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APPENDICES

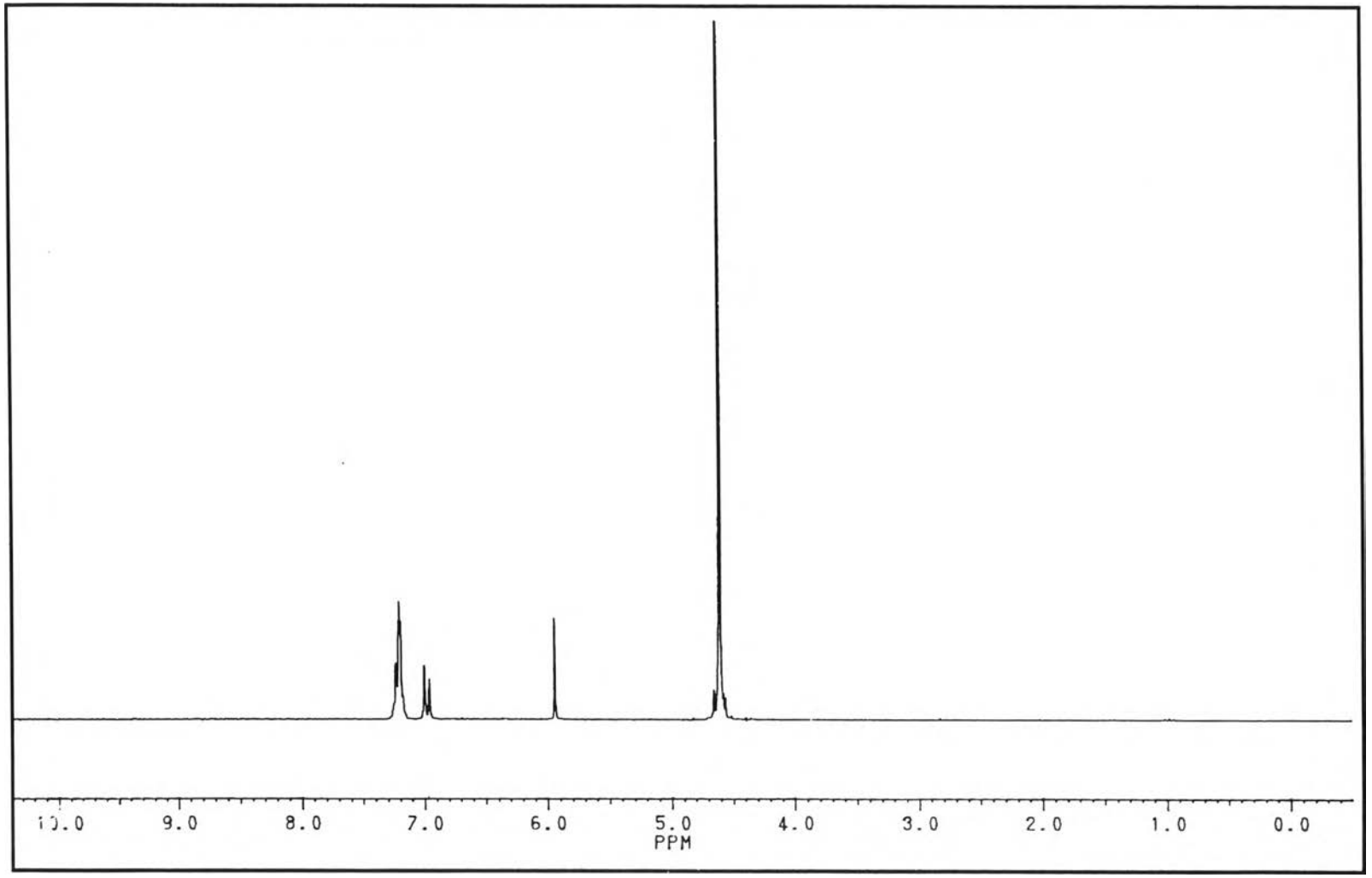


Figure 1 ^{1}H NMR spectrum (D_2O) of 1-(4′-chlorophenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(1)**

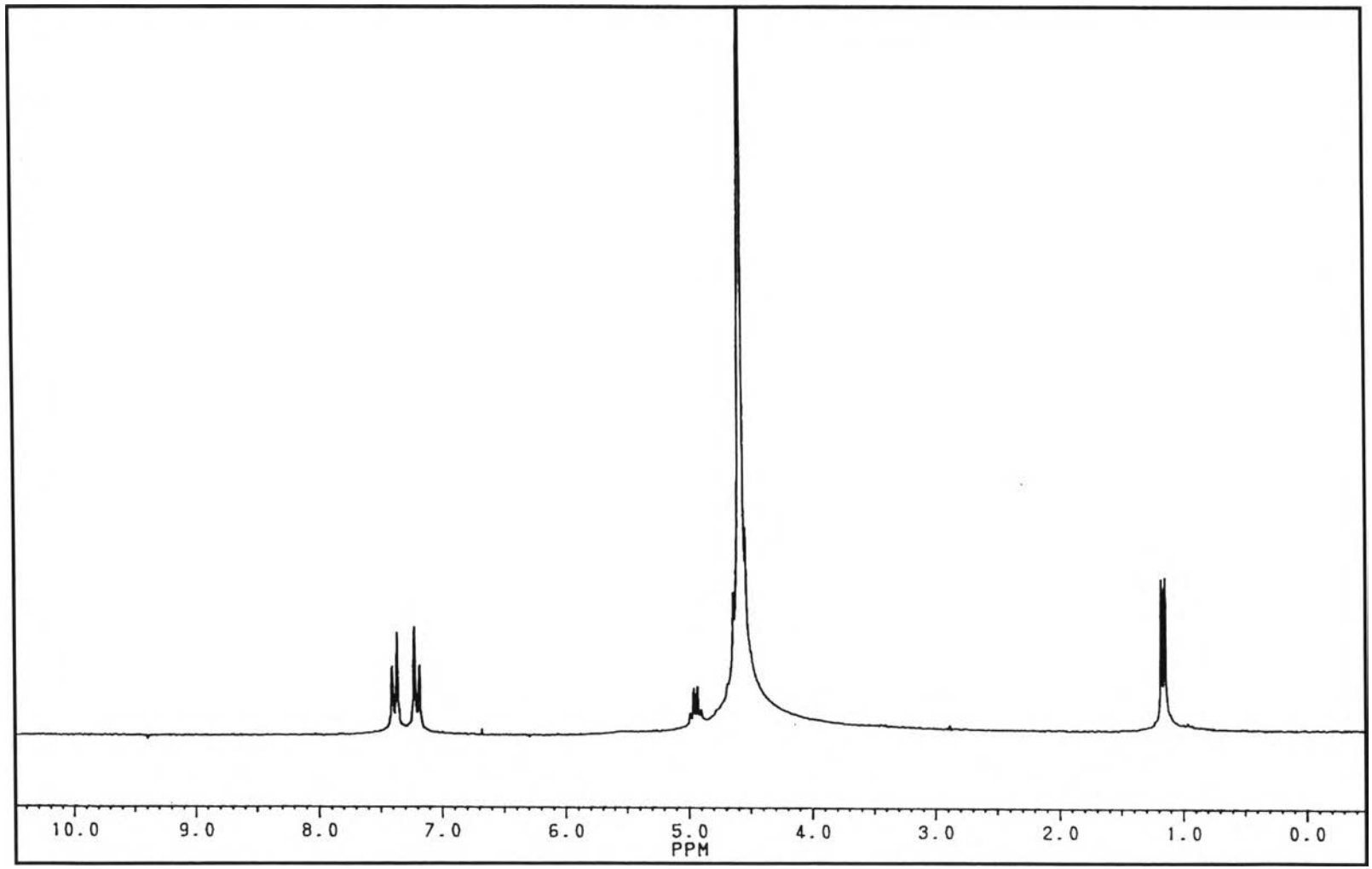


Figure 2 ^{1}H NMR spectrum (D_2O) of 1-(4′-chlorophenyl)-2-methyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(2)**

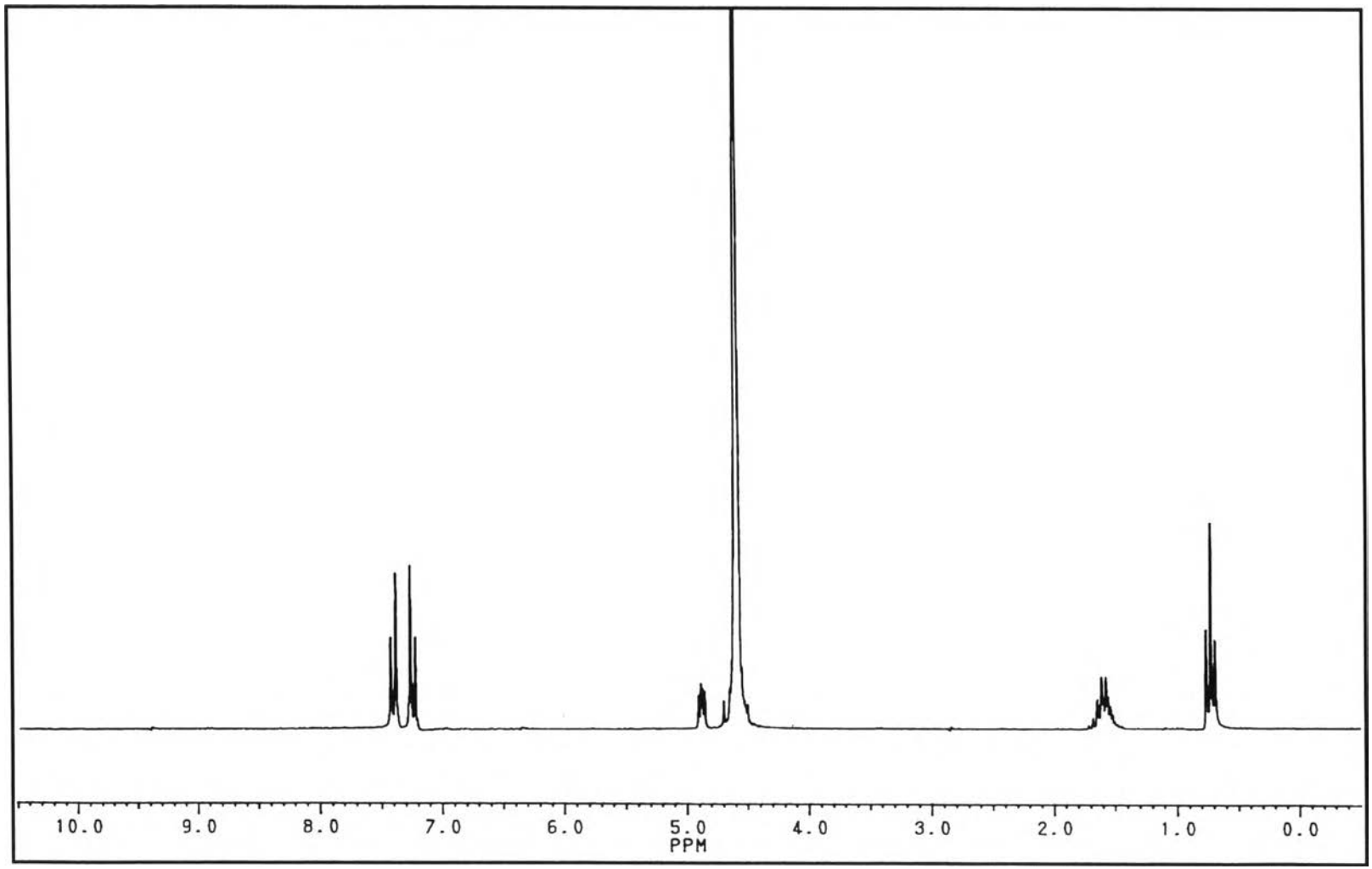


Figure 3 ^{1}H NMR spectrum (D_2O) of 1-(4′-chlorophenyl)-2-ethyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(3)**

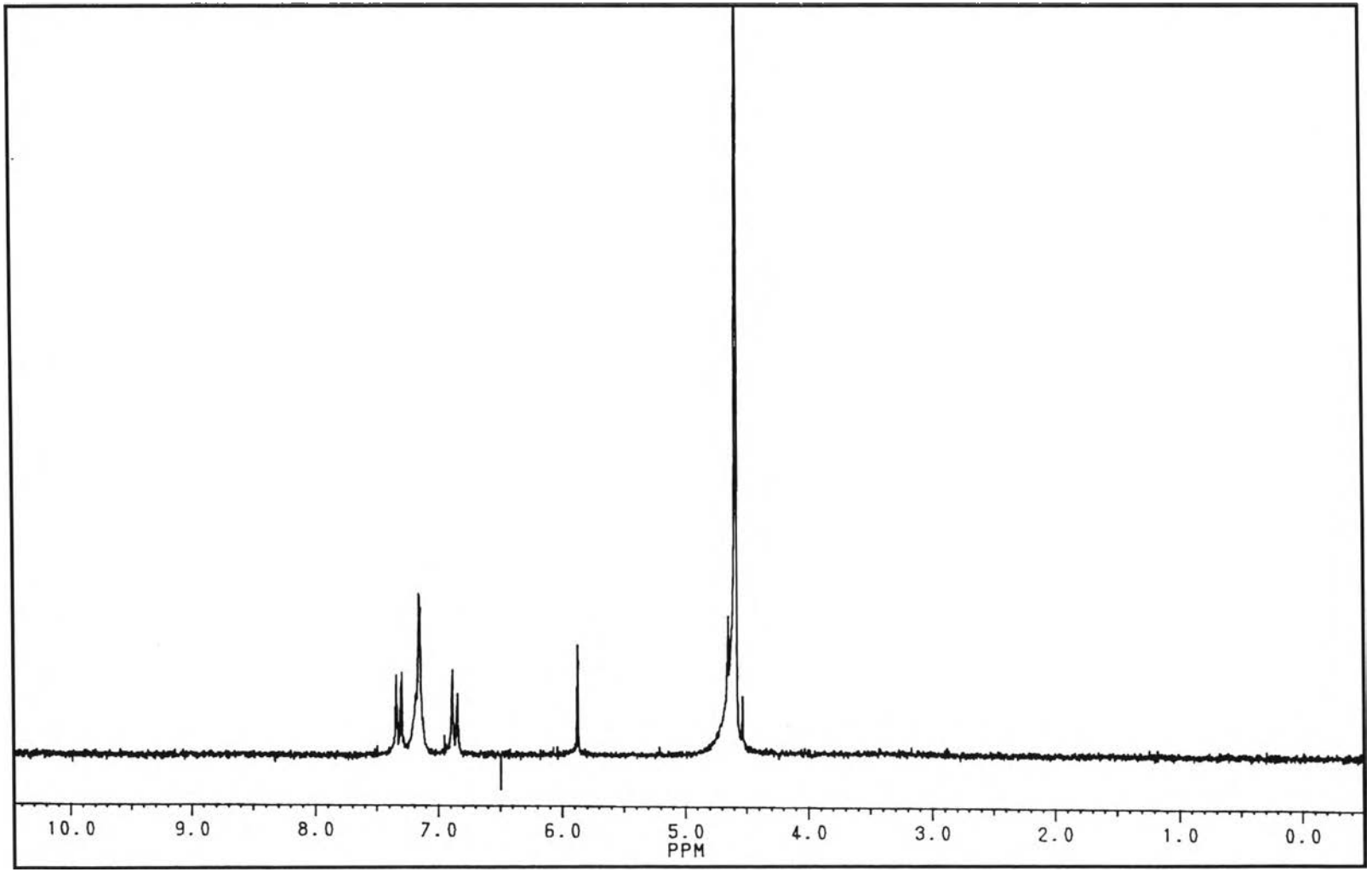


Figure 4 ^{1}H NMR spectrum (D_2O) of 1-(4′-bromophenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(4)**

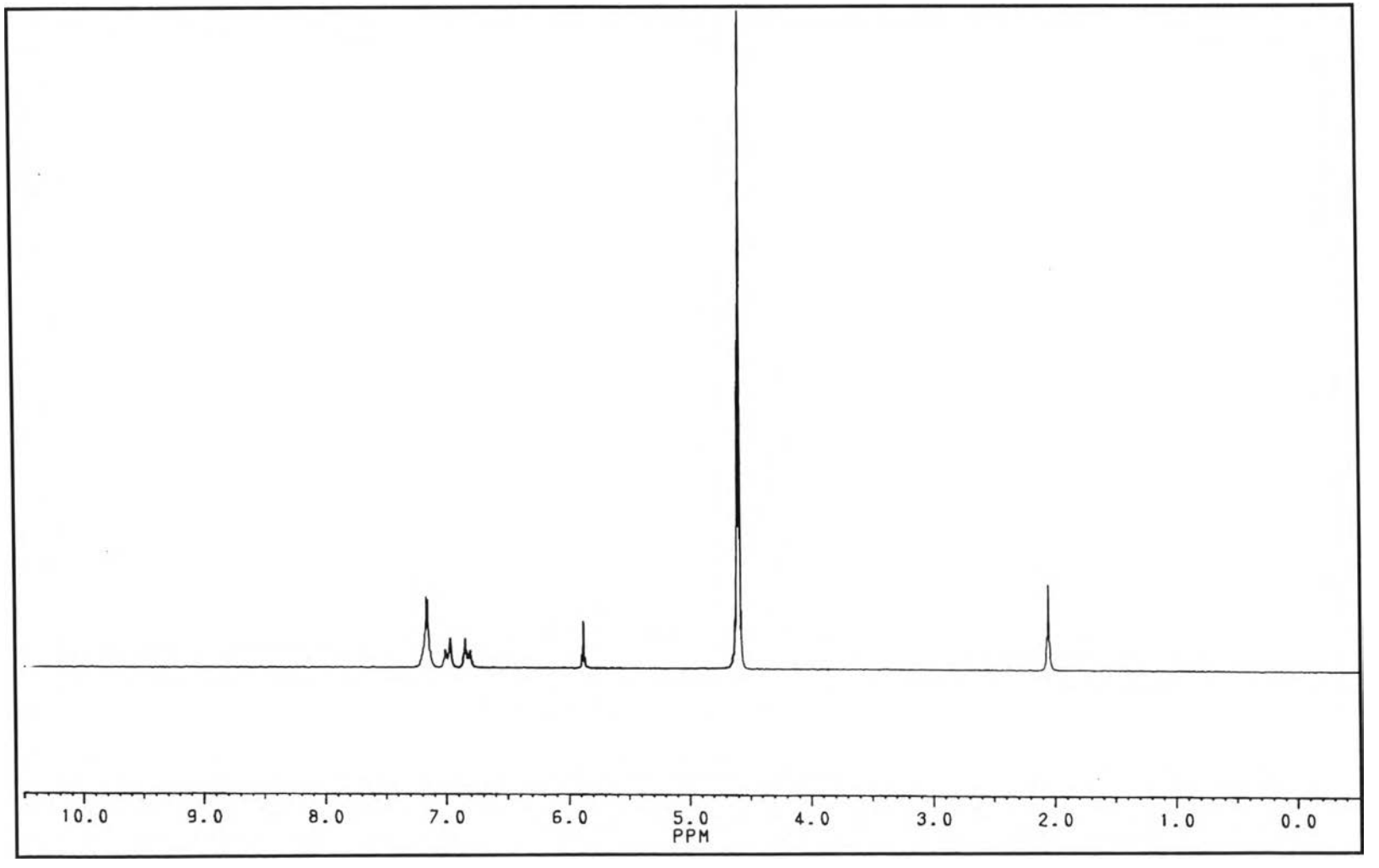


Figure 5 ^{1}H NMR spectrum (D_2O) of 1-(4′-methylphenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(5)**

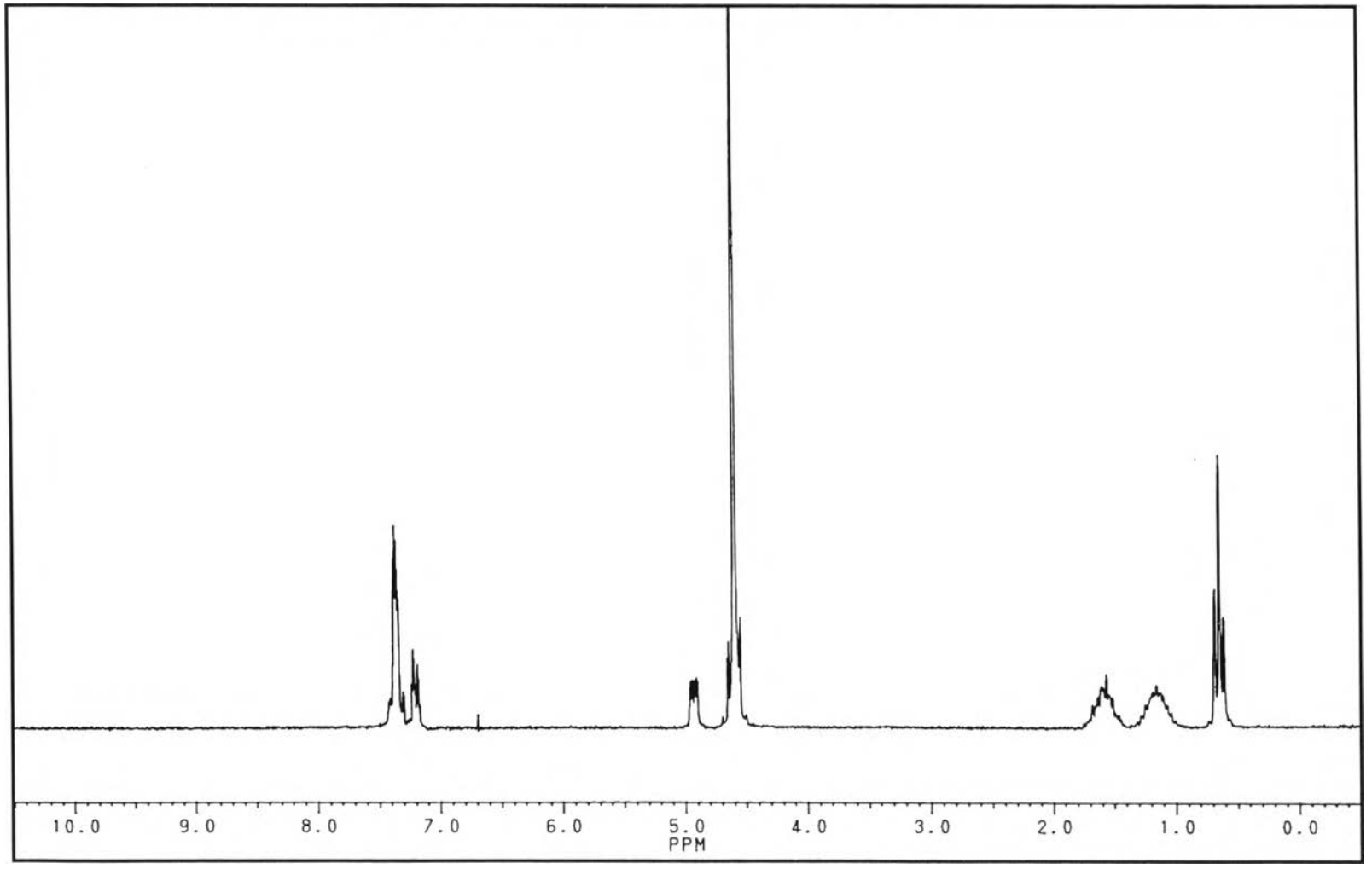


Figure 6 ^{1}H NMR spectrum (D_2O) of 1-(3′-chlorophenyl)-2-propyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(6)**

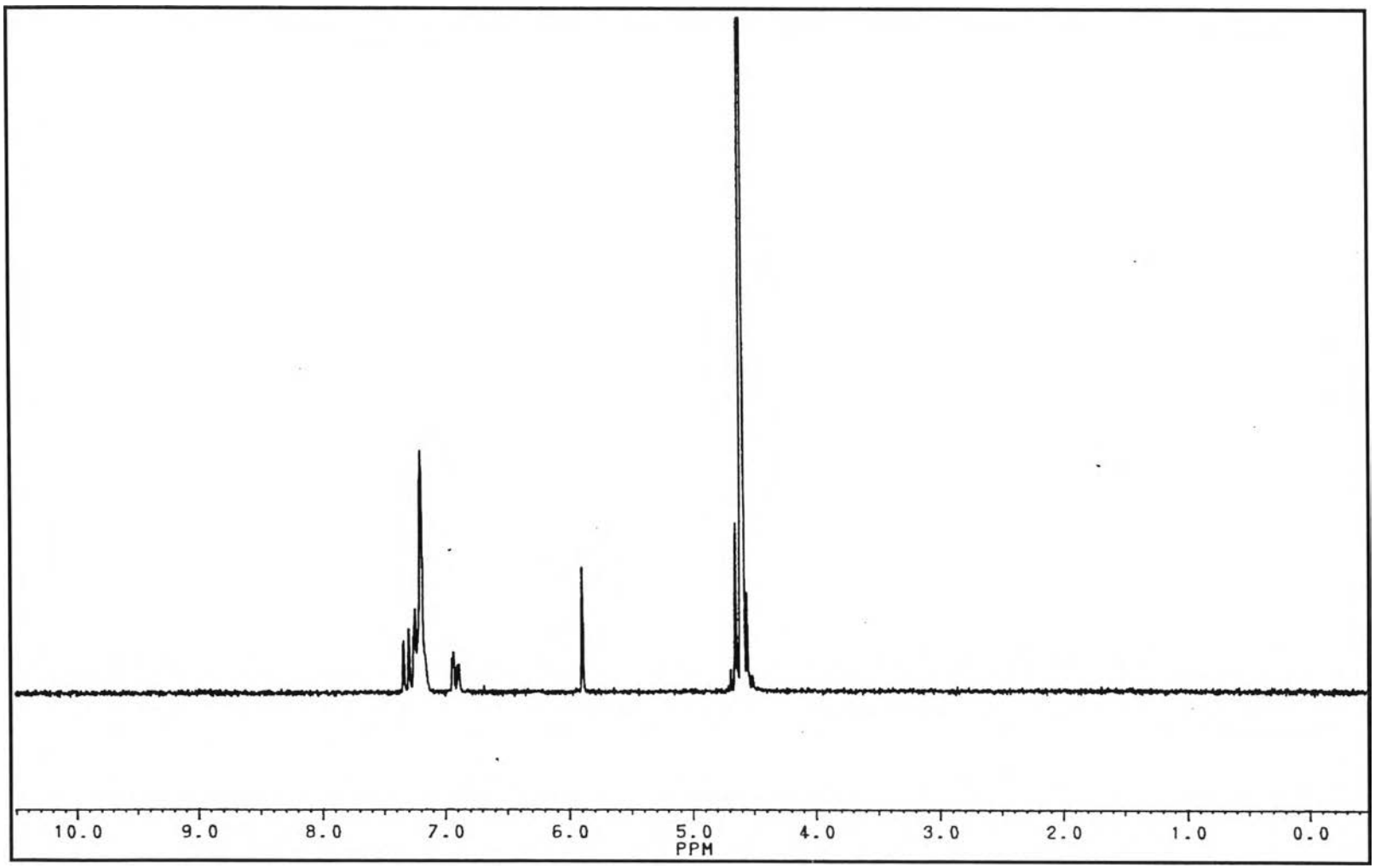


Figure 7 ^{1}H NMR spectrum (D_2O) of 1-(3′,4′-dichlorophenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(7)**

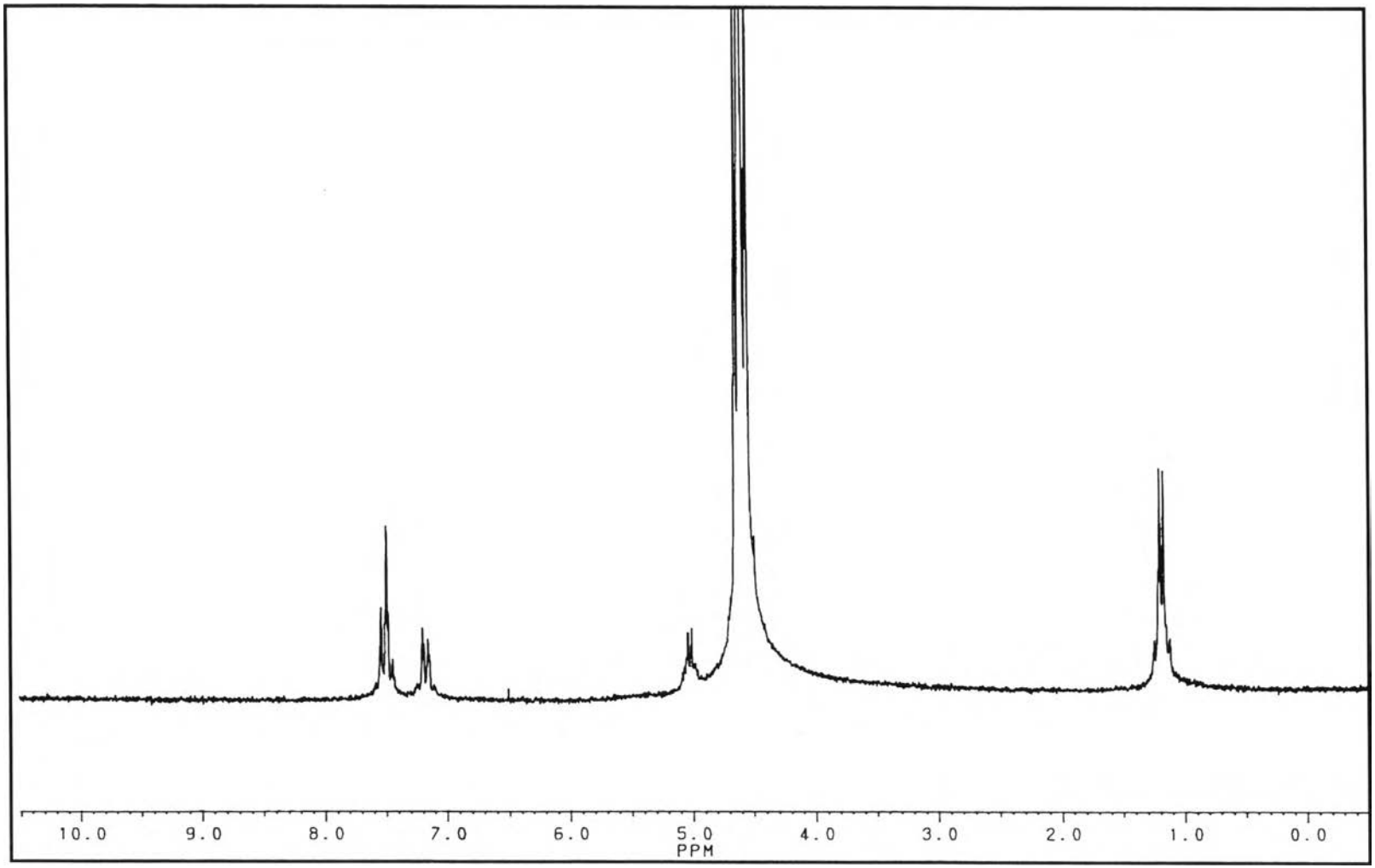


Figure 8 ^{1}H NMR spectrum (D_2O) of 1-(3′,4′-dichlorophenyl)-2-methyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(8)**

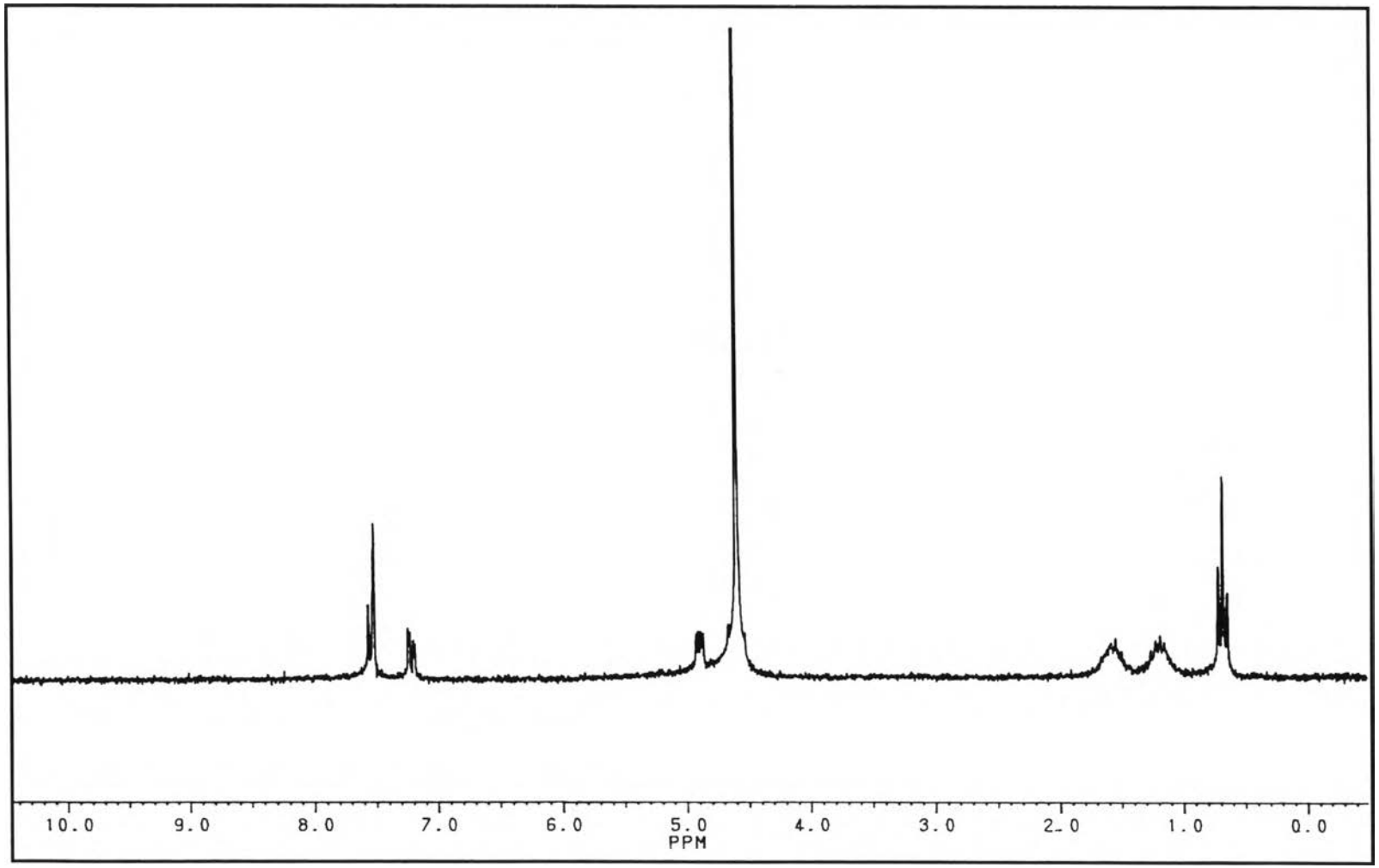


Figure 9 ^{1}H NMR spectrum (D_2O) of 1-(3′,4′-dichlorophenyl)-2-propyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(9)**

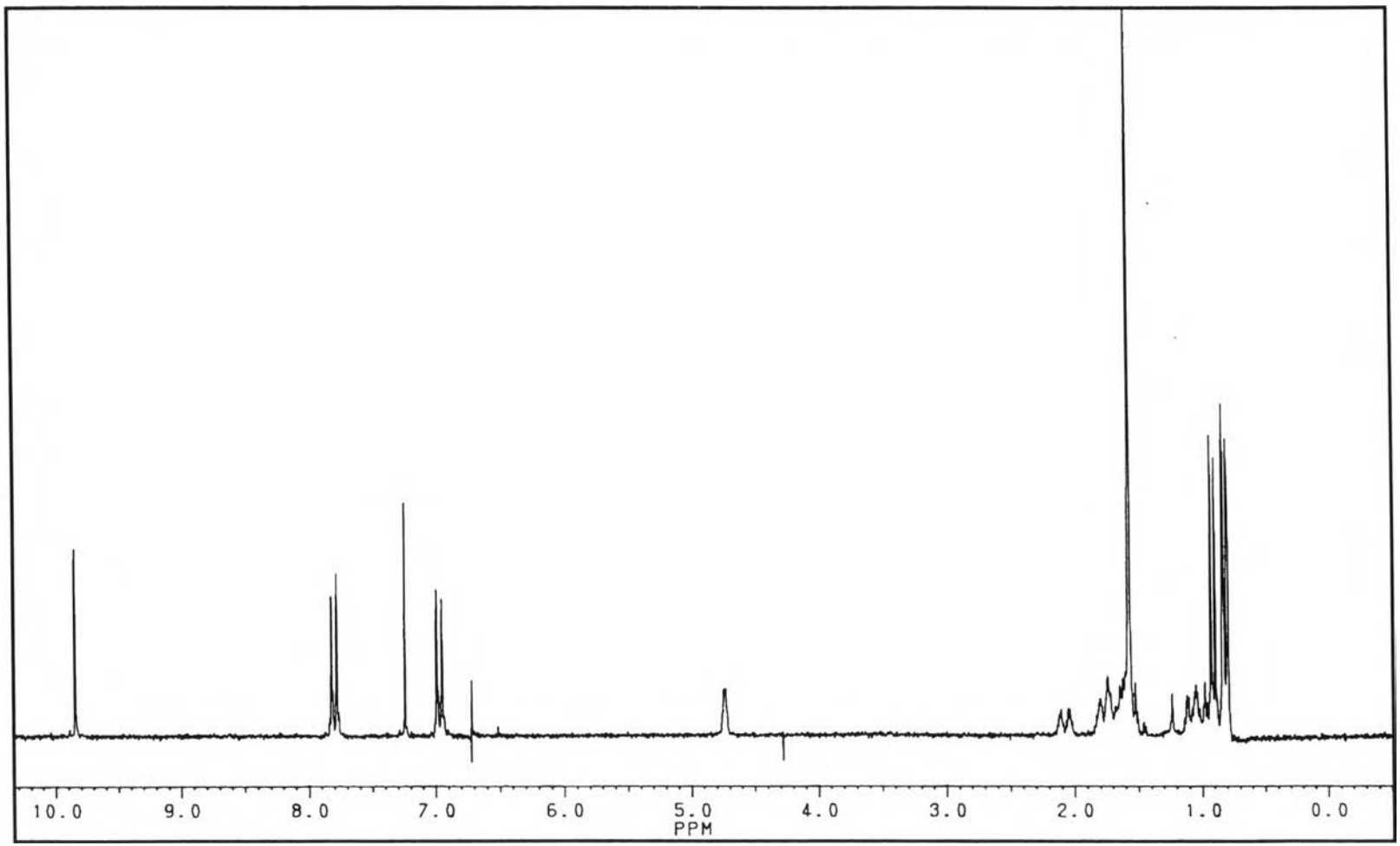


Figure 10 ^{1}H NMR spectrum ($CDCl_3$) of 4-(2′*S*-isopropyl-5′*R*-methyl-1′*S*-cyclohexyloxy)benzaldehyde **(46a)**

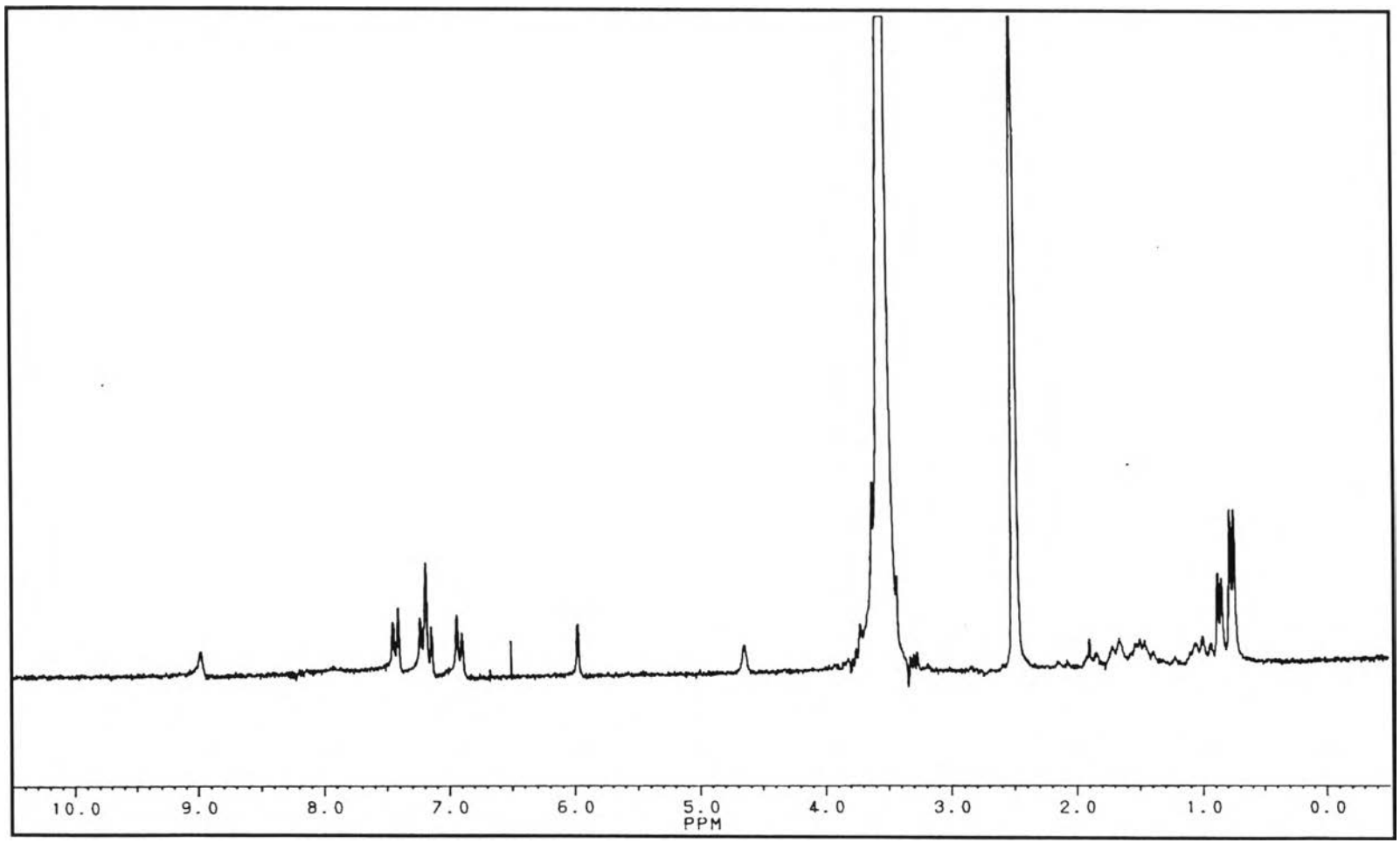


Figure 11 ^{1}H NMR spectrum (DMSO) of 1-(4′-chlorophenyl)-2-[4′-(2″*S*-isopropyl-5*R*″-methyl-1″*S*-cyclohexyloxy)phenyl]4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(46c)**

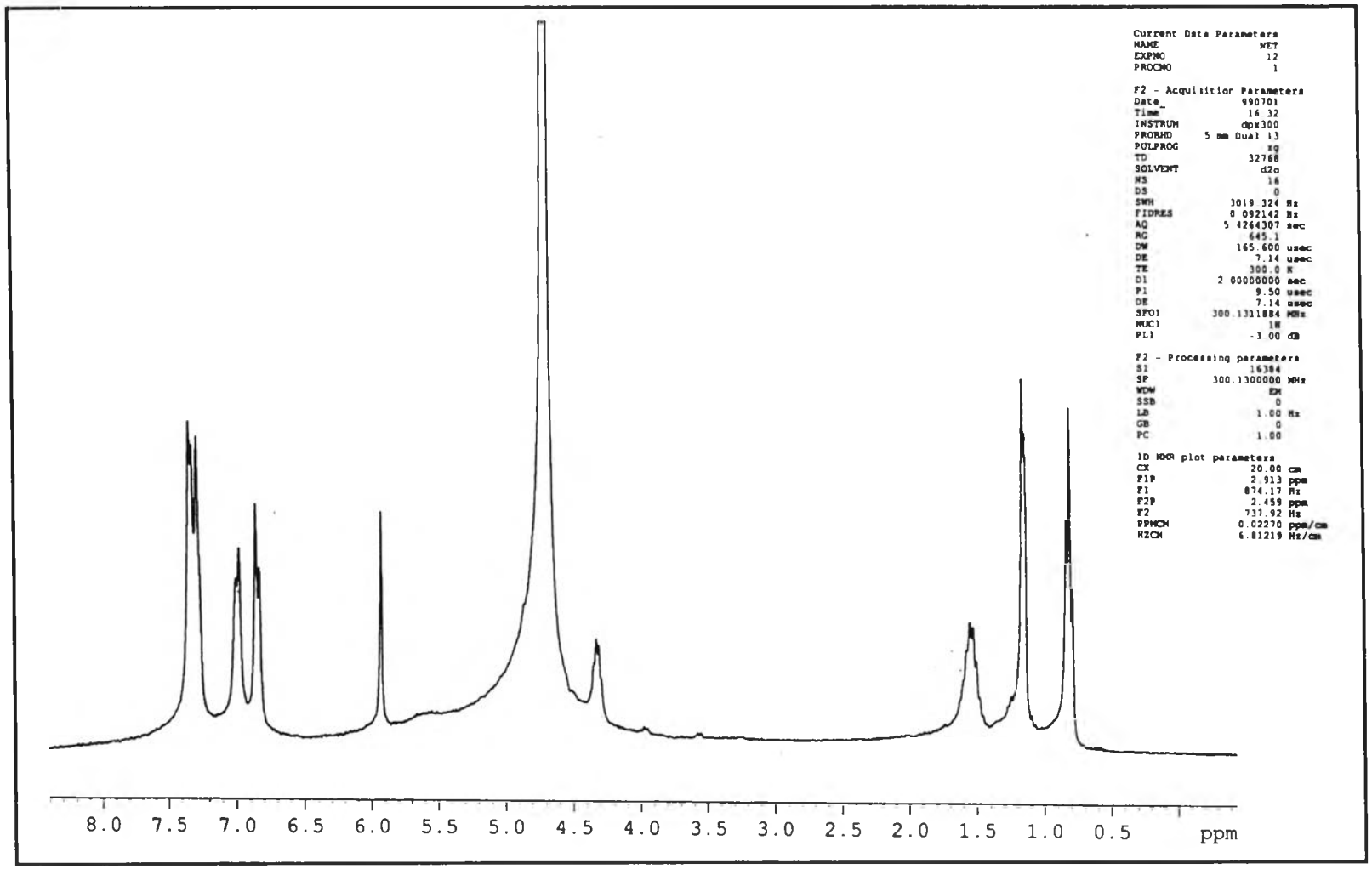


Figure 12 ^{1}H NMR spectrum (DMSO) of 1-(4′-sec-butoxyphenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(47c)**

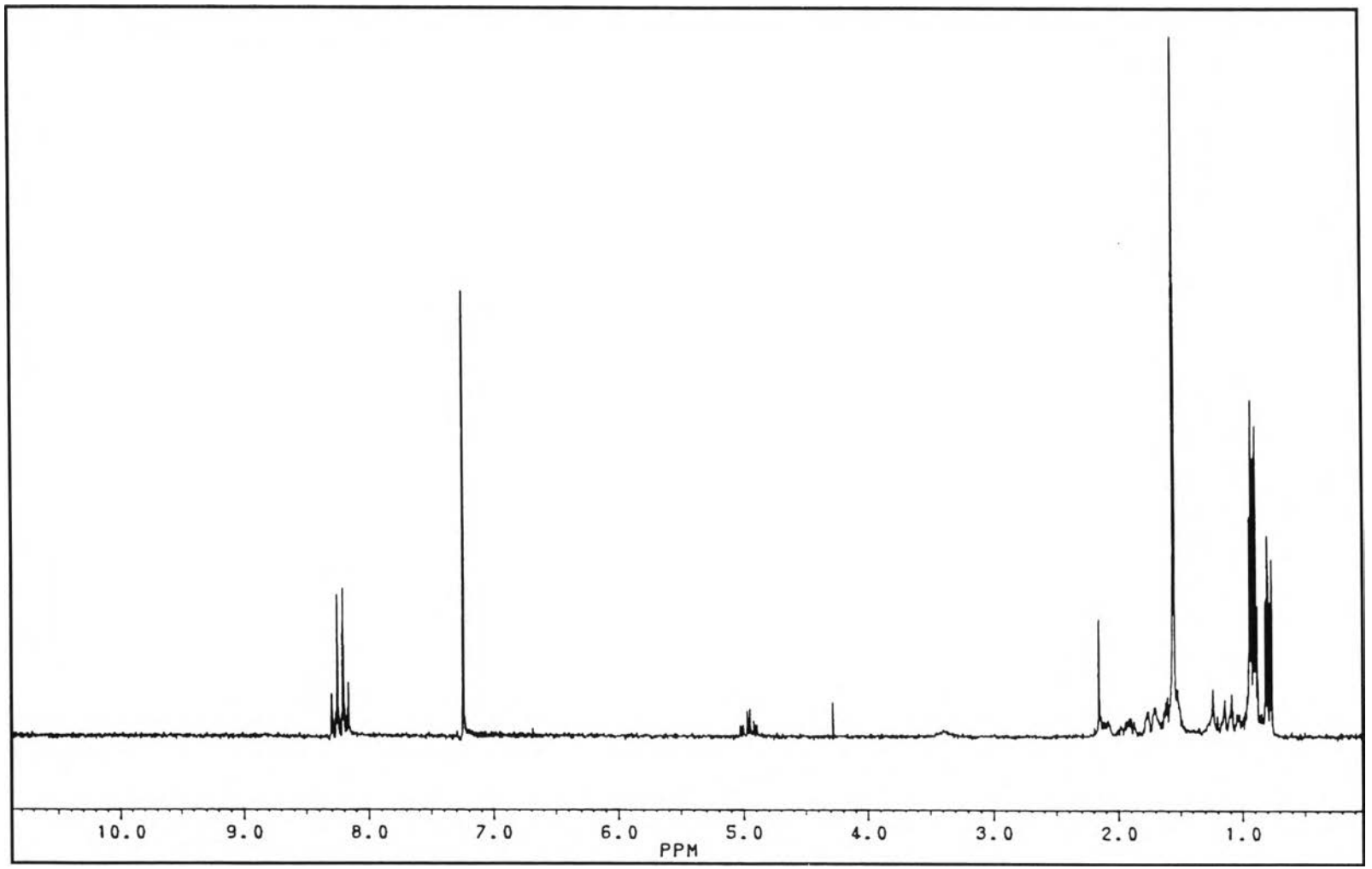


Figure 13 ^{1}H NMR spectrum ($CDCl_3$) of 4-nitrobenzoic acid (-)-menthyl ester **(49a)**

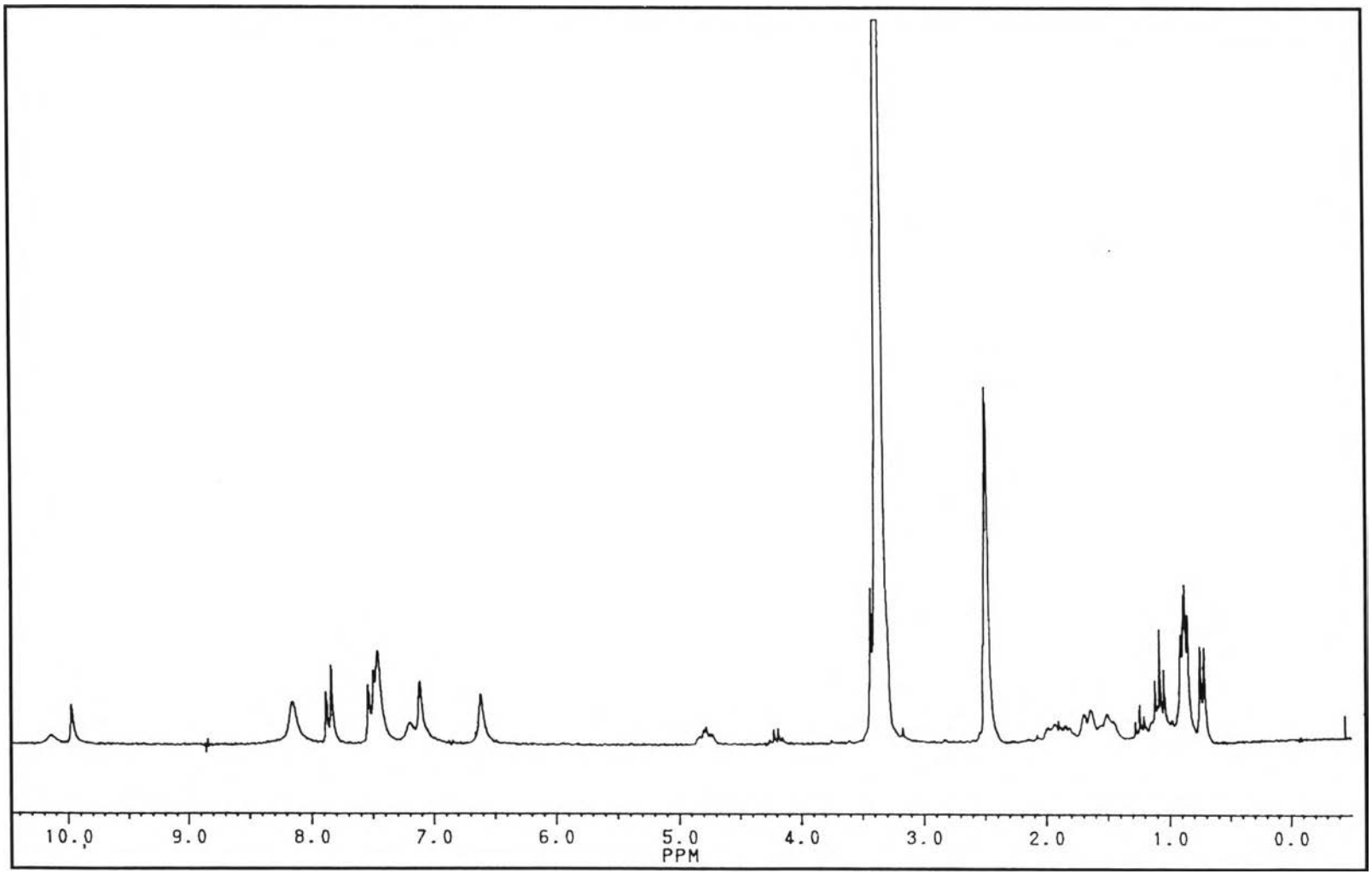


Figure 14 ^{1}H NMR spectrum (DMSO) of 4-(2′*S*-isopropyl-5′*R*-methyl-1′*R*-cyclohexyloxycarbonyl)phenylbiguanide hydrochloride **(49c)**

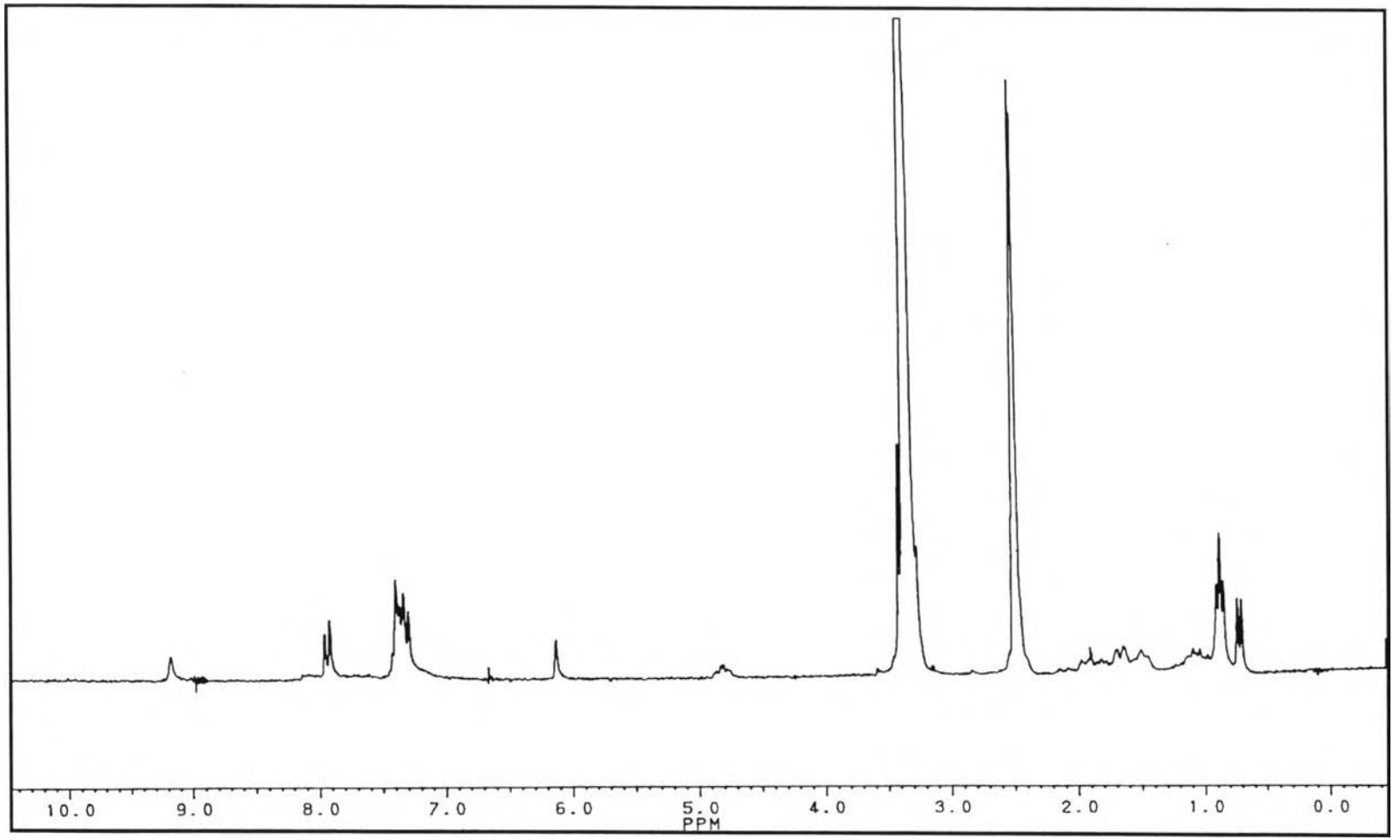


Figure 15 ^{1}H NMR spectrum (DMSO) of 1-[4′-(2″*S*-isopropyl-5″*R*-methyl-1″*R*-cyclohexyloxycarbonyl)phenyl]-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(49d)**

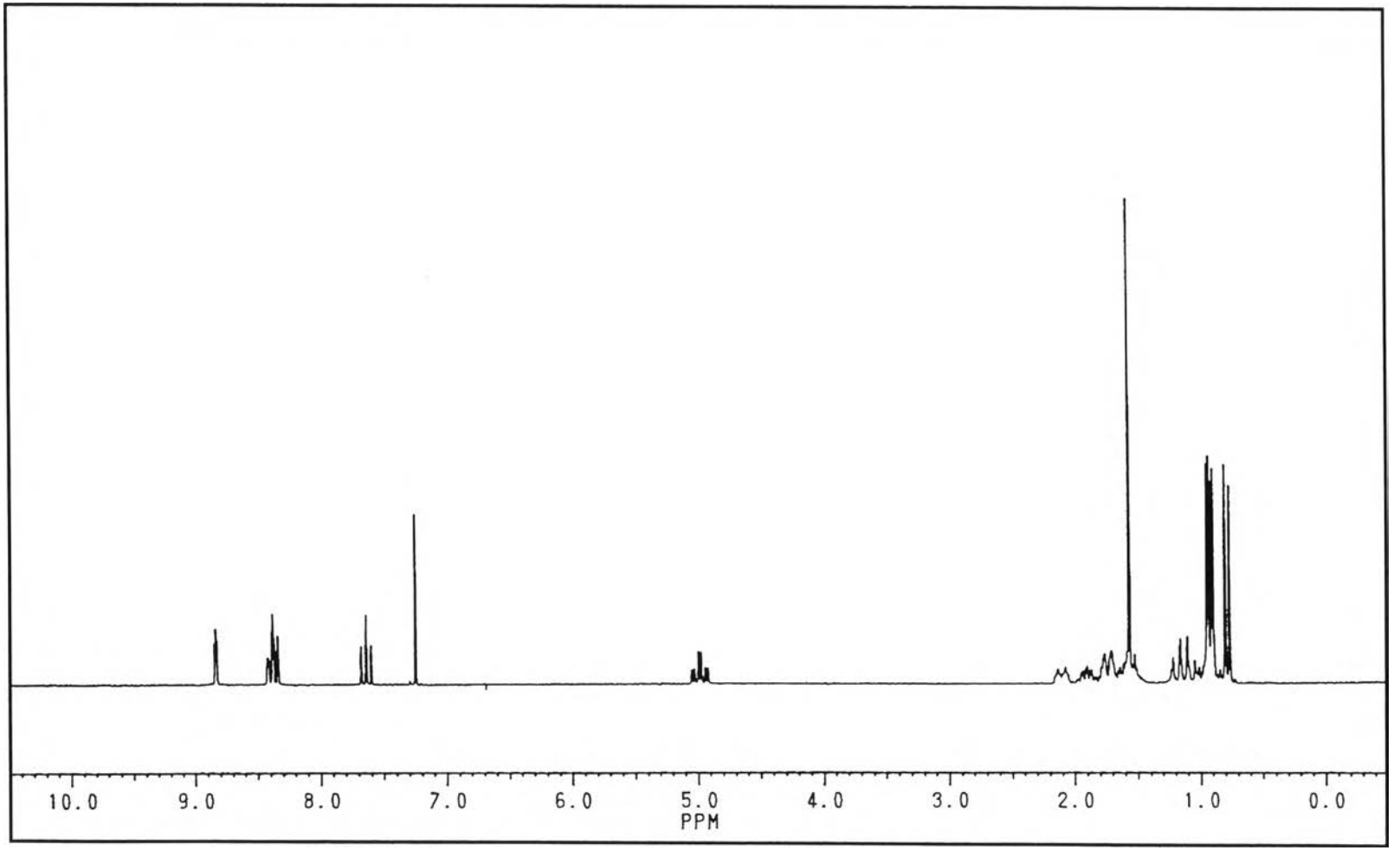


Figure 16 ^{1}H NMR spectrum ($CDCl_3$) of 3-nitrobenzoic acid (-)-menthyl ester **(50a)**

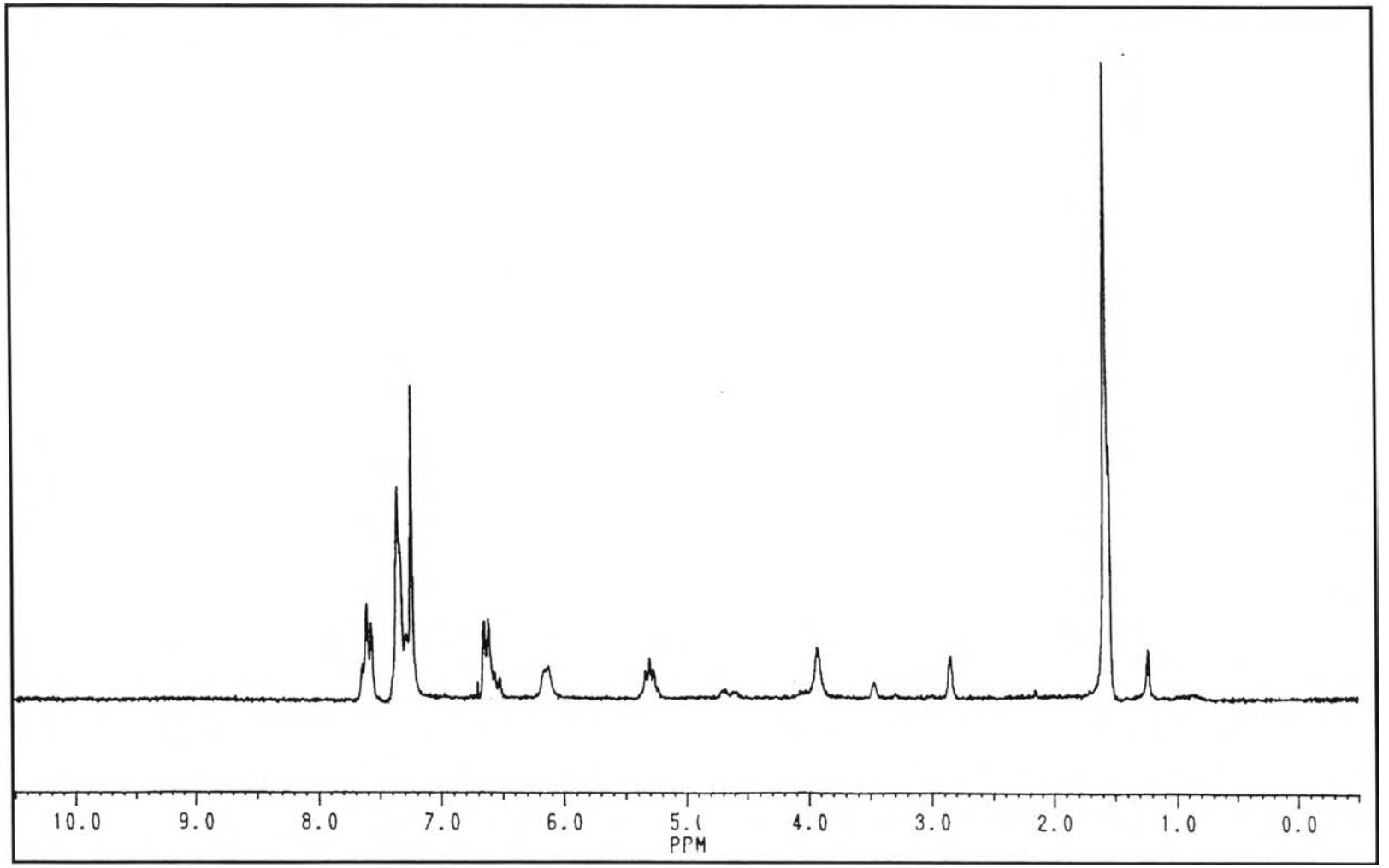


Figure 17 ^{1}H NMR spectrum ($CDCl_3$) of (±)-*N*-(α-methylbenzyl)-4-aminobenzamide **(51b)**

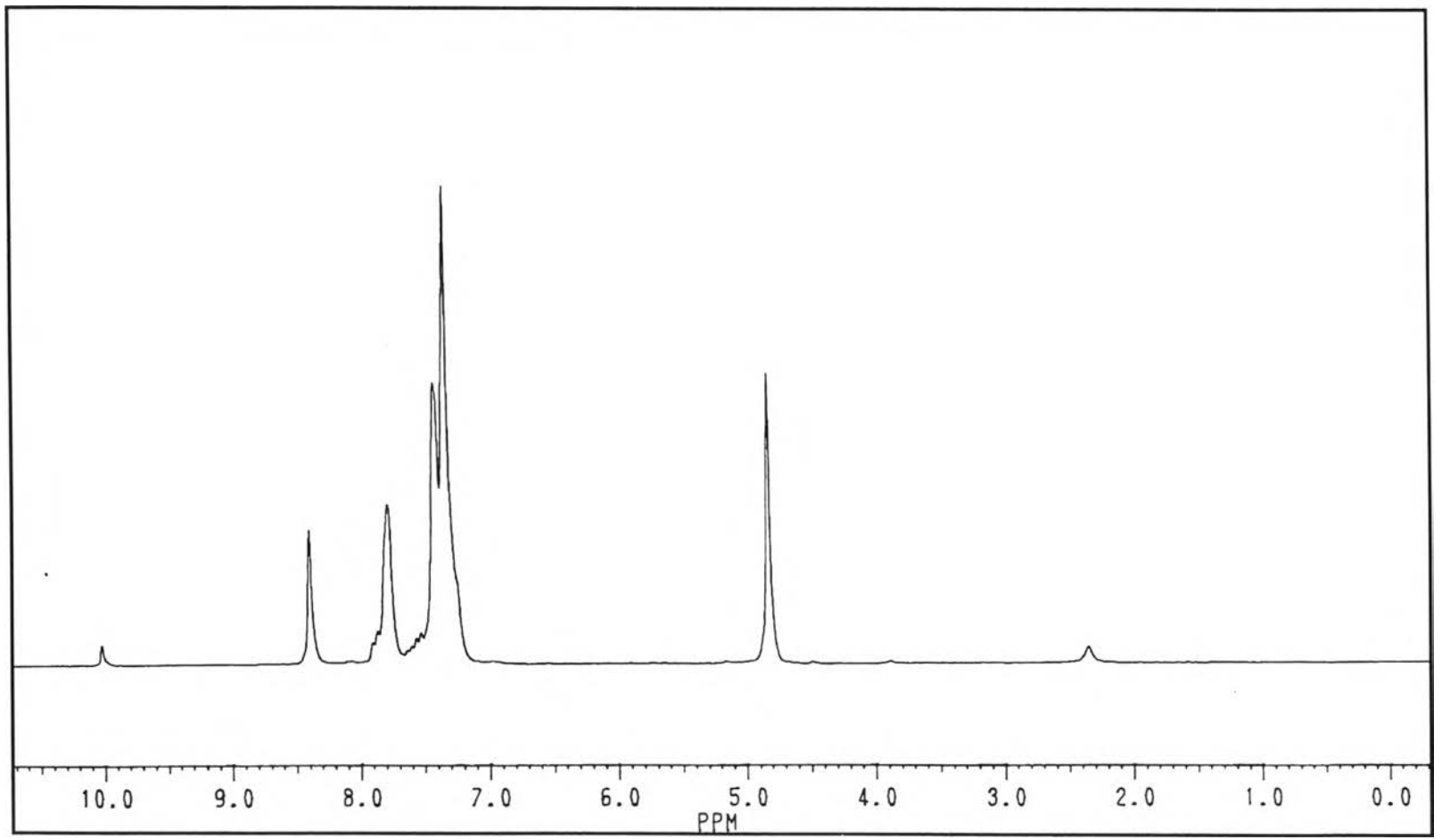


Figure 18 ^{1}H NMR spectrum ($CDCl_3$) of *N*-benzylidenebenzylamine **(52a)**

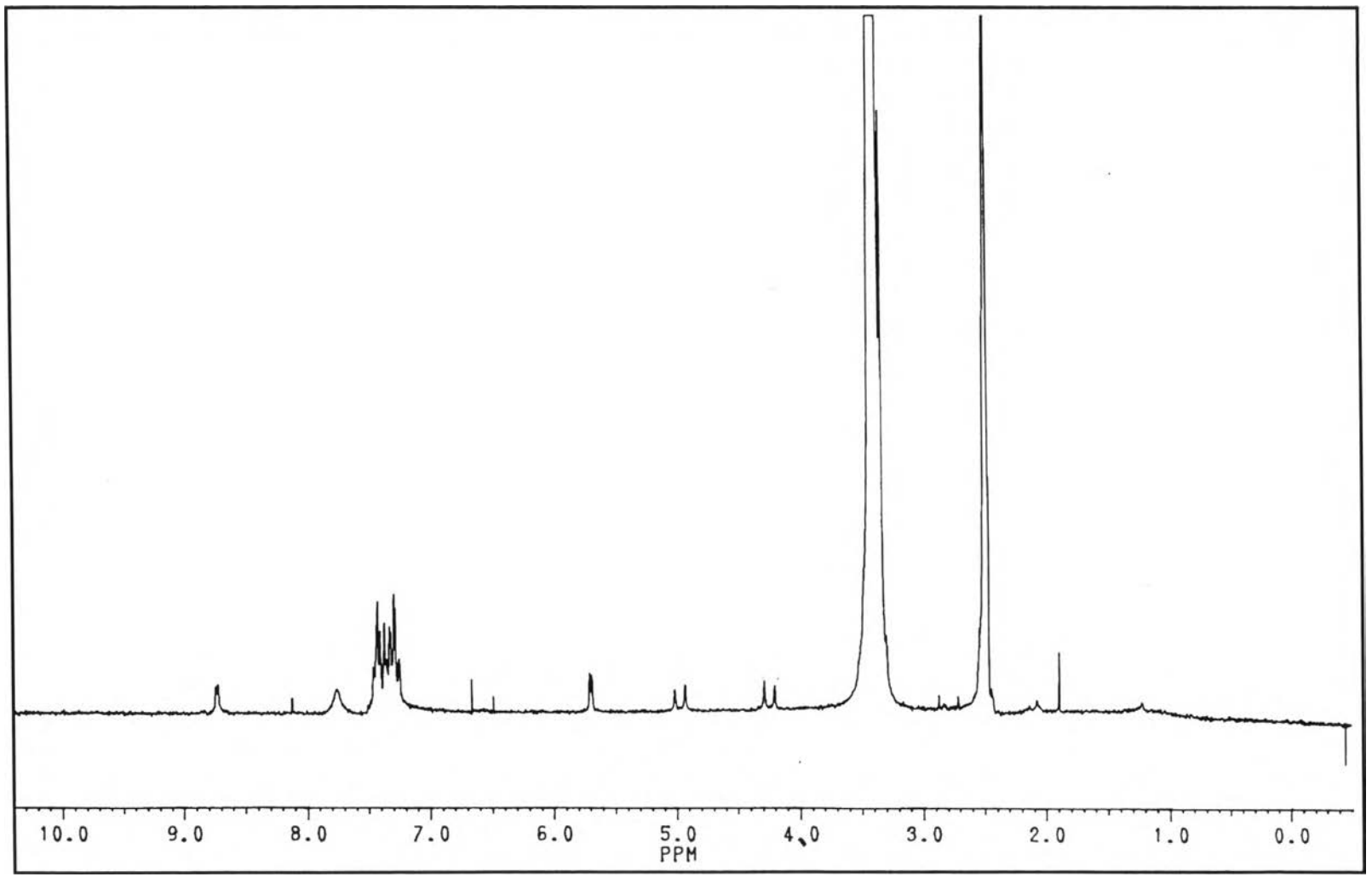


Figure 19 ^{1}H NMR spectrum (DMSO) of 1-benzyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(52b)**

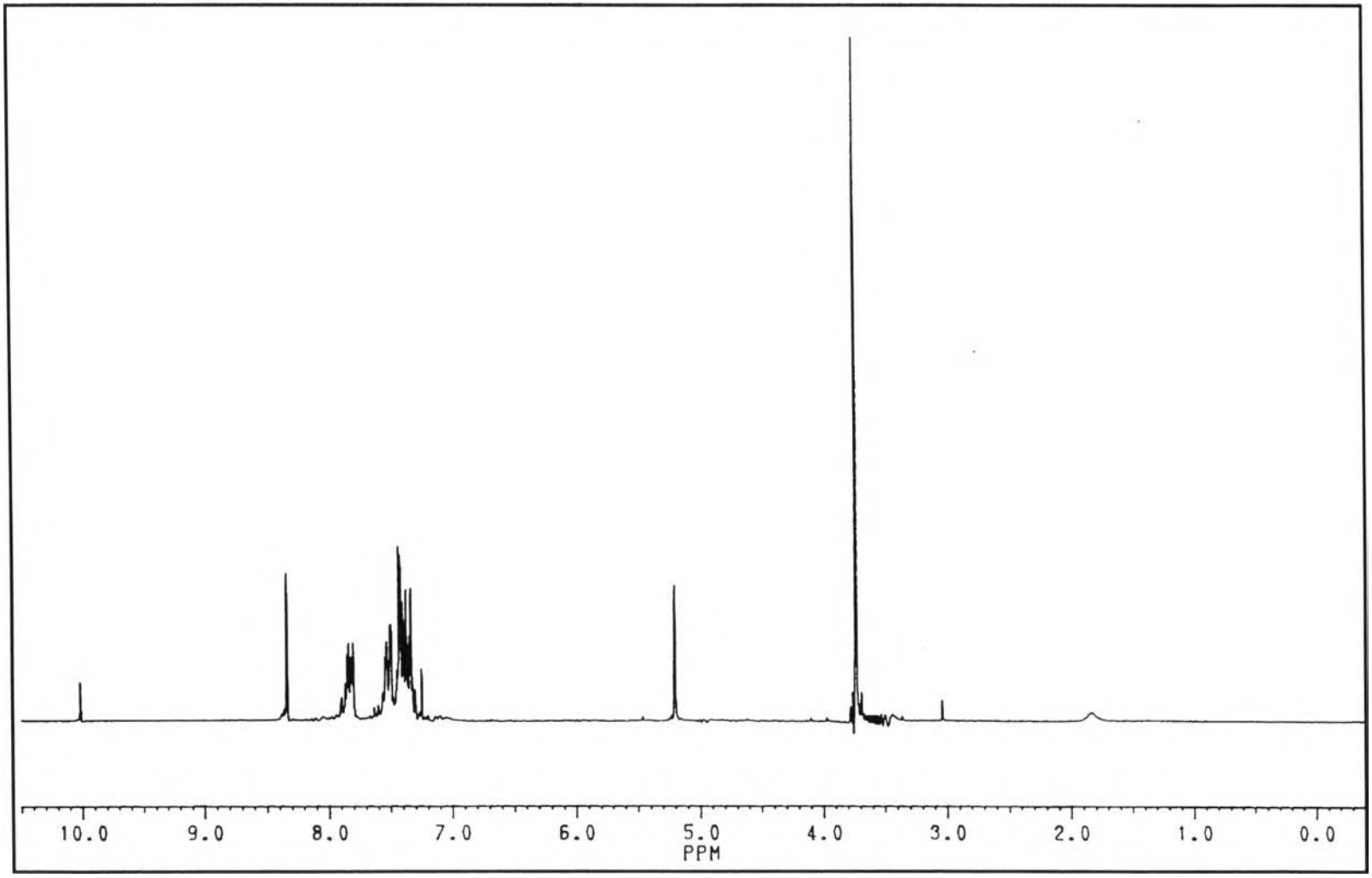


Figure 20 ^{1}H NMR spectrum ($CDCl_3$) of *N*-benzylidene-*R*-phenylglycine methyl ester **(53b)**

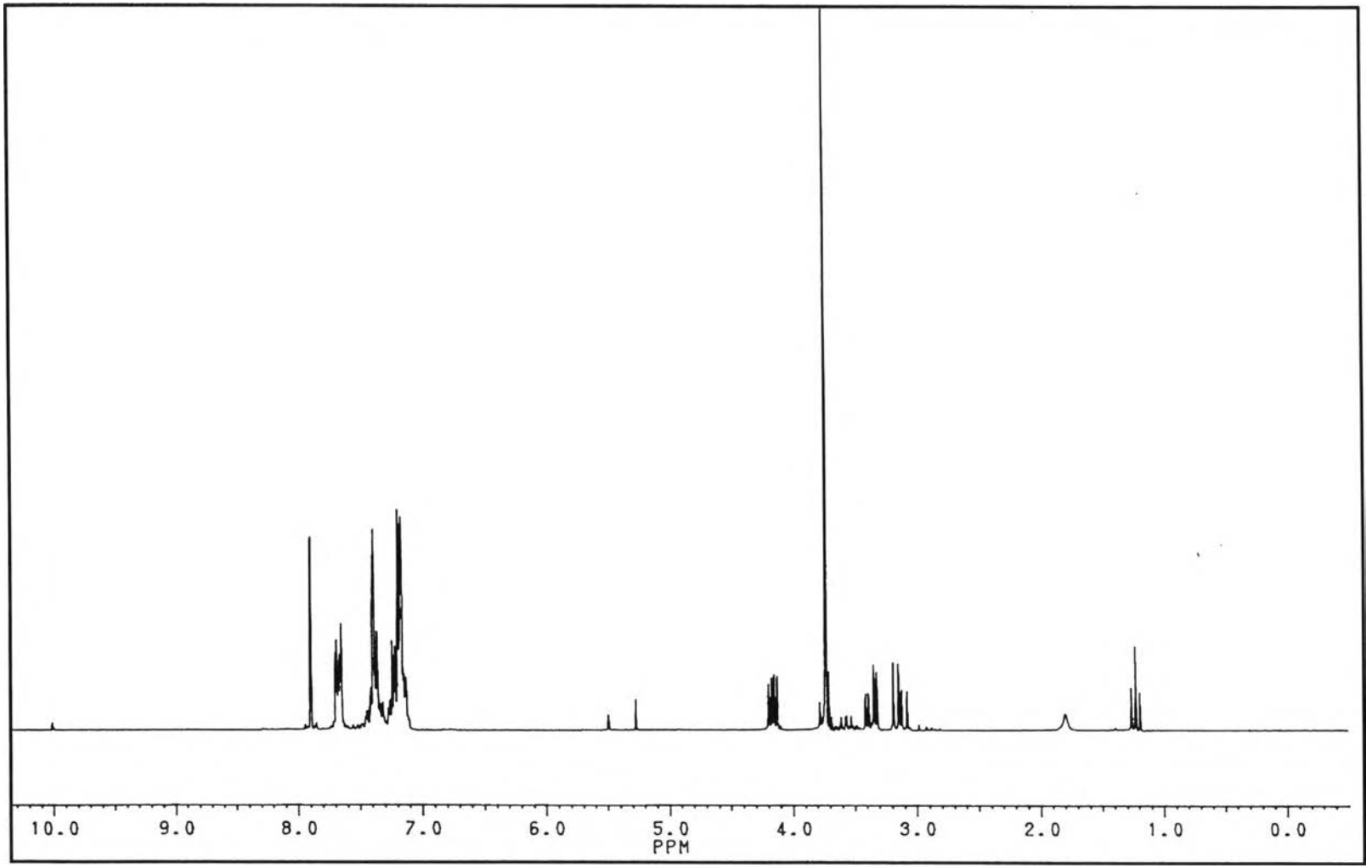


Figure 21 ^{1}H NMR spectrum ($CDCl_3$) of *N*-benzylidene-*S*-phenylalanine methyl ester **(54a)**

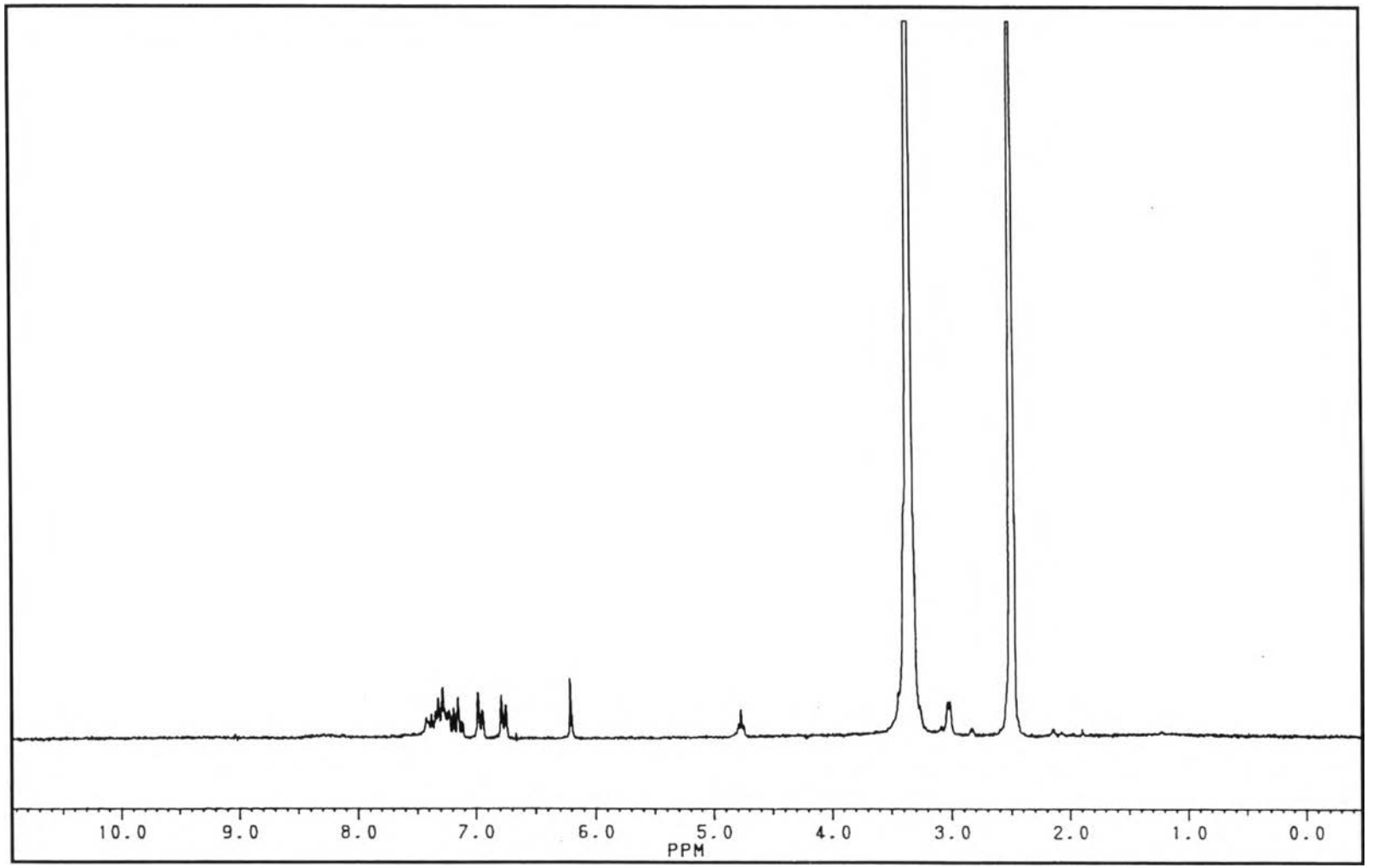


Figure 22 ^{1}H NMR spectrum (DMSO) of dihydrotriazine **(54d)**

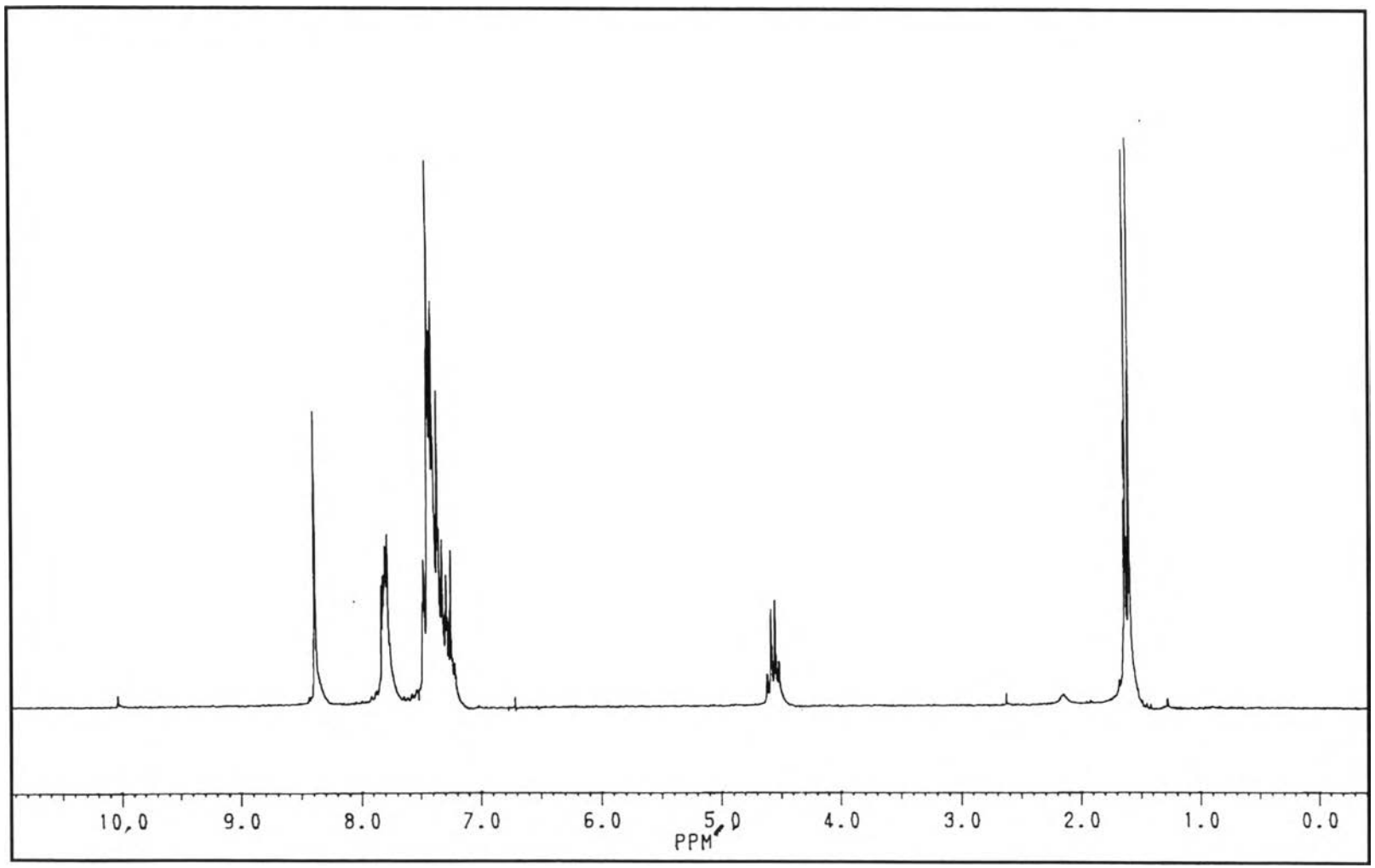


Figure 23 ^{1}H NMR spectrum ($CDCl_3$) of racemic *N*-benzylidene-2-methylbenzylamine**(55a)**

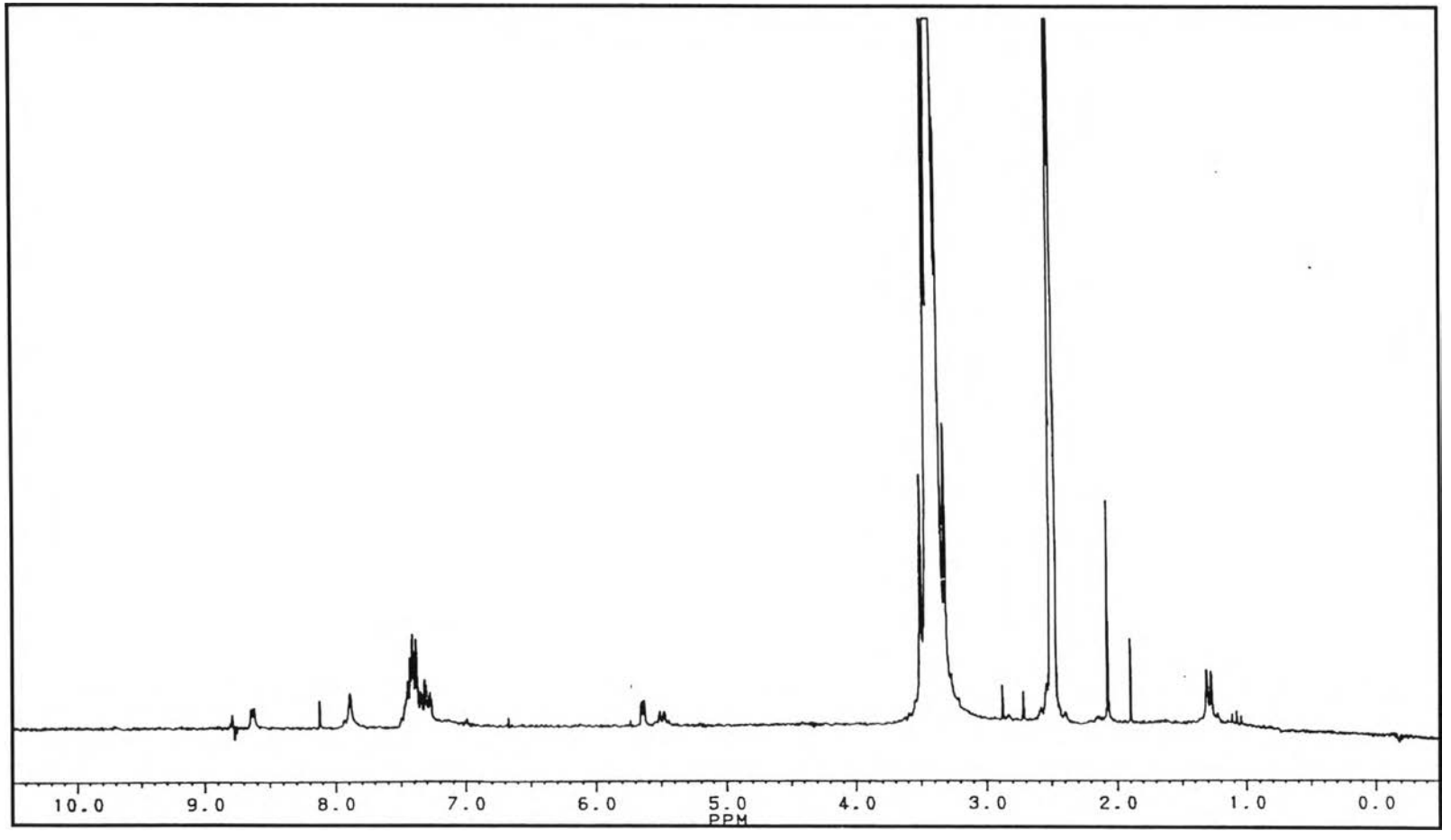


Figure 24 ^{1}H NMR spectrum (DMSO) of racemic 1-(1′*RS*-phenylethyl)-2*SR*-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(55b)**

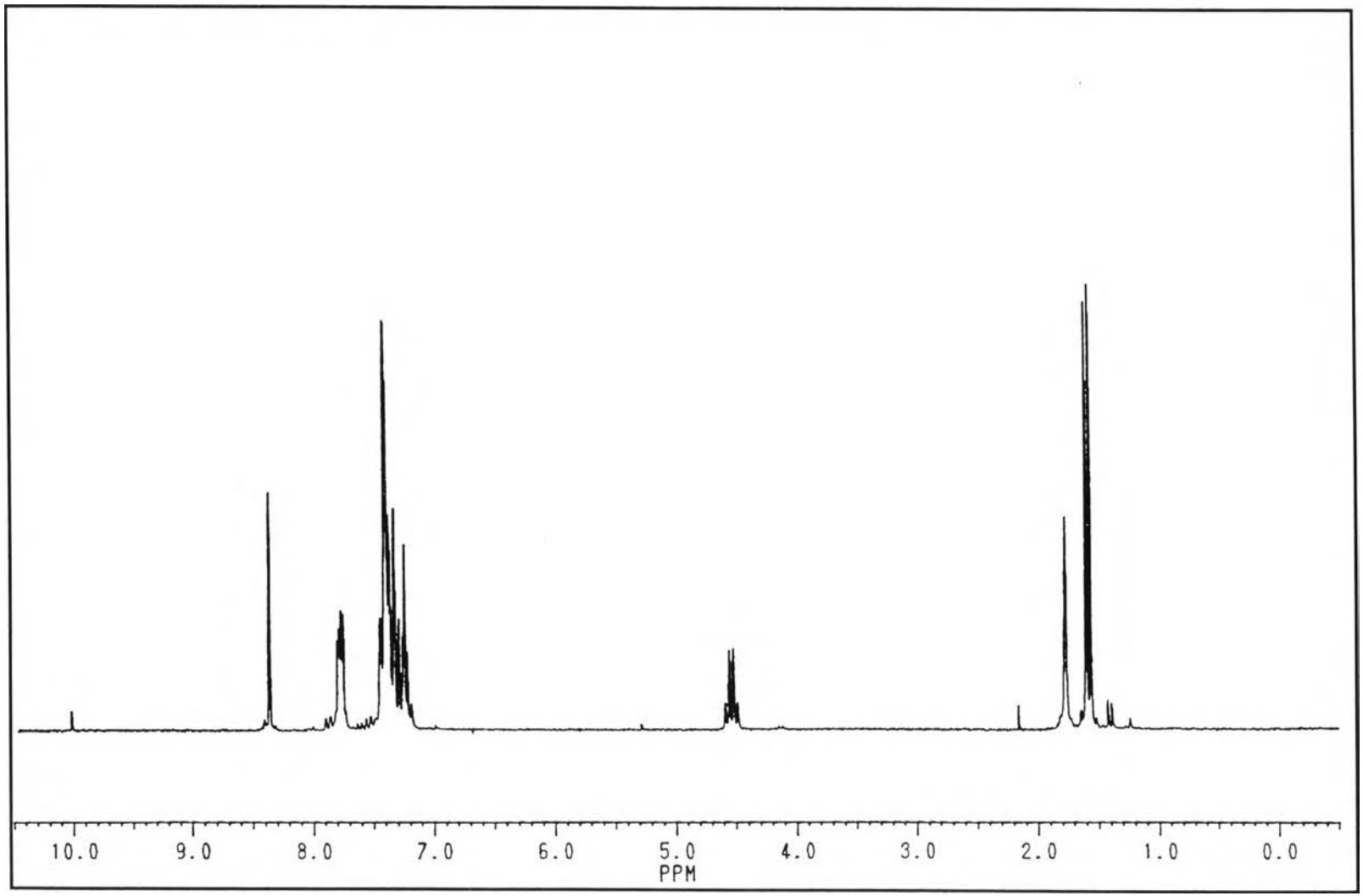


Figure 25 ^{1}H NMR spectrum ($CDCl_3$) of (*R*)-*N*-benzylidene-2-methylbenzylamine **(55a′)**

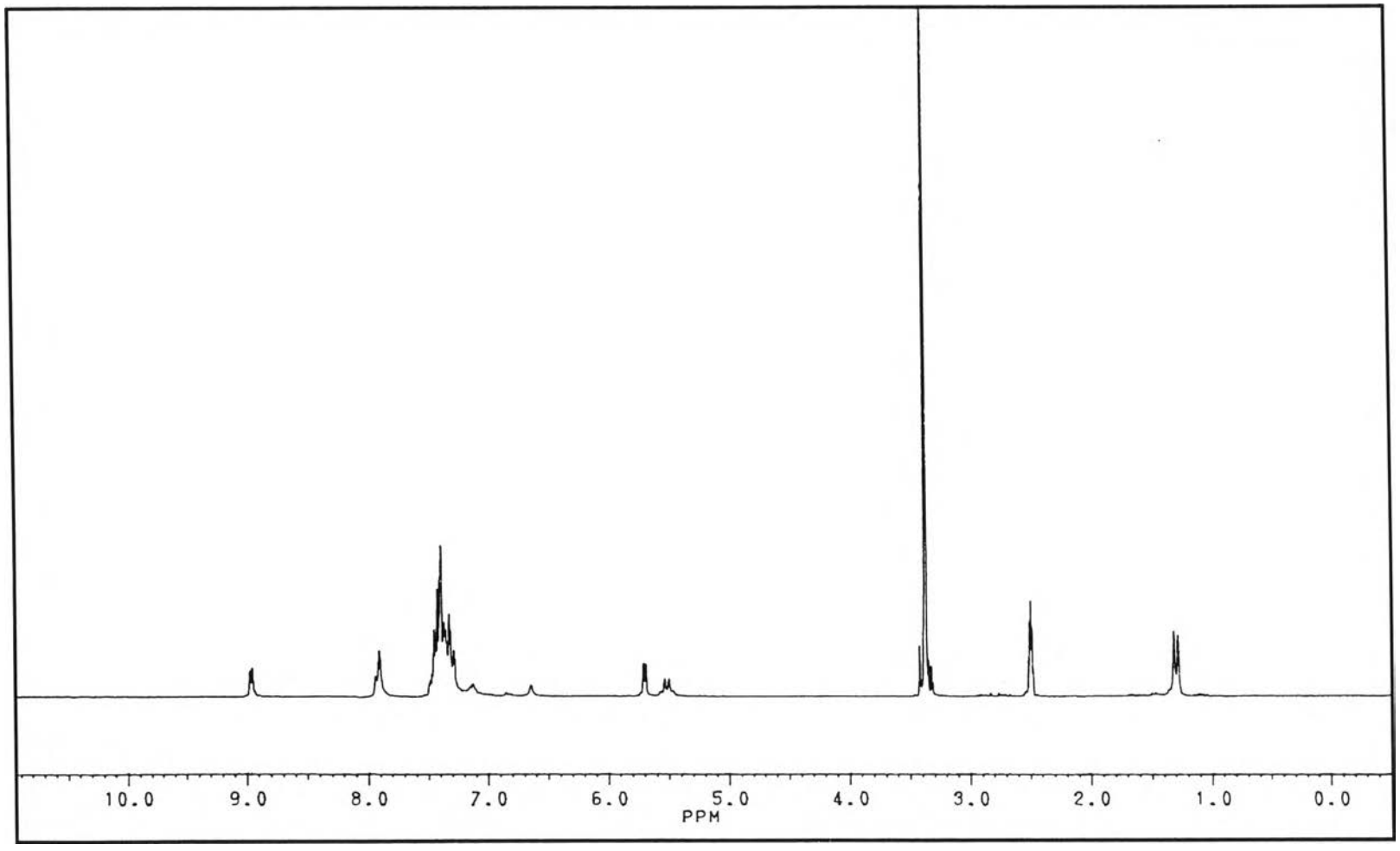


Figure 26 ^{1}H NMR spectrum (DMSO) of 1-(1′*R*-phenylethyl)-2*S*-phenyl-4,6-diamino-1,2-dihydro-1,3,5- triazine trifluoroacetate **(55b′)**

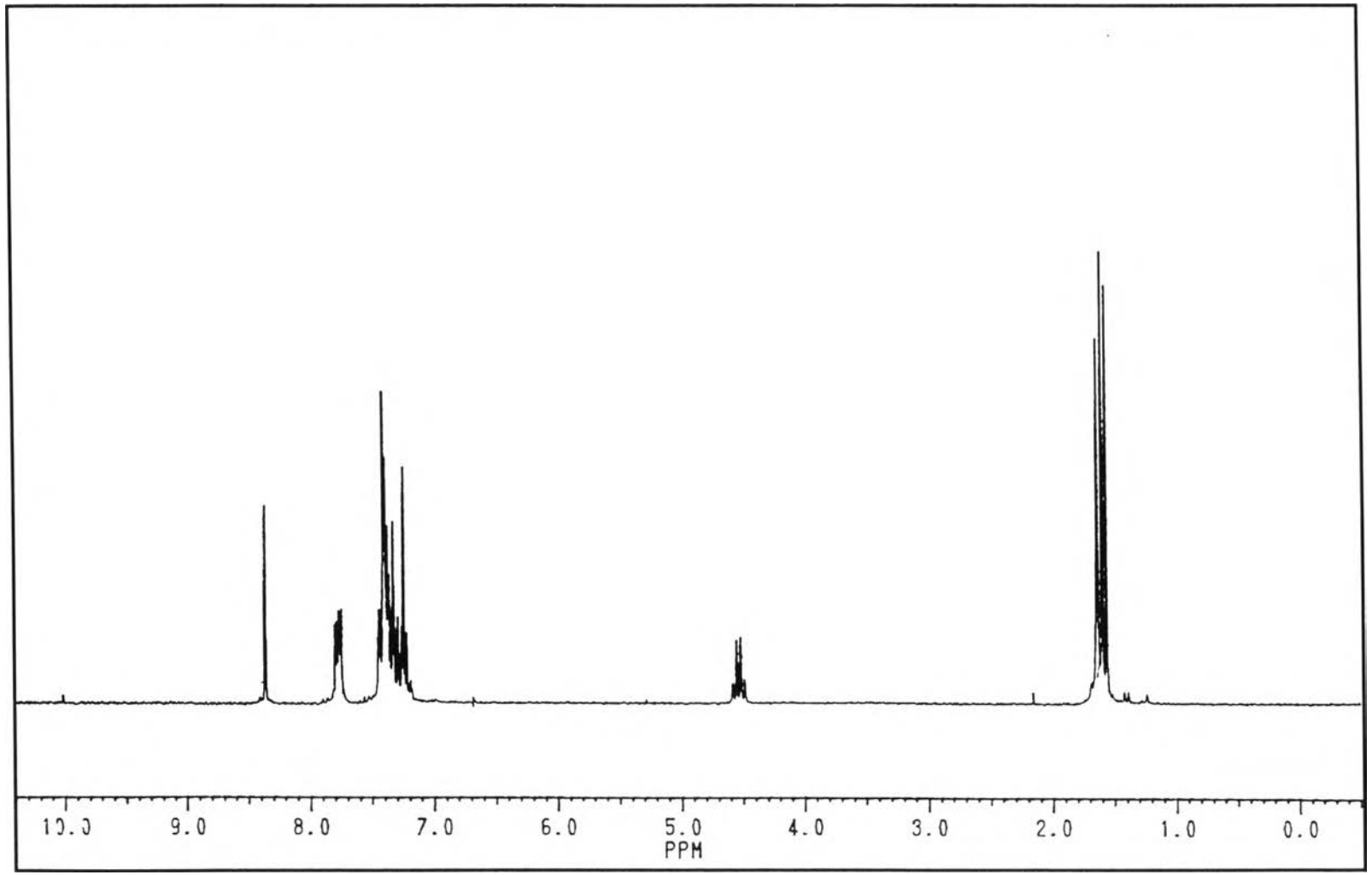


Figure 27 ^{1}H NMR spectrum ($CDCl_3$) of (*S*)-*N*-benzylidene-2-methylbenzylamine **(55a'')**

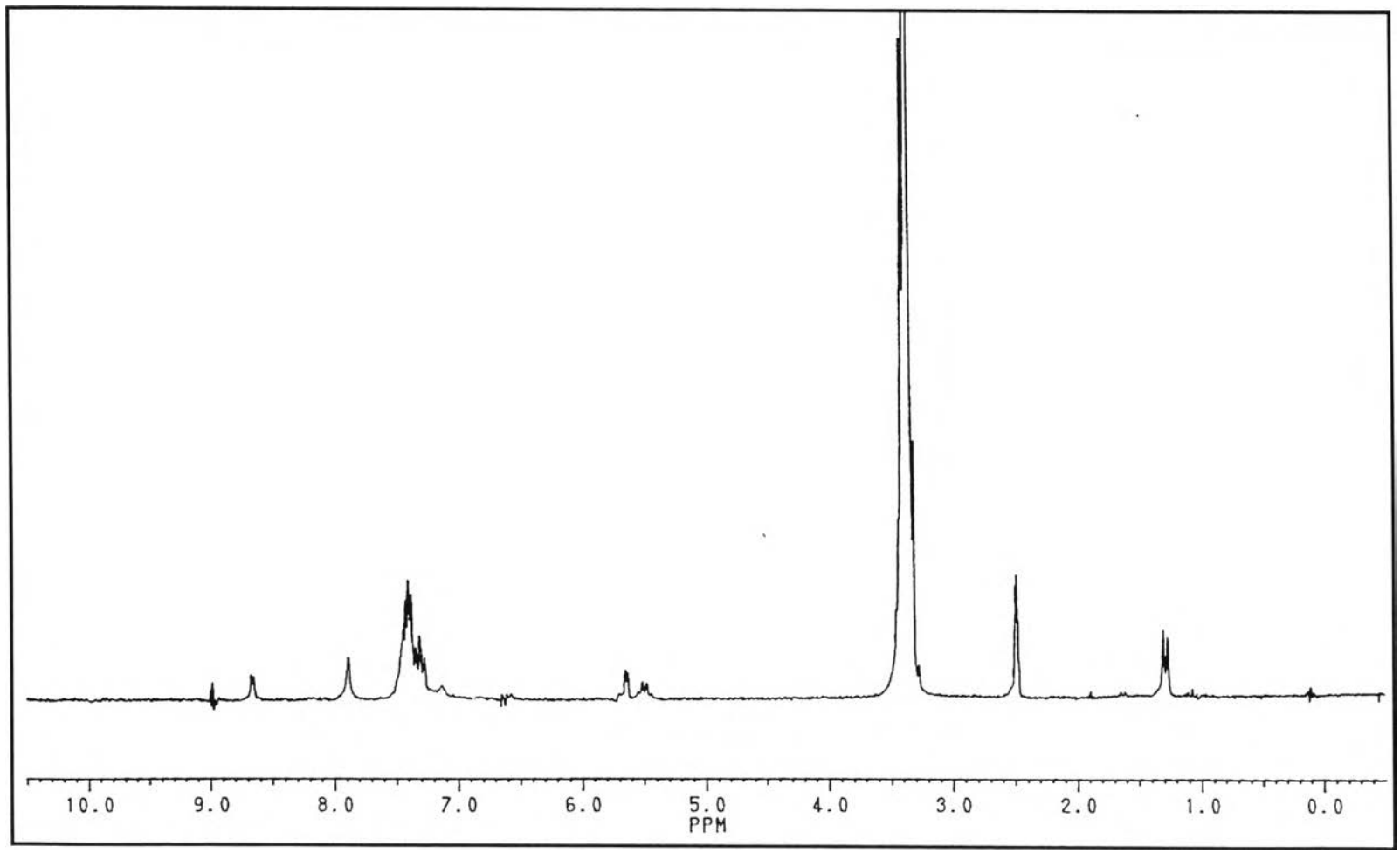


Figure 28 ^{1}H NMR spectrum (DMSO) of 1-(1′*S*-phenylethyl)-2*R*-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(55b′′)**

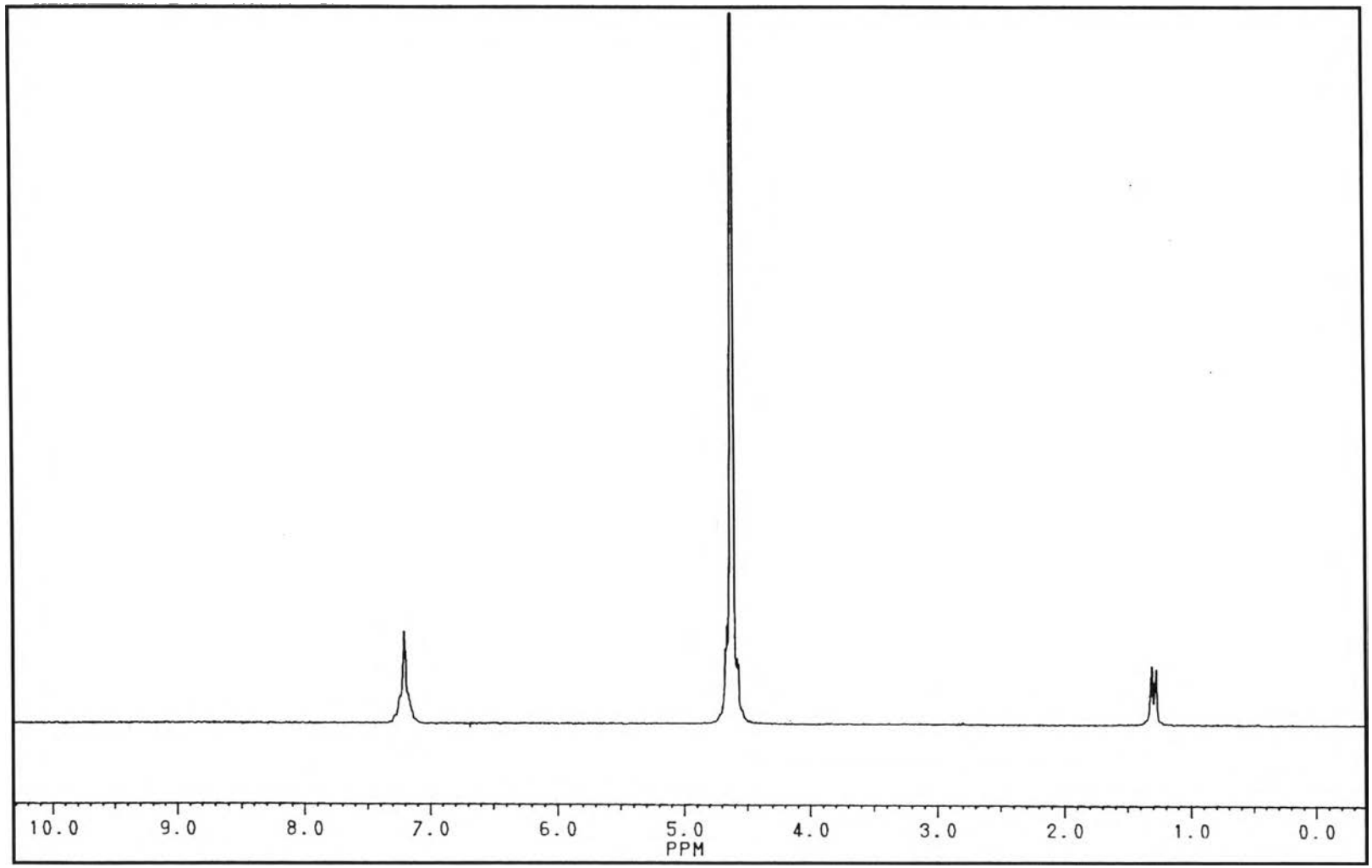


Figure 29 ^{1}H NMR spectrum (D_2O) of (*RS*)-α-methylbenzylbiguanide hydrochloride **(56a)**

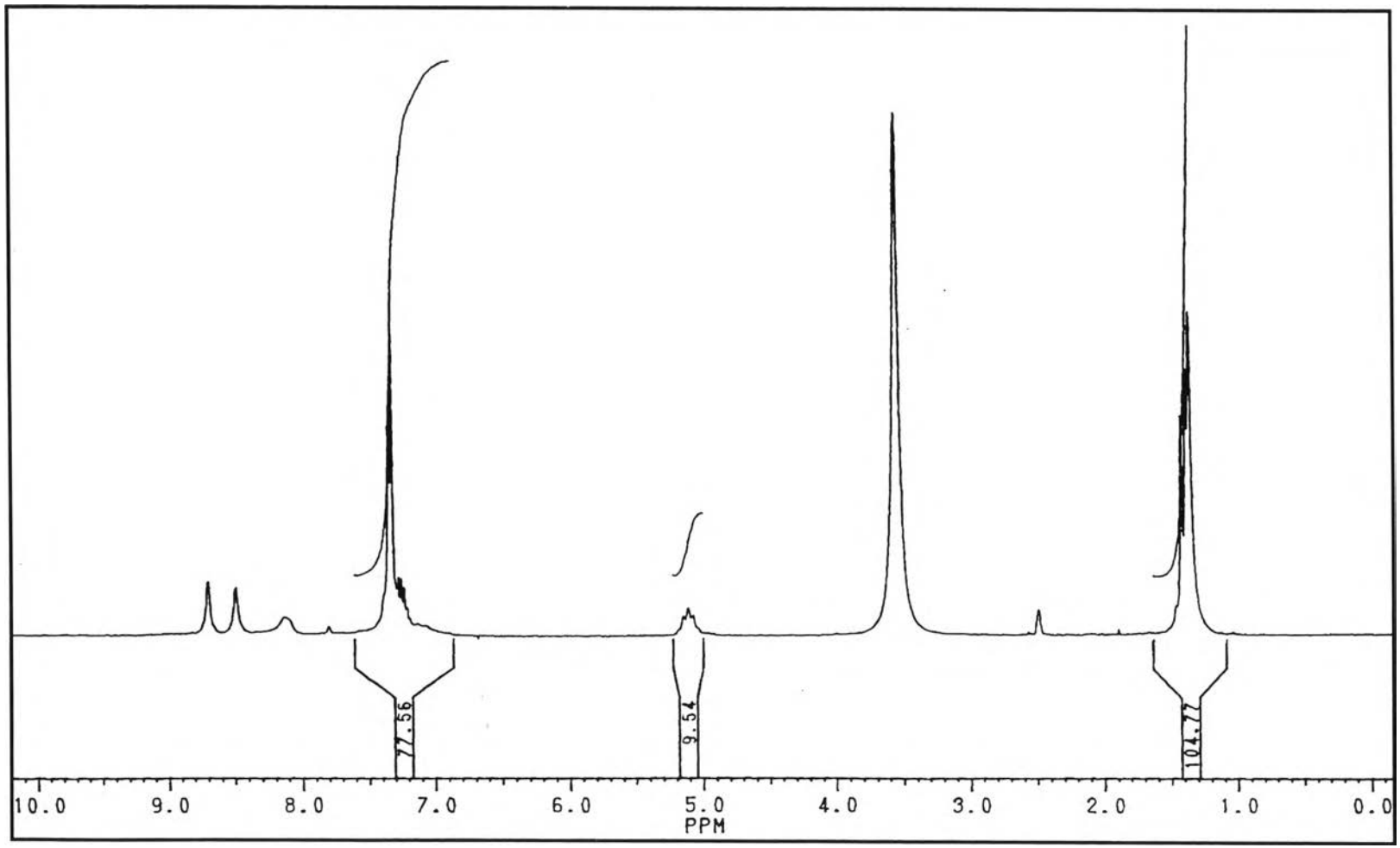


Figure 30 ^{1}H NMR spectrum (DMSO) of rearrangement product **(57b)**

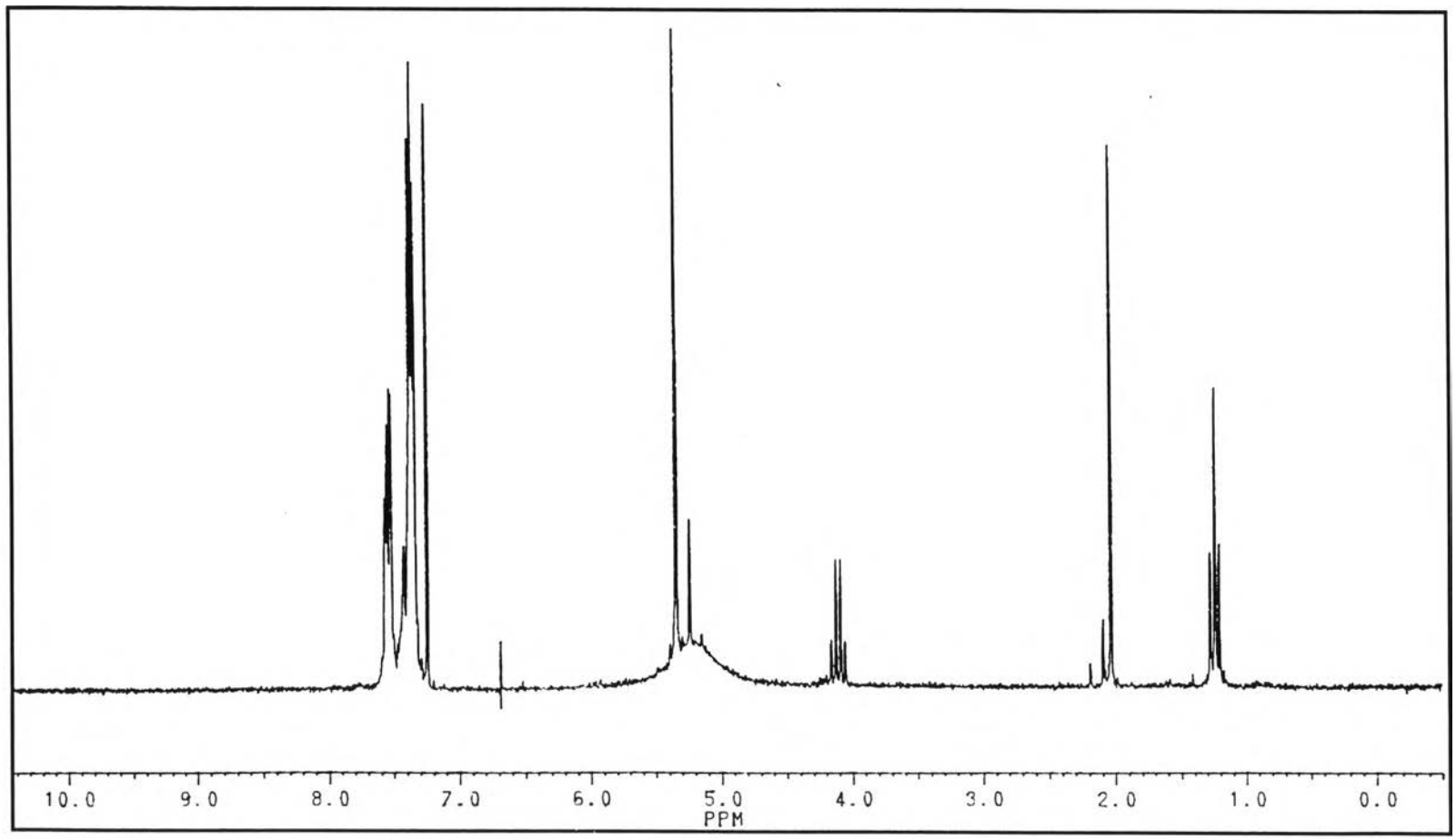


Figure 31 ^{1}H NMR spectrum ($CDCl_3$) of *R*-α-bromophenylacetic acid **(61a)**

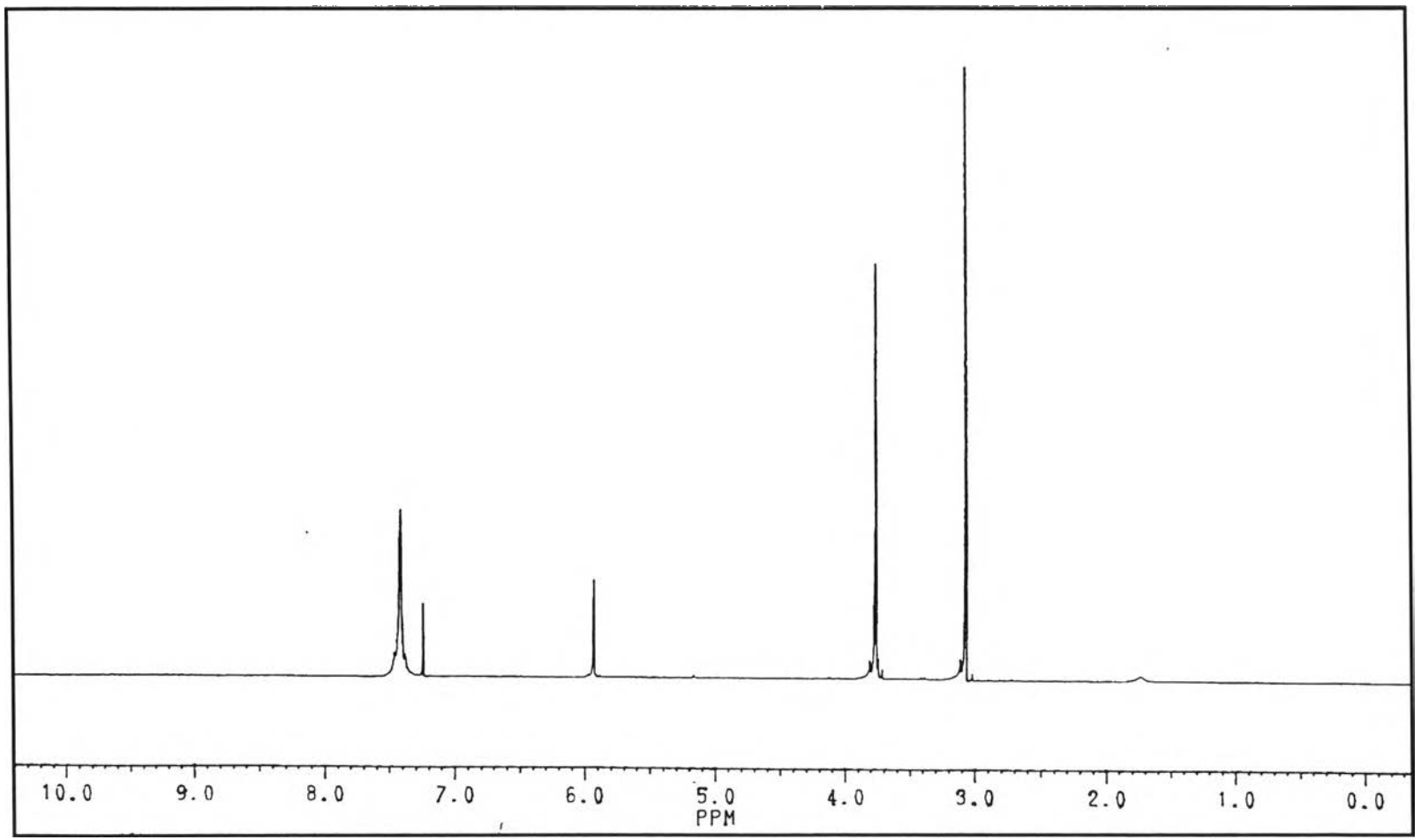


Figure 32 ^{1}H NMR spectrum ($CDCl_3$) of *(R)*-α-methanesulfonyloxyphenylacetic acid methyl ester **(62b)**

Dihydrotriazine **(4)** 1.8 mg / mL (MeOH)

stock solution (μL)	Volume (mL)	C (mg/mL)	A(254)
5	3005	0.003	0.074
10	3010	0.006	0.149
15	3015	0.009	0.222
20	3020	0.012	0.296
30	3030	0.018	0.446
40	3040	0.024	0.595
50	3050	0.030	0.743
60	3060	0.035	0.891
70	3070	0.041	1.040

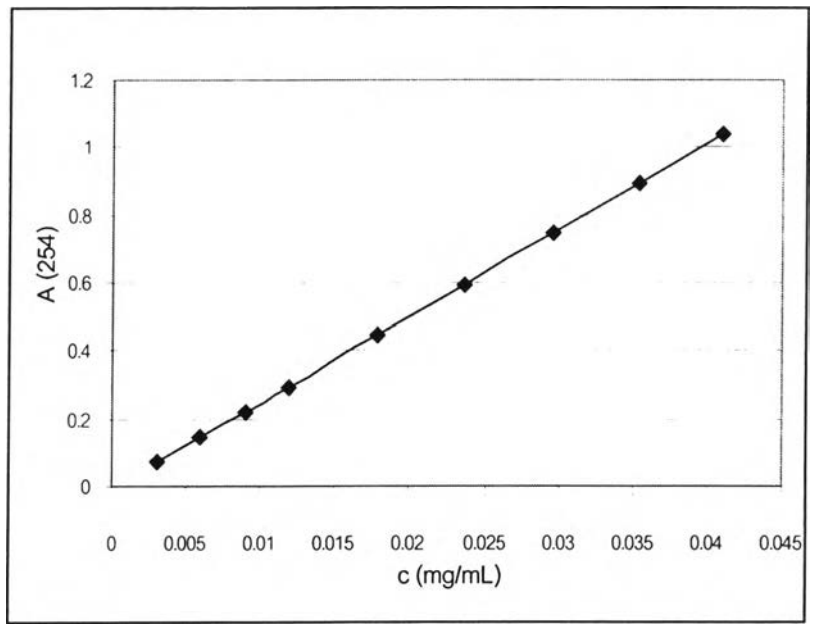


Figure 33 Calibration curve of 1-(4′-bromophenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(4)**

Dihydrotriazine **(5)** 2.5 mg / mL (MeOH)

Stock solution (μL)	Volume (mg/mL)	C (mg/mL)	A(254)
5	3005	0.004	0.102
10	3010	0.008	0.206
15	3015	0.012	0.311
20	3020	0.017	0.414
30	3030	0.025	0.624
40	3040	0.033	0.830
50	3050	0.0410	1.039

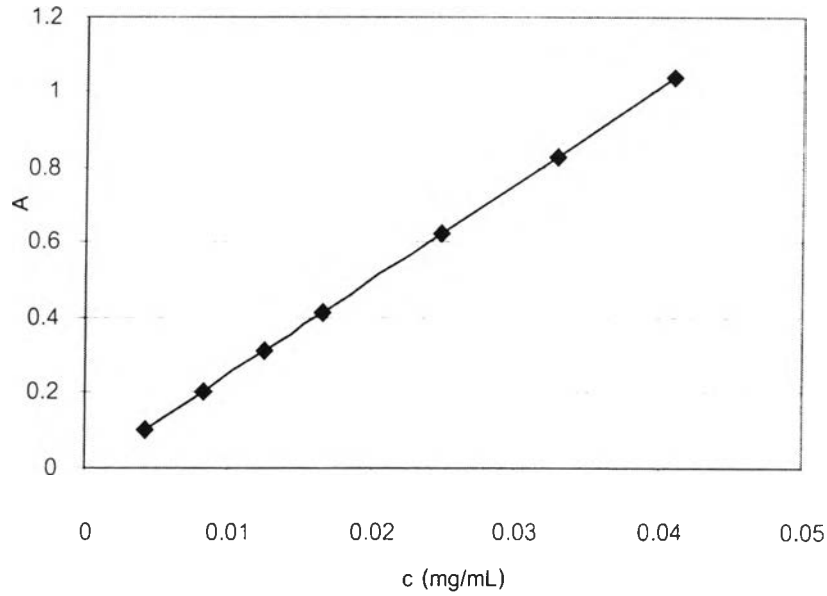


Figure 34 Calibration curve of 1-(4′-methylphenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(5)**

Dihydrotriazine **(55b″)** 2.0 mg in MeCN 10 mL

C (mg/mL)	C (mg/1000ml)	A (254)
0.003	3.0	0.101
0.006	6.0	0.172
0.010	10.0	0.244
0.014	14.0	0.332
0.018	18.0	0.418
0.024	24.0	0.561
0.030	30.0	0.701
0.034	34.0	0.791
0.040	40.0	0.941

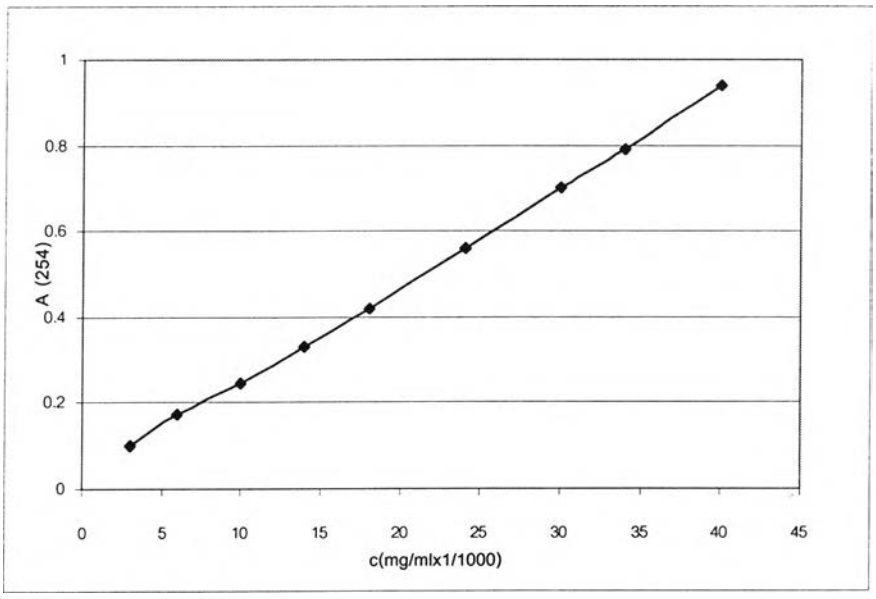


Figure 35 Calibration curve of 1-(1′*S*-phenylethyl)-2*R*-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(55b″)**

Time (hr)	% Deuterium incorperation
0.0	0.0
0.1	11.8
0.3	29.3
1.3	52.0
2.0	62.4
2.3	65.9
3.3	73.5
4.0	76.7
5.0	80.1
6.2	82.8
8.4	86.4
9.3	88.7
10.3	88.8
12.3	89.2
14.2	91.1
15.2	89.9
16.1	100.0

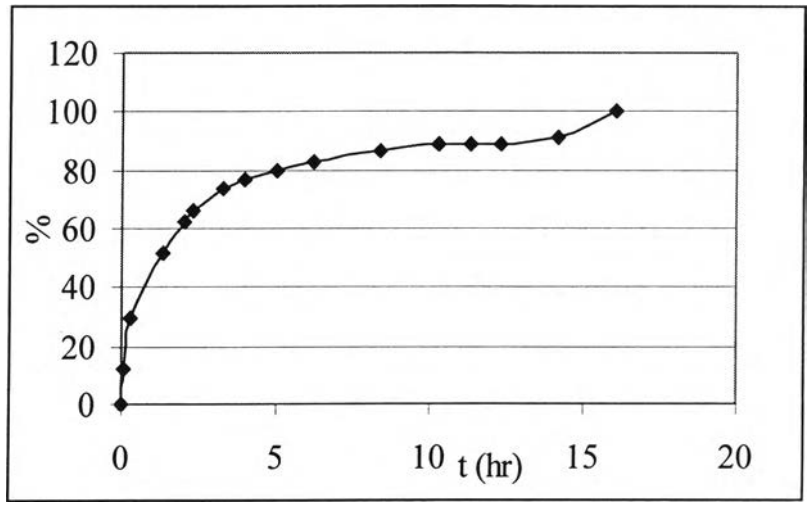
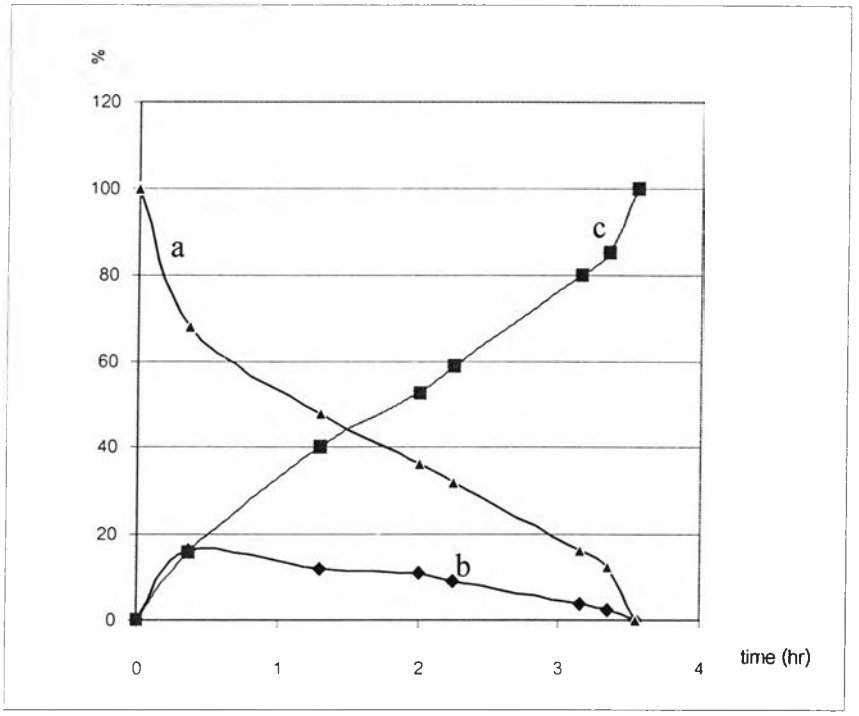


Figure 36 Measurement the racemization of the rate of deuterium exchange of **(54d)**

Time (hr)	(55b″)	Racemization	Rearrangement
0.0	0.20	0.00	0.00
0.4	0.23	0.06	0.05
1.3	0.20	0.05	0.17
2.0	0.16	0.05	0.24
2.3	0.13	0.04	0.24
3.2	0.07	0.02	0.33
3.4	0.03	0.01	0.22
4.0	0.00	0.00	0.23



a = starting material **(55b″)**
b = racemization product
d = rearrangement product

Figure 37 Racemization/rearrangement of 1-(1′*S*-phenylethyl)-2*R*-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine **(55b″)**

For first order reaction[44]

$$R.R. = -\frac{d[A]}{dt} = -k[A]$$

$$-\frac{d[A]}{[A]} = -kdt$$

integrate

$$\ln [A] = -kt + \ln [A]_o \qquad (1)$$

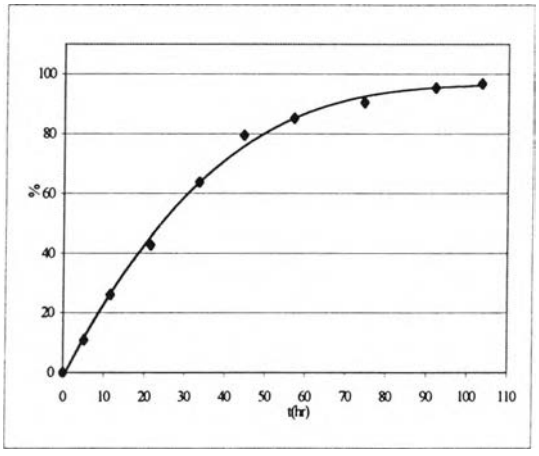
R.R = rate of reaction
k = spcific rate constant
[A] = the reactant concentration
$[A]_0$ = the reactant concentration at the begining

Half-life for a reaction, $t_{1/2}$, was the time taken for the reactant concentration falling to half their initial concentration. From derived the equation

$$t_{1/2} = \frac{\ln 2}{k} \qquad (2)$$

Time (hr)	% Rearrangement
0.0	0.0
5.2	11.0
12.0	26.2
21.4	42.8
33.5	63.9
44.5	79.5
57.0	85.2
74.5	90.4
92.0	95.4
103.4	96.7

rearrangement



rate of rearrangement

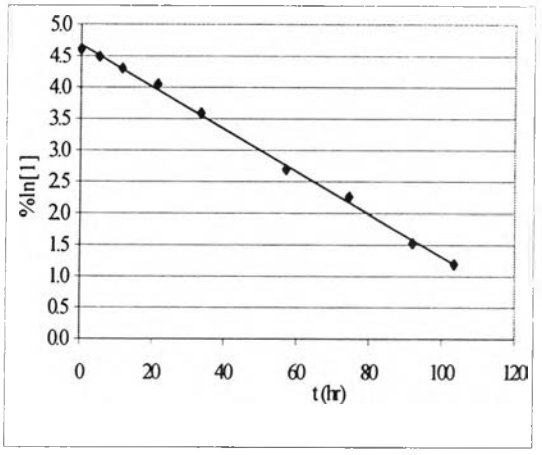


Figure 38 Rate of rearrangement of 1-(4′-chlorophenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(1)**

Time (hr)	% Rearrangement
0.0	0.0
4.4	10.4
7.0	15.3
15.3	32.8
20.4	42.4
33.3	64.4
37.4	71.8
56.4	90.9
67.2	95.1
79.4	100.0

rearrangement

rate of rearrangement

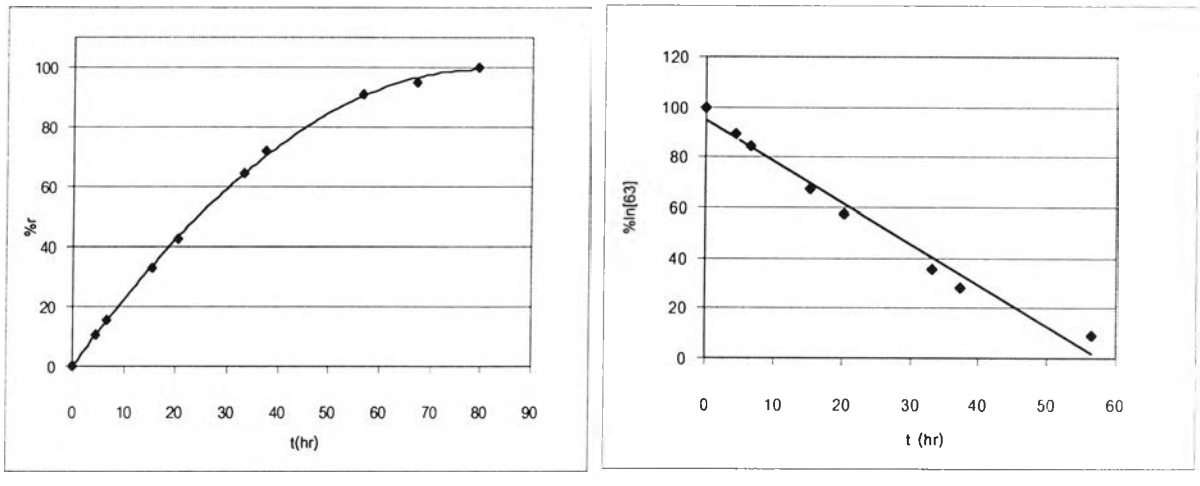


Figure 39 Rate of rearrangement of 1-benzyloxy-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine **(63)**

Time (hr)	%Rearrangement
0.0	0.0
2.3	25.3
9.1	27.0
16.0	26.3
44.0	26.4
56.5	30.3
67.3	35.9

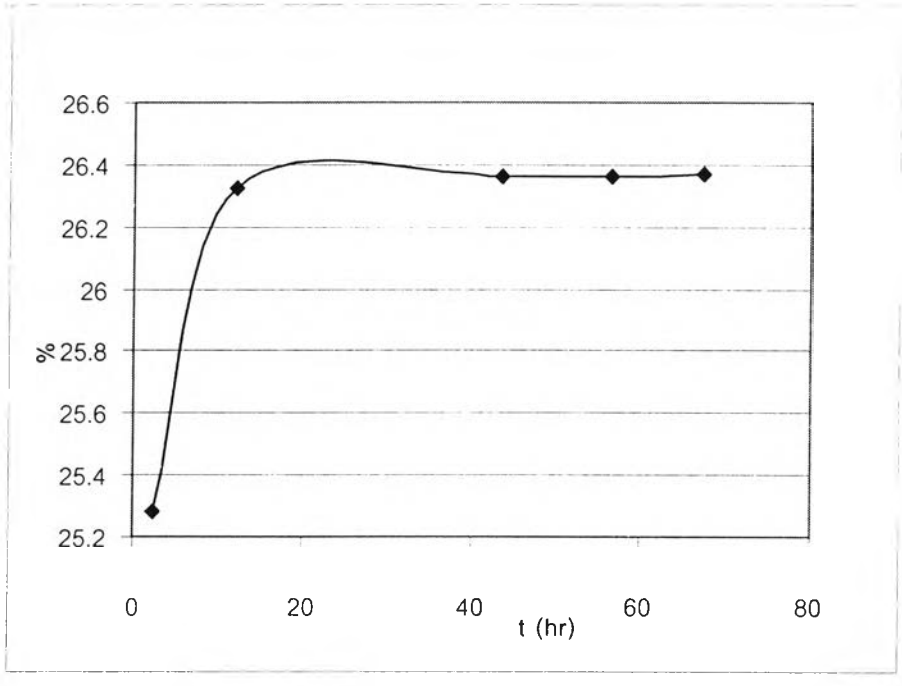
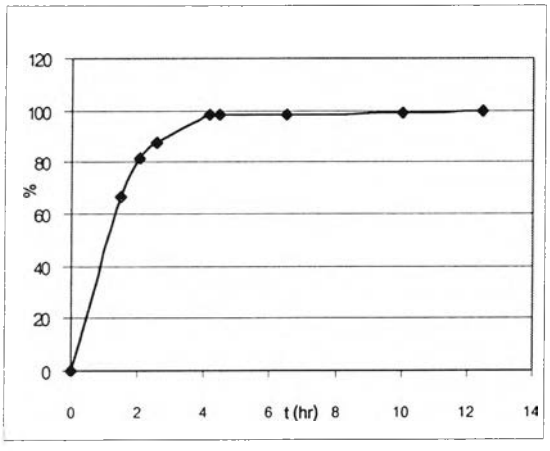


Figure 40 Rate of rearrangement of 1-benzyl-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(64)**

Time (hr)	% Rearrangement
0.0	0.0
1.5	66.9
2.1	81.3
3.0	87.5
4.2	98.4
4.5	98.4
6.5	98.5
10.0	99.3
12.5	100.0

rearrangement



rate of rearrangement

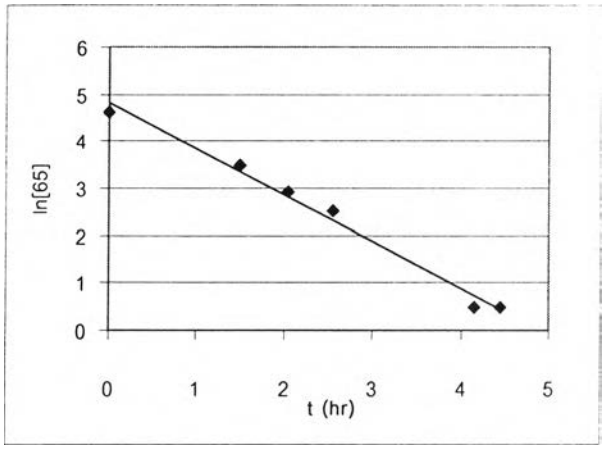
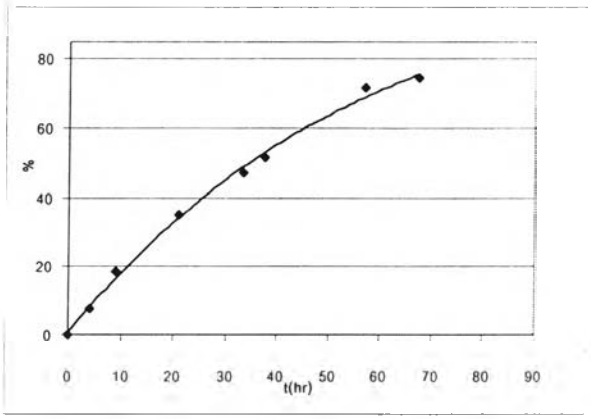


Figure 41 Rate of rearrangement of 1-benzyl-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluororacetate **(65)**

Time (hr)	% Rearrangement
0.0	0.0
4.2	7.6
9.15	18.7
21.1	35.2
33.5	47.3
38.0	51.5
57.0	71.8
67.4	74.4

rearrangement



rate of rearrangement

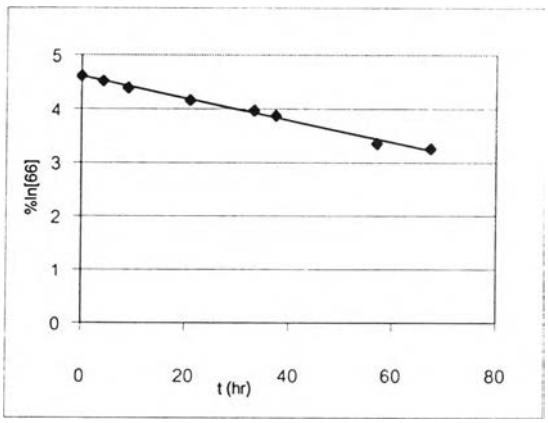
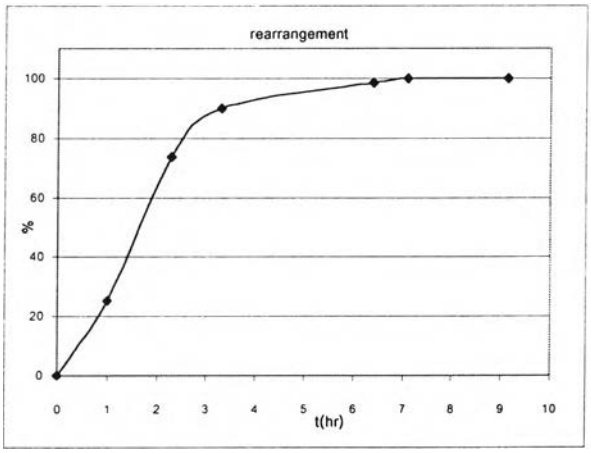


Figure 42 Rate of rearrangement of 1-benzyl-2-(4′-nitrophenyl)-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(66)**

Time (hr)	% Rearrangement
0.0	0
1.0	25.4
2.3	73.7
3.3	90.0
6.4	98.5
7.1	100.0

rearrangement



rate of rearrangement

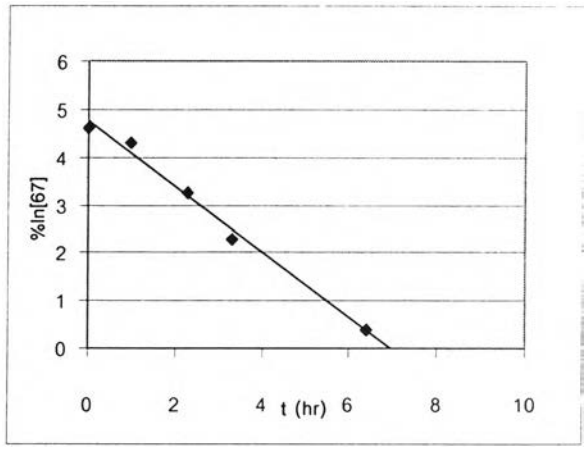
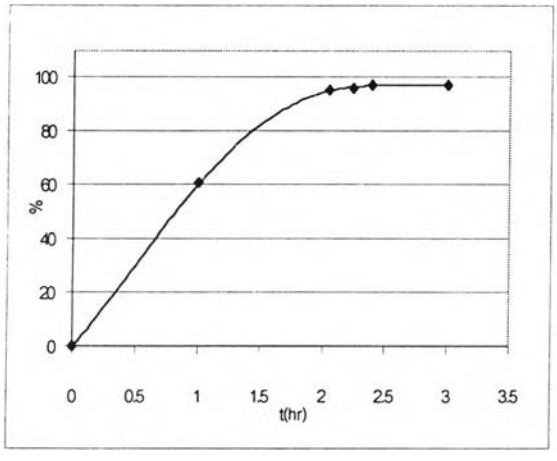


Figure 43 Rate of rearrangement of 1-benzyl-2-(4′-chlorophenyl)-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(67)**

Time (hr)	% Rearrangement
0.0	0.0
1.0	60.5
2.1	95.3
2.2	96.1
2.4	97.4
3.0	97.5
3.4	98.7

rearrangement



rate of rearrangement

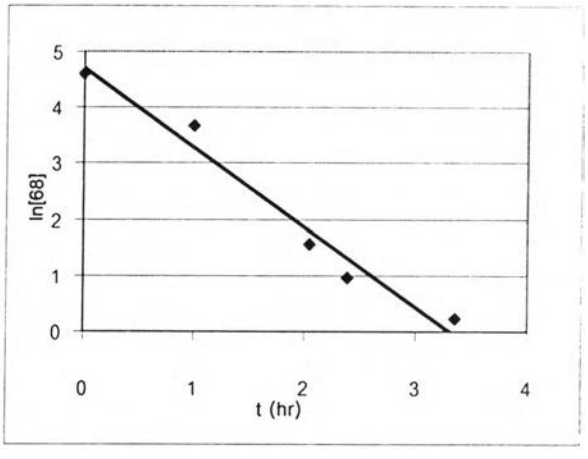


Figure 44 Rate of rearrangement of 1-benzyl-2-(4′-methoxyphenyl)-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(68)**

Table 1 Crystal data and structure refinement for 1-(4′-*sec*-butoxyphenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(47c)**.

Identification code	tv899x
Empirical formula	$C_{19}H_{24}ClN_5O$
Formula weight	373.88
Temperature	293 (2) K
Wavelength	0.70930 Å
Crystal system	Triclinic
Space group	p-1
Unit cell dimensions	*a* = 68.8660 (10) Å alpha = 77.582 (11) ° *b* = 12.559 (2) Å beta = 77.863 (9) ° *c* = 18.943 (2) Å gama = 82.338 (11) °
Volume, Z	2005.3 (4) $Å^3$, 4
Density (calculated)	1.238 Mg/m^3
Absorption coefficient	0.208 mm^{-1}
F (000)	790
Crystal size	0.2 x 0.2 x 0.2 mm
θ range for data collection	2.18 to 25.93°
Limiting indices	$-10 \leq h \leq 10, -15 \leq k \leq 15, -23 \leq l \leq 23$
Reflections collected	15724
Independent reflections	7862 (R_{int} = 0.1190)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7862 / 0 / 450
Goodness-of-fit on F^2	1.068
Final R indices [I>2 σ(I)]	R1 = 01047, wR2 = 0.2364
R indices (all data)	R1 = 0.3100, wR2 = 0.3076
Largest diff. peak and hole	0.740 and –0.505 $eÅ^{-3}$

Table 2 Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1-(4′-*sec*-butoxyphenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(47c)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(4)	6581 (7)	8224 (5)	-37 (3)	52 (2)
O(6)	3494 (9)	4958 (6)	2301 (4)	97 (2)
N(9)	8549 (8)	9375 (5)	-703 (4)	61 (2)
N(11)	8139 (8)	10562 (5)	-1774 (3)	58 (2)
N(12)	4170 (8)	8512 (6)	-390 (4)	74 (2)
N(14)	6081 (8)	9630 (5)	-1044 (4)	57 (2)
C(16)	9339 (9)	7754 (7)	130 (4)	50 (2)
C(17)	7589 (10)	9847 (7)	-1172 (5)	55 (2)
C(20)	5647 (10)	8807 (7)	-491 (4)	55 (2)
C(23)	8031 (9)	8661 (7)	-7 (4)	57 (2)
C(26)	6060 (10)	6323 (7)	493 (5)	60 (2)
C(27)	11780 (12)	6186 (9)	340 (7)	89 (3)
C(29)	5448 (10)	7655 (7)	1270 (5)	60 (2)
C(30)	5501 (11)	5538 (7)	1093 (5)	69 (3)
C(32)	9953 (12)	7624 (7)	736 (4)	73 (3)
C(34)	6002 (9)	7396 (7)	585 (4)	57 (2)
C(36)	4956 (11)	5787 (9)	1749 (5)	70 (5)
C(38)	4916 (11)	6842 (9)	1865 (5)	77 (3)
C(40)	9906 (11)	7101 (8)	-369 (5)	72 (3)
C(41)	11228 (13)	6837 (10)	848 (6)	97 (4)
C(45)	11108 (12)	6309 (8)	-260 (6)	93 (3)
C(46)	3670 (2)	5148 (12)	3031 (5)	137 (6)
C(47)	4720 (2)	3397 (15)	3494 (8)	169 (7)
C(49)	1964 (19)	5739 (14)	3077 (9)	161 (6)
C(50)	3320 (2)	4174 (18)	3506 (8)	187 (7)
O(3)	11541 (7)	3403 (5)	5502 (3)	78 (2)

	x	y	z	U(eq)
N(5)	8233 (7)	1443 (5)	3995 (3)	49 (2)
N(7)	6150 (7)	387 (5)	4066 (3)	56 (2)
N(8)	7756 (8)	1005 (6)	2911 (3)	66 (2)
N(55)	5578 (8)	146 (6)	2971 (3)	64 (2)
N(13)	6493 (7)	890 (5)	5100 (3)	55 (2)
C(15)	6988 (9)	898 (6)	4380 (4)	49 (2)
C(18)	6489 (10)	499 (6)	3329 (4)	54 (2)
C(19)	9942 (10)	2039 (7)	2786 (4)	55 (2)
C(21)	9140 (10)	1928 (7)	4370 (4)	53 (2)
C(22)	8638 (10)	2982 (7)	4528 (4)	62 (2)
C(24)	10803 (11)	1860 (7)	5123 (4)	59 (2)
C(25)	10483 (10)	1361 (6)	4579 (5)	59 (2)
C(28)	8994 (9)	1156 (7)	3268 (5)	60 (2)
C(31)	9478 (11)	3414 (7)	4906 (5)	65 (2)
C(33)	11327 (10)	1839 (7)	4951 (5)	62 (2)
C(35)	9267 (12)	3040 (9)	2534 (5)	76 (3)
C(37)	11737 (16)	3590 (11)	1881 (5)	101 (4)
C(39)	11525 (11)	1808 (8)	2584 (4)	70 (3)
C(42)	10142 (16)	3805 (9)	2090 (6)	97 (4)
C(43)	12393 (13)	2564 (12)	2127 (6)	99 (4)
Cl(1)	8089 (3)	136 (2)	1451 (1)	65 (1)
Cl(2)	2673 (3)	8752 (2)	3411 (1)	80 (1)
C(51)	12691 (15)	2754 (10)	5951 (9)	127 (5)
C(54)	13800 (13)	3565 (19)	5898 (13)	259 (10)
C(52)	11770 (3)	2413 (19)	6724 (14)	266 (11)

Table 3 Bond lengths [Å] and angles [°] for 1-(4′-*sec*-butoxyphenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(47c)**.

N(4)-C(20)	1.353 (9)	N(4)-C(34)	1.447 (9)
N(4)-C(23)	1.479 (9)	O(6)-C(36)	1.369 (10)
O(6)-C(46)	1.453 (12)	N(9)-C(17)	1.351 (9)
N(9)-C(23)	1.449 (9)	N(11)-C(17)	1.335 (9)
N(12)-C(20)	1.372 (10)	N(14)-C(20)	1.335 (9)
N(14)-C(17)	1.362 (9)	C(16)-C(32)	1.342 (10)
C(16)-C(40)	1.358 (11)	C(16)-C(23)	1.536 (11)
C(23)-H(23)	1.0016	C(26)-C(30)	1.386 (11)
C(26)-C(34)	1.389 (10)	C(26)-H(26)	0.9851
C(27)-C(45)	1.363 (13)	C(27)-C(41)	1.367 (14)
C(27)-H(27)	0.9981	C(29)-C(34)	1.378 (10)
C(29)-C(38)	1.396 (11)	C(29)-H(29)	1.0468
C(30)-C(36)	1.324 (12)	C(30)-H(30)	0.9805
C(32)-C(41)	1.419 (12)	C(32)-H(32)	0.9804
C(36)-C(38)	1.384 (12)	C(38)-H(38)	0.9491
C(40)-C(45)	1.375 (12)	C(40)-H(40)	1.0051
C(41)-H(41)	0.9803	C(45)-H(45)	1.0464
C(46)-C(50)	1.34 (2)	C(46)-C(49)	1.58 (2)
C(46)-H(46)	1.0150	C(47)-C(50)	1.47 (2)
C(47)-H(47A)	0.9668	C(47)-H(47B)	0.9763
C(47)-H(47C)	0.9984	C(49)-H(49A)	1.0693
C(49)-H(49B)	1.0011	C(49)-H(49C)	0.9405
C(50)-H(50A)	0.9271	C(50)-H(50B)	1.0591
O(3)-C(24)	1.392 (9)	O(3)-C(51)	1.508 (12)
N(5)-C(15)	1.367 (9)	N(5)-C(21)	1.441 (9)
N(5)-C(28)	1.497 (9)	N(7)-C(15)	1.340 (9)
N(7)-C(18)	1.346 (9)	N(8)-C(18)	1.375 (9)
N(8)-C(28)	1.456 (9)	N(55)-C(18)	1.328 (9)
N(13)-C(15)	1.339 (9)	C(19)-C(35)	1.352 (11)

C(19)-C(39)	1.384 (11)	C(19)-C(28)	1.503 (10)
C(21)-C(25)	1.390 (11)	C(21)-C(22)	1.413 (11)
C(22)-C(31)	1.364 (10)	C(22)-H(22)	0.9926
C(24)-C(31)	1.376 (11)	C(24)-C(33)	1.386 (11)
C(25)-C(33)	1.393 (10)	C(25)-H(25)	0.9828
C(28)-H(28)	1.0052	C(31)-H(31)	1.0058
C(33)-H(33)	1.0090	C(35)-C(42)	1.345 (13)
C(35)-H(35)	1.0077	C(37)-C(43)	1.37 (2)
C(37)-C(42)	1.39 (2)	C(37)-H(37)	0.9976
C(39)-C(43)	1.343 (13)	C(39)-H(39)	0.9753
C(42)-H(42)	0.9879	C(43)-H(43)	0.9931
C(51)-C(52)	1.52 (2)	C(51)-C(54)	1.48 (2)
C(51)-H(51) C(54)-H(54B)	0.9947 1.4074	C(54)-H(54A) C(53)-H(54C)	1.3296 1.3149
C(52)-H(52A)	1.3651	C(52)-H(52B)	1.1014
C(52)-H(52C)	1.0887		

C(20)-N(4)-C(34)	121.4 (7)	C(20)-N(4)-C(23)	119.3 (7)
C(34)-N(4)-C(23)	116.1 (6)	C(36)-O(6)-C(46)	121.8 (8)
C(17)-N(9)-C(23)	122.8 (7)	C(20)-N(14)-C(17)	116.9 (7)
C(32)-C(16)-C(40)	119.8 (8)	C(32)-C(16)-C(23)	119.9 (8)
C(40)-C(16)-C(23)	120.3 (7)	N(11)-C(17)-N(9)	118.6 (7)
N(11)-C(17)-N(14)	119.4 (7)	N(9)-C(17)-N(14)	121.9 (7)
N(14)-C(20)-N(4)	124.3 (8)	N(14)-C(20)-N(12)	117.9 (7)
N(4)-C(20)-N(12)	117.7 (8)	N(9)-C(23)-N(4)	109.1 (6)
N(9)-C(23)-C(16)	107.9 (6)	N(4)-C(23)-C(16)	112.5 (6)
N(9)-C(23)J-H(23)	108.4	N(4)-C(23)-H(23)	107.5
C(16)-C(23)-H(23)	111.3	C(30)-C(26)-C(34)	118.8 (8)
C(30)-C(26)-H(26)	121.2	C(34)-C(26)-H(26)	120.0
C(45)-C(27)-C(41)	119.7 (9)	C(45)-C(27)-CH(27)	118.6
C(41)-C(27)-H(27)	121.6	C(34)-C(29)-C(38)	119.9 (8)
C(34)-C(29)-H(29)	121.7	C(38)-C(29)-H(29)	118.4

C(36)-C(30)-C(26)	121.4 (9)	C(36)-C(30)-H(30)	120.1
C(26)-C(36)-H(30)	118.5	C(16)-C(32)-C(41)	120.7 (9)
C(16)-C(32)-H(32)	120.9	C(41)-C(32)-H(32)	118.4
C(29)-C(34)-C(26)	119.9 (8)	C(29)-C(34)-N(4)	120.7 (8)
C(26)-C(34)-N(4)	119.3 (7)	C(30)-C(36)-O(6)	116.7 (9)
C(30)-C(36)-C(38)	121.4 (9)	O(6)-C(36)-C(38)	121.8 (9)
C(36)-C(38)-C(29)	118.6 (8)	C(36)-C(38)-H(38)	119.2
C(29)-C(38)-H(38)	122.2	C(16)-C(40)-C(45)	120.5 (8)
C(16)-C(40)-H(40)	118.5	C(45)-C(40)-H(40)	121.0
C(27)-C(41)-C(32)	118.6 (9)	C(27)-C(41)-H(41)	119.6
C(32)-C(41)-H(41)	121.7	C(27)-C(45)-C(40)	120.6 (9)
C(27)-C(45)-H(45)	119.1	C(40)-C(45)-H(45)	120.2
C(50)-C(46)-O(6)	110.9 (13)	C(50)-C(46)-C(49)	99 (2)
O(6)-C(46)-C(49)	114.0 (11)	C(50)-C(46)-H(46)	109.3
O(6)-C(46)-H(46)	112.5	C(49)-C(46)-H(46)	110.7
C(50)-C(47)-H(47A)	117.9	C(50)-C(47)-H(47B)	109.2
H(47A)-C(47)-H(47B)	107.4	C(50)-C(47)-H(47C)	110.7
H(47A)-C(47)-H(47C)	105.9	H(47B)-C(47)-H(47C)	105.1
C(46)-C(49)-H(49A)	111.5	C(46)-C(49)-H(49B)	118.3
H(49A)-C(49)-H(49B)	98.3	C(46)-C(49)-H(49C)	116.4
H(49A)-C(49)-H(49C)	102.2	H(49B)-C(49)-H(49C)	107.5
C(46)-C(50)-C(47)	110 (2)	C(46)-C(50)-H(50A)	120.9
C(47)-C(50)-H(50A)	106.6	C(46)-C(50)-H(50B)	111.3
C(47)-C(50)-H(50B)	102.7	H(50A)-C(50)-H(50B)	104.0
C(24)-O(3)-C(51)	118.9 (7)	C(15)-N(5)-C(21)	120.5 (6)
C(15)-N(5)-C(28)	117.4 (6)	C(21)-N(5)-C(28)	117.8 (6)
C(15)-N(7)-C(18)	117.6 (7)	C(18)-N(8)-C(28)	119.2 (6)
N(13)-C(15)-N(7)	116.0 (7)	N(13)-C(15)-N(5)	120.9 (7)
N(7)-C(15)-N(5)	123.0 (7)	N(55)-C(18)-N(7)	120.8 (7)
N(55)-C(18)-N(8)	117.1 (7)	N(7)-C(18)-N(8)	122.1 (7)
C(35)-C(19)-C(39)	119.8 (8)	C(35)-C(19)-C(28)	121.1 (8)
C(39)-C(19)-C(28)	119.1 (8)	C(25)-C(21)-(22)	120.5 (7)

C(25)-C(21)-N(5)	120.4 (7)	C(22)-C(21)-N(5)	119.2 (8)
C(31)-C(22)-C(21)	118.5 (8)	C(31)-C(22)-H(22)	121.4
C(21)-C(22)-H(22)	120.1	C(31)-C(24)-C(33)	120.1 (8)
C(31)-C(24)-O(3)	115.4 (8)	C(33)-C(24)-O(3)	124.6 (8)
C(21)-C(25)-C(33)	119.3 (7)	C(21)-C(25)-H(25)	119.6
C(33)-C(25)-H(25)	121.0	N(8)-C(28)-C(19)	109.6 (7)
N(8)-C(28)-N(5)	106.7 (6)	C(19)-C(28)-N(5)	112.2 (7)
N(8)-C(28)-H(28)	113.8	C(19)-C(28)-H(28)	107.5
N(5)-C(28)-H(28)	107.1	C(24)-C(31)-C(22)	121.8 (8)
C(24)-C(31)-H(31)	118.5	C(22)-C(31)-H(31)	119.7
C(24)-C(33)-C(25)	119.8 (8)	C(24)-C(33)-H(33)	120.3
C(25)-C(33)-H(33)	119.8	C(19)-C(35)-C(42)	119.7 (10)
C(19)-C(35)-H(35)	121.8	C(42)-C(35)-H(35)	118.4
C(43)-C(37)-C(42)	118.1 (10)	C(43)-C(37)-H(37)	118.7
C(42)-C(37)-H(37)	123.2	C(43)-C(39)-C(19)	120.5 (10)
C(43)-C(39)-H(39)	121.3	C(19)-C(39)-H(39)	118.1
C(35)-C(42)-C(37)	121.4 (11)	C(35)-C(42)-H(42)	123.1
C(37)-C(42)-H(42)	115.5	C(37)-C(43)-C(39)	120.5 (11)
C(37)-C(43)-H(43)	118.4	C(39)-C(43)-H(43)	121.1
O(3)-C(51)-C(52)	106.0 (13)	O(3)-C(51)-C(54)	102.3 (13)
C(52)-C(51)-C(54)	114 (2)	O(3)-C(51)-H(51)	112.5
C952)-C(51)-H(51)	122.5	C(54)-C(51)-H(51)	98.3
C(51)-C(54)-H(54A)	156.1	C(51)-C(54)-H(54B)	88.1
H(54A)-C(54)-H(54B)	69.7	C(51)-C(54)-H(54C)	91.8
H(54A)-C(54)-H(54C)	72.7	H(54B)-C(54)-H(54C)	70.3
C(51)-C(52)-H(52A)	114.8	C(51)-C(52)-H(52B)	129.8
H(52A)-C(52)-H(52B)	78.1	C(51)-C(52)-H(52C)	137.7
H(52A)-C(52)-H(52C)	78.5	H(52B)-C(52)-H(52C)	91.4

Table 4 Anisotropic displacement parameters [$Å^2$ x 10^3] for 1-(4′-*sec*-butoxyphenyl)-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine hydrochloride **(47c)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
N(4)	44 (4)	71 (5)	42 (4)	2 (3)	-21 (3)	-6 (4)
O(6)	124 (4)	102 (5)	62 (4)	2 (4)	-11 (4)	-41 (5)
N(9)	54 (4)	72 (5)	54 (4)	9 (4)	-20 (4)	-10 (4)
N(11)	63 (5)	54 (4)	51 (4)	6 (3)	-10 (4)	-11 (4)
N(12)	44 (5)	89 (6)	91 (6)	-10(5)	-22 (4)	-10 (4)
N(14)	60 (5)	53 (4)	54 (4)	10 (4)	-22 (4)	-13 (4)
C(16)	42 (5)	57 (6)	51 (5)	-5 (4)	-18 (4)	-4 (4)
C(17)	50 (6)	56 (6)	61 (6)	-11 (5)	-16 (5)	-7 (5)
C(20)	62 (6)	57 (6)	50 (5)	-10 (4)	-24 (5)	2 (5)
C(23)	49 (5)	70 (6)	52 (5)	-11 (5)	-13 (4)	-3 (5)
C(26)	58 (6)	62 (6)	61 (6)	-15 (5)	-13 (5)	-3 (5)
C(27)	63 (7)	82 (8)	127 (10)	-20 (7)	-42 (7)	8 (6)
C(29)	64 (6)	60 (60	60 (6)	-26 (5)	-13 (5)	5 (5)
C(30)	85 (7)	56 (6)	56 (6)	-2 (5)	-1 (5)	-10 (5)
C(32)	104 (8)	71 (6)	46 (5)	-6 (5)	-29 (5)	-4 (6)
C(34)	58 (6)	55 (6)	52 (5)	-4 (4)	-14 (4)	10 (5)
C(36)	80 (7)	74 (7)	51 (6)	7 (5)	-7 (5)	-25 (6)
C(38)	75 (7)	102 (9)	50 (6)	-3 (6)	-7 (5)	-25 (6)
C(40)	70 (7)	81 (7)	72 (6)	-24 (6)	-28 (5)	11 (6)
C(41)	91 (9)	102 (9)	91 (8)	18 (7)	-56 (7)	16 (7)
C(45)	81 (8)	95 (8)	121 (9)	-62 (7)	-34 (7)	16 (7)
C(46)	233 (19)	141 (11)	34 (6)	14 (6)	-9 (8)	-86 (13)
C(47)	158 (16)	195 (18)	124 (13)	7 (11)	-8 (12)	-5 (13)
C(49)	129 (13)	198 (16)	166 (15)	-82 (13)	19 (11)	-48 (12)
C(50)	210 (2)	250 (2)	90 (11)	-37 (14)	-1 (13)	-25 (19)
O(3)	88 (5)	76 (4)	87 (4)	-22 (4)	-45 (4)	-18 (4)
N(5)	48 (4)	62 (4)	46 (4)	-26 (3)	-3 (3)	-17 (3)

	U11	U22	U33	U23	U13	U12
N(7)	57 (4)	74 (5)	35 (4)	-11 (3)	7 (3)	-31 (4)
N(8)	59 (5)	93 (6)	52 (4)	-11 (4)	-3 (4)	-42 (4)
N(55)	58 (5)	103 (6)	45 (4)	-32 (4)	-9 (3)	-28 (4)
N(13)	62 (5)	73 (5)	37 (4)	-20 (3)	-6 (3)	-18 (4)
C(15)	42 (5)	55 (5)	54 (5)	-14 (4)	-10 (4)	-12 (4)
C(18)	63 (6)	58 (6)	43 (5)	-17 (4)	-6 (4)	-2 (5)
C(19)	53 (6)	68 (6)	46 (5)	-9 (5)	3 (4)	-37 (5)
C(21)	58 (6)	61 (6)	47 (5)	-16 (4)	-8 (4)	-22 (5)
C(22)	62 (6)	67 (6)	59 (5)	-8 (5)	-19 (5)	-12 (5)
C(24)	69 (6)	52 (6)	62 (6)	-3 (5)	-26 (5)	-16 (5)
C(25)	68 (6)	42 950	74 (6)	-15 (4)	-27 (5)	-3 (5)
C(28)	46 (50	67 (6)	69 (6)	-16 (5)	-1 (5)	-18 (5)
C(31)	82 (7)	56 (6)	69 (6)	-27 (5)	-29 (5)	-6 (5)
C(33)	59 (6)	57 (6)	72 (6)	6 (5)	-34 (5)	-9 (5)
C(35)	88 (8)	70 (7)	65 (6)	-2 (5)	-12 (6)	-5 (6)
C(37)	134 (11)	135 (10)	45 (6)	-6 (6)	-2 (6)	-99 (10)
C(39)	74 (7)	96 (7)	46 (50	-10 (5)	-8 (5)	-35 (6)
C(42)	129 (11)	76 (8)	88 (8)	-4 (6)	-20 (8)	-40 (8)
C(43)	89 (8)	149 (11)	64 (8)	-13 (8)	3 (6)	-63 (9)
Cl(1)	59 (1)	91 (2)	52 (1)	-23 (1)	-12 (1)	-10 (1)
Cl(2)	93 (2)	101 (2)	55 (1)	1 (1)	-24 (1)	-45 (1)
C(51)	107 (9)	107 (9)	205 (16)	-85 (10)	-85 (11)	30 (8)

Table 5 Crystal data and structure refinement for 1-benzyl-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(52b)**.

Identification code	Shelxl
Empirical formula	$C_{18}H_{18}F_3N_5O_2$
Formula weight	393.37
Temperature	293 (2) K
Wavelength	0.70930 Å
Crystal system	Triclinic
Space group	p-1
Unit cell dimensions	a = 6.30 (5) Å alpha = 100.7 (2) ° b = 10.13 (5) Å beta = 96.5 (2) ° c = 15.20 (5) Å gama = 94.5 (2) °
Volume, Z	942 (9) $Å^3$, 2
Density (calculated)	1.387 Mg/m^3
Absorption coefficient	0.114 mm^{-1}
F (000)	408
Crystal size	0.2 x 0.2 x 0.2 mm
θ range for data collection	2.05 to 21.42°
Limiting indices	$0 \leq h \leq 6$, $-9 \leq k \leq 10$, $-15 \leq 1 \leq 14$
Reflections collected	2086
Independent reflections	1896 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1896 / 0 / 246
Goodness-of-fit on F^2	2.854
Final R indices [I>2 σ(I)]	R1 = 0.976, wR2 = 0.2922
R indices (all data)	R1 = 0.1106, wR2 = 0.3173
Largest diff. peak and hole	1.231 and –0.442 $eÅ^{-3}$

Table 6 Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1-benzyl.-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoro-acetate **(52b)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U (eq)
N (1)	-150 (7)	3115 (4)	4603 (3)	35 (1)
N (6)	-2611 (7)	14487 (4)	4845 (3)	38 (1)
N (7)	2202 (8)	4715 (5)	4297 (3)	45 (1)
N (9)	-176 (7)	867 (5)	3890 (3)	36 (1)
N (11)	2306 (6)	2520 (4)	3565 (3)	32 91)
C (10)	1821 (8)	1059 (5)	3526 (4)	31 (1)
C (12)	1482 (8)	3427 (5)	4146 (4)	33 92)
C (13)	4195 (8)	2873 (5)	3119 (4)	38 (2)
C (14)	1618 (8)	248 (5)	2579 (4)	33 (2)
C (15)	-944 (8)	1825 (5)	4448 (3)	28 (1)
C (17)	3656 (9)	3215 (6)	2205 (4)	41 (2)
C (19)	3129 (11)	-612 (7)	2349 (5)	61 (2)
C (20)	-65 (11)	295 (7)	1951(5)	62 (2)
C (21)	2017 (13)	3958 (8)	2003 (5)	70 (2)
C (22)	2966 (16)	-1400 (9)	1503 (6)	94 (3)
C (23)	4924 (12)	2881 (10)	1556 (6)	85 (4)
C (24)	-244 (15)	-483 (11)	1094 (5)	92 (30
C (25)	1316 (19)	-1317 (10)	887 (6)	100 (3)
C (26)	2906 (18)	3952 (11)	545 (6)	98 (3)
C (27)	1665 (16)	4312 (10)	1179 (7)	97 (3)
C (28)	4519 (19)	3236 (14)	727 (7)	125 (4)
F (2)	9821 (6)	7251 (5)	3194 (3)	87 (1)
F (3)	7893 (6)	5446 (4)	3134 (3)	84 (2)
F (8)	6933 (6)	6747 (6)	2278 (3)	106 (2)
O (4)	7021 (6)	8673 (4)	4067 (3)	49 (1)
O (5)	5074 (6)	6743 (4)	4018 (3)	56 (1)
C (16)	6477 (9)	7446 (6)	3802 (4)	38 (1)

	x	y	z	U (eq)
C (18)	7789 (10)	6743 (6)	3109 (4)	47 (2)

Table 7 Bond lengths [Å] and angles [°] for 1-benzyl-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoroacetate **(52b)**.

N (1)-C (15)	1.330 (9)	N (1)-C(12)	1.353 (10)
N(6)-C(15)	1.321 (10)	N(6)-H(6A)	0.9027
N(6)-H(6B)	0.9761	N(7)-C(12)	1.317 (9)
N(7)-H(7A)	0.8598	N(7)-H(7B)	0.8597
N(9)-C(15)	1.326 (8)	N(9)-C(10)	1.44 (10)
N(9)-H(9)	0.9819	N(11)-C(12)	1.332 (8)
N(11)-C(13)	1.486 (10)	N(11)-C(10)	1.476 (10)
C(10)-C(14)	1.505 (9)	C(10)-H(10)	0.9594
C(13)-C(17)	1.501 (9)	C(13)-H(13A)	0.9647
C(13)-H(13B)	0.9597	C(14)-C(19)	1.371 (11)
C(14)-C(20)	1.354 (11)	C(17)-C(23)	1.350 (11)
C(17)-C(21)	1.364 (11)	C(19)-C(22)	1.371 (12)
C(19)-H(19)	0.9973	C(20)-C(24)	1.381 (12)
C(20)-H(20)	1.0029	C(21)-C(27)	1.366 (12)
C(21)-H(21)	0.9555	C(22)-C(25)	1.336 (14)
C(22)-H(22)	0.9759	C(23)-C(28)	1.376 (14)
C(23)-H(23)	1.0214	C(24)-C(25)	1.371 (14)
C(24)-H(24)	0.9696	C(25)-H(25)	0.9609
C(26)-C(28)	1.33 (2)	C(26)-C(27)	1.33 (2)
C(26)-H(26)	0.9819	C(27)-H(27)	0.9432
C(28)-H(28)	0.9549	F(2)-C(18)	1.324 (12)
F(3)-C(18)	1.328 (10)	F(8)-C(18)	1.317 (9)
O(4)-C(16)	1.241 (9)	O(5)-C(16)	1.204 (9)
C(16)-C(18)	1.520 (11)		

C(15)-N(1)-C(12)	116.8 (5)	C(15)-N(6)-H(6A)	117.9
C(15)-N(6)-H(6B)	122.9	H(6A)-N(6)-H(6B)	119.2
C(12)-N(7)-H(7A)	119.8	C(12)-N(7)-H(7B)	120.2
H(7A)-N(7)-H(7B)	120.0	C(15)-N(9)-C(10)	123.6 (5)
C(15)-N(9)-H(9)	118.2	C(10)-N(9)-H(9)	117.6
C(12)-N(11)-C(13)	122.4 (5)	C(12)-N(11)-C(10)	121.1 (5)
C(13)-N(11)-C(10)	114.3	N(9)-C(10)-N(11)	107.7 (4)
N(9)-C(10)-C(14)	109.5 (5)	N(11)-C(10)-C(14)	112.5 (5)
N(9)-C(10)-H(10)	109.4	N(11)-C(10)-H(10)	109.1
C(14)-C(10)-H(10)	108.7	N(11)-C(12)-N(7)	121.0 (5)
N(11)-C(12)-N(1)	123.5 (5)	N(7)-C(12)-N(1)	115.5 (5)
N(11)-C(13)-C(17)	114.8 (5)	N(11)-C(13)-H(13A)	106.4
C(17)-C(13)-H(13A)	109.7	N(11)-C(13)-H(13B)	106.7
C(17)-C(13)-H(13B)	109.9	H(13A)-C(13)-H(13B)	109.1
C(19)-C(14)-C(20)	118.4 (7)	C(19)-C(14)-C(10)	119.5 (6)
C(2)-C(14)-C(10)	122.1 (6)	N(6)-C(15)-N(1)	118.8 (5)
N(6)-C(15)-N(9)	118.4 (5)	N(1)-C(15)-N(9)	122.8 (5)
C(23)-C(17)-C(21)	116.4 (7)	C(23)-C(17)-C(13)	120.1 (6)
C(21)-C(17)-C(13)	123.3 (5)	C(14)-C(19)-C(22)	121.3 (7)
C(14)-C(19)-H(19)	118.4	C(22)-C(19)-H(19)	120.2
C(24)-C(20)-C(14)	121. (8)	C(24)-C(20)-H(20)	119.7
C(14)-C(20)-H(20)	119.3	C(21)-C(21)-C(17)	121.3 (7)
C(27)-C(21)-H(21)	120.1	C(17)-C(21)-H(21)	118.5
C(25)-C(22)-C(19)	119.4 (8)	C(25)-C(22)-H(22)	116.6
C(19)-C(22)-H(22)	123.8	C(17)-C(23)-C(28)	121.2 (8)
C(17)-C(23)-H(23)	121.5	C(28)-C(23)-H(23)	117.3
C(20)-C(24)-C(25)	118.7 (8)	C(20)-C(24)-H(24)	121.2
C(25)-C(24)-H(24)	120.1	C(22)-C(25)-C(24)	121.1 (8)
C(22)-C(25)-H(25)	117.4	C(24)-C(25)-H(25)	121.4
C(28)-C(26)-C(27)	118.5 (9)	C(28)-C(26)-H(26)	122.1
C(27)-C(26)-H(26)	119.4	C(26)-C(27)-C(21)	121.3 (9)
C(26)-C(27)-H(27)	120.1	C(21)-C(27)-H(27)	118.5

C(26)-C(28)-C(23)	121.3 (8)	C(26)-C(28)-H(28)	116.1
C(23)-C(28)-H(28)	122.6	O(4)-C(16)-O(5)	129.2 (6)
O(4)-C(16)-C(18)	114.7 (6)	O(5)-C(16)-C(18)	116.0 (6)
F(8)-C(18)-F(2)	107.3 (6)	F(8)-C(18)-F(3)	104.5 (6)
F(2)-C(18)-F(3)	104.4 (6)	F(8)-C(18)-C(16)	111.7 (6)
F(2)-C(18)-C(16)	115.0 (6)	F(3)-C(18)-C(16)	113.1 (5)

Symmetry transformations used to generate equivalent atoms

Table 8 Anisotropic displacement parameters [$Å^2$ x 10^3] for 1-benzyl-2-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine trifluoro-acetate **(52b)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + 2hka $^*b^*U_{12}$].

	U11	U22	U33	U23	U13	U12
N(1)	46 (3)	16 (3)	41 (3)	2 (2)	16 (2)	-7 (2)
N(6)	40 (3)	21 (3)	51 (3)	2 (2)	17 (2)	-5 (2)
N(7)	58 (3)	24 (3)	55 (3)	5 (2)	27 (3)	-10 (2)
N(9)	34 (3)	25 (3)	46 (3)	-1 (2)	19 (2)	-11 (2)
N(11)	35 (2)	21 (3)	42 (3)	3 (2)	20 (2)	-3 (2)
C(10)	33 (3)	21 (3)	42 (4)	12(3)	7 (2)	4 (2)
C(12)	34 (3)	26 (4)	39 (3)	10 (3)	7 (3)	-12 (3)
C(13)	30 (3)	31 (3)	54 (4)	21 (3)	18 (3)	-3 (2)
C(14)	40 (3)	26 (3)	33 (3)	0 (3)	13 (3)	2 (3)
C(15)	32 (3)	25 (3)	26 (3)	5 (3)	7 (2)	-5 (3)
C(17)	45 (4)	36 (3)	43 (4)	7 (3)	19 (3)	-6 (3)
C(19)	64 (4)	64 (5)	58 (5)	7 (4)	17 (4)	12 (4)
C(20)	68 (5)	68 (5)	44 (4)	3 (4)	0 (4)	8 (4)
C(21)	90 (6)	79 (5)	52 (5)	25 (4)	22 (4)	34 (5)
C(22)	122 (7)	82 (6)	75 (7)	-14 (5)	26 (6)	37 (5)
C(23)	71 (5)	133 (8)	65 (6)	29 (5)	36 (4)	43 (5)
C(24)	99 (6)	126 (8)	46 (5)	18 (5)	-9 (4)	4 (6)
C(25)	135 (8)	101 (7)	50 (6)	-298 (5)	21 (6)	11 (6)
C(26)	108 (7)	132 (8)	62 (6)	48 (6)	5 (6)	3 (6)

C(27)	112 (7)	109 (7)	82 (7)	43 (6)	9 (6)	34 (6)
C(28)	119 (8)	210 (12)	69 (7)	43 (7)	62 (6)	48 (8)
F(2)	50	89 (3)	113 (4)	-8 (3)	44 (2)	-22 (2)
F(3)	50	55 (3)	144 (4)	-5 (3)	41 (2)	6 (2)
F(8)	50	192 (5)	70 (3)	5 (3)	11 (2)	24 (3)
O(4)	50	22 (2)	71 (3)	-1 (2)	20 (2)	-14 (2)
O(5)	50	27 (2)	94 (3)	8 (2)	39 (2)	-15 (2)
C(16)	50	25 (4)	39 (3)	5 (3)	10 (3)	-3 (3)
C(18)	50	36 (4)	50 (4)	4 (3)	7 (3)	-8 (3)

Table 9 Crystal data and structure refinement for dihydrotriazine **(54d)**.

Identification code	tvgala
Empirical formula	$C_{23}H_{20}N_{12}O_4$
Formula weight	528.51
Temperature	293 (2) K
Wavelength	0.70930 Å
Crystal system	Monoclinic
Space group	$P2_1/C$
Unit cell dimensions	*A* = 25.03 (5) Å alpha = 90.0 (2) ° *b* = 6.06 (5) Å beta = 149.4 (2) ° *c* = 32.09 (5) Å gamma = 90.0 (2) °
Volume, Z	2478 (21) $Å^3$, 4
Density (calculated)	1.416 Mg/m^3
Absorption coefficient	0.104 mm^{-1}
F (000)	1096
Crystal size	0.2 x 0.2 x 0.2 mm
θ range for data collection	2.49 to 22.85°
Limiting indices	$0 \leq h \leq 27$, $0 \leq k \leq 6$, $-34 \leq 1 \leq 17$
Reflections collected	4045
Independent reflections	3295
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3295 / 0 / 361
Goodness-of-fit on F^2	1.049
Final R indices [I>2 σ(I)]	R1 = 0.0671, wR2 = 0.1574
R indices (all data)	R1 = 0.1736, wR2 = 0.2139
Largest diff. peak and hole	0.266 and –0.304 $eÅ^{-3}$

Table 10 Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for dihydrotriazine **(54d)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(20)	296 (3)	7326 (7)	4863 (2)	43 (1)
N(22)	998 (3)	4012 (7)	5045 (3)	44(1)
N(17)	1994 (3)	6044 (8)	6188 (3(	51 (1)
N(19)	1333 (3)	9223 (8)	6015 (3)	52 (1)
O(30)	1173 (3)	744 (6)	4804 (3)	64 (1)
N(33)	-581 (3)	5057 (7)	3792 (3)	52 (1)
C(24)	2876 (4)	4583 (9)	6153 (3)	42 (1)
C(21)	226 (4)	5599 (9)	4567 (3)	44 (1)
C(23)	2046 (4)	4227 (8)	5924 (3)	43 (1)
C(18)	1214 (4)	7506 (9)	5689 (3)	42 (1)
C(26)	3596 (5)	2972 (10)	6558 (4)	62 (2)
C(35)	100 (5)	4634 (10)	3330 (3)	51 (2)
C(31)	665 (4)	2338 (10)	4553 (3)	48 (1)
C(32)	-426 (4)	2966 (9)	3680 (3)	52 (2)
C(25)	2889 (5)	6496 (10)	5937 (4)	59 (2)
C(34)	-580 (4)	3021 (10)	3107 (3)	58 (2)
C(28)	4346 (5)	5210 (16)	6527 (5)	81 (2)
C(40)	-332 (6)	6576 (12)	2885 (4)	74 (2)
C(36)	1134 (5)	4219 (13)	3940 (4)	79 (2)
C(27)	4348 (5)	3306 (14)	6749 (4)	78 (2)
C(37)	1735 (6)	5638 (19)	4114 (5)	102 (3)
C(29)	3619 (6)	6816 (13)	6121 (5)	82 (2)
C(39)	288 (10)	8030 (13)	3073 (7)	106 (3)
C(38)	1306 (10)	7520 (2)	3674 (8)	118 (4)
O(11)	4359 (4)	4953 (8)	8145 (3)	86 (2)
N(7)	5063 (5)	5610 (10)	8841 (4)	71 (2)
C(2)	3995 (4)	10858 (10)	8584 (3)	57 (2)

	x	y	z	U(eq)
C(4)	5708 (5)	10191 (12)	9978 (4)	65 (2)
O(12)	3264 (4)	8441 (9)	7598 (3)	113 (2)
C(6)	4940 (4)	7683 (11)	8996 (3)	57 (2)
C(1)	3990 (5)	8914 (11)	8318 (4)	61 (2)
C(5)	5767 (4)	8278 (11)	9793 (3)	60 (2)
O(15)	6565 (4)	12699 (12)	10970 (3)	138 (3)
O(13)	2283 (4)	11781 (9)	7278 (3)	118 (2)
N(8)	3072 (4)	12298 (10)	7985 (4)	73 (2)
O(16)	7359 (4)	9659 (11)	11362 (3)	126 (2)
O(14)	3134 (4)	14022 (10)	8209 (3)	124 (2)
O(10)	5886 (4)	4610 (10)	9432 (3)	116 (2)
N(9)	6620 (5)	10909 (14)	10832 (4)	94 (2)
C(3)	4834 (5)	11495 (11)	9383 (4)	63 (2)

Table 11 Bond lengths [Å] and angles [°] for dihydrotriazine **(54d)**.

N(20)-C(21)	1.318 (10)	N(20)-C(18)	1.356 (10)
N(22)-C(21)	1.382 (11)	N(22)-C(31)	1.397 (10)
N(22)-C(23)	1.456 (11)	N(17)-C(18)	1.333 (11)
N(17)-C(23)	1.462 (10)	N(17)-H(17)	0.8597
N(19)-C(18)	1.314 (10)	N(19)-H(19A)	0.8595
N(19)-H(19B)	0.8597	O(30)-C(31)	1.198 (10)
N(33)-C(21)	1.351 (10)	N(33)-C(32)	1.457 (11)
N(33)-H(33)	0.8600	C(24)-C(26)	1.363 (11)
C(24)-C(25)	1.366 (11)	C(24)-C(23)	1.506 (8)
C(23)-H(23)	0.9838	C(26)-C(27)	1.404 (10)
C(26)-H(26)	0.9778	C(35)-C(36)	1.368 (11)
C(35)-C(40)	1.390 (13)	C(35)-C(34)	1.506 (11)
C(31)-C(32)	1.511 (12)	C(32)-C(34)	1.522 (8)
C(32)-H(32)	0.9766	C(25)-C(29)	1.365 (10)
C(25)-H(25)	0.9535	C(34)-H(34A)	0.9679
C(34)-H(34B)	0.9588	C(28)-C(27)	1.353 (13)
C(28)-C(29)	1.369 (13)	C(28)-H(28)	1.0058
C(40)-C(39)	1.393 (13)	C(40)-H(40)	0.9791
C(36)-C(37)	1.366 (12)	C(36)-H(36)	1.0223
C(27)-H(27)	1.0352	C(37)-C(38)	1.36 (2)
C(37)-H(37)	0.9601	C(29)-H(29)	1.0096
C(39)-C(38)	1.36 (2)	C(39)-H(39)	0.9758
C(38)-H(38)	0.9321	O(11)-N(7)	1.215 (9)
N(7)-O(10)	1.218 (10)	N(7)-C(6)	1.476 (12)
C(2)-C(3)	1.366 (11)	C(2)-C(1)	1.450 (12)
C(2)-N(8)	1.466 (12)	C(4)-C(5)	1.366 (12)
C(4)-C(3)	1.366 (12)	C(4)-N(9)	1.465 (12)
O(12)-C(1)	1.222 (10)	C(6)-C(5)	1.359 (11)
C(6)-C(1)	1.428 (12)	C(5)-H(5)	0.9837
O(15)-N(9)	1.222 (11)	O(13)-N(8)	1.198 (10)

N(8)-O(14)	1.200 (10)	O(16)-N(9)	1.213 (11)
C(3)-H(3)	1.0125		

C(21)-N(20)-C(18)	115.1 (6)	C(21)-N(22)-C(31)	110.2 (6)
C(21)-N(22)-C(23)	123.8 (6)	C(21)-N(22)-C(23)	125.6 (6)
C(18)-N(17)-C(23)	125.0 (6)	C(18)-N(17)-H(17)	117.6
C(23)-N(17)-H(17)	117.4	C(18)-N(19)-H(19A)	120.1
C(18)-N(19)-H(19B)	119.8	H(19A)-N(19)-H(19B)	120.1
C(21)-N(33)-C(32)	112.4 (6)	C(21)-N(33)-H(33)	123.7
C(32)-N(33)-H(33)	123.9	C(26)-C(24)-C(25)	120.2 (7)
C(26)-C(24)-(23)	120.0 (6)	C(25)-C(24)-C(23)	119.9 (6)
N(33)-C(21)-N(20)	126.6 (6)	N(33)-C(21)-N(22)	109.3 (7)
N(20)-C(21)-N(22)	124.0 (6)	N(22)-C(23)-N(17)	106.2 (6)
N(22)-C(23)-C(24)	112.8 (5)	N(17)-C(23)-C(24)	112.5 (6)
N(22)-C(23)-H(23)	108.8	N(17)-C(23)-H(23)	108.7
C(24)-C(23)-H(23)	107.7	N(19)-C(18)-N(17)	118.4 (6)
N(19)-C(18)-N(20)	117.5 (6)	N(17)-C(18)-N(20)	124.0 (6)
C(24)-C(26)-C(27)	119.3 (7)	C(24)-C(26)-H(26)	120.8
C(27)-C(26)-H(26)	119.8	C(36)-C(35)-C(40)	117.9 (8)
C(36)-C(35)-C(34)	122.2 (7)	C(40)-C(35)-C(34)	119.9 (7)
O(32)-C(31)-N(22)	124.7 (7)	O(30)-C(31)-C(32)	129.0 (7)
N(22)-C(31)-C(32)	106.4 (7)	N(33)-C(32)-C(31)	101.7 (6)
N(33)-C(32)-C(34)	115.7 (6)	C(31)-C(32)-C(34)	114.8 (5)
N(33)-C(32)-H(32)	108.5	C(31)-C(32)-H(32)	109.8
C(334)-C(32)-H(32)	106.2	C(29)-C(25)-C(24)	120.6 (7)
C(29)-C(25)-H(25)	121.1	C(24)-C(25)-H(25)	118.3
C(35)-C(34)-C(32)	115.7 (6)	C(35)-C(34)-H(34A)	106.3
C(32)-C(34)-H(34A)	109.2	C(35)-C(34)-H(34B)	106.6
C(32)-C(34)-H(34B)	109.8	H(34A)-C(34)-H(34B)	108.9
C(27)-C(28)-C(29)	120.4 (7)	C(27)-C(28)-H(28)	118.9
C(29)-C(28)-H(28)	120.7	C(39)-C(40)-C(35)	119.9 (8)
C(39)-C(40)-H(40)	118.3	C(35)-C(40)-H(40)	121.

C(37)-C(36)-C(35)	122.0 (8)	C(37)-C(36)-H(36)	118.7
C(35)-C(36)-H(36)	119.3	C(28)-C(27)-C(26)	119.7 (7)
C(28)-C(27)-H(27)	119.3	C(26)-C(27)-H(27)	121.0
C(38)-C(37)-C(36)	119.9 (9)	C(38)-C(37)-H(37)	112.0
C(36)-C(37)-H(37)	128.1	C(25)-C(29)-C(28)	119.9 (7)
C(25)-C(29)-H(29)	117.8	C(28)-C(29)-H(29)	122.3
C(38)-C(39)-C(40)	120.0 (9)	C(38)-C(39)-H(39)	124.1
C(40)-C(39)-H(39)	115.4	C(39)-C(38)-C(37)	120.4 (9)
C(39)-C(38)-H(38)	117.8	C(37)-C(38)-H(38)	121.6
O(11)-N(7)-O(10)	122.2 (7)	O(11)-N(7)-C(6)	120.3 (7)
O(10)-N(7)-C(6)	117.5 (7)	C(3)-C(2)-C(1)	123.7 (7)
C(3)-C(2)-N(8)	115.9 (7)	C(1)-C(2)-N(8)	120.3 (7)
C(5)-C(4)-C(3)	121.7 (7)	C(5)-C(4)-N(9)	119.2 (8)
C(3)-C(4)-N(9)	119.1 (8)	C(5)-C(6)-C(1)	124.8 (7)
C(5)-C(6)-N(7)	116.0 (7)	C(1)-C(6)-CN(7)	119.2 (7)
O(12)-C(1)-C(6)	125.1 (7)	O(12)-C(1)-C(2)	123.3 (7)
C(6)-C(1)-C(2)	111.6 (7)	C(6)-C(5)-C(4)	118.9 (7)
C(6)-C(5)-H(5)	119.6	C(4)-C(5)-H(5)	121.4
O(14)-N(8)-O(13)	121.0 (7)	O(14)-N(8)-C(2)	119.0 (7)
O(13)-N(8)-C(2)	119.9 (7)	O(16)-N(9)-O(15)	123.8 (8)
O(16)-N(9)-C(4)	118.6 (9)	O(15)-N(9)-C(4)	117.5 (9)
C(2)-C(3)-C(4)	119.1 (7)	C92)-C93)-H(3)	124.7
C(4)-C(3)-H(3)	116.1		

Symmetry transformations used to generate equivalent atoms:

Table 12 Anisotropic displacement parameters [$Å^2$ x 10^3] for dihydrotriazine **(54d)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
N(20)	40 (3)	40 (3)	43 (3)	-9 (2)	35 (30	0 (2)
N(22)	46 (3)	38 (3)	49 (3)	-6 (2)	41 (3)	-3 (2)
N(17)	52 (3)	57 (3)	47 (3)	1 (3)	43 (3)	9 (3)
N(19)	52 (3)	52 (3)	43 (3)	-6 (2)	39 (3)	2 (2)
O(30)	84 (3)	36 (2)	79 (3)	-2 (2)	71 (3)	5 (2)
N(33)	41 (3)	58 (3)	43 (3)	-8 (2)	34 (3)	1(2)
C(24)	41 (3)	37 (3)	43 (3)	-2 (3)	36 (3)	0 (3)
C(21)	44 (3)	43 (3)	53 (3)	0 (3)	43 (3)	-3 (3)
C(23)	45 (3)	35 (3)	41 (3)	5 (3)	36 (3)	7 (3)
C(18)	45 (3)	44 (3)	52 (4)	-7 (3)	44 (3)	-7 (3)
C(26)	53 (4)	57 (4)	61 (4)	5 93)	47 (4)	13 (3)
C(35)	60 (4)	56 (4)	46 (3)	-1 (3)	47 (3)	8 (3)
C(31)	57 (4)	40 (3)	65 (4)	-1 (3)	56 (4)	-2 (3)
C(32)	49 (3)	54 (4)	62 (4)	-19 (3)	49 (3)	-15 (3)
C(25)	58 (4)	57 (4)	68 (4)	11 (3)	55 (4)	11 (3)
C(34)	49 (3)	66 (4)	50 (3)	-17 (3)	42 (3)	-5 (3)
C(28)	67 (5)	115 (7)	79 (5)	-32 (5)	66 (5)	-27 (5)
C(40)	96 (5)	73 (5)	89 (5)	12 (4)	85 (5)	19 (4)
C(36)	67 (5)	108 (6)	66 (4)	21 (4)	57 (4)	17 (5)
C(27)	50 (4)	98 (6)	69 (5)	0 (4)	48 (4)	16 (4)
C(37)	83 (6)	155 (9)	81 (6)	-1 (6)	73 (5)	-18 (6)
C(29)	93 (5)	73 (5)	104 (6)	-9 (5)	88 (5)	-18 (5)
C(39)	202 (10)	61 (5)	162 (9)	21 (6)	173 (9)	25 (7)
C(38)	167 (10)	126 (9)	159 (10)	-47 (8)	155 (10)	-54 (8)
O(11)	89 (4)	83 (4)	79 (3)	-16 (3)	71 (3)	3 (3)
N(7)	81 (4)	82 (4)	73 (4)	4 (4)	70 (4)	8 (4)
C(2)	50 (4)	64 (4)	44 (3)	-3 (3)	38 (3)	3 (3)

	U11	U22	U33	U23	U13	U12
C(4)	51 (4)	79 (5)	50 (4)	-14 (4)	41 (4)	-8 (4)
O(12)	80 (3)	119 (4)	43 (3)	-8 (3)	39 (3)	42 (3)
C(6)	54 (4)	73 (4)	50 (4)	3 (3)	45 (3)	12 (3)
C(1)	48 (4)	71 (4)	44 (4)	-7 (3)	36 (4)	6 (3)
C(5)	51 (4)	76 (5)	49 (4)	5 (3)	42 (4)	5 (3)
O(15)	89 (4)	158 (6)	72 (4)	-56 (4)	55 (4)	-14 (4)
O(13)	61 (3)	114 (4)	50 (3)	-17 (3)	28 (3)	31 (3)
N(8)	57 (4)	74 (4)	61 (4)	-14 (3)	47 (3)	-1 (3)
O(16)	68 (40	156 (6)	52 (3)	-7 (4)	36 (3)	14 (4)
O(14)	95 (4)	102 (4)	95 (4)	-28 (4)	70 (4)	18 (3)
O(10)	97 (4)	124 (5)	81 (4)	20 (4)	70 (4)	52 (4)
N(9)	60 (4)	126 (6)	57 (4)	-29 (4)	45 (4)	-15 (4)
C(3)	59 (4)	67 (4)	56 (4)	-19 (4)	49 (4)	-8 (4)

Table 13 Crystal data and structure refinement for 1*RS*-phenylethyl-2*SR*-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine picrate **(55b)**.

Identification code	Tvka4a
Empirical formula	$C_{29}H_{25}N_{11}O_{14}$
Formula weight	751.60
Temperature	293 (2) K
Wavelength	0.70930 Å
Crystal system	Monoclinic
Space group	$P2_1/C$
Unit cell dimensions	*A* = 14.83 (5) Å alpha = 90.0 (2) ° *b* = 15.19 (5) Å beta = 105.2 (2) ° *c* = 15.48 (5) Å gama = 90.0 (2) °
Volume, Z	3365 (19) $Å^3$, 4
Density (calculated)	1.484 Mg/m^3
Absorption coefficient	0.121 mm^{-1}
F (000)	1552
Crystal size	0.2 x 0.2 x 0.2 mm
θ range for data collection	2.15 to 19.86°
Limiting indices	$0 \leq h \leq 14$, $0 \leq k \leq 13$, $-14 \leq l \leq 14$
Reflections collected	3271
Independent reflections	2857
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2857 / 0 / 487
Goodness-of-fit on F^2	1.142
Final R indices [I>2 σ(I)]	R1 = 0.0690, wR2 = 0.1682
R indices (all data)	R1 = 0.1477, wR2 = 0.2065
Largest diff. peak and hole	0.439 and –0.296 $eÅ^{-3}$

Table 14 Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1*RS*-phenylethyl-2*SR*-phenyl-4,6- diamino-1,2-dihydro-1,3,5-triazine picrate **(55b)**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	3343 (4)	1716 (4)	2226 (4)	64 (2)
N(2)	2888 (5)	3 (4)	2298 (4)	49 (2)
N(3)	2501 (4)	-1505 (4)	2034 (4)	45 (2)
N(4)	3775 (4)	-1086 (5)	3158 (4)	46 (2)
N(5)	3608 (4)	-2544 (4)	2771 (4)	54 (2)
N(6)	1582 (5)	2217 (6)	1018 (5)	63 (2)
O(7)	4815 (4)	2850 (4)	983 (4)	82 (2)
O(8)	985 (5)	2520 (4)	387 (5)	90 (2)
O(9)	1739 (5)	5469 (4)	1239 (5)	94 (2)
O(10)	1634 (4)	1441 (5)	1210 (4)	85 (2)
N(11)	4339 (5)	364 (4)	3196 (4)	57 (2)
O(12)	4779 (5)	2263 (5)	3531 (5)	91 (2)
N(13)	3615 (6)	4201 (6)	31 (5)	67 (2)
O(14)	1041 (5)	2561 (5)	-1978 (5)	95 (2)
O(15)	3116 (6)	5783 (4)	2083 (5)	111 (3)
N(16)	4641 (5)	2979 (6)	3206 (5)	64 (2)
O(17)	5237 (5)	3555 (4)	3339 (5)	102 (3)
O(18)	4369 (6)	4451 (4)	457 (5)	122 (3)
O(19)	3022 (50	4733 (5)	-290 (5)	115 (3)
C(20)	2121 (6)	-626 (5)	2106 (5)	47 (2)
C(21)	3126 (6)	2509 (6)	2127 (5)	46 (2)
C(22)	1988 (6)	-2120 (5)	1308 (6)	57 (2)
C(23)	1868 (6)	-1662 (5)	412 (6)	57 (2)
N(24)	2502 (7)	5253 (6)	1721 (6)	70 (2)
N(25)	4325 (7)	1034 (6)	681 (6)	90 (3)
O(26)	5070 (5)	1128 (4)	1174 (5)	108 (3)

	x	y	z	U(eq)
C(27)	2084 (6)	3718 (7)	1419 (5)	50 (2)
C(28)	3273 (6)	-1737 (6)	2634 (6)	47 (2)
C(29)	1558 (5)	-593 (6)	2812 (5)	47 (2)
C(30)	3543 (6)	4078 (6)	2459 (6)	55 (2)
C(31)	3739 (6)	3202 (6)	2576 (5)	48 (2)
C(32)	2268 (6)	2841 (6)	1535 (5)	46 (2)
C(33)	3675 (7)	-226 (7)	2897 (5)	51 (2)
C(34)	3435 (6)	3270 (6)	-116 (5)	44 (2)
N(35)	1511 (6)	1972 (7)	-1550 (5)	76 (2)
C(36)	2943 (7)	1531 (6)	-419 (6)	63 (3)
C(37)	2715 (7)	4330 (6)	1876 (6)	54 (2)
C(38)	2389 (5)	2190 (7)	-875 (5)	56 (2)
C(39)	3760 (6)	1757 (7)	187 (5)	56 (2)
O(40)	1294 (5)	1207 (6)	-1648 (5)	126 (3)
C(41)	1111 (7)	-2448 (6)	1491 (6)	76 (3)
C(42)	1047 (6)	149 (6)	2812 (6)	63 (3)
C(43)	2612 (6)	3059 (7)	-736 (6)	58 (2)
C(44)	4080 (7)	2635 (7)	404 (6)	58 (2)
C(45)	2628 (7)	-1541 (7)	89 (7)	80 (3)
C(46)	2555 (11)	-1159 (9)	-725 (10)	103 (4)
C(47)	1546 (7)	-1256 (6)	3397 (7)	75 (3)
C(48)	1034 (7)	-1362 (7)	-99 (8)	91 (3)
C(49)	488 (8)	-426 (11)	4000 (8)	96 (4)
O(50)	3964 (7)	332 (6)	639 (7)	200 (6)
C(51)	513 (7)	251 (7)	3424 (9)	85 (3)
C(52)	1003 (10)	-1166 (8)	3996 (7)	97 (4)
C(53)	1720 (17)	-861 (9)	-1202 (9)	128 (6)
C(54)	962 (10)	-953 (10)	-906 (9)	131 (5)

Table 15 Bond lengths [Å] and angles [°] for 1*RS*-phenylethyl-2*SR*-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine picrate **(54b)**.

O(1)-C(21)	1.247 (10)	N(2)-C(33)	1.331 (10)
N(2)-C(20)	1.456 (10)	N(2)-H(2)	1.2288
N(3)-C(28)	1.3189(10)	N(3)-C(20)	1.466 (10)
N(3)-C(22)	1.505 (11)	N(4)-C(28)	1.368 (10)
N(4)-C(33)	1.363 (10)	N(4)-H(4)	1.1269
N(5)-C(28)	1.320 (10)	N(5)-H(5A)	1.2190
N(5)-H(5B)	1.0235	N(6)-O(10)	1.213 (9)
N(6)-O(8)	1.222 (9)	N(6)-C(32)	1.465 (11)
O(7)-C(44)	1.258 (10)	O(9)-N(24)	1.225 (9)
N(11)-C(33)	1.323 (10)	N(11)-H(11A)	1.1354
N(11)-H(11B)	1.0938	O(12)-H(16)	1.193 (9)
N(13)-O(18)	1.201 (9)	N(13)-O(19)	1.202 (9)
N(13)-C(34)	1.446 (11)	O(14)-C(35)	1.217 (9)
O(15)-N(24)	1.235 (9)	N(16)-O(17)	1.222 (9)
N(16)-C(31)	1.473 (11)	C(20)-C(29)	1.541 (11)
C(20)-H(20)	0.9799	C(21)-C(31)	1.442 (11)
C(21)-C(32)	1.449 (11)	C(22)-C(41)	1.488 (12)
C(22)-C(23)	1.520 (12)	C(22)-H(22)	0.9929
C(23)J-C(48)	1.360 (13)	C(23)-C(45)	1.360 (13)
N(24)-C(37)	1.444 (12)	N(25)-O(26)	1.176 (10)
N(25)-O(50)	1.187 (11)	N(25)-C(39)	1.469 (12)
C(27)-C(32)	1.363 (11)	C(27)-C(37)	1.375 (11)
C(27)-H(27)	1.0068	C(29)-C(42)	1.359 (11)
C(29)-C(47)	1.358 (12)	C(30)-C(31)	1.364 (11)
C(30)-C(37)	1.373 (12)	C(30)-H(30)	1.0050
C(34)-C(43)	1.378 (11)	C(34)-C(44)	1.446 (12)
N(35)-O(40)	1.205 (10)	N(35)-C(38)	1.477 (11)
C(36)-C(38)	1.369 (12)	C(36)-C(39)	1.366 (11)
C(36)-H(36)	1.0100	C(38)-C(43)	1.364 (12)

C(39)-C(44)	1.426 (12)	C(41)-H(41A)	0.9773
C(41)-H(41B)	0.9580	C(41)-H(41C)	0.9973
C(42)-C(51)	1.394 (13)	C(42)-H(42)	1.0036
C(43)-H(43)	0.9388	C(45)-C(46)	1.36 (2)
C(45)-H(45)	1.0021	C(46)-C(53)	1.34 (2)
C(46)-H(46)	1.0302	C(47)-C(52)	1.385 (14)
C(47)-H(47)	0.9981	C(48)-C(54)	1.37 (2)
C(48)-H(48)	0.9986	C(49)-C(52)	1.36 (2)
C(49)-C(51)	1.37 (2)	C(49)-H(49)	1.0141
C(51)-H(51)	1.0082	C(52)-H(52)	0.9956
C(53)-C(54)	1.33 (2)	C(53)-H(53)	0.9806
C(54)-H(54)	1.0114		

C(33)-N(2)-C(20)	117.7 (7)	C(33)-N(2)-H(2)	127.3
C(20)-N(2)-H(2)	114.6	C(28)-N(3)-C(20)	118.0 (7)
C(28)-N(3)-C(22)	122.4 (7)	C(20)-N(3)-C(22)	119.5 (6)
C(28)-N(4)-C(33)	121.1 (7)	C(28)-N(4)-H(4)	111.0
C(33)-N(4)-H(4)	124.9	C(28)-N(5)-H(5A)	114.7
C(28)-N(5)-H(5B)	112.5	H(5A)-N(5)-H(5B)	128.8
O(10)-N(6)-O(8)	123.2 (8)	O(10)-N(6)-C(32)	120.2 (8)
O(8)-N(6)-C(32)	116.6 (8)	C(33)-N(11)-H(11A)	122.8
C(33)-N(11)-H(11B)	121.7	H(11A)-N(11)-H(11B)	112.6
O(18)-N(13)-O(19)	119.3 (9)	O(18)-N(13)-C(34)	120.1 (8)
O(19)-N(13)-C(34)	120.6 (8)	O(12)-N(16)-O(17)	123.0 (8)
O(12)-N(16)-C(31)	120.9 (8)	O(17)-N(16)-C(31)	115.9 (8)
N(2)-C(20)-N(3)	108.5 (6)	N(2)-C(20)-C(29)	112.0 (7)
N(3)-C(20)-C(29)	112.0 (7)	N(2)-C(20)-H(20)	109.0
N(3)-C(20)-H(20)	109.1	C(29)-C(20)-H(20)	106.2
O(1)-C(21)-C(31)	122.5 (8)	O(1)-C(21)-C(32)	124.6 (8)
C(31)-C(21)-C(32)	112.9 (8)	N(3)-C(22)-C(41)	11.2 (8)
N(3)-C(22)-C(23)	108.2 (7)	C(41)-C(22)-C(23)	115.4 (7)
N(3)-C(22)-H(22)	107.2	C(41)-C(22)-H(22)	106.1

C(23)-C(22)-H(22)	108.4	C(48)-C(23)-C(45)	117.2 (9)
C(48)-C(23)-C(22)	123.6 (9)	C(45)-C(23)-C(22)	119.2 (9)
O(9)-N(24)-O(15)	123.8 (8)	O(9)-N(24)-C(37)	119.2 (9)
O(15)-N(24)-C(37)	117.0 (9)	O(26)-N(25)-O(50)	118.6 (10)
O(26)-N(25)-C(39)	123.9 (9)	O(50)-N(25)-C(39)	117.1 (10)
C(32)-C(27)-C(37)	120.5 (8)	C(32)-C(27)-H(27)	121.4
C(37)-C(27)-H(27)	118.0	N(5)-C(28)-N(3)	125.5 (8)
N(5)-C(28)-N(4)	117.0 (8)	N(3)-C(28)-N(4)	117.5 (8)
C(42)-C(29)-C(47)	120.7 (8)	C(42)-C(29)-C(20)	115.7 (9)
C(47)-C(29)-C(20)	123.7 (8)	C(31)-C(30)-C(37)	118.8 (8)
C(31)-C(30)-H(30)	123.5	C(37)-C(30)-H(30)	117.7
C(30)-C(31)-C(21)	124.2 (8)	C(30)-C(31)-N(16)	11539 (8)
C(21)-C(31)-N(16)	119.9 (8)	C(27)-C(32)-C(21)	122.3 (8)
C(27)-C(32)-N(6)	118.3 (8)	C(21)-C(32)-N(6)	119.4 (8)
N(11)-C(33)-N(2)	120.1 (9)	N(11)-C(33)-N(4)	122.2 (8)
N(2)-C(33)J-N(4)	117.7 (8)	C(43)-C(43)-C(44)	124.6 (9)
C(43)-C(34)-N(13)	115.5 (9)	C(44)-C(34)-N(13)	119.8 (8)
O(40)-N(35)-O(14)	123.0 (9)	O(40)-N(35)-C(38)	117.5 (10)
O(14)-N(35)-C(38)	119.5 (9)	C(38)-C(36)-C(39)	118.3 (8)
C(38)-C(36)-H(36)	121.6	C(39)-C(36)-H(36)	120.1
C(27)-C(37)-C(30)	121.3 (8)	C(27)-C(37)-N(24)	118.8 (9)
C(30)-C(37)-N(24)	119.9 (9)	C(36)-C(38)-C(43)	122.6 (8)
C(36)-C(38)-N(35)	120.0 (10)	C(43)-C(38)-N(35)	117.4 (9)
C(36)-C(39)-C(44)	125.3 (9)	(36)-C(39)-N(25)	116.8 (9)
C(44)-C(39)-N(25)	117.9 (8)	C(22)-C(41)-H(41A)	113.1
C(22)-C(41)-H(41B)	113.2	H(41A)-C(41)-H(41B)	108.2
C(22)-C(41)-H(41C)	110.1	H(41A)-C(41)-H(41C)	105.1
H(41B)-C(41)-H(41C)	106.6	C(29)-C(42)-C(51)	120.7 (9)
C(29)-C(42)-H(42)	120.1	C(51)-C(42)-H(42)	119.1
C(38)-C(43)-C(34)	118.0 (8)	C(38)-C(43)-H(43)	119.4
C(34)-C(43)-H(43)	122.6	O(7)-C(44)-C(39)	125.7 (8)
O(7)-C(44)-C(34)	123.1 (9)	C(39)-C(44)-C(34)	111.2 (9)

C(46)-C(45)-C(23)	121.6 (10)	C(46)-C(45)-H(45)	119.5
C(23)-C(45)-H(45)	118.9	C(53)-C(46)-C(45)	119.3 (12)
C(53)-C(46)-H(46)	118.1	C(45)-C(46)-H(46)	122.6
C(29)-C(47)-C(52)	119.0 (9)	C(29)-C(47)-H(47)	122.5
C(52)-C(47)-H(47)	118.5	C(54)-C(48)-C(23)	121.4 (11)
C(54)-C(48)-H(48)	118.6	C(23)-C(48)-H(48)	120.0
C(52)-C(49)-C(51)	12.0.5 (10)	C(52)-C(49)-H(49)	121.6
C(51)-C(49)-H(49)	117.9	C(49)-C(51)-C(42)	118.4 (9)
C(49)-C(51)-H(51)	121.0	C(42)-C(51)-H(51)	120.5
C(49)-C(52)-C(47)	120.8 (10)	C(49)-C(52)-H(52)	118.1
C(47)-C(52)-H(52)	121.2	C(54)-C(53)-C(46)	121.1 (13)
C(54)-C(53)-H(53)	123.8	C(46)-C(53)-H(53)	115.1
C(53)-C(54)-C(48)	119.4 (13)	C(53)-C(54)-H(54)	117.6
C(48)-C(54)-H(54)	123.0		

Symmetry transformations used to generate equivalent atoms:

Table 16 Anisotropic displacement parameters [$Å^2$ x 10^3] for 1*RS*-phenylethyl-2*SR*-phenyl-4,6-diamino-1,2-dihydro-1,3,5-triazine picrate **(54b)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + 2hka $^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
O(1)	67 (4)	30 (4)	86 (4)	4 (3)	2 (3)	-2 (3)
N(2)	54 (5)	31 (4)	54 (4)	3 (4)	1 (4)	-3 (4)
N(3)	40 (4)	34 (5)	50 (4)	-1 (4)	-7 (4)	2 (4)
N(4)	58 (5)	18 (5)	57 (5)	14 (4)	6 (4)	9 (4)
N(5)	55 (4)	17 (4)	76 (5)	-5 (4)	-8 (4)	-4 (4)
N(6)	64 (6)	52 (6)	68 (6)	-2 (5)	10 (5)	-6 (6)
O(7)	70 (4)	56 (4)	95 (5)	1 (4)	-24 (4)	-15 (4)
O(8)	78 (5)	74 (5)	99 (5)	4 (4)	-14 (4)	-7 (4)
O(9)	100 (6)	49 (5)	121 (6)	-1 (4)	7 (5)	14 (4)
O (10)	90 (5)	38 (4)	112 (6)	6 (4)	3 (4)	-15 (4)
N(11)	64 (5)	35 (5)	59 (5)	1 (4)	-6 (4)	-12 (4)
O(12)	84 (5)	55 (5)	110 (6)	22 (4)	-14 (4)	-12 (4)
N(13)	62 (6)	64 (8)	66 (5)	6 (5)	3 (5)	-7 (6)
O(14)	72 (5)	102 (6)	89 (5)	9 (5)	-16 (4)	3 (4)
O(15)	132 (6)	26 (4)	147 (7)	-9 (4)	-16 (5)	-16 (4)
N(16)	52 (6)	43 (6)	97 (6)	-3 (5)	21 (5)	-6 (5)
O(17)	72 (5)	57 (5)	157 (7)	-5 (5)	-6 (4)	-18 (4)
O(18)	104 (6)	63 (5)	148 (7)	4 (5)	-55 (3)	-13 (5)
O(19)	102 (6)	60 (5)	150 (7)	13 (5)	-28 (5)	16 (5)
C(20)	56 (6)	28 (6)	48 (5)	4 (4)	-1 (4)	11 (5)
C(21)	61 (7)	31 (7)	52 (6)	-4 (5)	26 (5)	-10 (6)
C(22)	46 (6)	44 (6)	72 (7)	-2 (5)	2 (5)	-2 (5)
C(23)	57 (6)	51 (6)	56 (6)	-12 (5)	6 (6)	-20 (5)
N(24)	86 (7)	35 (7)	84 (6)	-2 (5)	14 (5)	-5 (6)
N(25)	99 (8)	45 (7)	105 (7)	-9 (6)	-13 (6)	-9 (7)
O(26)	87 (5)	65 (5)	138 (7)	0 (4)	-28 (5)	-4 (4)
C(27)	53 (6)	40 (7)	54 (6)	12 (5)	7 (4)	6 (6)

	U11	U22	U33	U23	U13	U12
C(28)	52 (6)	23 (6)	62 (6)	-19 (5)	11 (5)	-17 (6)
C(29)	49 (5)	37 (6)	51 (6)	-6 (5)	6 (4)	-1 (5)
C(30)	54 (6)	39 (7)	69 (6)	-10 (5)	13 (5)	-2 (5)
C(31)	47 (6)	30 (7)	64 (6)	-4 (5)	12 (5)	-3 (5)
C(32)	48 (6)	41 (7)	47 (6)	0 (5)	10 (5)	-3 (5)
C(33)	67 (7)	42 (8)	42 (5)	-16 (5)	8 (5)	-2 (6)
C(34)	43 (6)	48 (7)	43 (5)	-7 (5)	14 (5)	-9 (5)
N(35)	68 (7)	80 (8)	73 (6)	-5 (6)	6 (5)	-14 (6)
C(36)	68 (7)	61 (7)	57 (6)	-7 (6)	11 (6)	-21 (6)
C(37)	67 (7)	28 (7)	67 (6)	2 (5)	18 (6)	-6 (6)
C(38)	40 (6)	67 (8)	51 (6)	-3 (6)	-7 (5)	-7 (6)
C(39)	67 (7)	39 (7)	54 (6)	4 (6)	3 (5)	-3 (6)
O(40)	120 (7)	83 (6)	136 (7)	5 (5)	-35 (5)	-37 (5)
C(41)	79 (7)	64 (7)	76 (6)	1 (5)	4 (5)	-26 (6)
C(42)	53 (6)	52 (7)	78 (7)	5 (5)	9 (5)	10 (5)
C(43)	56 (6)	64 (8)	50 (6)	6 (5)	10 (5)	4 (6)
C(44)	63 (7)	51 (8)	58 (6)	10 (6)	15 (5)	9 (6)
C(45)	71 (8)	106 (9)	56 (7)	-12 (6)	7 (6)	-13 (6)
C(46)	131 (12)	118 (11)	78 (10)	-27 (8)	56 (9)	-33 (9)
C(47)	102 (8)	55 (7)	76 (7)	9 (6)	40 (6)	18 (6)
C(48)	56 (7)	121 (9)	82 (8)	17 (7)	-4 (6)	-5 (6)
C(49)	97 (9)	119 (11)	88 (9)	-33 (9)	53 (7)	-12 (9)
O(50)	192 (10)	65 (6)	254 (12)	24 (7)	-102 (9)	-6 (7)
C(51)	69 (7)	75 (8)	118 (9)	-19 (8)	38 (7)	16 (6)
C(52)	150 (11)	85 (9)	70 (8)	8 (7)	52 (8)	-9 (9)
C(53)	210 (12)	105 (11)	64 (9)	11 (8)	33 (12)	-51 (13)
C(54)	127 (12)	155 (13)	76 (11)	44 (9)	-36 (8)	1 (10)

VITA

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