SADTLER
STANDARD SPECTRA

SADTLER SPECTRA

NUCLEAR MAGNETIC RESONANCE SPECTRA

BIO-RAD

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SADTLER NUCLEAR MAGNETIC RESONANCE SPECTRA

Volumes 95-99

With this 1991 supplement of 2,000 spectra to the Sadtler Standard Nuclear Magnetic Resonance Spectra collection, the catalog now contains 54,000 proton NMR spectra.

INTRODUCTION

Protons give rise to signals of varying position, intensity and complexity. The actual position of the signal, the so-called chemical shift, is dependent on the immediate electronic environment of a proton and therefore is an index of its chemical nature. The intensity, which can be obtained by integration, is a measure of the number of protons of that kind which cause the signal. The resonances of protons are often complex with multiplicity arising from nuclear spin interaction between the proton yielding the signal and other protons nearby. It is known that coupling between protons which are two, three and four or more bonds apart (geminal, vicinal and long range coupling respectively) is peculiarly dependent on the geometric relation between the protons in question. Consequently, signal multiplicity characterizes the local molecular geometry of a proton.

In practice, the chemical shift and intensity parameters are readily obtained by inspection of the scanned and integrated spectra. However, the elucidation of spin multiplicity requires more time and in many cases can only be determined unambiguously by spin decoupling experiments or calculation.

ASSIGNMENTS

The center positions of signals in the spectrum (the chemical shifts δ), have been expressed in terms of a dimensionless field-independent scale on which the frequency of TMS is taken as zero.

$$\delta = \frac{\nu \text{ sample} - \nu \text{ TMS}}{80 \text{ MHz}} \times \text{million}$$

ν = resonance frequency of protons in the substance

The chemical shift δ is then cited in parts per million (p.p.m.). Chemical shifts are considered to be accurate to +/- 3 Hz or +/- 0.05 p.p.m.

Whenever possible, the chemical shift assignments have been made by first order analysis. In the case of non-first order multiplets, the shift was taken as the estimated weighted center. Alternative assignments have been noted; however, if a chemical shift could not be attributed with reasonable certainity due to overlapping, then no precise assignment was attempted. In several cases, protons have been assigned within a range or about a certain value of chemical shift.

Low intensity multiplets have been enlarged and separately positioned on the chart.

INSTRUMENTATION & TECHNIQUE

All spectra have been scanned in the Sadtler Research Laboratories at 80 MHz on a Varian CFT-20 Fourier Transform NMR spectrometer.

Samples are dissolved in deuterochloroform as the solvent of choice together with added tetramethylsilane (TMS) as an internal standard. Solute concentrations are roughly 5% to 20%. 3-trimethylsilyltetradeuteriopropionate, sodium salt (TSP) is used as an internal standard when deuterium oxide (D2O) is used as the solvent.

For those samples which are found to be insoluble in deuterochloroform, other solvents were used; such as dimethyl sulfoxide, polysol-D (DMSO-D6/CDCl3) and deuterium oxide.

In certain cases, a second spectrum may have been scanned after the addition of D2O or trifluoroacetic acid to the sample solution.

As in the previous volumes of the NMR Standard Spectra collection, coupling constants have been measured for some of the less usual spin-spin coupling patterns and are printed on the spectra page at the end of the assignments section.

Your comments and suggestions, as well as samples whose spectra require replacement, are always welcome. Samples of new 98% pure compounds (accompanied by structure and/or name, physical data, solubility, and journal reference) are continually being sought and it is only because of the generous contributions of those whose names appear as the "source" that we can offer these spectra to scientists. Our sincere thanks is expressed to these donors.

N-[p-(BENZYLOXY)BENZYLIDENE]-p-TOLUIDINE **52001 M**

$C_{21}H_{19}NO$ **MOL. WT.** 301.39 **PRISM NO.** 79001

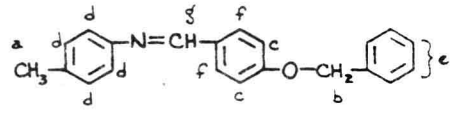
SOLVENT $CDCl_3$

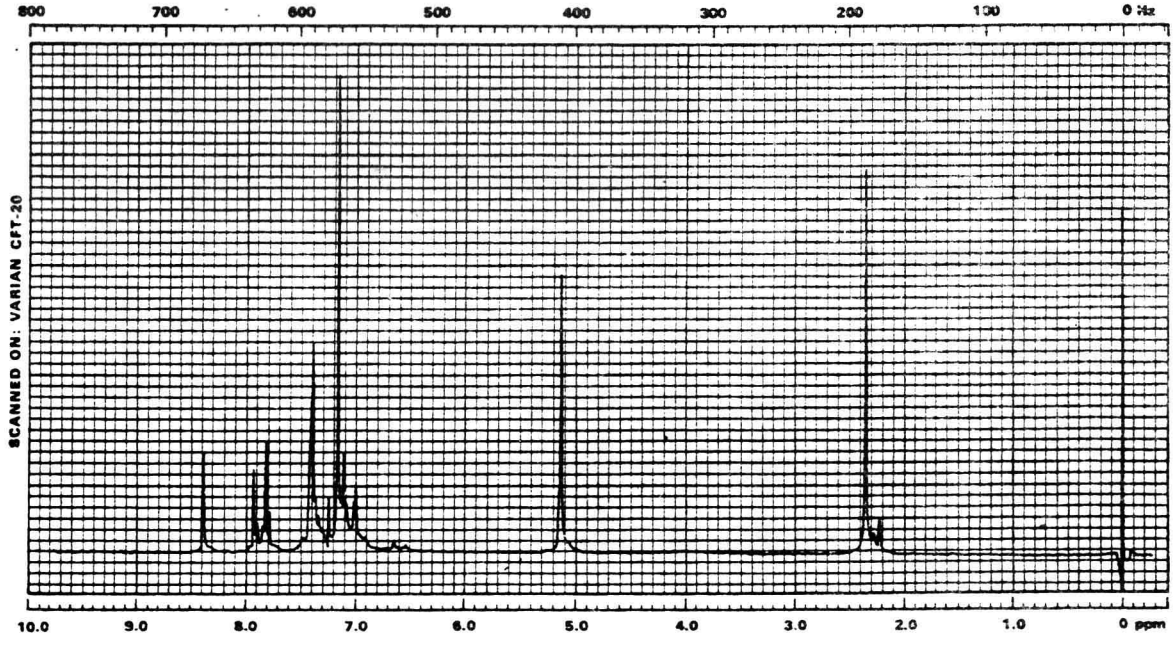
REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	2.37	h	2.22, 6.60 imps	o		v	
b	5.12	i		p		w	
c	7.06	j		q		x	
d	ca7.18	k		r		y	
e	ca7.40	l		s		z	
f	7.87	m		t		1	
g	8.39	n		u		2	





52002 M N-[p-(BENZYLOXY)BENZYLIDENE]-3,4-XYLIDINE

$C_{22}H_{21}NO$ **MOL. WT.** 315.42

PRISM NO. 79002

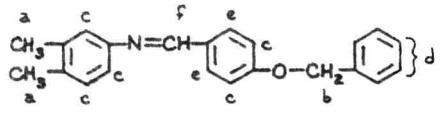
SOLVENT $CDCl_3$

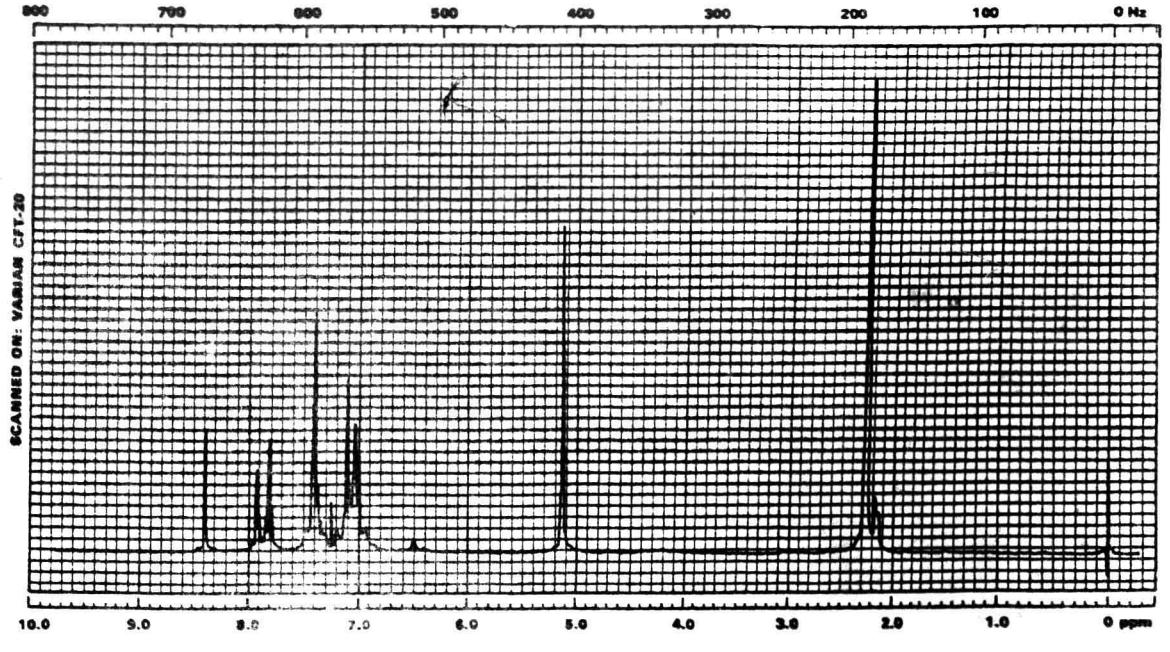
REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	2.29	h	7.26 $CHCl_3$	o		v	
b	5.14	i		p		w	
c	6.80-7.25	j		q		x	
d	ca7.40	k		r		y	
e	7.86	l		s		z	
f	8.39	m		t		1	
g	2.18, 6.50 imps	n		u		2	





α-CHLORO-o-TOLUNITRILE

52003 M

C_8H_6ClN **MOL. WT.** 151.60

PRISM NO. 79003

SOLVENT $CDCl_3$

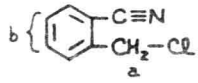
REFERENCE TMS

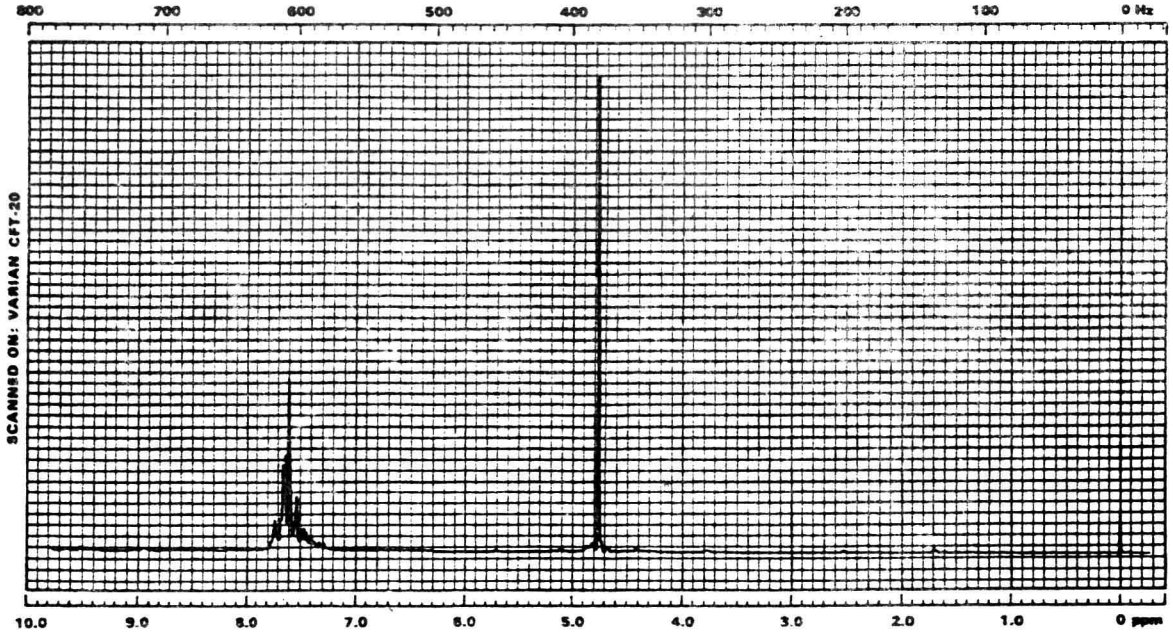
SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

BIO-RAD Sadtler Division

ASSIGNMENTS

a	4.79	h		o		v	
b	7.25-7.80	i		p		w	
c		j		q		x	
d		k		r		y	
e		l		s		z	
f		m		t		1	
g		n		u		2	





52004 M o-(HEXADECYLSULFONYL)ANILINE

$C_{22}H_{39}NO_2S$ **MOL. WT.** 381.63

PRISM NO. 79004

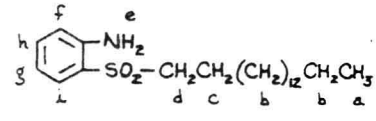
SOLVENT $CDCl_3$

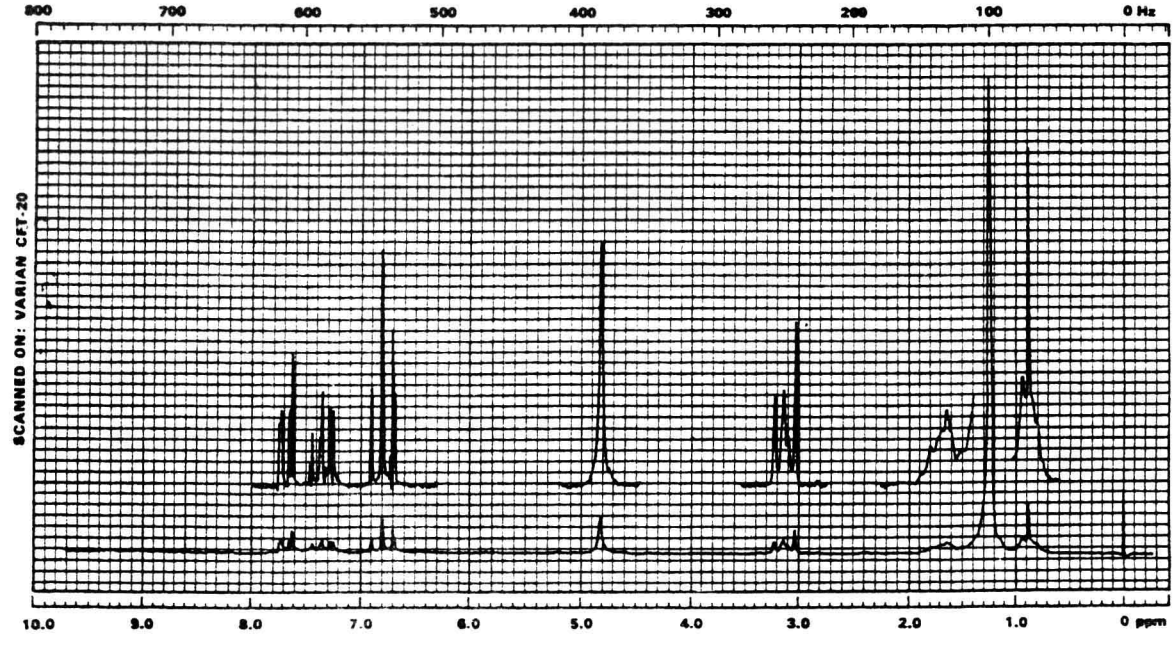
REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	0.90	h	7.35	o		v	
b	1.05-1.55	i	7.68	p		w	
c	1.68	j		q		x	
d	3.13	k		r		y	
e	4.81	l		s		z	
f	6.76	m		t		1	
g	6.80	n		u		2	





4-ETHOXYMETANILYL FLUORIDE

52005 M

$C_8H_{10}FNO_3S$ **MOL. WT.** 219.24

PRISM NO. 79005

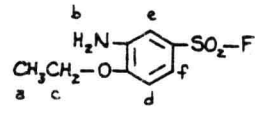
SOLVENT $CDCl_3$

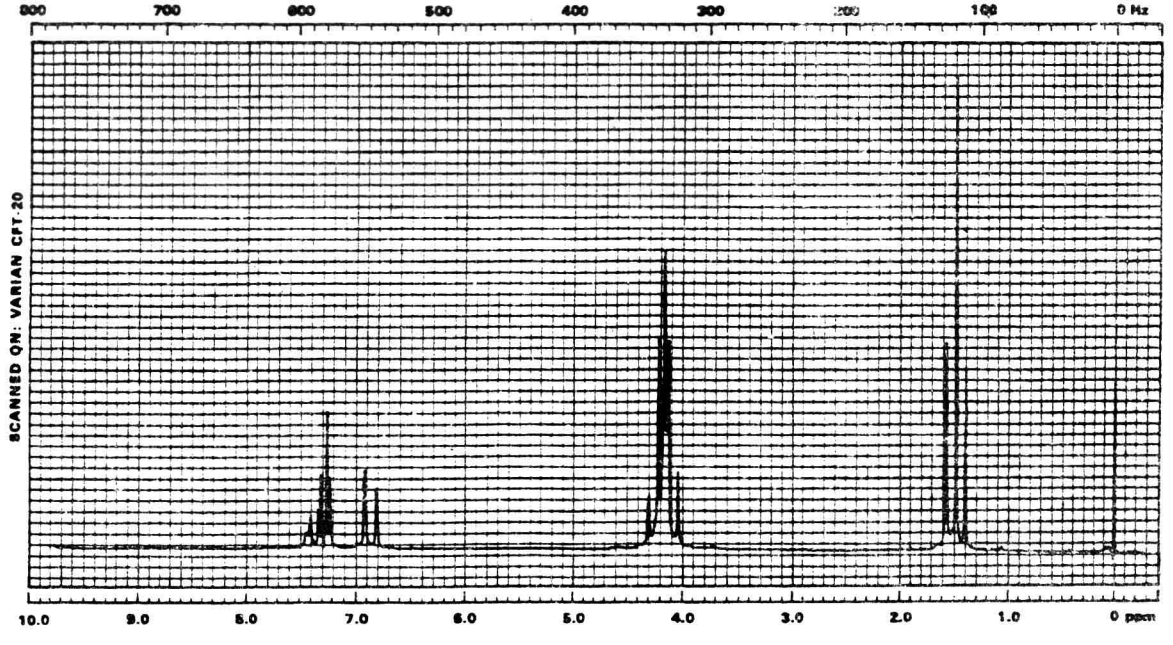
REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	1.50	h		o		v	
b	4.18	i		p		w	
c	4.19	j		q		x	
d	6.86	k		r		y	
e	7.28	l		s		z	
f	7.37	m		t		1	
g		n		u		2	





52006 M 2,6-DIAMINO-3-(PHENYLAZO)PYRIDINE, 1,2-ETHANEDISULFONATE (1:1)

$C_{11}H_{11}N_5 \cdot C_2H_6O_6S_2$ **MOL. WT.** 403.44

PRISM NO. 79006

SOLVENT Polysol

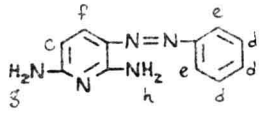
REFERENCE TMS

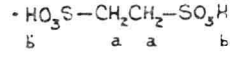
SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

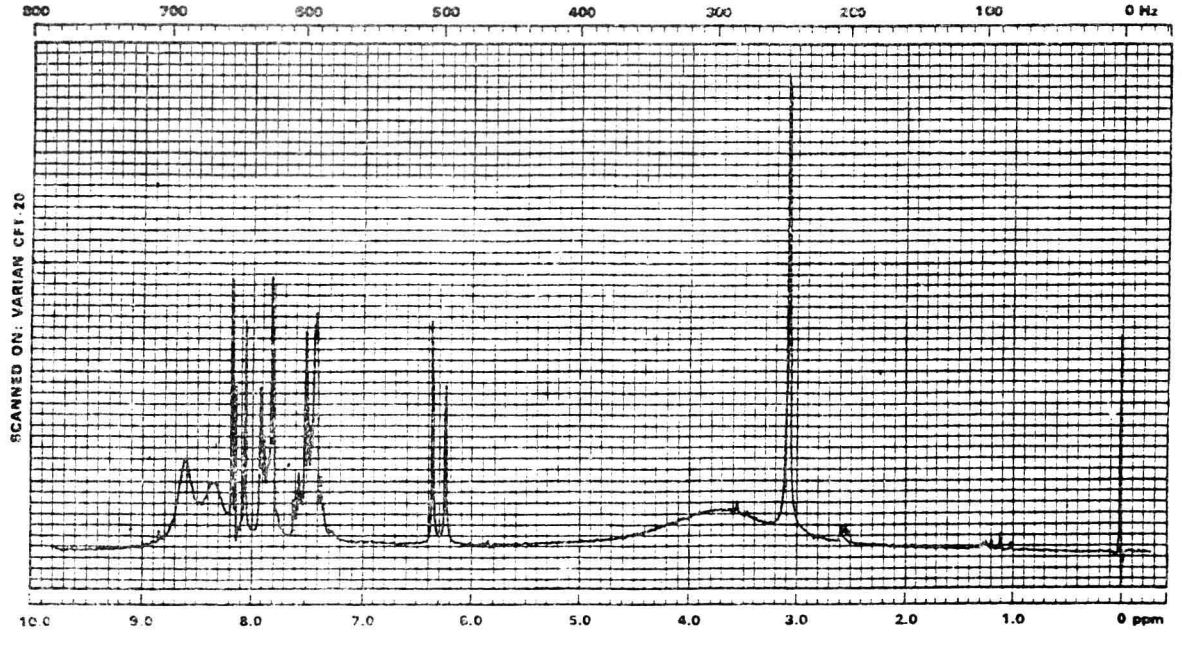
ASSIGNMENTS

a	3.10	h	8.60/g	o		v	
b	3.00-5.50*	i	1.10, 1.28 imps	p		w	
c	6.31	j	2.55 DMSO-d_5	q		x	
d	7.30-7.65	k	8.19 $CHCl_3$	r		y	
e	7.86	l		s		z	
f	8.11	m		t		1	
g	8.35/h	n		u		2	

*Plus H_2O







o-(CHLOROMETHYL)ANISOLE **52007 M**

C_8H_9ClO **MOL. WT.** 156.61 **PRISM NO.** 79007

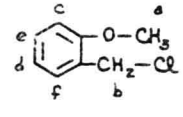
SOLVENT $CDCl_3$

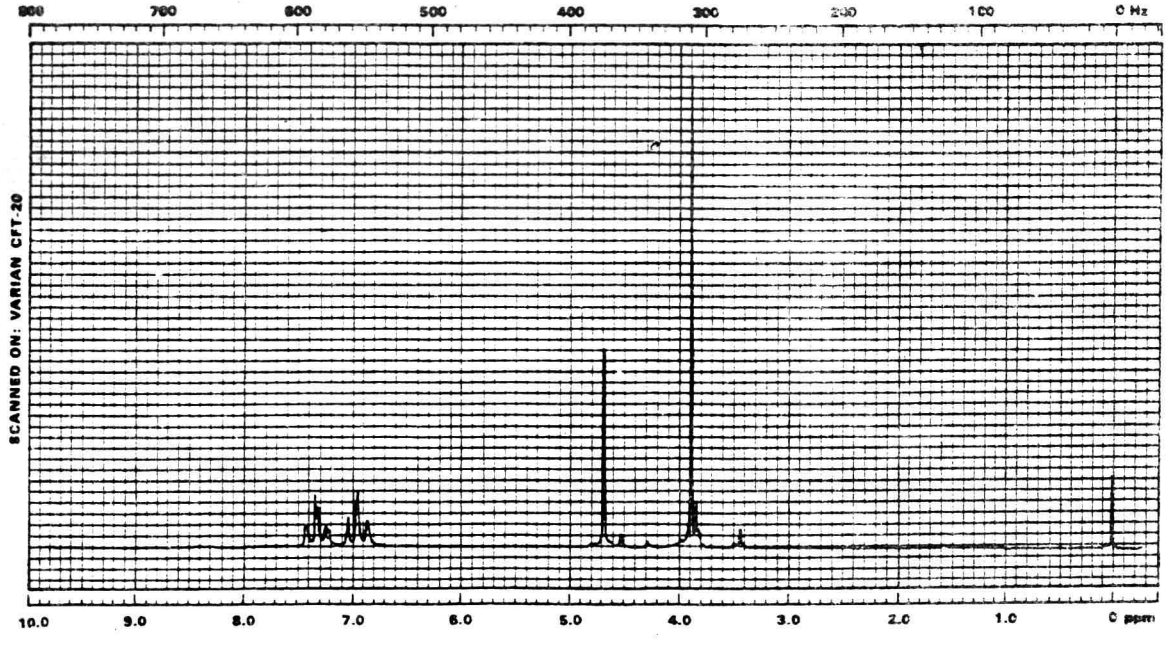
SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

REFERENCE TMS

ASSIGNMENTS

a	3.90	h	4.51 imp	o		v	
b	4.69	i		p		w	
c	6.91	j		q		x	
d	6.97	k		r		y	
e	7.33	l		s		z	
f	7.37	m		t		1	
g	3.42, 3.85 imps	n		u		2	





52008 M p-UREIDOBENZOIC ACID

$C_8H_8N_2O_3$ MOL. WT. 180.16

PRISM NO. 79008

SOLVENT Polysol

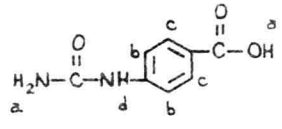
REFERENCE TMS

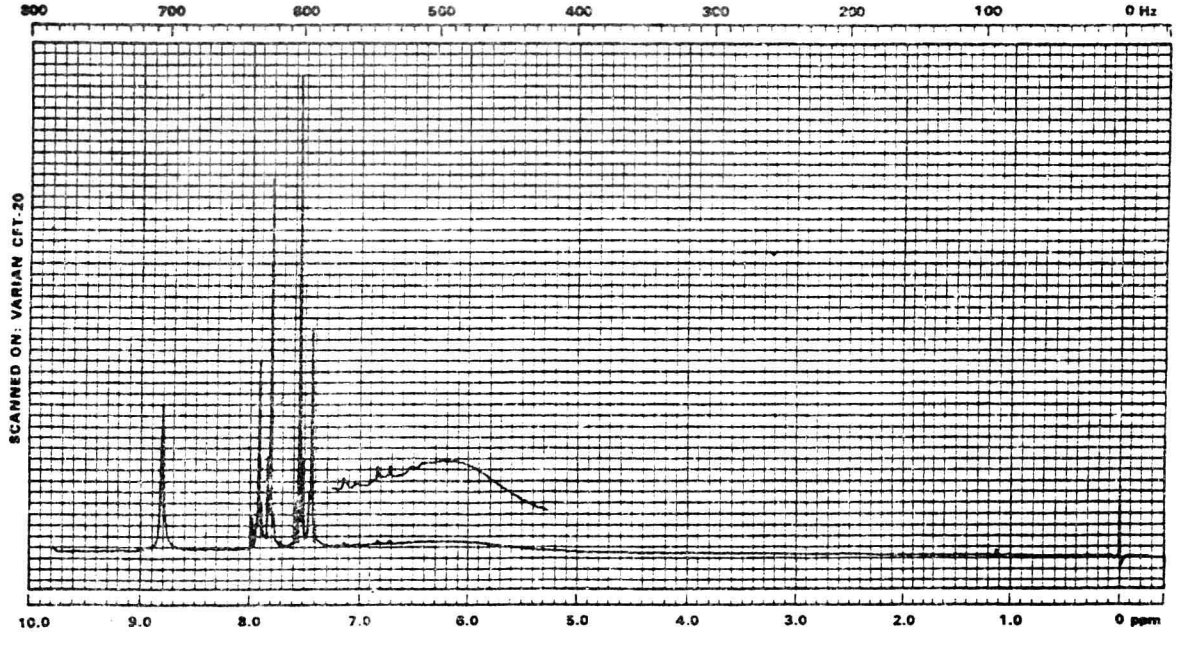
SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	5.00-7.30*	h		o		v	
b	7.49	i		p		w	
c	7.84	j		q		x	
d	8.80	k		r		y	
e	6.70-7.20 imps	l		s		z	
f		m		t		1	
g		n		u		2	

*Plus H_2O





m-ACETYLBENZENESULFONIC ACID, SODIUM SALT

52009 M

$C_8H_7NaO_4S$ MOL. WT. 222.20

PRISM NO. 79009

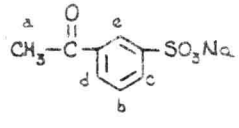
SOLVENT Polysol

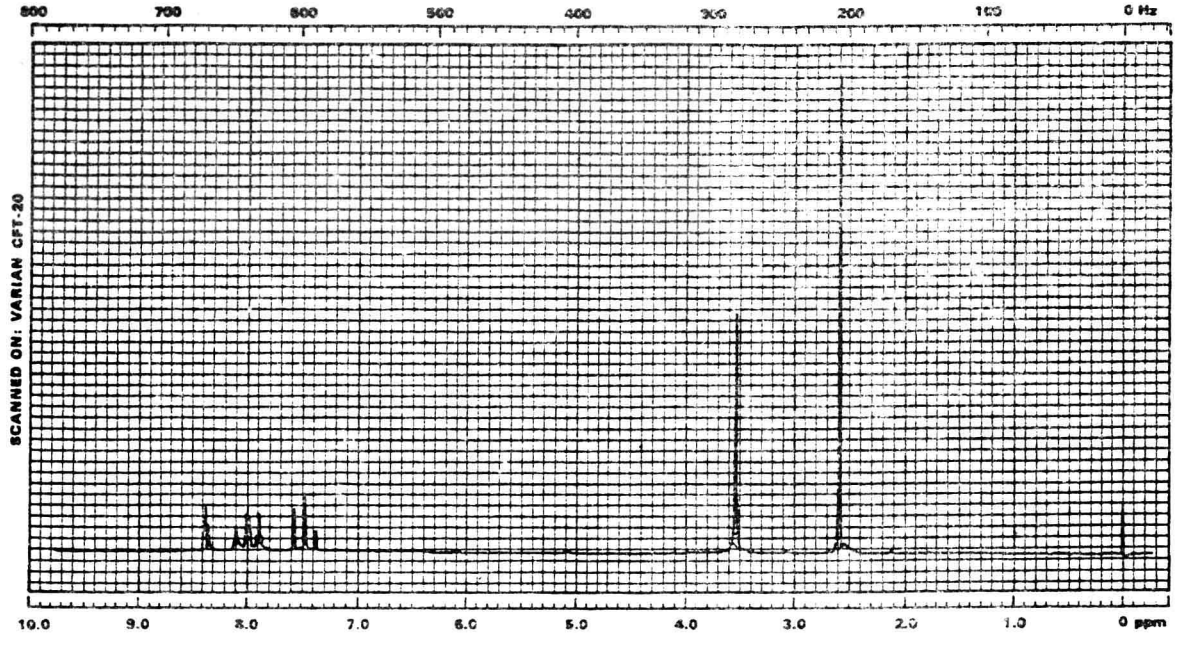
REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	2.60	h		o		v	
b	7.49	i		p		w	
c	7.95	j		q		x	
d	8.05	k		r		y	
e	8.38	l		s		z	
f	3.53 H_2O	m		t		1	
g		n		u		2	





52010 M 2-METHYL-5-(TRIFLUOROMETHYL)BENZOTHIAZOLE

$C_9H_6F_3NS$ **MOL. WT.** 217.21

PRISM NO. 79010

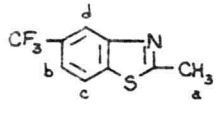
SOLVENT $CDCl_3$

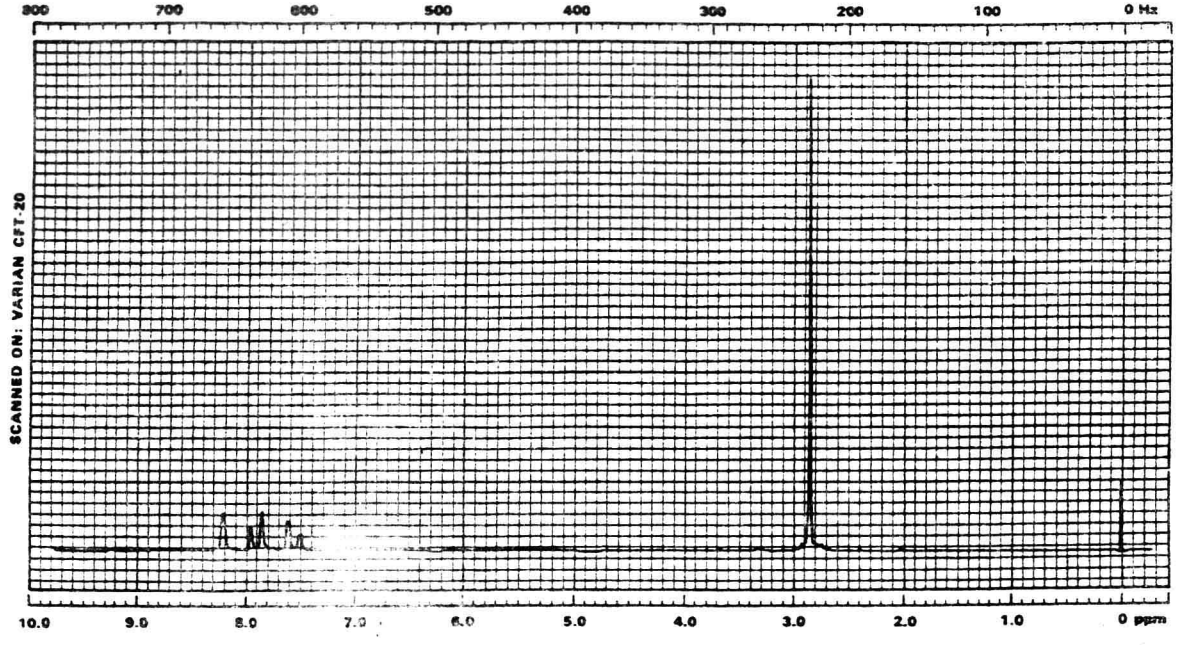
REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	2.88	h		o		v	
b	7.56	i		p		w	
c	7.90	j		q		x	
d	8.21	k		r		y	
e		l		s		z	
f		m		t		1	
g		n		u		2	





3-AMINO-4-(HEXADECYLTHIO)BENZOIC ACID, METHYL ESTER

52011 M

$C_{24}H_{41}NO_2S$ MOL. WT. 407.66

PRISM NO. 79011

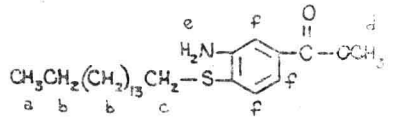
SOLVENT $CDCl_3$

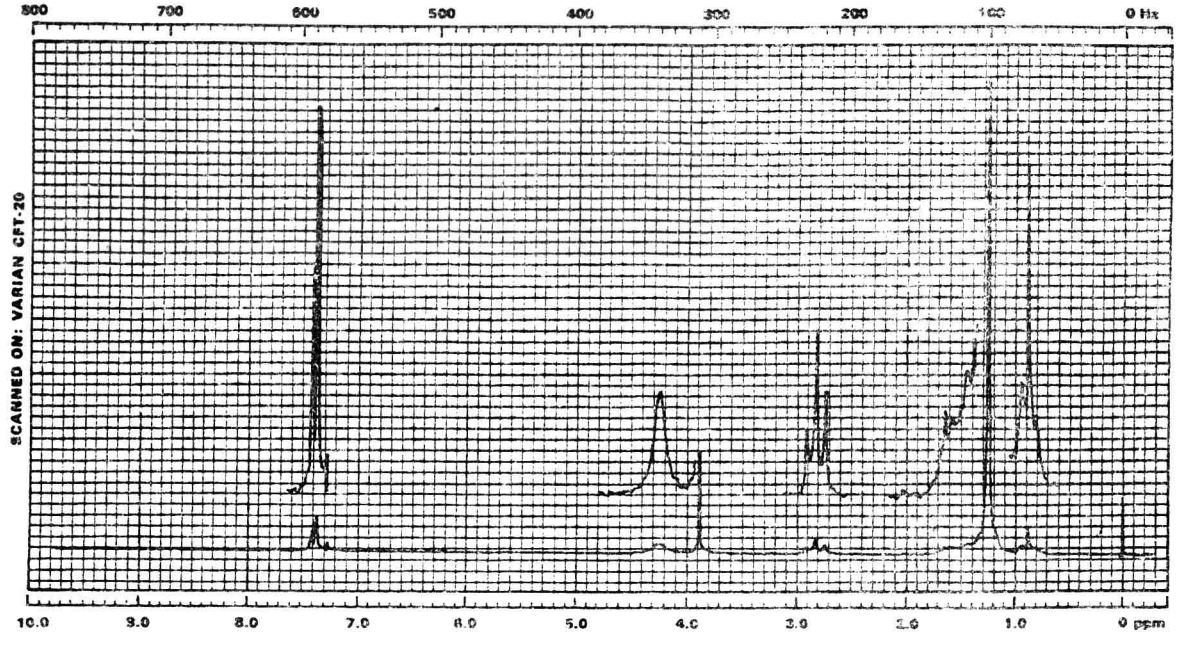
REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	0.90	h		o		v	
b	1.05-1.90	i		p		w	
c	2.81	j		q		x	
d	3.89	k		r		y	
e	4.23	l		s		z	
f	ca7.39	m		t		1	
g	7.28 $CHCl_3$	n		u		2	





52012 M 1-METHYL-3-(1-NAPHTHYL)-1-PHENYLUREA

$C_{18}H_{16}N_2O$ **MOL. WT.** 276.34 **PRISM NO.** 79012

SOLVENT $CDCl_3$

REFERENCE TMS

SOURCE OF SAMPLE
Aldrich Chemical Company, Inc.,
Milwaukee, Wisconsin

ASSIGNMENTS

a	3.40	h		o		v	
b	6.67	i		p		w	
c	7.20-7.65	j		q		x	
d	7.76	k		r		y	
e	7.97	l		s		z	
f		m		t		1	
g		n		u		2