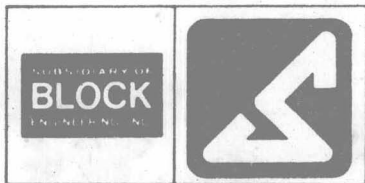


**Standard
Infrared
Grating Spectra
Volume 35-36
34001 - 36000**



SADTLER RESEARCH LABORATORIES, INC.

STANDARD GRATING SPECTRA

Vol. 35

CREATIVE CHEMISTS SINCE 1874

3316 SPRING GARDEN ST., PHILADELPHIA, PA. 19104
TEL. 215 382-7800 • TWX 710 - 670-1186 • CABLE SADTLABS

The publication of the physical data of the Sadtler Standard Spectra and the Sadtler Commercial Spectra is intended to be descriptive. The samples of the materials represented have come generally from other sources than our own laboratories and frequently without the donors' knowledge of their part in this publication.

On the other hand every effort is made by Sadtler Research Laboratories, Inc. to assure the reliability of the published spectra. When improved data is available or errors are called to our attention we revise and reissue the proper replacement spectra.

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SADTLER STANDARD GRATING SPECTRA

This 1975 supplement of 4,000 spectra to the Sadtler Standard Grating Spectra collection brings the total collection to 37,000 infrared grating spectra determined in the 2.5 - 40 micron region (4000 to $\sim 200\text{ cm}^{-1}$). The last 1000 spectra of this supplement, numbered 37001P to 38000P, are previously published prism spectra which are now re-issued and renumbered to form an integral part of the Grating Spectra collection. Inclusion of the infrared prism spectra is intended to provide the widest selection of spectral data to Grating Spectra subscribers, grating format spectra are not available at this time since many of the compounds are no longer obtainable.

Presently all grating spectra are prepared at Sadtler Research Laboratories on a Perkin-Elmer 621 instrument using samples donated by scientists in universities and in industry throughout the world.

Standard techniques have been developed in our laboratories to insure that the spectra published are of the best possible quality and reproducible for comparison and identification purposes. The preferred sample preparation methods are the capillary cell for liquids and the KBr wafer for solids, the spectra obtained are qualitative only. The KBr method is used for solids since it is a standard technique and requires a small sample amount for preparation of good spectra, leaving the remainder for further analytical investigation. A paper describing the preparation procedure entitled Improved KBr Techniques by Traudé and Philip Sadtler is available from our laboratories.

When the KBr method cannot be used for solids due to reaction with the sample, the Split Mull technique is used; the sample is mullied in mineral oil and the entire spectrum is scanned, then a perfluorinated hydrocarbon mull is prepared and scanned in the 3.0 - 3.8 and 6.6 - 7.4 micron regions. This provides a complete spectrum of the compound.

Liquid samples and low melting solids are generally determined using capillary cells.

Each spectrum is clearly labelled with the sample preparation technique used.

Continuous updating of the collection is taking place to provide the best possible data. Although the spectra at the beginning of the collection, published over 15 years ago, do not always appear to be of optimum quality, it should be remembered that more recent advances in instrumentation and techniques have improved spectra quality. Earlier spectra are continuously reviewed and replaced when necessary, if a sample is available.

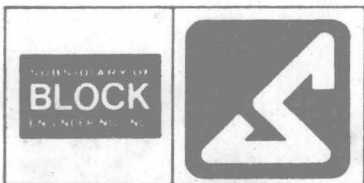
Samples of 98% pure compounds are continually being sought, it is only due to the generosity of those donors whose names appear as the "Source of Sample" that we can offer these spectra to scientists. Our continued thanks are expressed to these donors.

The following five indexes accompany the Sadtler Standard Spectra:

- Alphabetical Index
- Molecular Formula Index
- Chemical Classes Index
- Numerical Index
- Spec-Finder

THE FIRST THREE ARE COMPOSITE INDEXES CONTAINING ENTRIES FOR 49,000 PRISM SPECTRA AND CORRESPONDING SPECTRUM NUMBERS FOR THE 38,000 Sadtler Standard Grating Spectra, the 38,000 Sadtler Ultraviolet Spectra and the 22,000 Sadtler Nuclear Magnetic Resonance Spectra. The last two indexes are specific to the Sadtler Standard Grating Spectra, the numerical index is according to the sequence of the publication and the Spec-Finder provides a means of identifying grating spectra of unknown compounds by comparison with the coded peaks of the references.

WE SUGGEST THAT THE INTRODUCTIONS TO THE VARIOUS INDEXES BE READ CAREFULLY TO ASSURE THE BEST UTILIZATION OF THEIR APPLICATIONS.



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STANDARD GRATING SPECTRA

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WE SUGGEST THAT THE INTRODUCTIONS TO THE VARIOUS INDEXES BE READ CAREFULLY TO ASSURE THE BEST UTILIZATION OF THEIR APPLICATIONS.

2-(o-CHLOROSTYRYL) -5-NITROIMIDAZOLE-1-ETHANOL

34001K

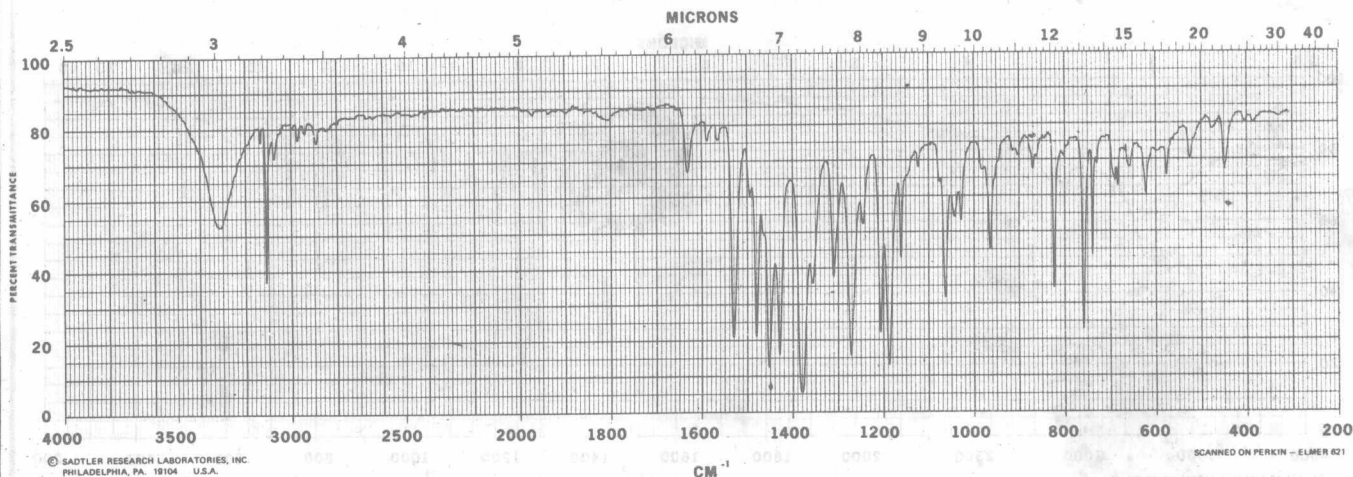
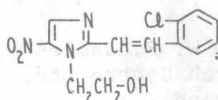
$C_{13}H_{12}ClN_3O_3$

Mol. Wt. 293.71

M.P. 188-189°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



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2-(p-CHLOROSTYRYL) -5-NITROIMIDAZOLE-1-ETHANOL

34002K

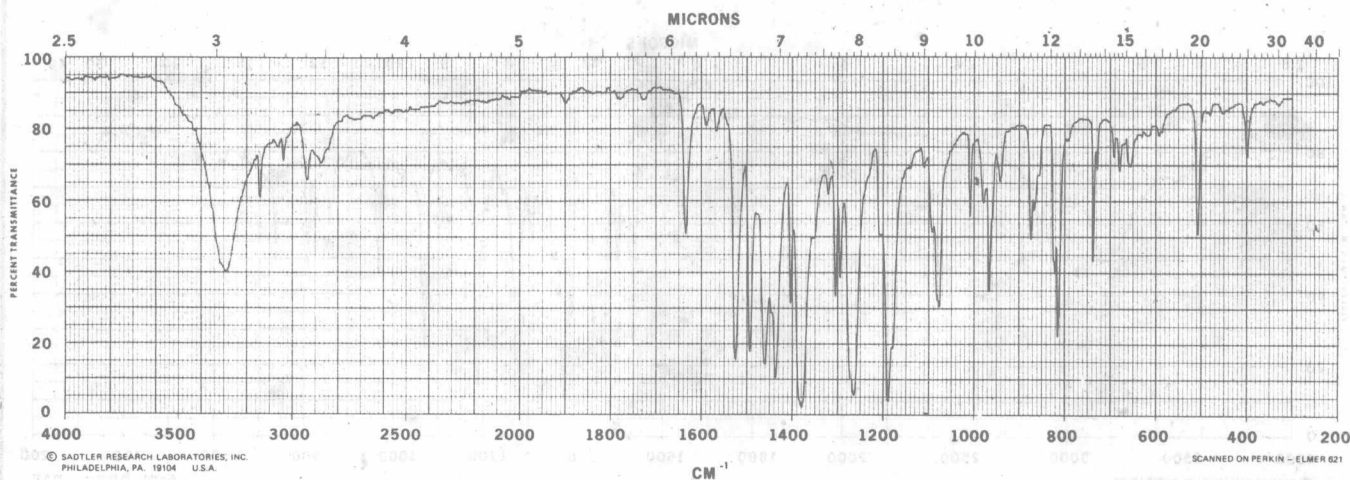
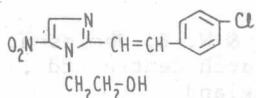
$C_{13}H_{12}ClN_3O_3$

Mol. Wt. 293.71

M.P. 194-195°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



34003K

2-(p-METHYLSTYRYL)-5-NITROIMIDAZOLE-1-ETHANOL

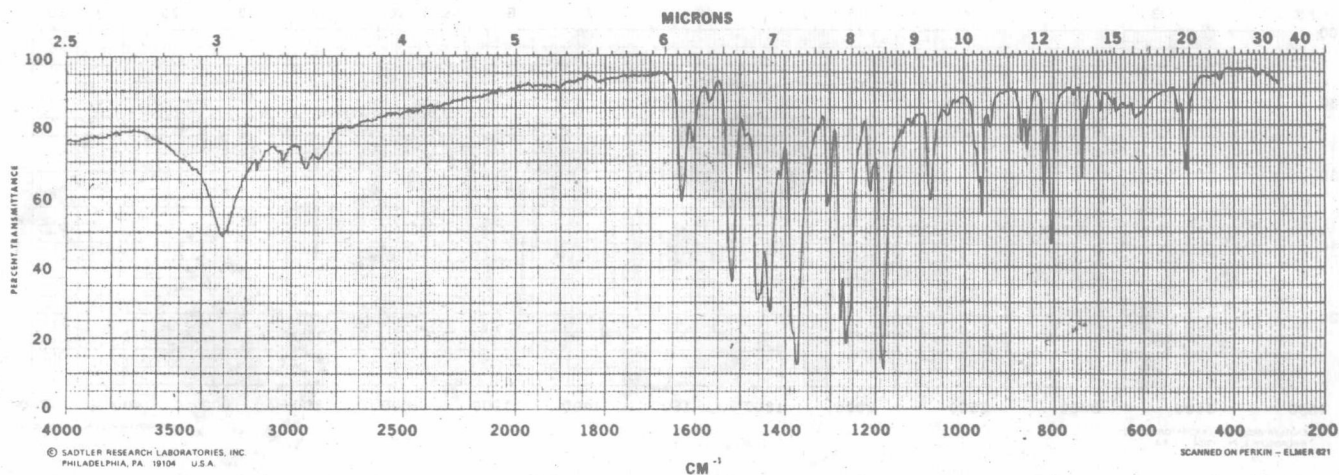
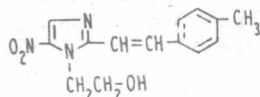
 $C_{14}H_{15}N_3O_3$

Mol. Wt. 273.29

M.P. 145-146°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



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34004K

2-(3,4-DIMETHYLSTYRYL)-5-NITROIMIDAZOLE-1-ETHANOL

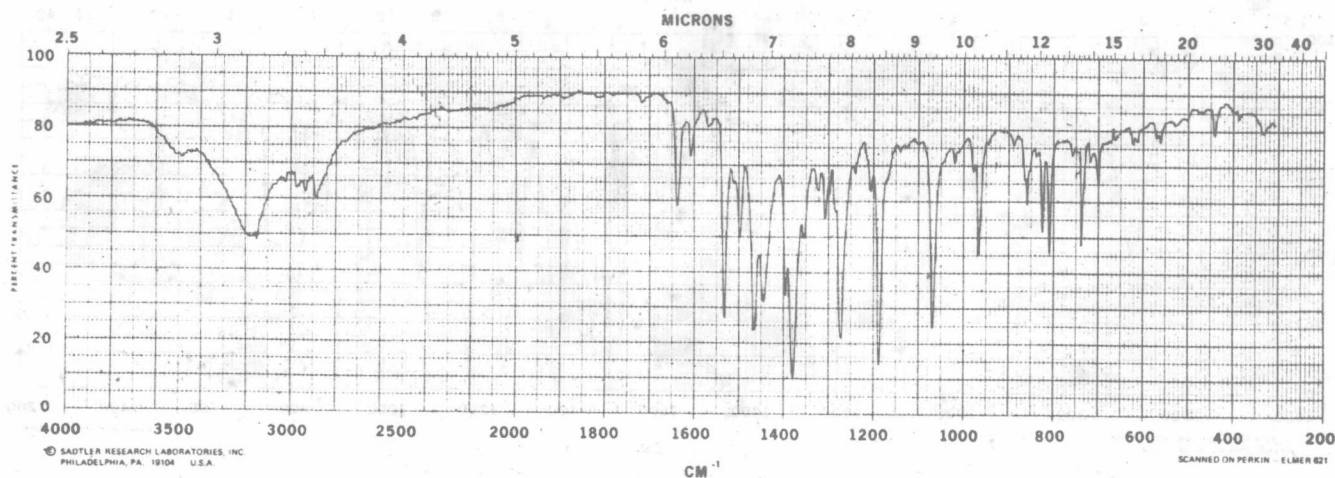
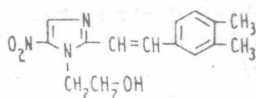
 $C_{15}H_{17}N_3O_3$

Mol. Wt. 287.32

M.P. 159-160°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



2-(p-ETHYLSTYRYL) -5-NITROIMIDAZOLE-1-ETHANOL

34005K

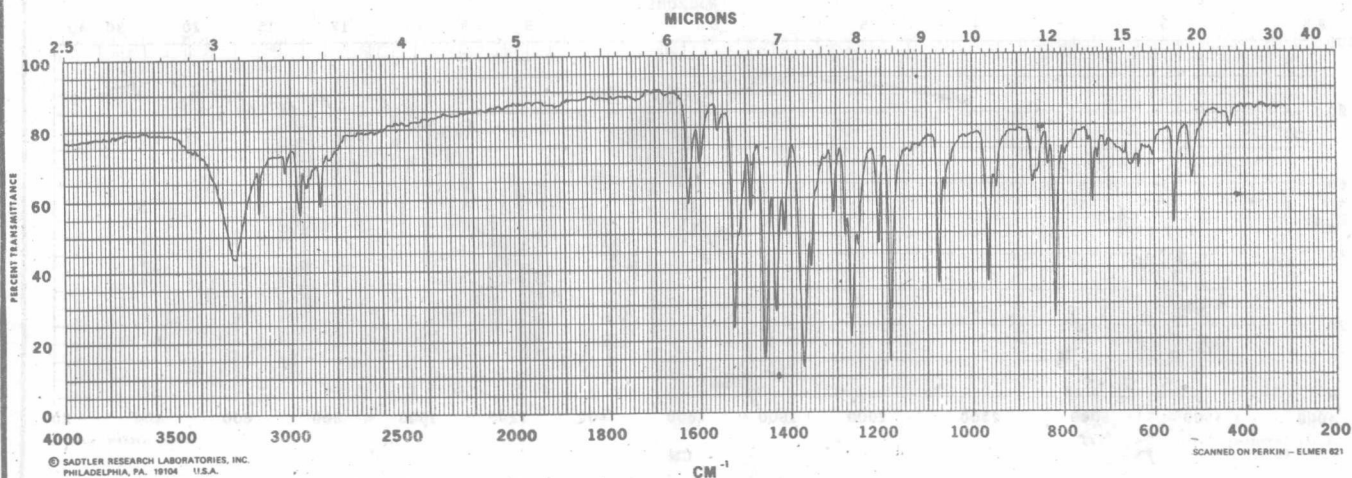
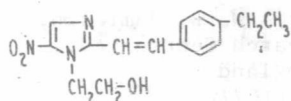
$C_{15}H_{17}N_3O_3$

Mol. Wt. 287.32

M.P. 187-188°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



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2-(p-ISOPROPYLSTYRYL) -5-NITROIMIDAZOLE-1-ETHANOL

34006K

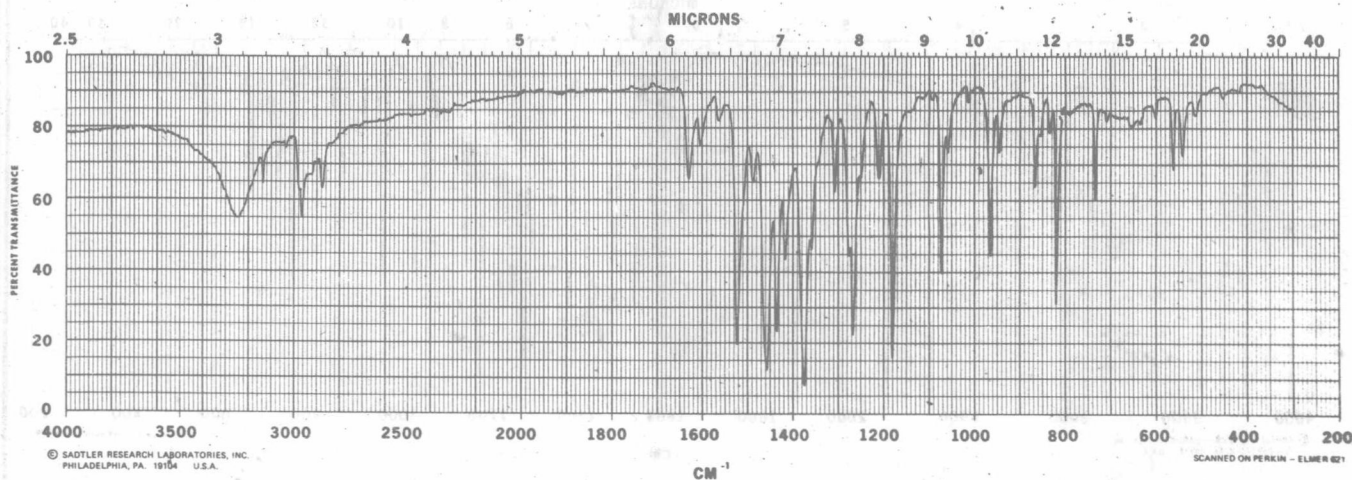
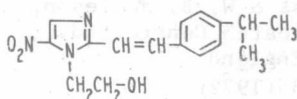
$C_{16}H_{19}N_3O_3$

Mol. Wt. 301.35

M.P. 171-172°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer

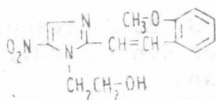


34007K

2-(o-METHOXYSTYRYL)-5-NITROIMIDAZOLE-1-ETHANOL

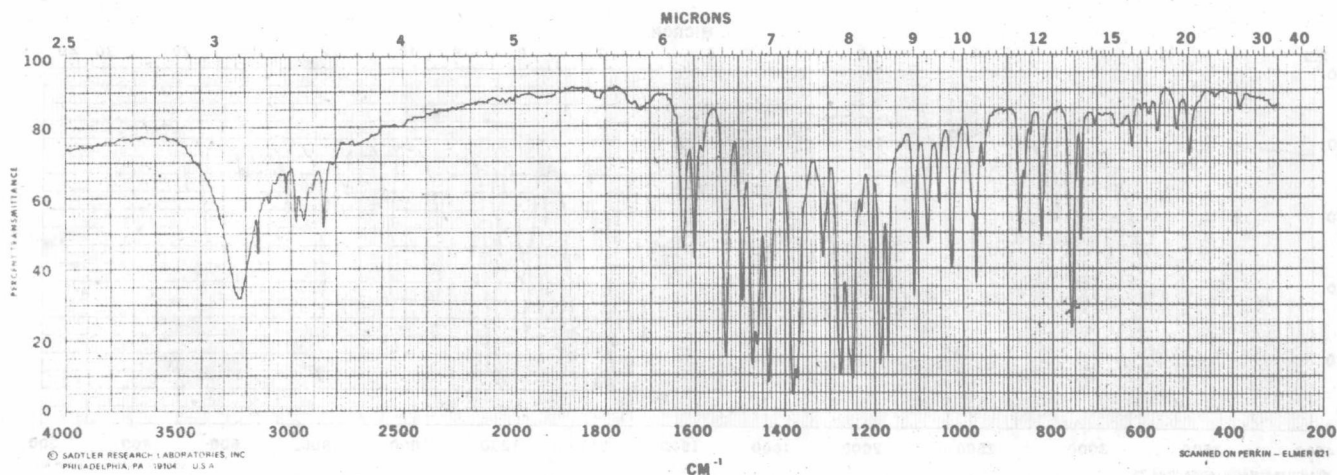
 $C_{14}H_{15}N_3O_4$ Mol. Wt. 289.29

M.P. 199-200°C



Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



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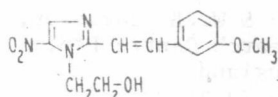
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34008K

2-(m-METHOXYSTYRYL)-5-NITROIMIDAZOLE-1-ETHANOL

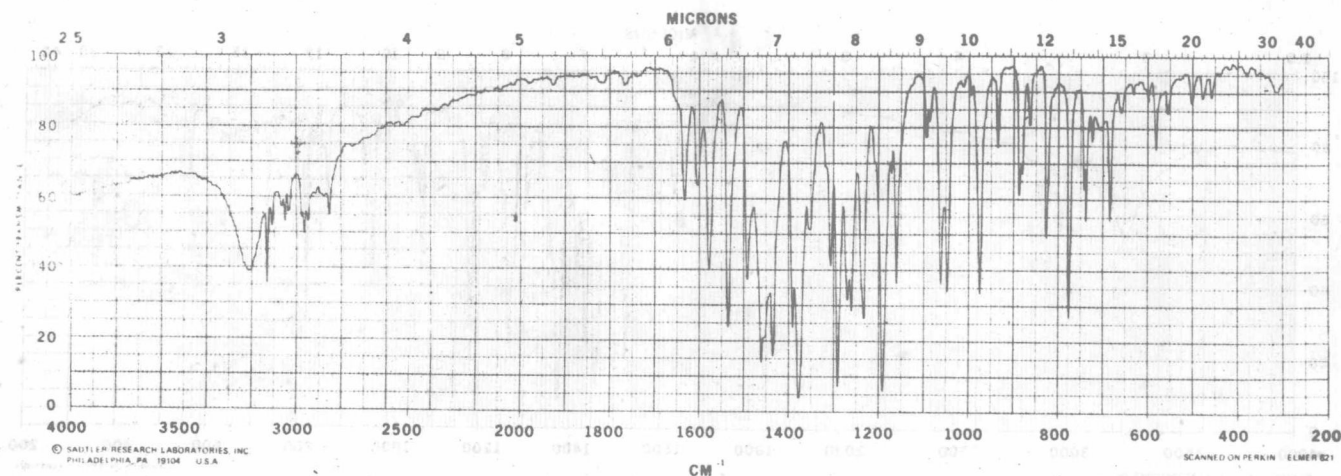
 $C_{14}H_{15}N_3O_4$ Mol. Wt. 289.29

M.P. 134-135°C



Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer

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2-(p-METHOXYSTYRYL) -5-NITROIMIDAZOLE-1-ETHANOL

34009K

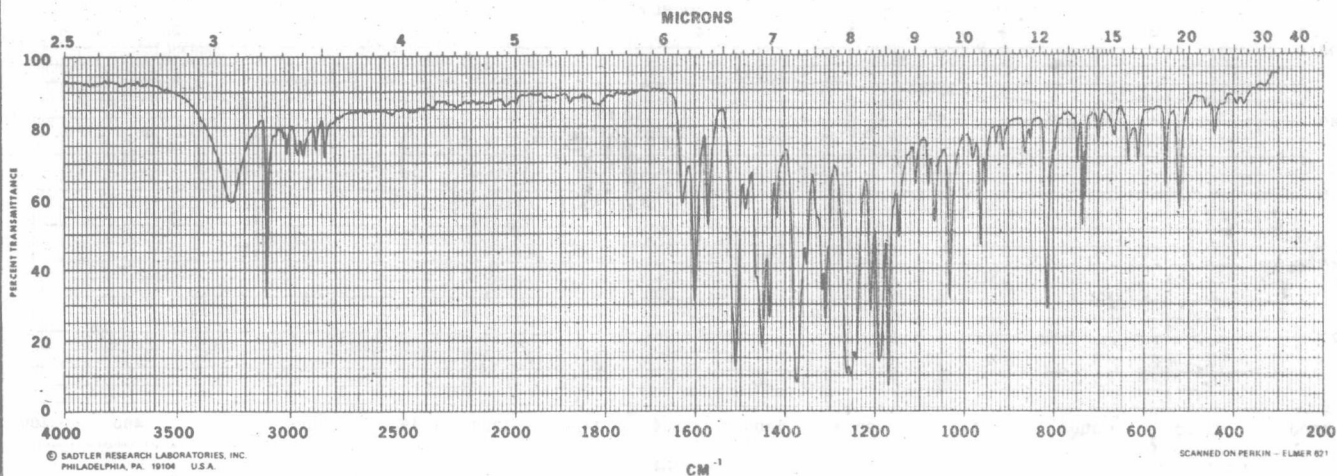
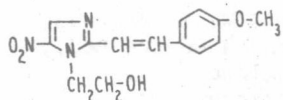
$C_{14}H_{15}N_3O_4$

Mol. Wt. 289.29

M.P. 152-153°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



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2-(p-METHYLSTYRYL) -5-NITROIMIDAZOLE-1-ETHANOL, p-TOLUENE-SULFONATE (ESTER)

34010K

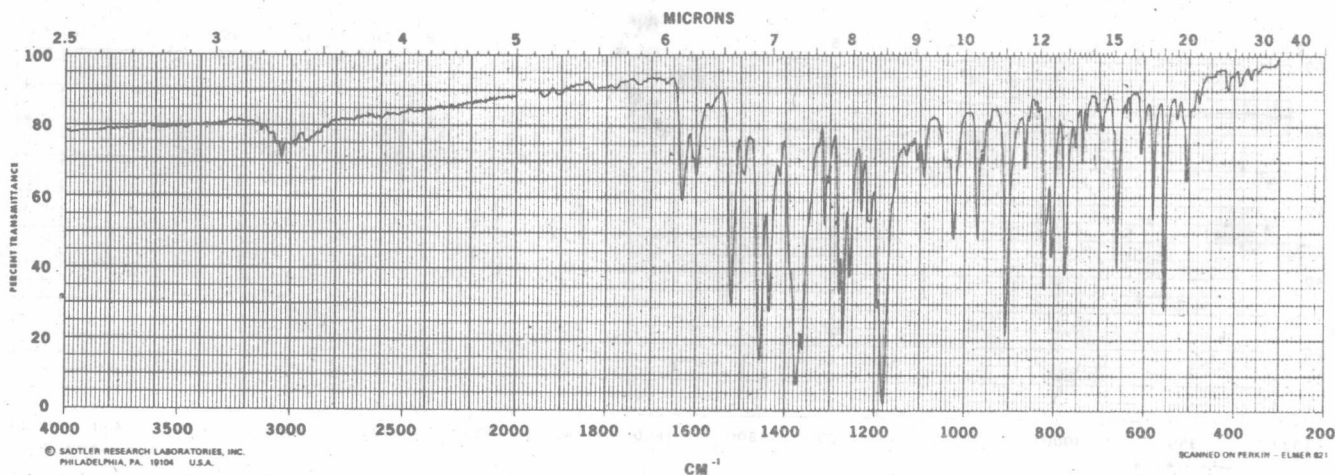
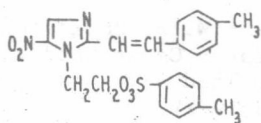
$C_{21}H_{21}N_3O_5S$

Mol. Wt. 427.48

M.P. 155-156°C

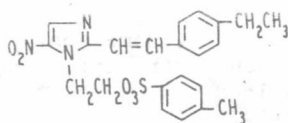
Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



34011K

2-(p-ETHYLSTYRYL)-5-NITROIMIDAZOLE-1-ETHANOL, p-TOLUENE-SULFONATE (ESTER)

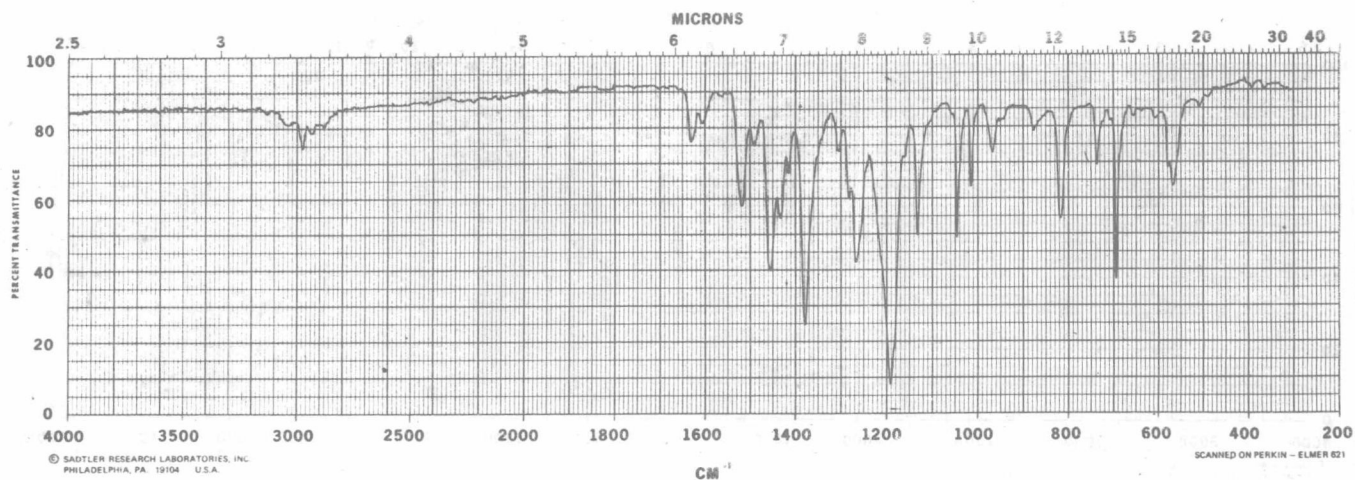
 $C_{22}H_{23}N_3O_5S$

Mol. Wt. 441.51

M.P. 134.5-135.5°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer

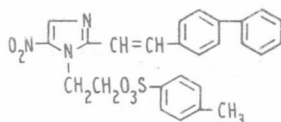


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34012K

5-NITRO-2-(p-PHENYLSTYRYL) IMIDAZOLE-1-ETHANOL, p-TOLUENE-SULFONATE (ESTER)

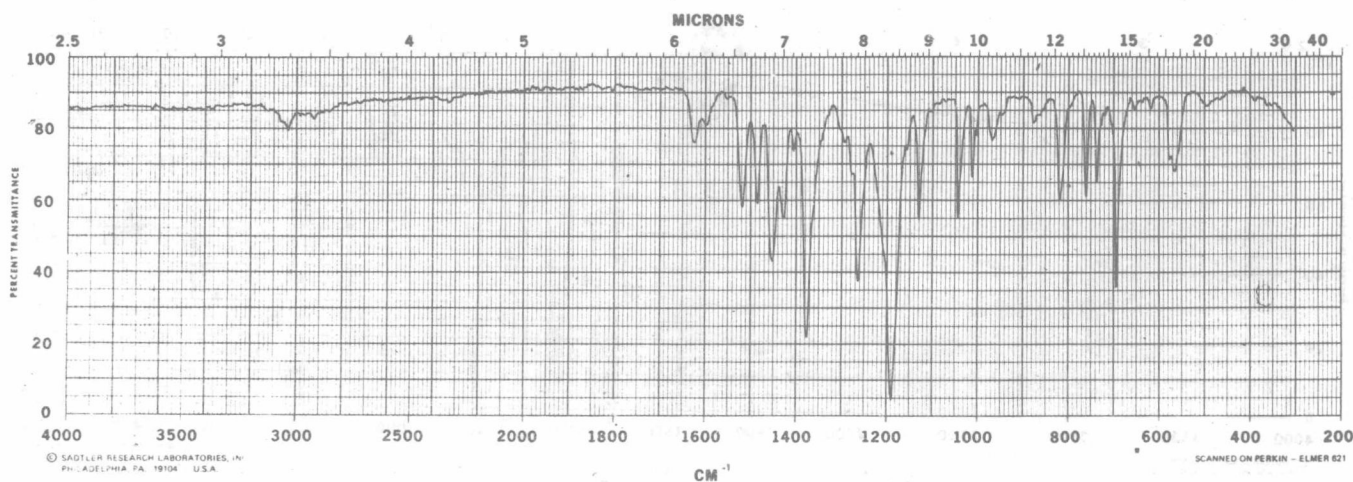
 $C_{26}H_{23}N_3O_5S$

Mol. Wt. 489.55

M.P. 169-170°C

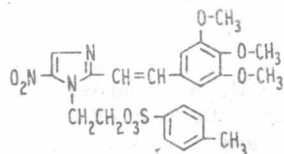
Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



5-NITRO-2-(3,4,5-TRIMETHOXYSTYRYL)IMIDAZOLE-1-ETHANOL,
p-TOLUENESULFONATE (ESTER)

34013K



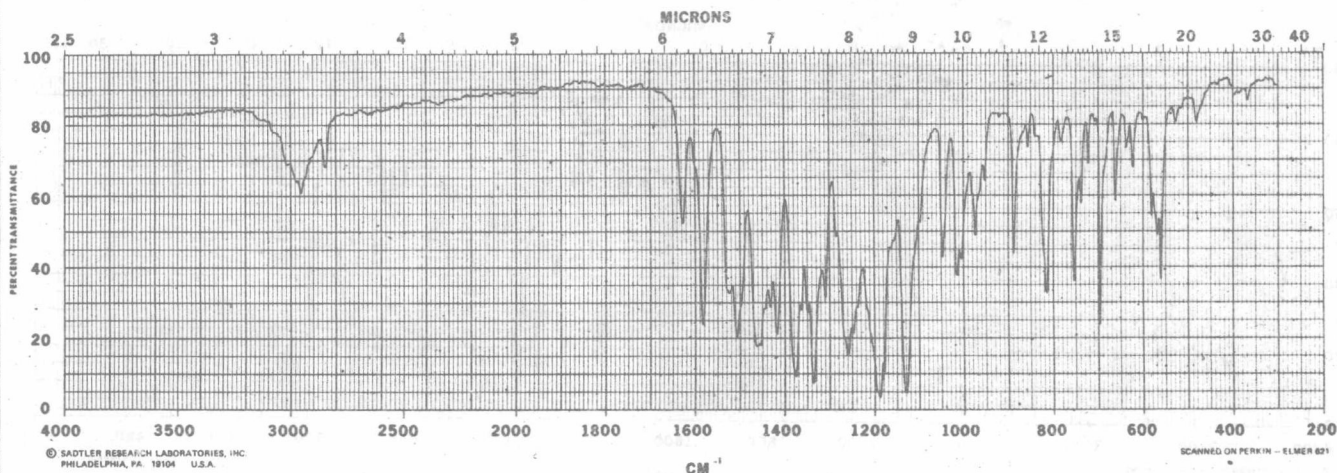
$C_{23}H_{25}N_3O_8S$

Mol. Wt. 503.54

M.P. 159-160°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer

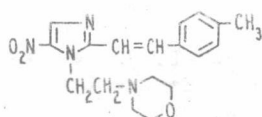


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4-[2-[2-(p-METHYLSTYRYL)-5-NITROIMIDAZOL-1-YL]ETHYL]-
MORPHOLINE

34014K



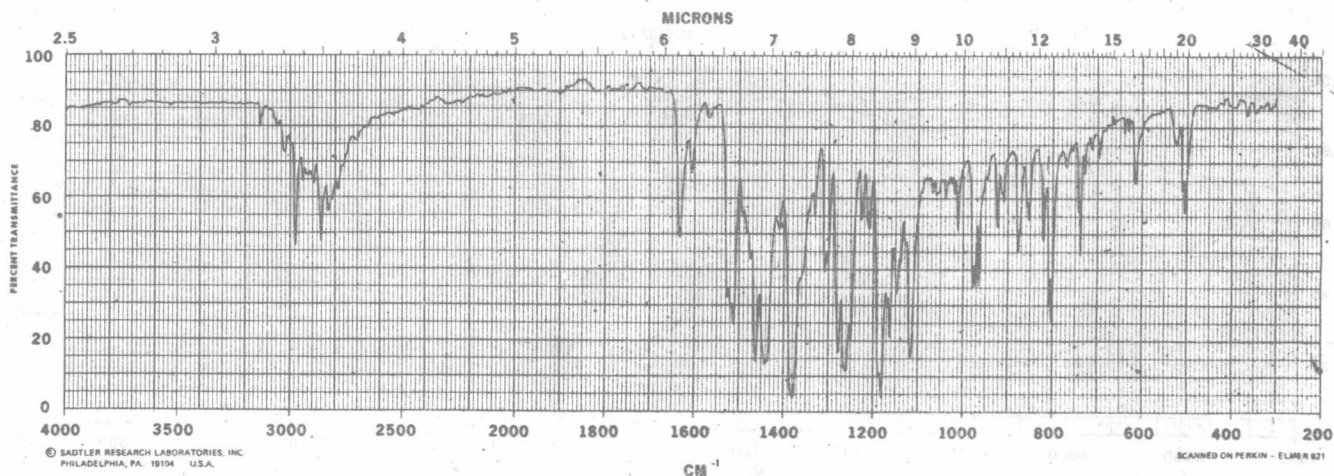
$C_{18}H_{22}N_4O_3$

Mol. Wt. 342.40

M.P. 125-126°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)
KBr Wafer



34015K

1-(2-CHLOROETHYL)-2-(p-METHYLSTYRYL)-5-NITROIMIDAZOLE

 $C_{14}H_{14}ClN_3O_2$

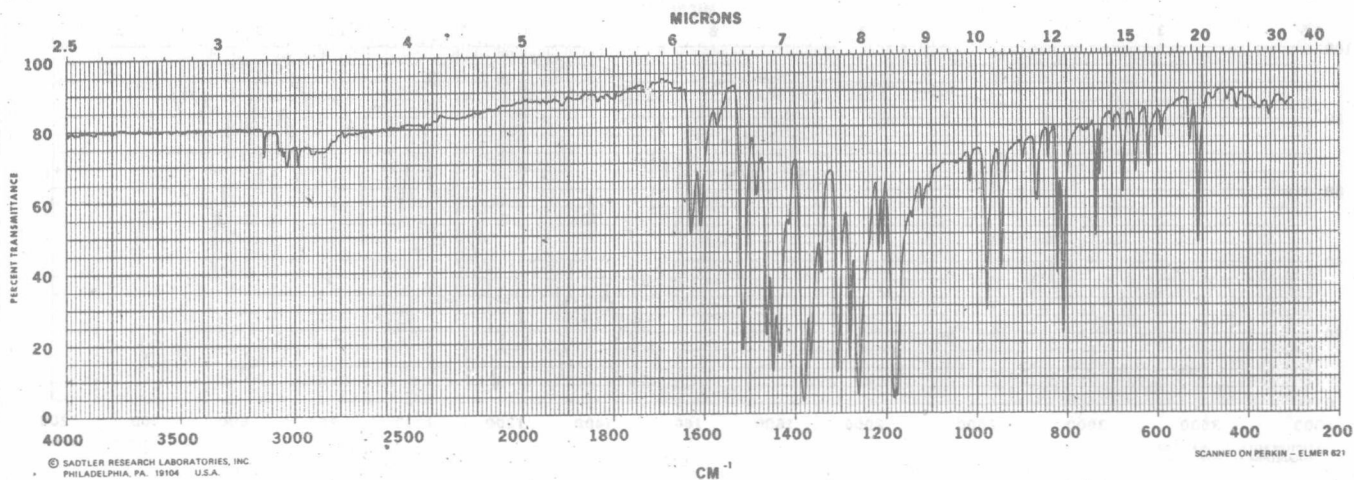
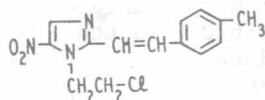
Mol. Wt. 291.74

M.P. 159-160°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)

KBr Wafer



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34016K

5-NITRO-2-STYRYL-1-VINYLMIDAZOLE

 $C_{13}H_{11}N_3O_2$

Mol. Wt. 241.25

M.P. 159-160°C

Source of Sample: W. J. Ross & W. B. Jamieson,
Lilly Research Centre Ltd.,
Surrey, England

Ref.: J. Med. Chem. 15, 1035(1972)

KBr Wafer

