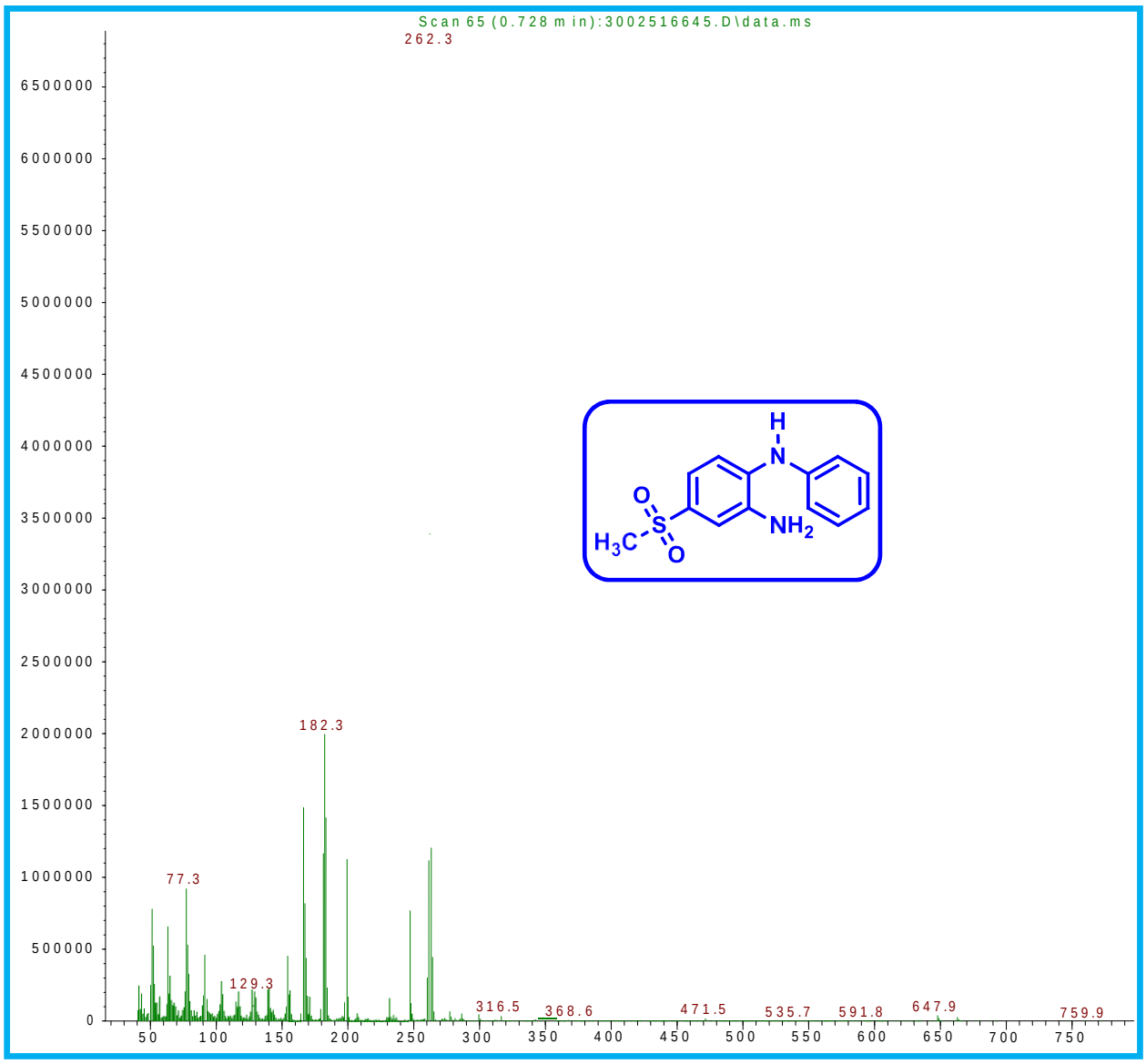
^{13}C NMR spectrum of 3d



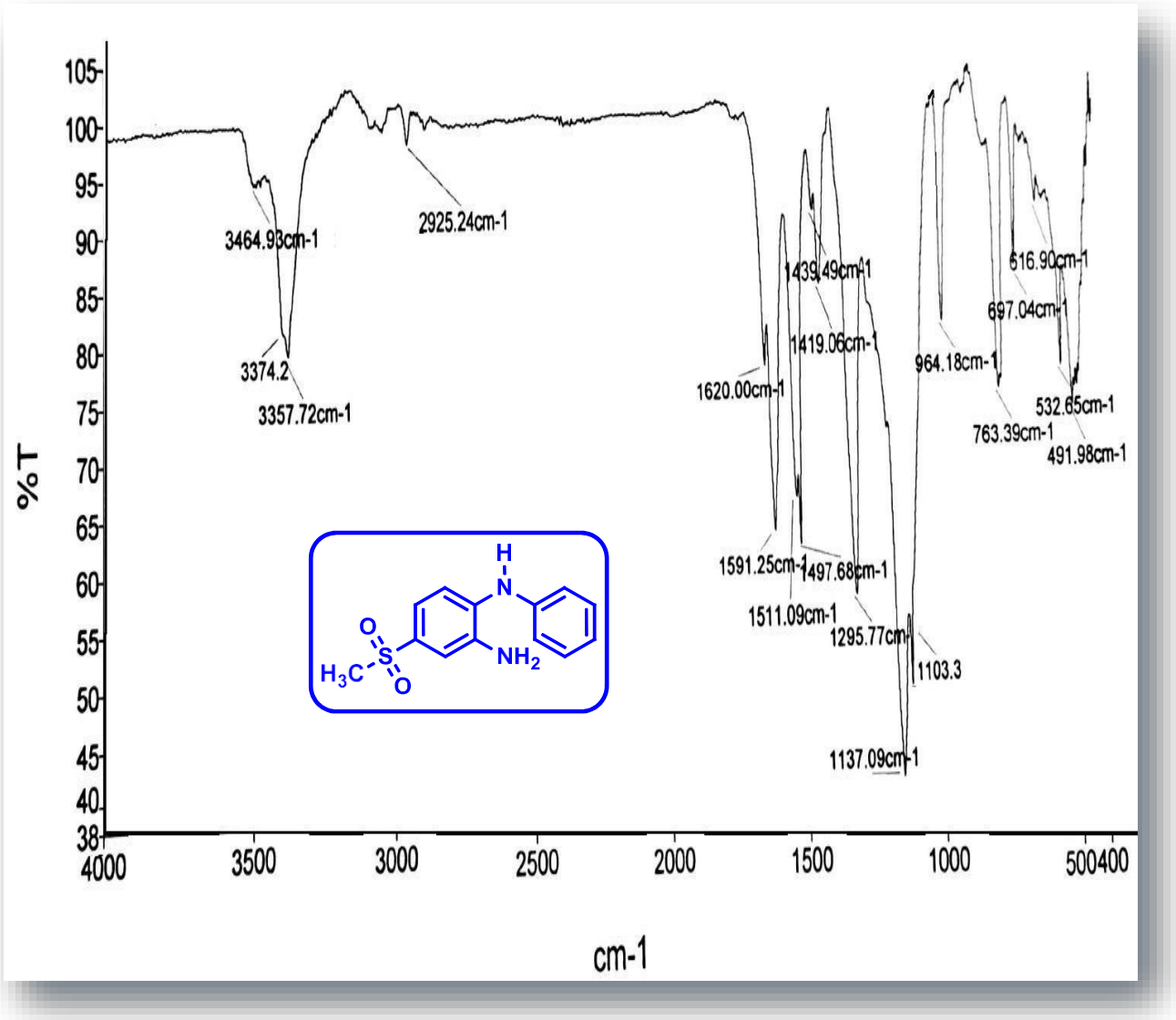
Expanded ^{13}C NMR spectrum of 3d

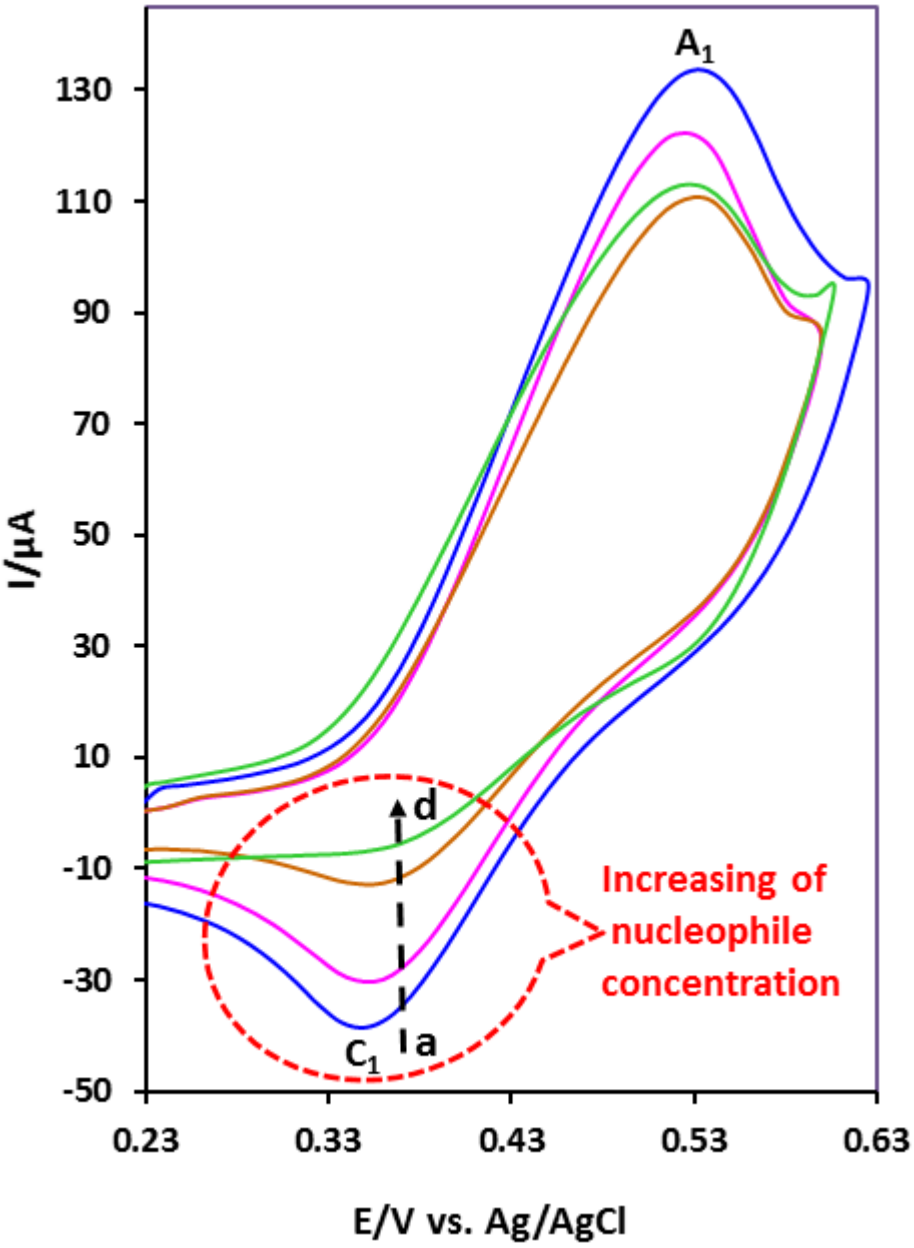


Mass spectrum of 3d



FTIR spectrum of 3d





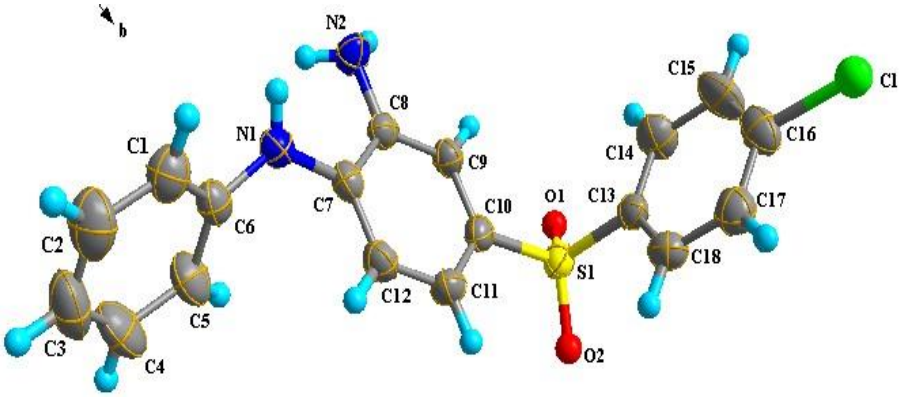
Cyclic voltammograms of **2ADPA** (0.1 mM) in the presence of different concentration of benzenesulfinic acid: (a) 0.00 mM, (b) 0.025 mM, (c) 0. 05 mM and (d) 0.10 mM at glassy carbon electrode in water (phosphate buffer, *c* = 0.2 M, pH= 2.0)/ethanol (70/30, v/v) mixture. Scan rate 5 V s^{-1}. Temperature = 25 ^{o}C.

Dear Depositor,
Thank you for depositing your crystal structure(s) at the Cambridge Crystallographic Data Centre.
The data have been assigned to the following deposition numbers.
CCDC 1407863

Summary of Data CCDC1407863

Compound Name:
Formula: C18 H15 Cl1 N2 O2 S1
Unit Cell Parameters: a 19.109(4) b 8.8080(18) c 20.086(4) Pna21

If we have any queries relating to the data then we will contact you later.
Data submitted as a Private Communication will be processed and added to the Cambridge Structural Database (CSD).
Please note, if the data have not appeared in a journal publication 1 year after the date of deposition, and the CCDC cannot contact you to discuss the matter, then the CCDC will automatically include the data
in the CSD as a Private Communication.
Kind regards,
Data Acquisition Team



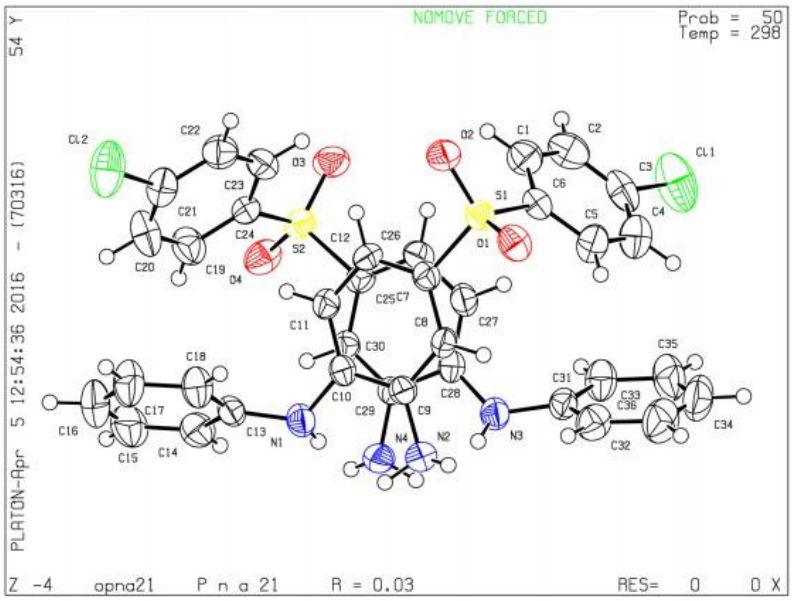


Table 1. Crystal data and structure refinement for o+pna21.

Identification code	o+pna21
Empirical formula	C18 H15 Cl N2 O2 S
Formula weight	358.83
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 19.109(4) A alpha = 90 deg. b = 8.8080(18) A beta = 90 deg. c = 20.086(4) A gamma = 90 deg.
Volume	3380.7(12) A^3
Z, Calculated density	8, 1.410 Mg/m^3
Absorption coefficient	0.362 mm^-1
F(000)	1488
Crystal size	? x ? x ? mm
Theta range for data collection	2.52 to 26.99 deg.
Limiting indices	-23<=h<=24, -10<=k<=11, -25<=l<=25
Reflections collected / unique	25341 / 7373 [R(int) = 0.0482]
Completeness to theta = 26.99	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7373 / 2 / 457
Goodness-of-fit on F^2	0.852
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0617
R indices (all data)	R1 = 0.0549, wR2 = 0.0654
Largest diff. peak and hole	0.241 and -0.242 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropicdisplacement parameters (A^2 x 10^3) for o+pna21.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(2)	-588(1)	5683(1)	6838(1)	41(1)
S(1)	3088(1)	5548(1)	7143(1)	38(1)
Cl(1)	2333(1)	5998(1)	4125(1)	94(1)
Cl(2)	236(1)	7236(1)	9774(1)	81(1)
O(2)	2959(1)	6988(2)	7453(1)	52(1)
N(3)	1454(1)	987(3)	5992(1)	43(1)
N(2)	2131(2)	108(3)	7427(1)	45(1)
O(1)	3765(1)	4852(2)	7206(1)	49(1)
N(4)	268(1)	161(2)	6657(1)	45(1)
C(25)	21(1)	4314(3)	6554(1)	37(1)
C(30)	-106(1)	2795(3)	6697(1)	37(1)
C(6)	2900(1)	5725(3)	6280(1)	39(1)
C(13)	481(1)	1479(3)	8610(1)	40(1)
C(31)	1955(1)	1100(3)	5476(1)	41(1)
C(12)	1854(1)	4786(3)	7725(1)	42(1)
C(21)	22(1)	6735(3)	8956(1)	51(1)
C(28)	977(1)	2143(3)	6157(1)	36(1)
C(24)	-337(1)	6079(3)	7674(1)	37(1)
C(7)	2458(1)	4247(3)	7429(1)	36(1)
C(10)	1448(1)	2223(3)	7855(1)	35(1)
N(1)	946(1)	1150(3)	8074(1)	43(1)
O(3)	-487(1)	7052(2)	6457(1)	53(1)
C(9)	2058(1)	1667(3)	7547(1)	35(1)
C(11)	1355(1)	3775(3)	7936(1)	40(1)
C(23)	187(1)	7103(3)	7794(1)	46(1)
C(22)	375(2)	7450(3)	8444(1)	51(1)
C(29)	361(1)	1691(3)	6493(1)	36(1)
C(8)	2561(1)	2689(3)	7341(1)	35(1)
C(19)	-674(2)	5349(4)	8189(1)	57(1)
C(26)	613(1)	4760(3)	6216(1)	43(1)
C(20)	-487(2)	5705(4)	8846(1)	66(1)
C(2)	2264(2)	6903(3)	5398(1)	60(1)
C(5)	3203(1)	4722(3)	5838(1)	54(1)
C(18)	738(1)	2076(3)	9197(1)	53(1)
C(4)	3027(2)	4811(4)	5170(1)	63(1)
C(27)	1088(1)	3656(3)	6019(1)	43(1)
C(14)	-217(1)	1105(3)	8565(1)	53(1)
C(36)	1759(2)	1581(3)	4845(1)	55(1)
C(17)	295(2)	2277(4)	9742(2)	74(1)
C(3)	2556(2)	5884(4)	4964(1)	56(1)
C(1)	2433(2)	6811(3)	6071(1)	53(1)
C(33)	3102(2)	542(4)	5073(2)	72(1)
C(32)	2635(1)	620(3)	5589(1)	53(1)
C(15)	-654(2)	1308(4)	9111(2)	75(1)
C(35)	2246(2)	1531(4)	4332(1)	72(1)
C(34)	2920(2)	1006(4)	4455(2)	77(1)
C(16)	-391(2)	1873(4)	9698(2)	83(1)
O(4)	-1263(1)	4983(2)	6859(1)	53(1)

Table 3. Bond lengths [A] and angles [deg] for o+pna21.

S(2)-O(4)	1.4297(19)
S(2)-O(3)	1.4413(19)
S(2)-C(25)	1.770(2)
S(2)-C(24)	1.782(2)
S(1)-O(2)	1.4342(18)
S(1)-O(1)	1.4360(18)
S(1)-C(7)	1.759(2)
S(1)-C(6)	1.777(2)
Cl(1)-C(3)	1.740(2)
Cl(2)-C(21)	1.749(3)
N(3)-C(28)	1.405(3)
N(3)-C(31)	1.415(3)
N(3)-H(3)	0.84(2)
N(2)-C(9)	1.401(3)
N(2)-H(2B)	0.85(3)
N(2)-H(2A)	0.90(3)
N(4)-C(29)	1.398(3)
N(4)-H(4A)	0.83(3)
N(4)-H(4B)	0.878(17)
C(25)-C(26)	1.376(3)
C(25)-C(30)	1.390(3)
C(30)-C(29)	1.382(3)
C(30)-H(30)	0.9300
C(6)-C(1)	1.374(3)
C(6)-C(5)	1.381(3)
C(13)-C(14)	1.377(3)
C(13)-C(18)	1.381(3)
C(13)-N(1)	1.425(3)
C(31)-C(32)	1.385(4)
C(31)-C(36)	1.388(3)
C(12)-C(11)	1.372(3)
C(12)-C(7)	1.382(3)
C(12)-H(12)	0.9300
C(21)-C(20)	1.347(4)
C(21)-C(22)	1.383(4)
C(28)-C(27)	1.378(3)
C(28)-C(29)	1.415(3)
C(24)-C(23)	1.369(3)
C(24)-C(19)	1.378(3)
C(7)-C(8)	1.397(3)
C(10)-C(11)	1.387(3)
C(10)-C(9)	1.409(3)
C(10)-N(1)	1.416(3)
N(1)-H(1)	0.86(3)
C(9)-C(8)	1.381(3)
C(11)-H(11)	0.9300
C(23)-C(22)	1.388(4)
C(23)-H(23)	0.9300
C(22)-H(22)	0.9300
C(8)-H(8)	0.9300
C(19)-C(20)	1.402(4)
C(19)-H(19)	0.9300
C(26)-C(27)	1.388(4)
C(26)-H(26)	0.9300
C(20)-H(20)	0.9300
C(2)-C(3)	1.370(4)
C(2)-C(1)	1.392(4)
C(2)-H(2)	0.9300
C(5)-C(4)	1.385(4)
C(5)-H(5)	0.9300
C(18)-C(17)	1.395(4)
C(18)-H(18)	0.9300
C(4)-C(3)	1.369(4)
C(4)-H(4)	0.9300
C(27)-H(27)	0.9300
C(14)-C(15)	1.391(4)
C(14)-H(14)	0.9300

C(36)-C(35)	1.390(4)
C(36)-H(36)	0.9300
C(17)-C(16)	1.361(5)
C(17)-H(17)	0.9300
C(1)-H(1A)	0.9300
C(33)-C(34)	1.352(5)
C(33)-C(32)	1.369(4)
C(33)-H(33)	0.9300
C(32)-H(32)	0.9300
C(15)-C(16)	1.374(5)
C(15)-H(15)	0.9300
C(35)-C(34)	1.390(5)
C(35)-H(35)	0.9300
C(34)-H(34)	0.9300
C(16)-H(16)	0.9300

O(4)-S(2)-O(3)	119.87(11)
O(4)-S(2)-C(25)	108.00(11)
O(3)-S(2)-C(25)	108.10(11)
O(4)-S(2)-C(24)	107.42(11)
O(3)-S(2)-C(24)	107.44(11)
C(25)-S(2)-C(24)	105.07(10)
O(2)-S(1)-O(1)	119.59(11)
O(2)-S(1)-C(7)	108.44(11)
O(1)-S(1)-C(7)	108.00(11)
O(2)-S(1)-C(6)	108.14(12)
O(1)-S(1)-C(6)	107.81(11)
C(7)-S(1)-C(6)	103.74(11)
C(28)-N(3)-C(31)	124.1(2)
C(28)-N(3)-H(3)	116.3(17)
C(31)-N(3)-H(3)	114.7(18)
C(9)-N(2)-H(2B)	110.3(19)
C(9)-N(2)-H(2A)	109.4(17)
H(2B)-N(2)-H(2A)	114(3)
C(29)-N(4)-H(4A)	111.3(17)
C(29)-N(4)-H(4B)	109(2)
H(4A)-N(4)-H(4B)	113(3)
C(26)-C(25)-C(30)	121.3(2)
C(26)-C(25)-S(2)	120.35(19)
C(30)-C(25)-S(2)	118.29(18)
C(29)-C(30)-C(25)	120.2(2)
C(29)-C(30)-H(30)	119.9
C(25)-C(30)-H(30)	119.9
C(1)-C(6)-C(5)	121.3(2)
C(1)-C(6)-S(1)	119.45(18)
C(5)-C(6)-S(1)	119.18(19)
C(14)-C(13)-C(18)	119.4(2)
C(14)-C(13)-N(1)	120.4(2)
C(18)-C(13)-N(1)	120.1(2)
C(32)-C(31)-C(36)	119.8(2)
C(32)-C(31)-N(3)	119.5(2)
C(36)-C(31)-N(3)	120.5(2)
C(11)-C(12)-C(7)	119.3(2)
C(11)-C(12)-H(12)	120.3
C(7)-C(12)-H(12)	120.3
C(20)-C(21)-C(22)	122.5(2)
C(20)-C(21)-Cl(2)	119.6(2)
C(22)-C(21)-Cl(2)	117.9(2)
C(27)-C(28)-N(3)	123.6(2)
C(27)-C(28)-C(29)	119.7(2)
N(3)-C(28)-C(29)	116.6(2)
C(23)-C(24)-C(19)	121.1(2)
C(23)-C(24)-S(2)	119.52(17)
C(19)-C(24)-S(2)	119.4(2)
C(12)-C(7)-C(8)	120.7(2)
C(12)-C(7)-S(1)	119.20(18)
C(8)-C(7)-S(1)	120.11(18)
C(11)-C(10)-C(9)	120.0(2)
C(11)-C(10)-N(1)	122.3(2)
C(9)-C(10)-N(1)	117.7(2)
C(10)-N(1)-C(13)	121.4(2)

C(10)-N(1)-H(1)	112.4(18)
C(13)-N(1)-H(1)	115.8(19)
C(8)-C(9)-N(2)	121.2(2)
C(8)-C(9)-C(10)	118.8(2)
N(2)-C(9)-C(10)	119.9(2)
C(12)-C(11)-C(10)	121.0(2)
C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(24)-C(23)-C(22)	120.0(2)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(21)-C(22)-C(23)	118.2(3)
C(21)-C(22)-H(22)	120.9
C(23)-C(22)-H(22)	120.9
C(30)-C(29)-N(4)	121.8(2)
C(30)-C(29)-C(28)	118.7(2)
N(4)-C(29)-C(28)	119.2(2)
C(9)-C(8)-C(7)	120.3(2)
C(9)-C(8)-H(8)	119.9
C(7)-C(8)-H(8)	119.9
C(24)-C(19)-C(20)	118.8(3)
C(24)-C(19)-H(19)	120.6
C(20)-C(19)-H(19)	120.6
C(25)-C(26)-C(27)	118.6(2)
C(25)-C(26)-H(26)	120.7
C(27)-C(26)-H(26)	120.7
C(21)-C(20)-C(19)	119.3(3)
C(21)-C(20)-H(20)	120.3
C(19)-C(20)-H(20)	120.3
C(3)-C(2)-C(1)	119.0(3)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(6)-C(5)-C(4)	119.1(3)
C(6)-C(5)-H(5)	120.4
C(4)-C(5)-H(5)	120.4
C(13)-C(18)-C(17)	120.2(3)
C(13)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
C(3)-C(4)-C(5)	119.4(3)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(28)-C(27)-C(26)	121.3(2)
C(28)-C(27)-H(27)	119.3
C(26)-C(27)-H(27)	119.3
C(13)-C(14)-C(15)	120.0(3)
C(13)-C(14)-H(14)	120.0
C(15)-C(14)-H(14)	120.0
C(31)-C(36)-C(35)	119.1(3)
C(31)-C(36)-H(36)	120.5
C(35)-C(36)-H(36)	120.5
C(16)-C(17)-C(18)	120.0(3)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(4)-C(3)-C(2)	121.9(2)
C(4)-C(3)-Cl(1)	119.5(2)
C(2)-C(3)-Cl(1)	118.6(2)
C(6)-C(1)-C(2)	119.3(3)
C(6)-C(1)-H(1A)	120.4
C(2)-C(1)-H(1A)	120.4
C(34)-C(33)-C(32)	120.8(3)
C(34)-C(33)-H(33)	119.6
C(32)-C(33)-H(33)	119.6
C(33)-C(32)-C(31)	120.2(3)
C(33)-C(32)-H(32)	119.9
C(31)-C(32)-H(32)	119.9
C(16)-C(15)-C(14)	120.2(3)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(34)-C(35)-C(36)	119.9(3)
C(34)-C(35)-H(35)	120.0
C(36)-C(35)-H(35)	120.0

C(33)-C(34)-C(35)	120.2(3)
C(33)-C(34)-H(34)	119.9
C(35)-C(34)-H(34)	119.9
C(17)-C(16)-C(15)	120.2(3)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for o+pna21. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(2)	44(1)	35(1)	43(1)	-2(1)	-1(1)	4(1)
S(1)	38(1)	38(1)	38(1)	0(1)	1(1)	-3(1)
Cl(1)	84(1)	154(1)	45(1)	15(1)	-13(1)	-25(1)
Cl(2)	65(1)	136(1)	43(1)	-11(1)	-4(1)	11(1)
O(2)	64(1)	41(1)	51(1)	-7(1)	5(1)	-9(1)
N(3)	46(1)	45(1)	38(1)	4(1)	6(1)	5(1)
N(2)	53(2)	37(1)	47(1)	-2(1)	6(1)	1(1)
O(1)	35(1)	59(1)	53(1)	7(1)	-2(1)	-4(1)
N(4)	43(1)	37(1)	55(1)	-1(1)	8(1)	-3(1)
C(25)	45(1)	34(1)	31(1)	-3(1)	-2(1)	2(1)
C(30)	33(1)	41(1)	36(1)	-1(1)	6(1)	-2(1)
C(6)	38(1)	43(1)	35(1)	5(1)	1(1)	-6(1)
C(13)	38(1)	41(2)	41(1)	7(1)	8(1)	-1(1)
C(31)	41(1)	43(1)	38(1)	-7(1)	5(1)	-4(1)
C(12)	53(2)	31(1)	41(1)	-2(1)	7(1)	7(1)
C(21)	46(2)	65(2)	41(1)	-1(1)	1(1)	11(1)
C(28)	37(1)	43(2)	29(1)	-2(1)	1(1)	1(1)
C(24)	38(1)	33(1)	39(1)	0(1)	4(1)	4(1)
C(7)	40(1)	38(2)	31(1)	3(1)	2(1)	1(1)
C(10)	36(1)	42(1)	28(1)	2(1)	0(1)	-1(1)
N(1)	47(1)	48(1)	36(1)	-3(1)	5(1)	-9(1)
O(3)	74(1)	40(1)	46(1)	4(1)	-3(1)	9(1)
C(9)	43(1)	35(1)	28(1)	3(1)	-1(1)	1(1)
C(11)	38(1)	40(2)	42(1)	2(1)	8(1)	6(1)
C(23)	54(2)	41(1)	43(1)	6(1)	4(1)	-3(1)
C(22)	52(2)	49(2)	52(2)	-3(1)	-3(1)	-3(1)
C(29)	41(1)	34(1)	32(1)	-1(1)	-2(1)	-3(1)
C(8)	34(1)	40(1)	32(1)	-1(1)	4(1)	6(1)
C(19)	52(2)	63(2)	55(2)	-1(1)	6(1)	-16(2)
C(26)	53(2)	35(2)	42(1)	1(1)	5(1)	-7(1)
C(20)	60(2)	93(2)	44(1)	11(2)	12(1)	-9(2)
C(2)	60(2)	59(2)	60(2)	15(2)	-14(2)	-2(2)
C(5)	54(2)	62(2)	44(1)	-2(1)	3(1)	12(1)
C(18)	46(2)	73(2)	39(1)	1(1)	1(1)	-1(1)
C(4)	62(2)	81(2)	47(2)	-6(1)	6(1)	2(2)
C(27)	42(1)	47(2)	38(1)	0(1)	9(1)	-5(1)
C(14)	47(2)	52(2)	61(2)	0(1)	3(1)	-7(1)
C(36)	50(2)	74(2)	39(1)	-7(1)	0(1)	-3(1)
C(17)	81(2)	97(3)	43(1)	-8(2)	16(2)	-2(2)
C(3)	55(2)	78(2)	37(1)	11(1)	-1(1)	-24(2)
C(1)	59(2)	52(2)	48(2)	5(1)	-3(1)	4(2)
C(33)	45(2)	84(2)	86(2)	-12(2)	12(2)	3(2)
C(32)	42(2)	56(2)	62(2)	-5(1)	0(1)	2(1)
C(15)	46(2)	79(2)	99(2)	8(2)	22(2)	-7(2)
C(35)	81(2)	96(3)	38(1)	-6(1)	9(2)	-16(2)
C(34)	66(2)	90(3)	76(2)	-20(2)	33(2)	-5(2)
C(16)	77(2)	100(3)	73(2)	-2(2)	41(2)	-2(2)
O(4)	39(1)	51(1)	69(1)	-11(1)	-4(1)	4(1)