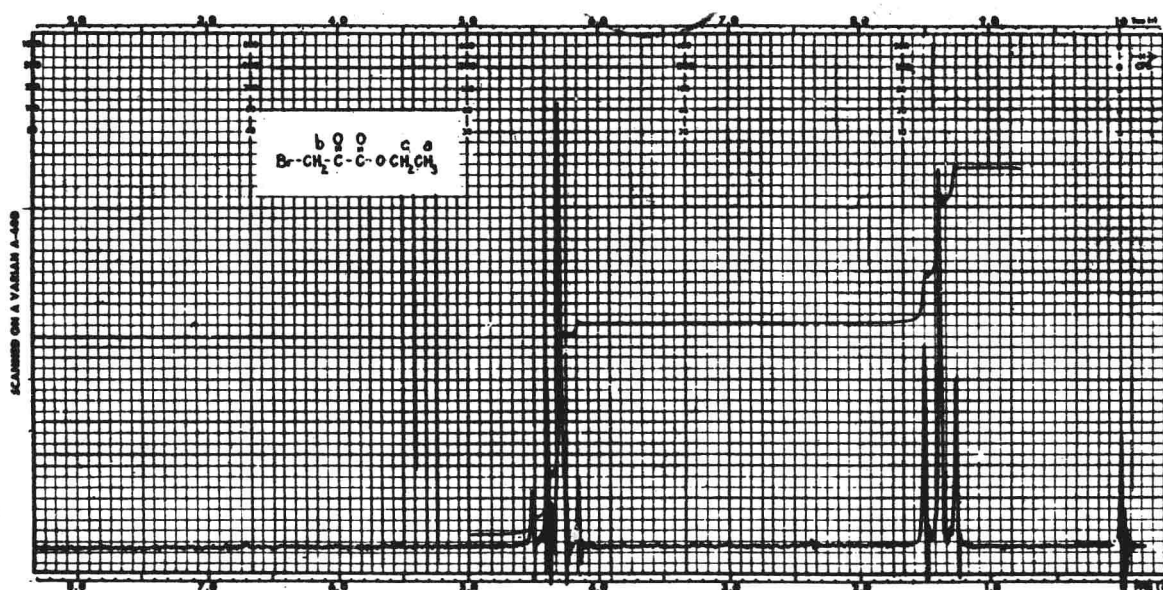


SADTLER RESEARCH LABORATORIES, INC.

NUCLEAR MAGNETIC RESONANCE SPECTRA



CREATIVE CHEMISTS SINCE 1874

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PROTON MAGNETIC RESONANCE SPECTRA

Volumes 43 - 46

With this 1978 supplement of 2,000 spectra to the Sadtler Standard Nuclear Magnetic Resonance Spectra collection, the catalog now contains 28,000 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, multiplicity arises 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.

$$\delta = \frac{\nu_{\text{sample}} - \nu_{\text{TMS}}}{60 \text{ mc}} \quad \times \text{ million}$$

$$\nu = \text{resonance frequency of protons in the substance}$$

The chemical shift δ is then cited in parts per million (p.p.m.). Chemical shifts are considered as being 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 certainty 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 deuteriochloroform as the solvent of choice together with added tetramethylsilane (TMS) as an internal standard. Solute concentrations are roughly 5% to 20%.

For those samples which are found to be insoluble in deuteriochloroform, other solvents were used; such as carbon tetrachloride, dimethyl sulfoxide, polysol-D and heavy water.

In certain cases special techniques have been used to simplify the spectra of certain compounds. Several compounds in this group of spectra contain functional groups which can co-ordinate with the transition metal shift reagents. To illustrate the dramatic effect these reagents have on the chemical shifts of proton spectra, certain samples were scanned before and after the addition of the reagent EU-FOD-d₂₇. The "before" and "after" spectra are printed on the same page for comparison purposes. Examples of such spectra are numbers 21569 and 21570.

In other cases, a second spectrum may have been scanned after the addition of D₂O or trifluoroacetic acid.

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 are always welcome as well as samples whose spectra require replacement. 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 always expressed to these donors.

26001 M

N-(4-CHLORO-o-TOLYL)-3,4,5,6-TETRAPHENYLPHthalimide

 $C_{39}H_{28}ClNO_2$

Mol. Wt. 576.10

PRISM NO.

53001

SOLVENT

 $CDCl_3$

REFERENCE

TMS

SWEEP OFFSET

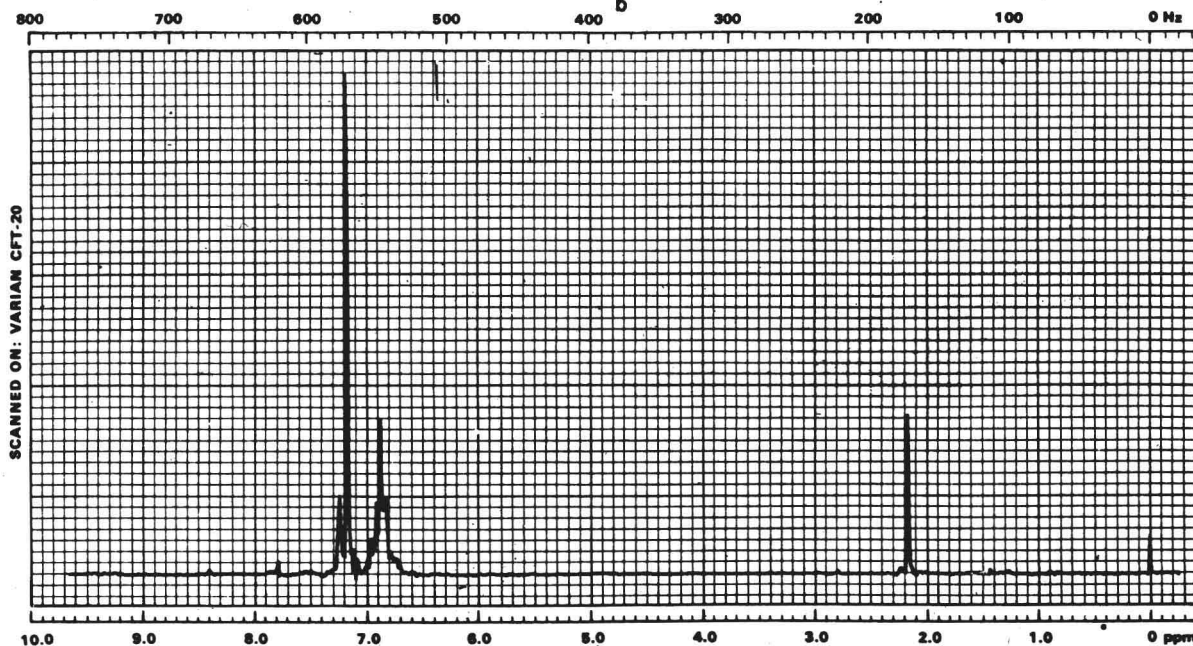
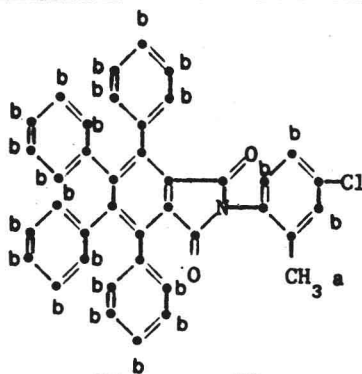
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Source of Sample:
M. Khalifa,
Cairo University,
Cairo, Egypt

NMR ©1978 Sadtler Research Laboratories, Inc., subsidiary of Block Engineering, Inc.

ASSIGNMENTS

a	2.18	f		k		p	
b	6.65-7.35	g		l		q	
c		h		m		r	
d		i		n		s	
e		j		o		t	



26002 M

3-[4-(p-METHOXYPHENYL)-2-THIAZOLYL]-2-METHYL-4(3H)-QUINAZOLINONE

$C_{19}H_{15}N_3O_2S$

Mol. Wt. 349.41

PRISM NO.

53004

M.P. 155°C

SOLVENT

$CDCl_3$

Source of Sample:

REFERENCE

TMS

M. Badr,
Assiut University,
Assiut, Egypt

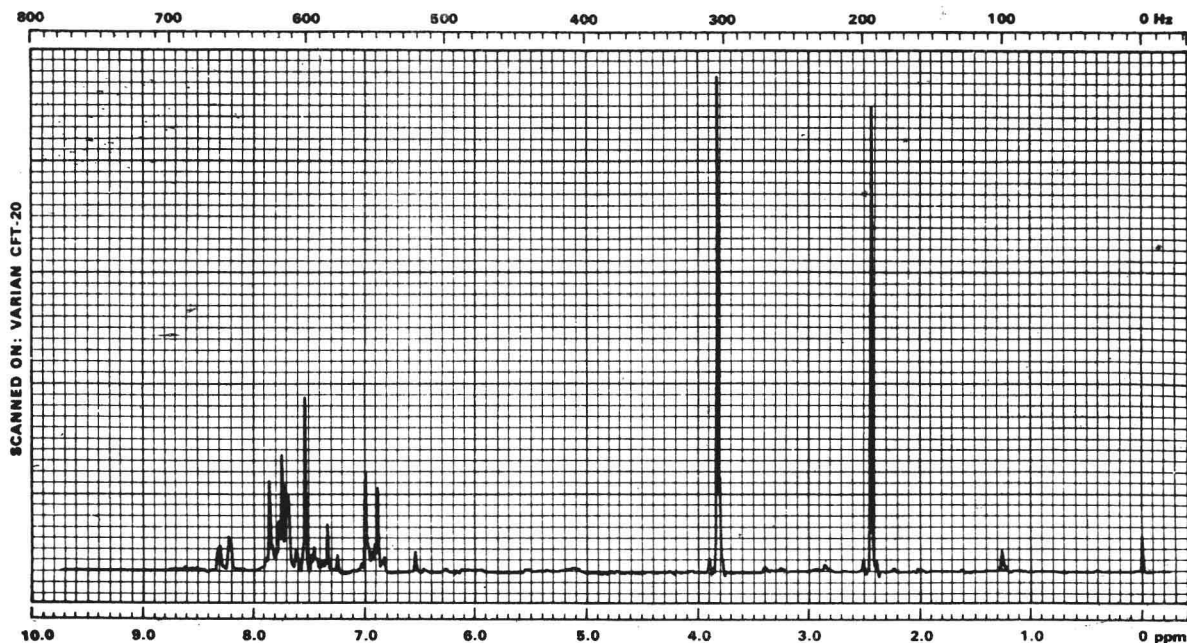
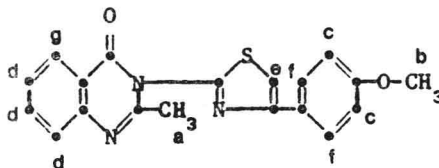
SWEEP OFFSET

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ASSIGNMENTS

a	2.43	f	7.80	k		p	
b	3.83	g	8.25	l		q	
c	6.95	h		m		r	
d	7.20-7.80	i		n		s	
e	7.53	j		o		t	



26003 M

2-(α,β -DIBROMO-p-METHOXYPHENETHYL)-3-PHENYL-4(3H)-QUINAZOLINONE $C_{23}H_{18}Br_2N_2O_2$

Mol. Wt. 514.23

PRISM NO.

53006

M.P. 166°C

SOLVENT

 $CDCl_3$

Source of Sample:
M. Badr,
Assiut University,
Assiut, Egypt

REFERENCE

TMS

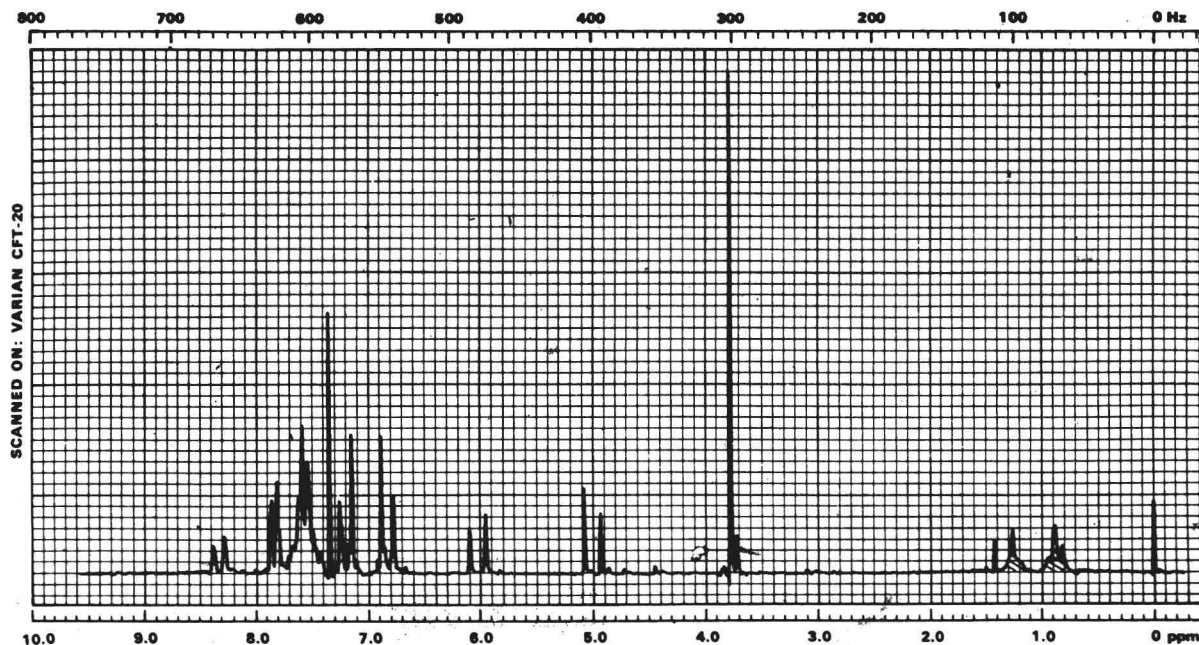
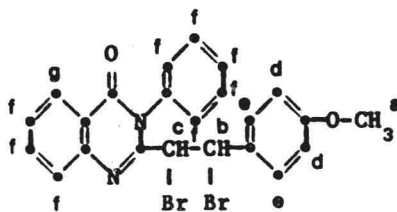
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ASSIGNMENTS

a	3.80	f	7.40-7.95	k		p	
b	5.01	g	8.33	l		q	
c	6.03	h	7.37 $CHCl_3$	m		r	
d	6.84	i	0.90, 1.27 imp.	n		s	
e	7.19	j	1.42 imp.	o		t	



26004 M

2-(α,β -DIAMINO-p-METHOXYPHENETHYL)-3-PHENYL-4(3H)-QUINAZOLINONE

$C_{23}H_{22}N_4O_2$

Mol. Wt. 386.46

PRISM NO.

53007

M.P. 172°C

SOLVENT

$CDCl_3$

Source of Sample:

REFERENCE

TMS

M. Badr,
Assiut University,
Assiut, Egypt

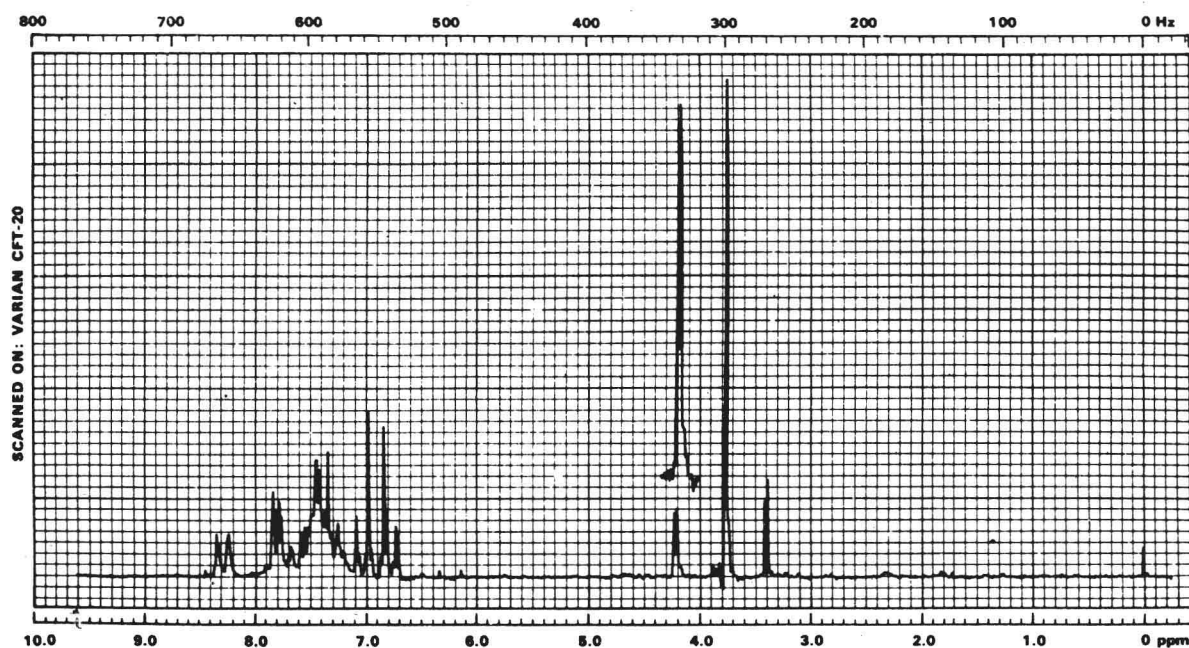
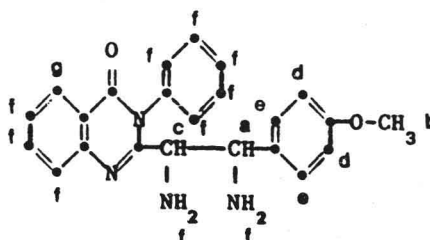
SWEEP OFFSET

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ASSIGNMENTS

a	3.40	f	7.10-8.00	k		p	
b	3.76	g	8.28	l		q	
c	4.19	h		m		r	
d	6.78	i		n		s	
e	7.04	j		o		t	



26005 M

2-MERCAPTO-4'-NITROACETANILIDE

 $C_8H_8N_2O_3S$

Mol. Wt. 212.23

PRISM NO.

53017

M.P. 172°C

SOLVENT

Polyso1

Source of Sample:

REFERENCE

TMS

C. Bhandari,

University of Rajasthan,

SWEEP OFFSET

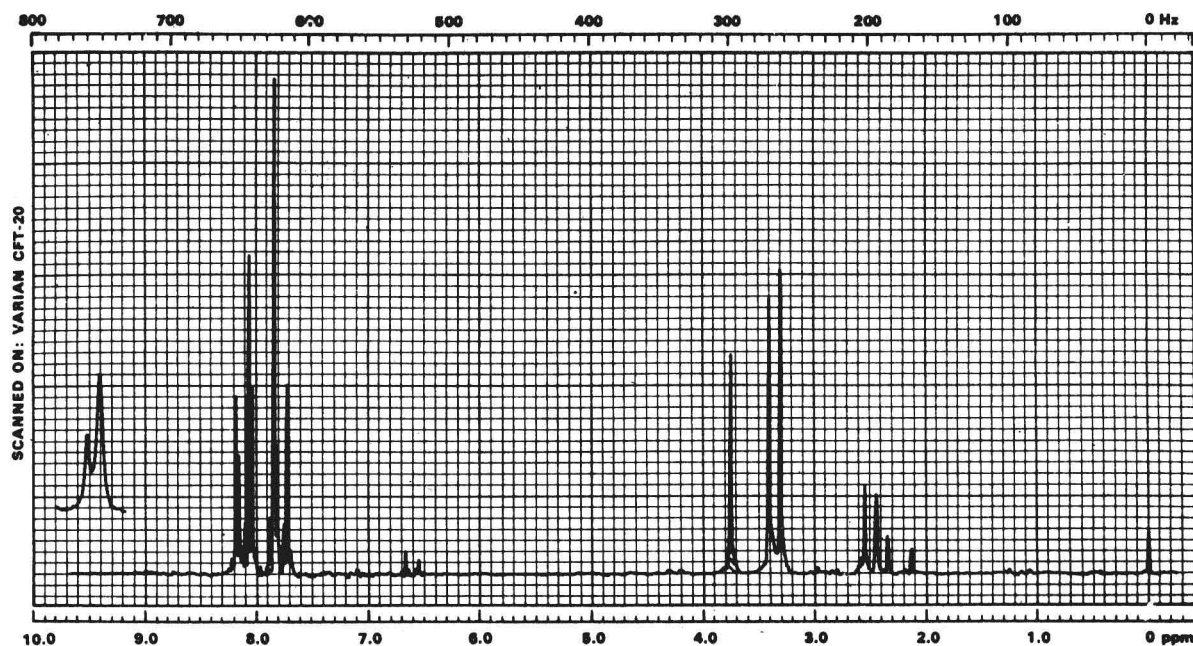
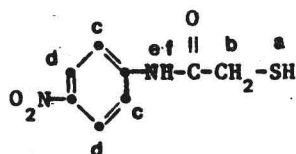
1 ppm

Jaipur, India

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ASSIGNMENTS

a	2.44	f	10.52	k		p	
b	3.35	g	2.13, 6.66 imps.	l		q	
c	7.79	h	3.74 H ₂ O	m		r	
d	8.12	i		n		s	
e	10.40	j		o		t	



26006 M

2-MERCAPTOPROPIONANILIDE

$C_9H_{11}NOS$

Mol. Wt. 181.26

PRISM NO.

53018

M.P. 88°C

SOLVENT

$CDCl_3$

Source of Sample:

REFERENCE

TMS

C. Bhandari,
University of Rajasthan,
Jaipur, India

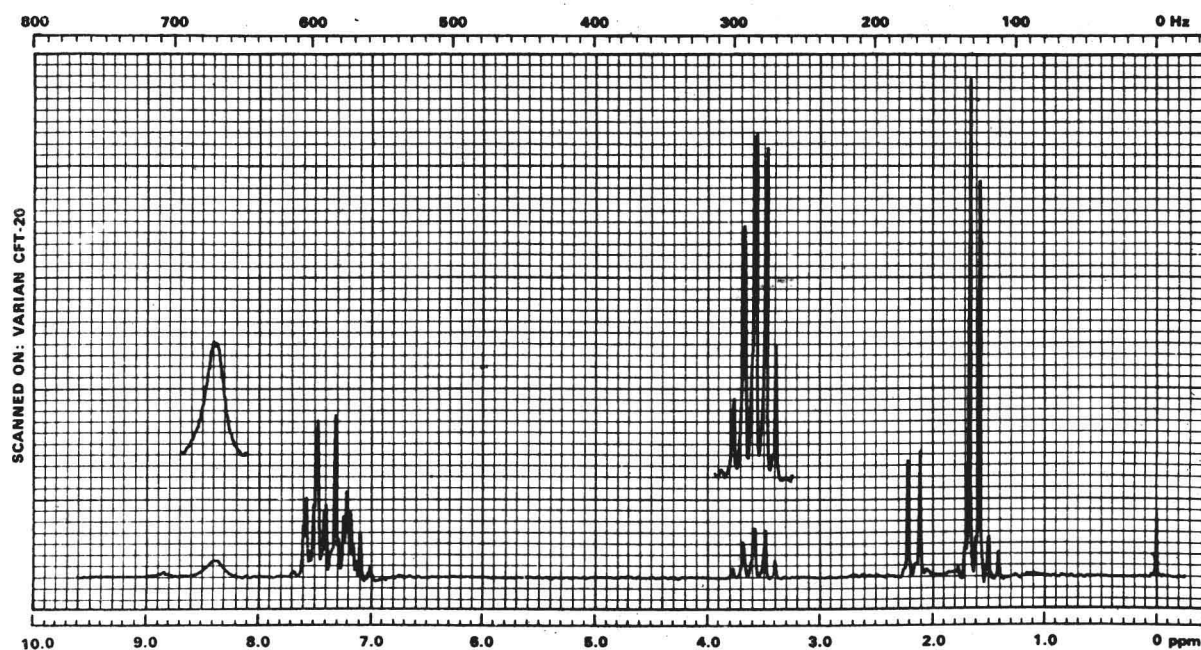
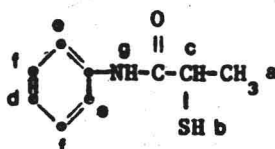
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ASSIGNMENTS

a	1.62	f	7.48	k		p	
b	2.17	g	8.40	l		q	
c	3.58	h	1.40, 1.50 imps.	m		r	
d	7.12	i		n		s	
e	7.27	j		o		t	



26007 M

CHLOROMETHYL 10-(PHENOXYACETYL) PHENOTHIAZIN-2-YL KETONE

 $C_{22}H_{16}ClNO_3S$

Mol. Wt. 409.89

PRISM NO.

53025

M.P. 139°C

SOLVENT

 $CDCl_3$

Source of Sample:

REFERENCE

TMS

H. Abu-Shady,
Cairo University,
Cairo, Egypt

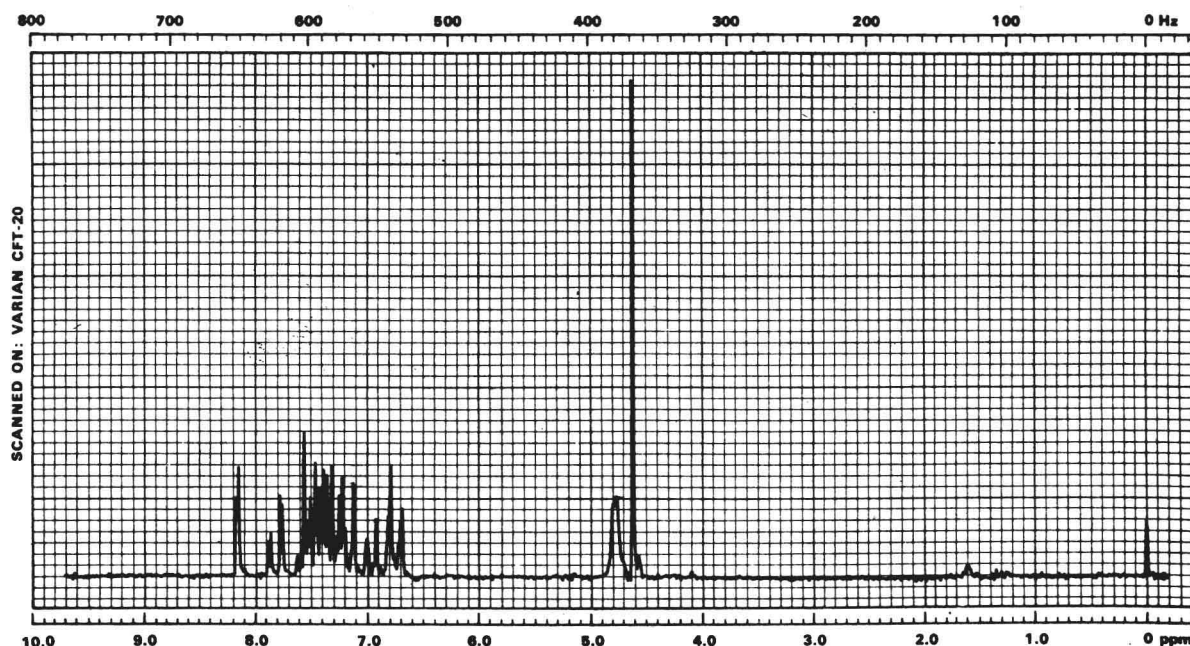
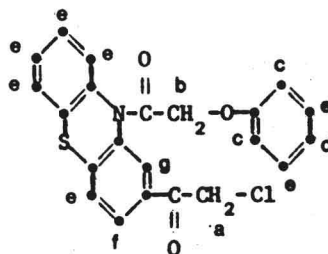
SWEEP OFFSET

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ASSIGNMENTS

a	4.62	f	7.83	k		p	
b	ca 4.78	g	8.17	l		q	
c	6.76	h		m		r	
d	6.91	i		n		s	
e	7.05-7.70	j		o		t	



26008 M

5-(BENZYLOXY)-N-(2-HYDROXYETHYL) INDOLE-2-CARBOXAMIDE

$C_{18}H_{18}N_2O_3$

Mol. Wt. 310.36

PRISM NO.

53027

M.P. 184-186°C

SOLVENT

Polysol

Source of Sample:

P. Nantka-Namirski & Z. Ozdowska,

Polish Academy of Sciences,

Warsaw, Poland

REFERENCE

TMS

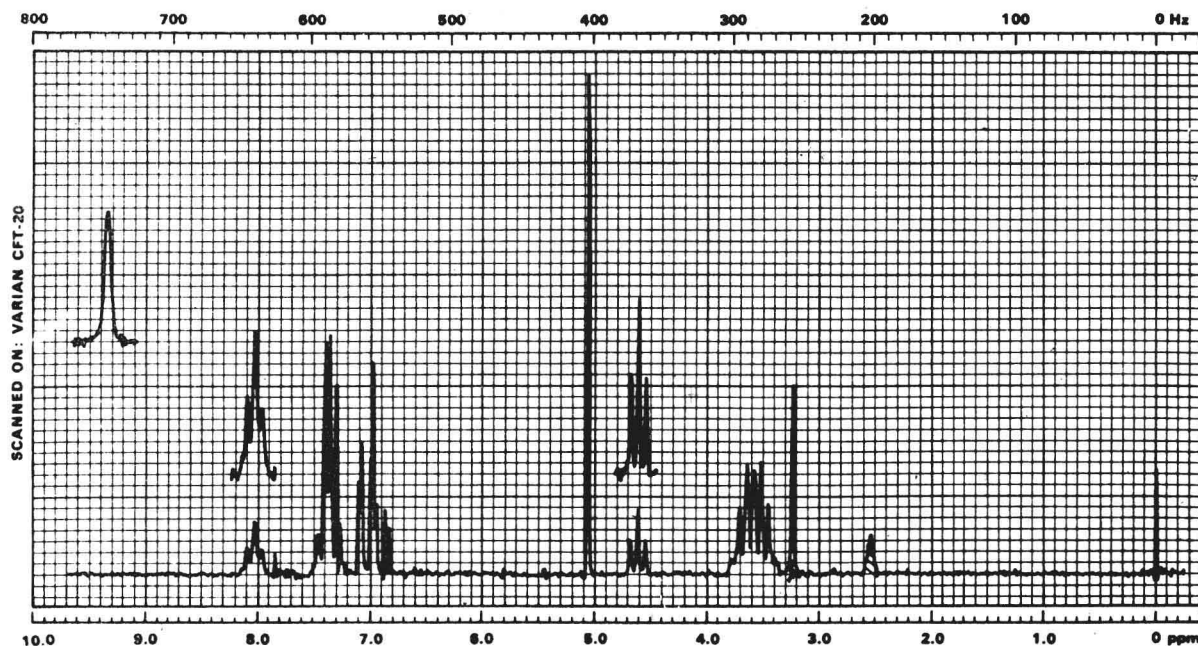
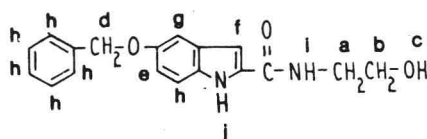
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1.75 ppm

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ASSIGNMENTS

a	3.52	f	6.98	k	2.54 DMSO-d ₅	p	
b	3.65	g	7.09	l	3.23 H ₂ O	q	
c	4.61	h	7.15-7.50	m		r	
d	5.07	i	8.03	n		s	
e	6.92	j	11.10	o		t	



26009M

1-BENZYL-5-(BENZYLOXY)INDOLE-2-CARBOXYLIC ACID, ETHYL ESTER

 $C_{25}H_{23}NO_3$

Mol. Wt. 385.47

PRISM NO.

53028

M.P. 153°C

SOLVENT

 $CDCl_3$

Source of Sample:

P. Nantka-Namirski & Z. Ozdowska,
Polish Academy of Sciences,
Warsaw, Poland

REFERENCE

TMS

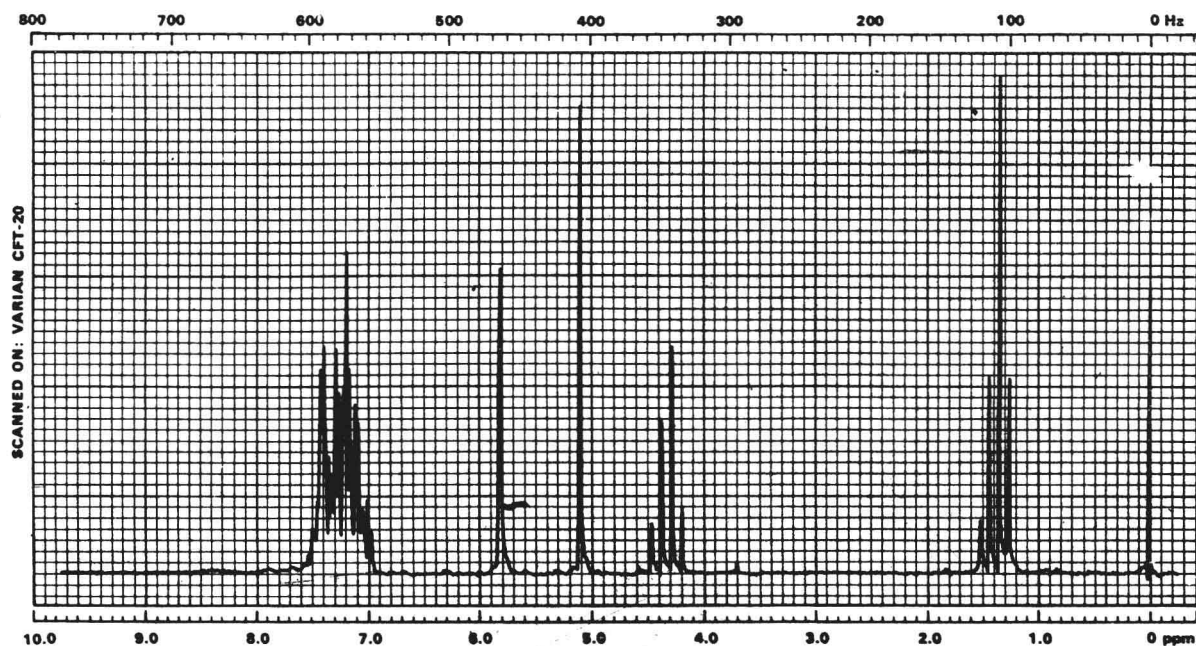
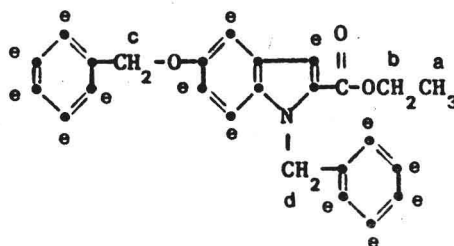
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ASSIGNMENTS

a	1.36	f		k		p	
b	4.34	g		l		q	
c	5.11	h		m		r	
d	5.81	i		n		s	
e	6.90-7.60	j		o		t	



26010 M

5-(BENZYLOXY)-2-CARBOXYINDOLE-1-ACETIC ACID, DIETHYL ESTER

$C_{22}H_{23}NO_5$

Mol. Wt. 381.43

PRISM NO.

53030

M.P. 120°C

SOLVENT

$CDCl_3$

Source of Sample:

P. Nantka-Namirski & Z. Ozdowska,
Polish Academy of Sciences,
Warsaw, Poland

REFERENCE

TMS

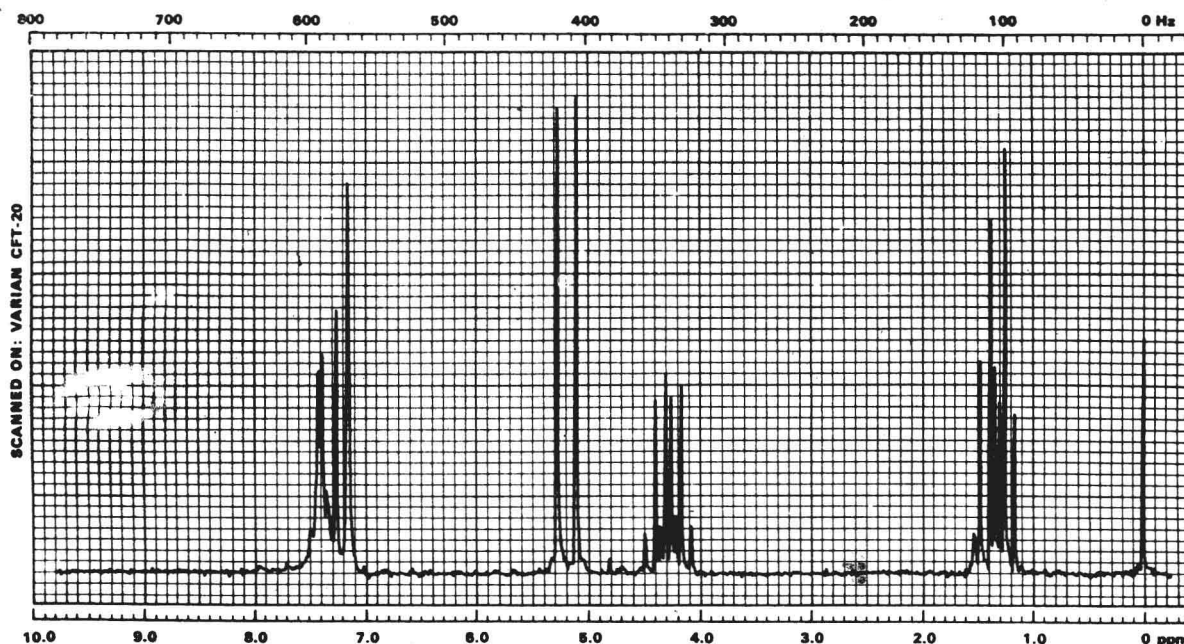
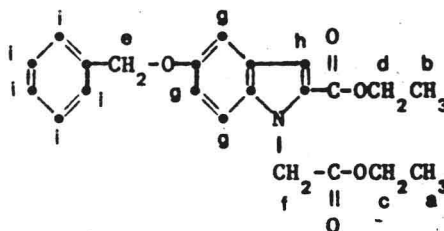
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ASSIGNMENTS

a	1.25	f	5.58	k		p	
b	1.39	g	7.16	l		q	
c	4.23	h	7.27	m		r	
d	4.34	i	7.20-7.60	n		s	
e	5.11	j		o		t	



26011 M

5-(p-TOLUIDINO)-1-p-TOLYL-1H-1,2,3-TRIAZOLE

 $C_{16}H_{16}N_4$

Mol. Wt. 264.33

PRISM NO.

53032

M.P. 166-166.5°C

SOLVENT

Polysol

Source of Sample:

REFERENCE

TMS

J. Svetlik,
Slovak Technical University,
Bratislava, Czechoslovakia

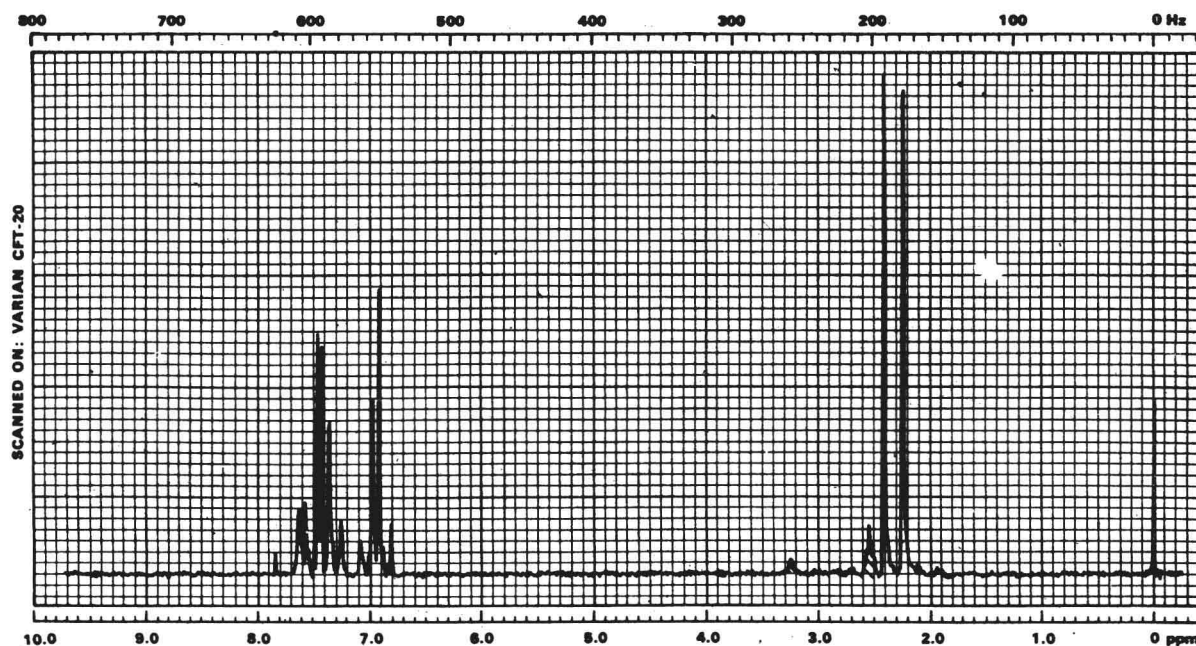
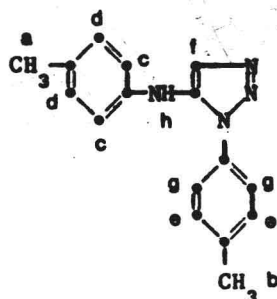
SWEEP OFFSET

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ASSIGNMENTS

a	2.23	f	7.42	k		p	
b	2.40	g	7.50	l		q	
c	6.87	h	7.63	m		r	
d	7.03	i	2.53 DMSO-d ₅	n		s	
e	7.31	j	3.24 H ₂ O	o		t	



26012 M

5-(p-ANISIDINO)-1-(p-METHOXYPHENYL)-1H-1,2,3-TRIAZOLE

$C_{16}H_{16}N_4O_2$

Mol. Wt. 296.33

PRISM NO.

53033

M.P. 176-176.5°C

SOLVENT

PolySol

Source of Sample:

REFERENCE

TMS

J. Svetlik,
Slovak Technical University,
Bratislava, Czechoslovakia

SWEEP OFFSET

-

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ASSIGNMENTS

a	3.73	f	7.32	k		p	
b	3.86	g	7.52	l		q	
c	6.78	h	unobserved	m		r	
d	6.97	i	2.55 DMSO- d_5	n		s	
e	7.05	j		o		t	

