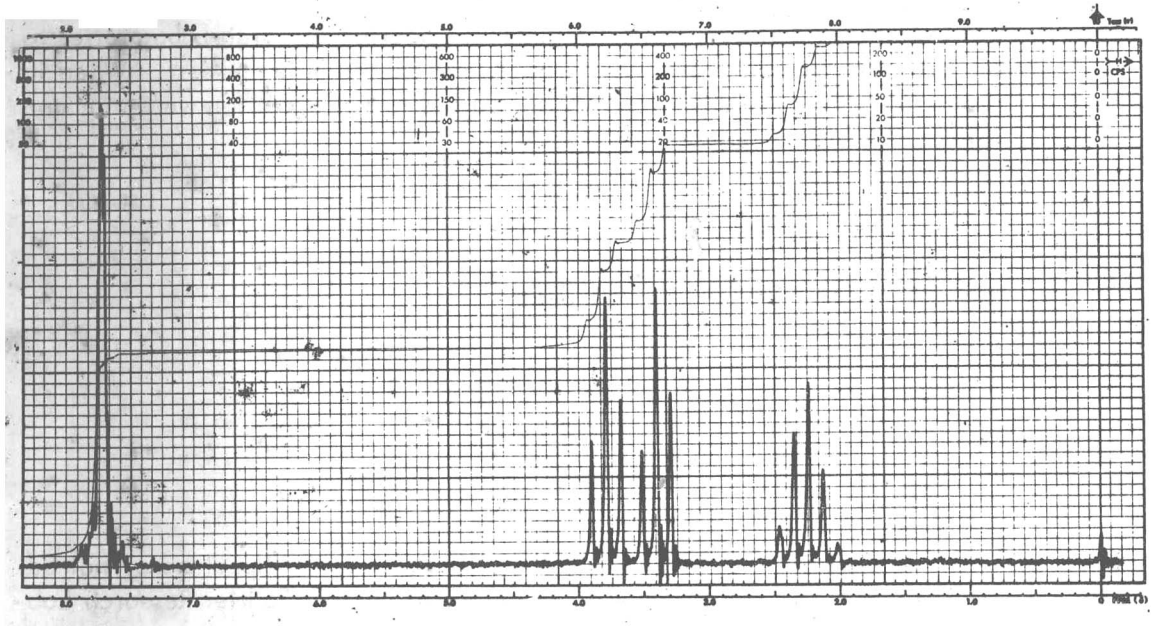




NUCLEAR MAGNETIC RESONANCE SPECTRA

Vol. 4



2001 M - 2666 M

LEGAL NOTICE

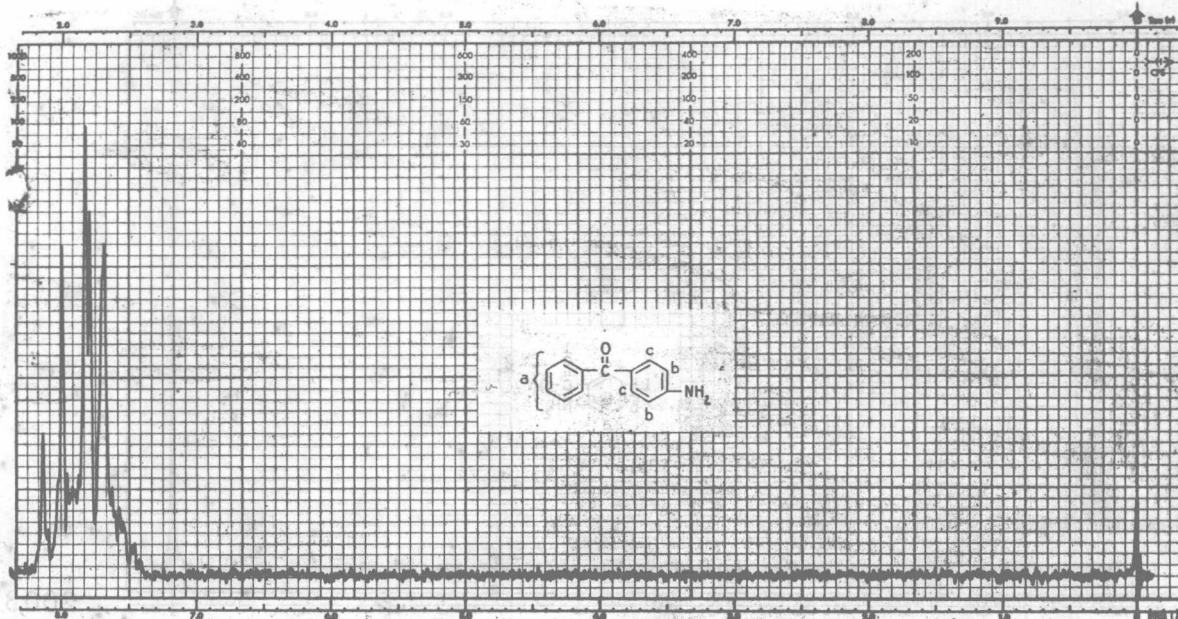
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2001 M

4-AMINO BENZOPHENONE

IR 18120

$C_{13}H_{11}NO$

Mol. Wt. 197.24

Source: Aldrich Chemical Company, Milwaukee, Wis.

ASSIGNMENTS

Filter Bandwidth: 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 63
 Integral amp: -

a 7.38-8.08 f _____
 b 7.75 or c g _____
 c 8.06 or b h _____
 d _____ i _____
 e _____ i _____

NH₂ is unobserved

Conc. Sat'd. sol'n./0.5ml Trifluoroacetic acid at 68°C

α, α, α -TRIFLUORO-o-TOLUIDINE

IR 18122

$C_7H_6F_3N$

Mol. Wt. 161.11

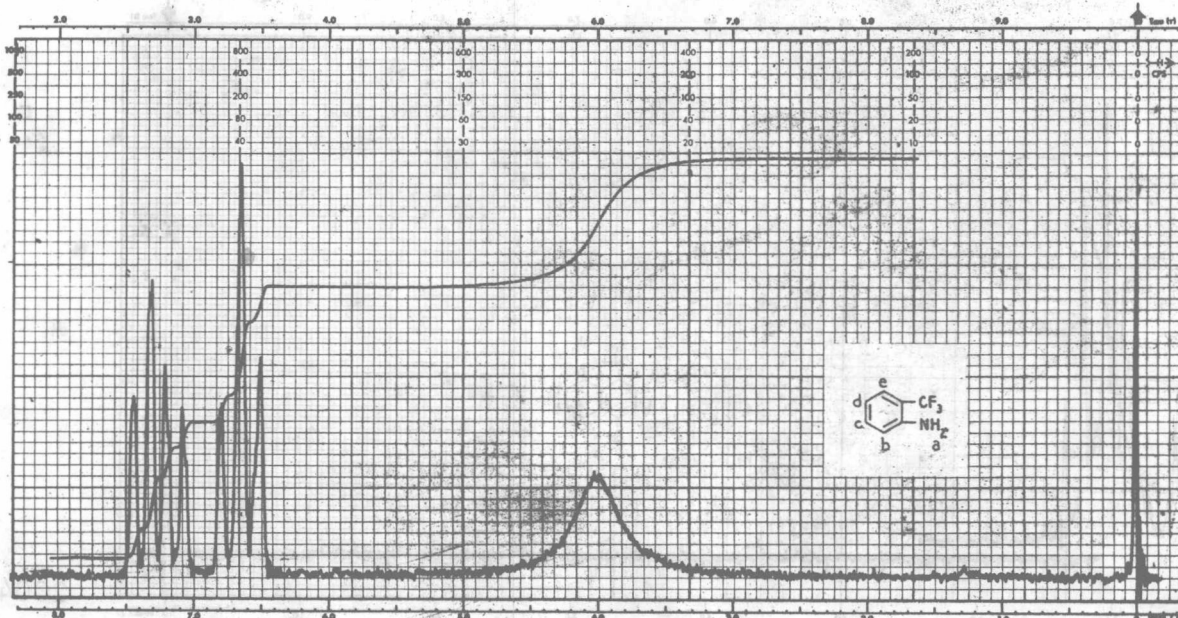
Source: Aldrich Chemical Company, Milwaukee, Wis.



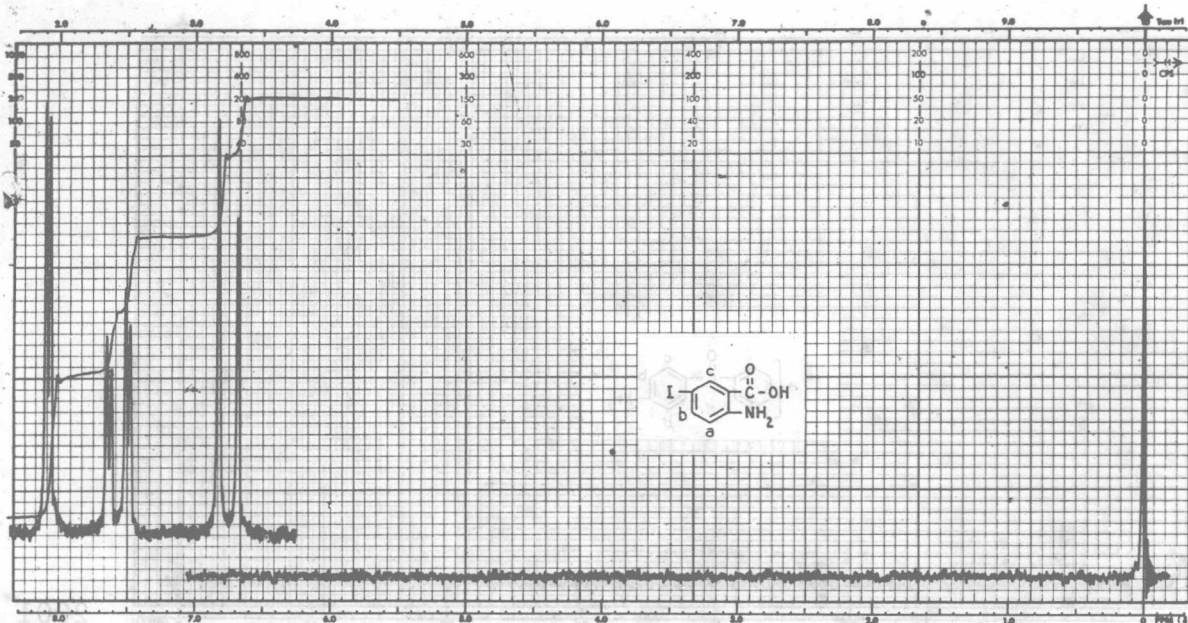
ASSIGNMENTS

Filter Bandwidth: 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 50
 Integral amp: 80 (spec. amp. 5)
 Conc. 100mg/0.5ml CCl₄

a 4.00 f _____
 b 6.58 g _____
 c 6.65 h _____
 d 7.21 i _____
 e 7.39 j _____



2002 M



2003 M

5-IODOANTHRANILIC ACID

IR 18123

$C_7H_6INO_2$

Mol. Wt. 263.04

Source: Aldrich Chemical Company, Milwaukee, Wis.

ASSIGNMENTS

Filter Bandwidth: 2 cps
 Sweep time: 250/500 sec
 Sweep width: 500 cps
 Sweep offset: - / 42 cps
 Spectrum amp: 50/ 80
 Integral amp: 80 (spec. amp. 20)
 Conc. Sat'd. sol'n/0.5ml Trifluoroacetic acid

a	<u>7.45</u>	f	_____
b	<u>8.26</u>	g	_____
c	<u>8.78</u>	h	_____
d	_____	i	_____
e	_____	j	_____

OH, NH₂ unobserved

4-BROMO-1-NAPHTHYLAMINE

IR 18124

$C_{10}H_8BrN$

Mol. Wt. 222.09

Source: Aldrich Chemical Company, Milwaukee, Wis.

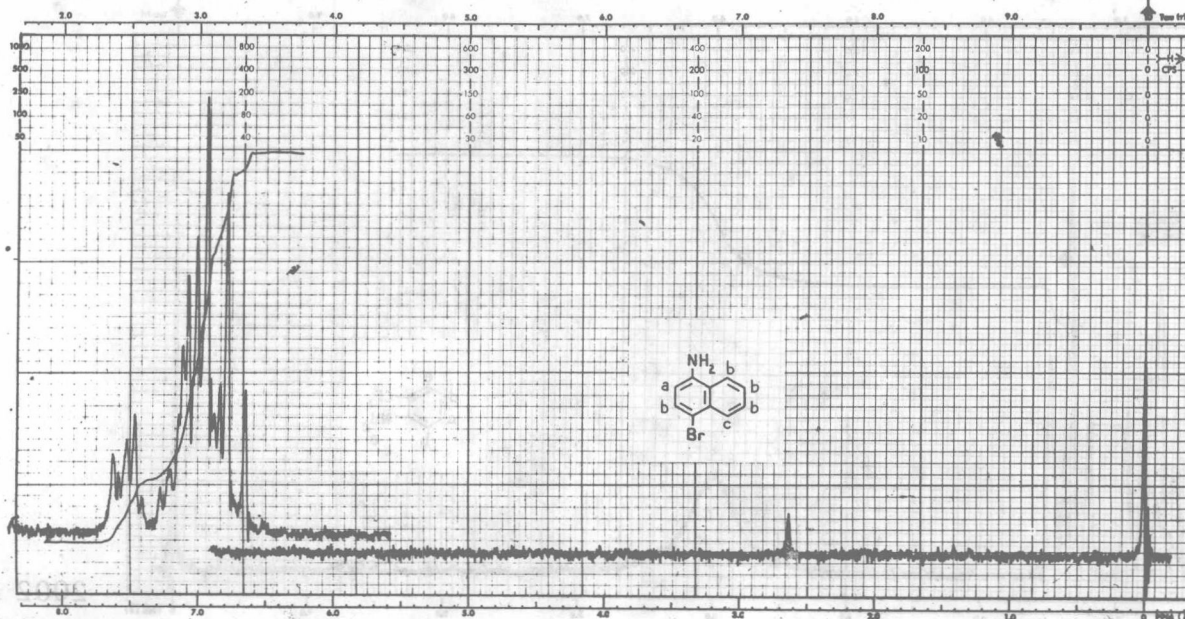


ASSIGNMENTS

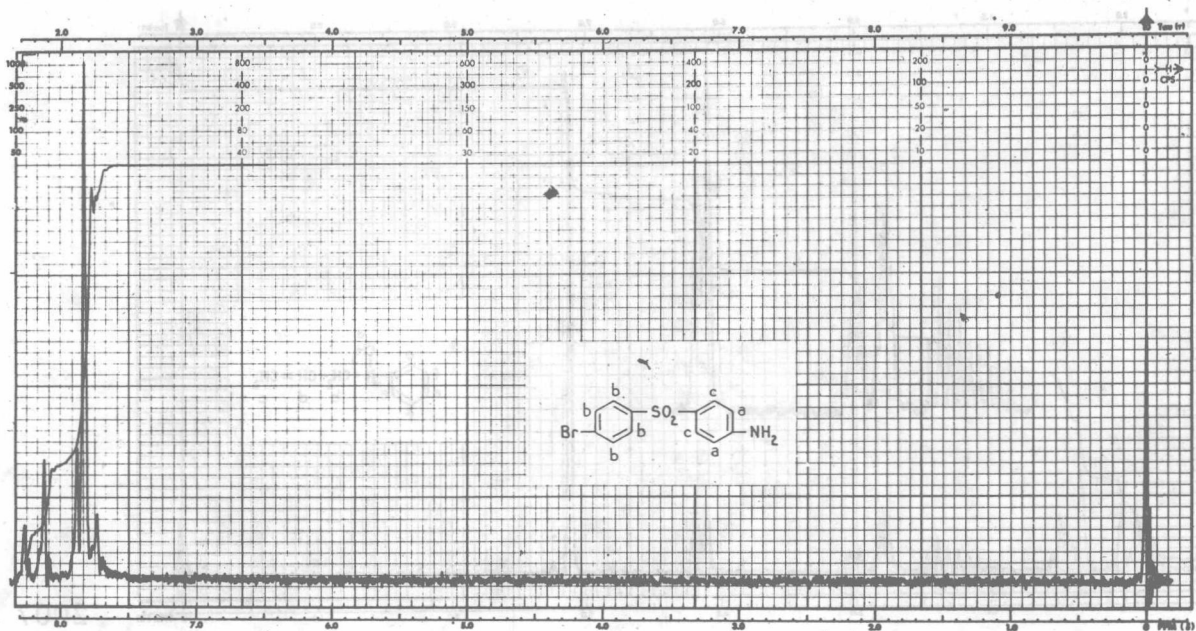
Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - / 48 cps
 Spectrum amp: 40
 Integral amp: 80 (spec. amp. 6.3)
 Conc. Sat'd. sol'n/0.5ml Trifluoroacetic acid

a	<u>7.50</u>	f	_____
b	<u>7.61-8.12</u>	g	_____
c	<u>ca 8.36</u>	h	_____
d	<u>2.64 imp.</u>	i	_____
e	_____	j	_____

NH₂ is unobserved



2004 M



2005 M

4- (4-BROMOPHENYLSULFONYL) ANILINE

IR 18126

$C_{12}H_{10}BrNO_2S$

Mol. Wt. 312.19

Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 25
 Integral amp: 80 (spec. amp. 16)

ASSIGNMENTS

a 7.80 f _____
 b 7.82 g _____
 c 8.20 h _____
 d _____ i _____
 e _____ i _____
 NH₂ is unobserved

Conc. Sat'd. sol'n/0.5ml Trifluoroacetic acid

2-AMINO-4,6-PYRIMIDINEDIOL

IR 18127

$C_4H_5N_3O_2$

Mol. Wt. 127.10

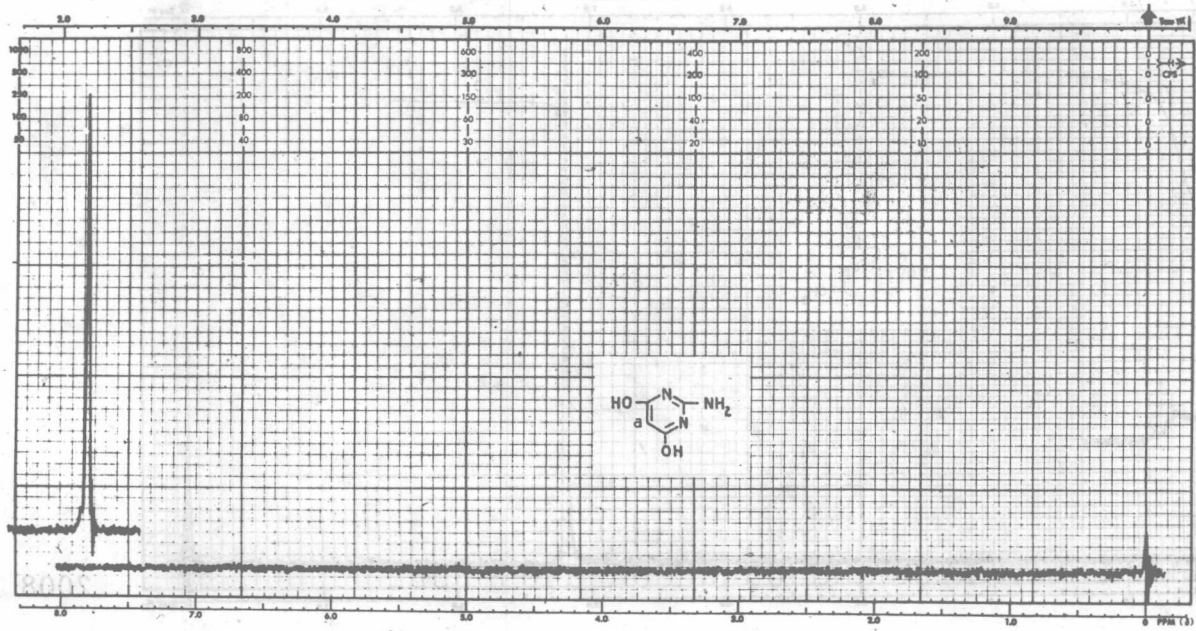
Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - /30 cps
 Spectrum amp: 20
 Integral amp: -

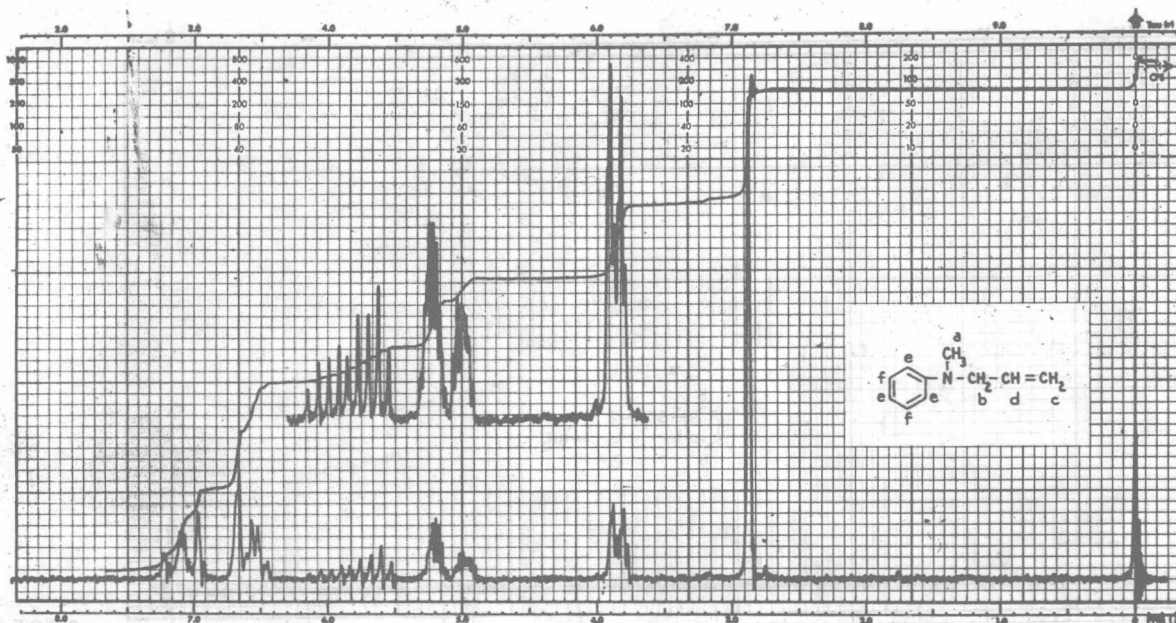
ASSIGNMENTS

a 8.30 f _____
 b _____ g _____
 c _____ h _____
 d _____ i _____
 e _____ i _____
 OH, NH₂ unobserved

Conc. Sat'd. sol'n./1.0ml Trifluoroacetic acid



2006 M



2007 M

N-ALLYL-N-METHYLANILINE

IR 18130

$C_{10}H_{13}N$

Mol. Wt. 147.22

Source: Aldrich Chemical Company, Milwaukee, Wis.

ASSIGNMENTS

Filter Bandwidth: 4/ 1 cps
 Sweep time: 250/500 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 16/100
 Integral amp: 80 (spec. amp. 6.3)
 Conc. 100mg/0.5ml CCl₄

a 2.87 f 7.08
 b 3.84 g _____
 c ca 5.10 h _____
 d ca 5.75 i _____
 e 6.42-6.75 j _____

4-AMINO-2-METHYL-5-PYRIMIDINECARBONITRILE

IR 18138

$C_6H_6N_4$

Mol. Wt. 134.14

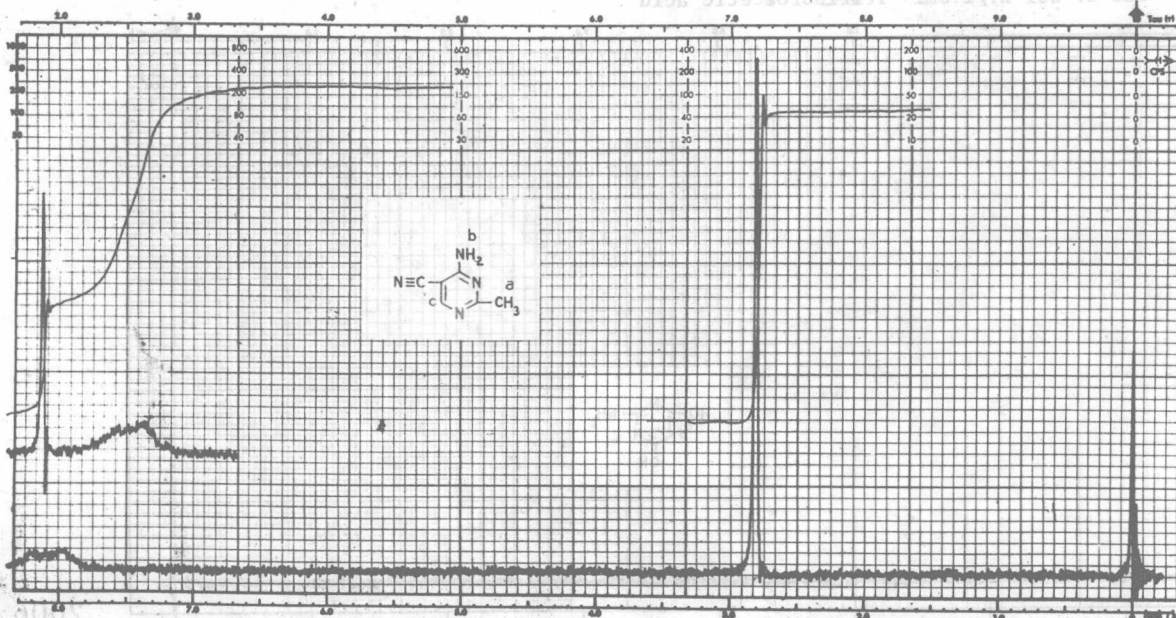
Source: Aldrich Chemical Company, Milwaukee, Wis.



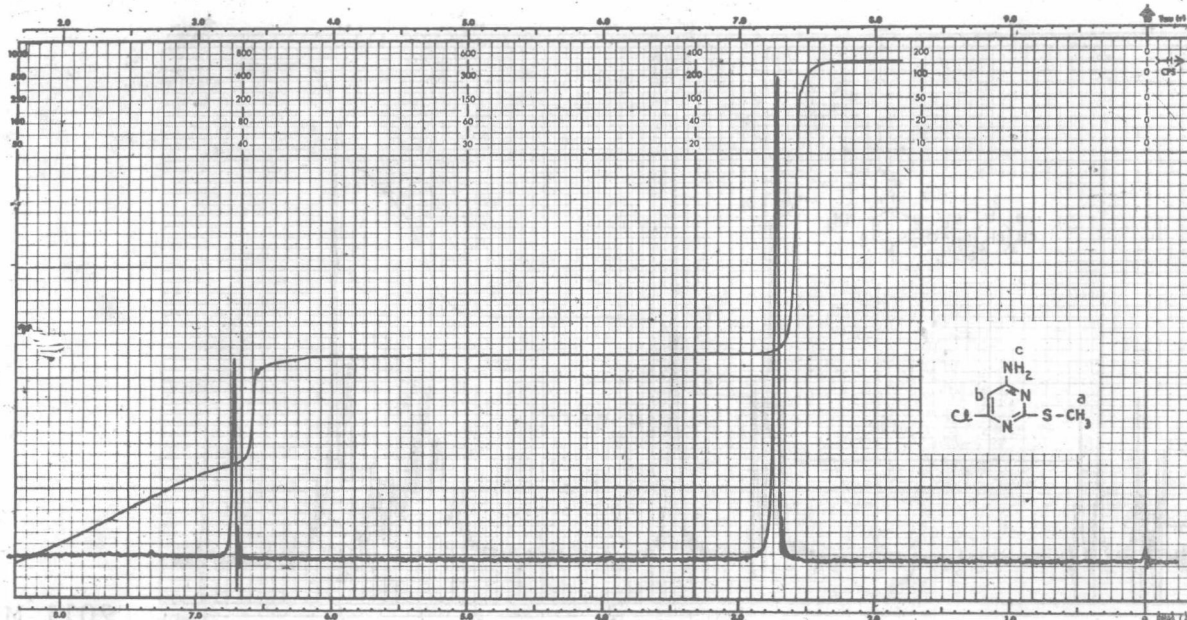
ASSIGNMENTS

Filter Bandwidth: 4/ 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - /36 cps
 Spectrum amp: 25/40
 Integral amp: 80 (spec. amp. 8)
 Conc. Sat'd. sol'n./0.5ml Trifluoroacetic acid

a 2.80 f _____
 b ca 8.06 g _____
 c 8.73 h _____
 d _____ i _____
 e _____ j _____



2008 M



2009 M

4-AMINO-6-CHLORO-2-(METHYLTHIO)PYRIMIDINE

IR 18141

C₅H₆ClN₃S

Mol. Wt. 175.64

Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 8
 Integral amp: 80 (spec. amp. 5)

ASSIGNMENTS

a 2.72 f _____
 b 6.72 g _____
 c ca 7.65 h _____
 d _____ i _____
 e _____ j _____

NH₂ is spread out

Solvent Trifluoroacetic acid

8-AMINO-6-METHOXYQUINOLINE

IR 18144

C₁₀H₁₀N₂O

Mol. Wt. 174.20

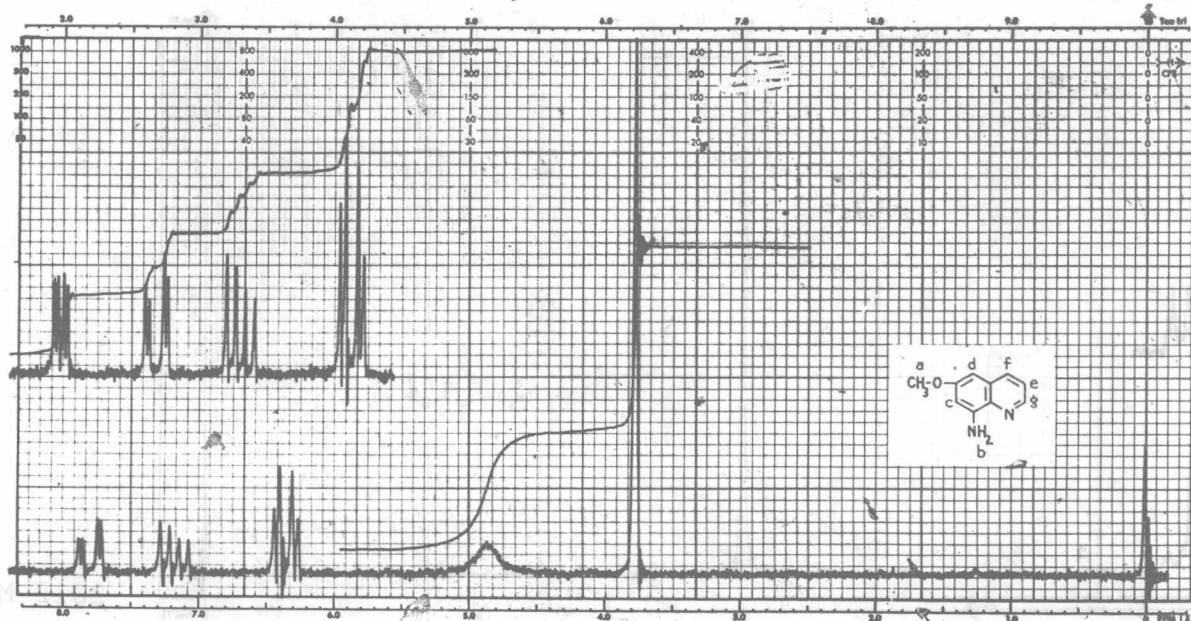
Source: Aldrich Chemical Company, Milwaukee, Wis.



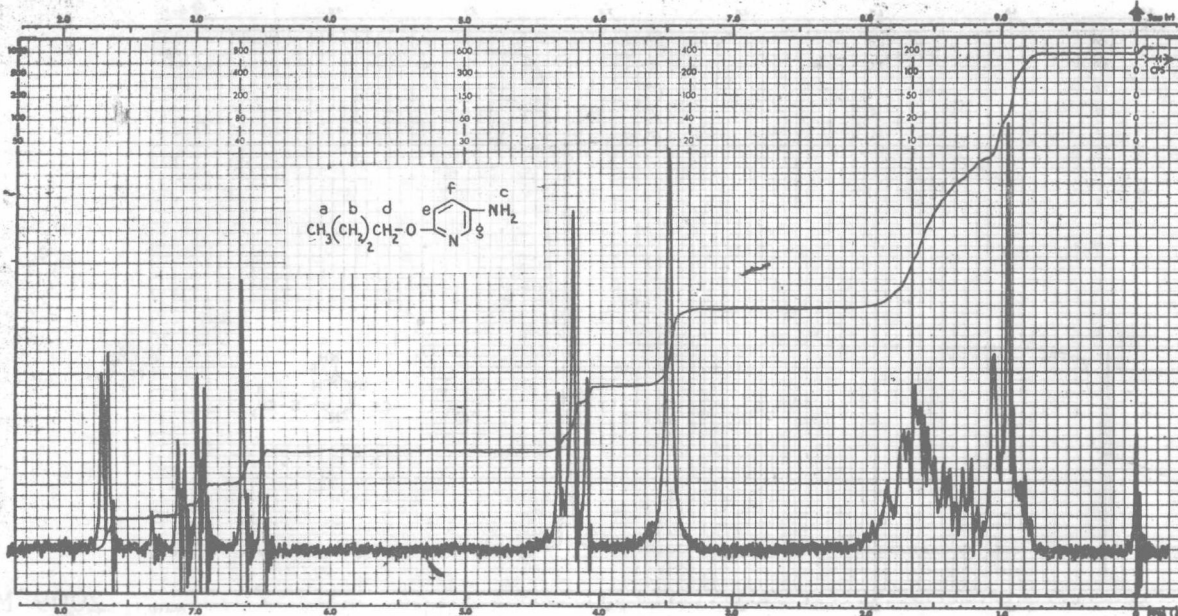
Filter Bandwidth: 4/2 cps
 Sweep time: 250/500 sec
 Sweep width: 500 cps
 Sweep offset: - / 30 cps
 Spectrum amp: 25/63
 Integral amp: 80 (spec. amp. 16)
 Conc. 100mg/0.5ml CCl₄

ASSIGNMENTS

a 3.78 f 7.80
 b 4.86 g 8.52
 c 6.28 h _____
 d 6.42 i _____
 e 7.18 j _____



2010 M



2011 M

5-AMINO-2-BUTOXYPYRIDINE

IR 18145

$C_9H_{14}N_2O$ Mol. Wt. 166.23
Source: Aldrich Chemical Company, Milwaukee, Wis.

ASSIGNMENTS

Filter Bandwidth: 4 cps
Sweep time: 250 sec
Sweep width: 500 cps
Sweep offset: - cps
Spectrum amp: 63
Integral amp: 80 (spec. amp. 6.3)
Conc. 100mg/0.5ml $CDCl_3$

a	0.95	f	7.03
b	ca 1.64	g	7.67
c	3.47	h	
d	4.20	i	
e	6.57	j	

2-AMINO-6-METHOXYBENZOTHAZOLE

IR 18146

$C_8H_8N_2OS$ Mol. Wt. 180.23
Source: Aldrich Chemical Company, Milwaukee, Wis.

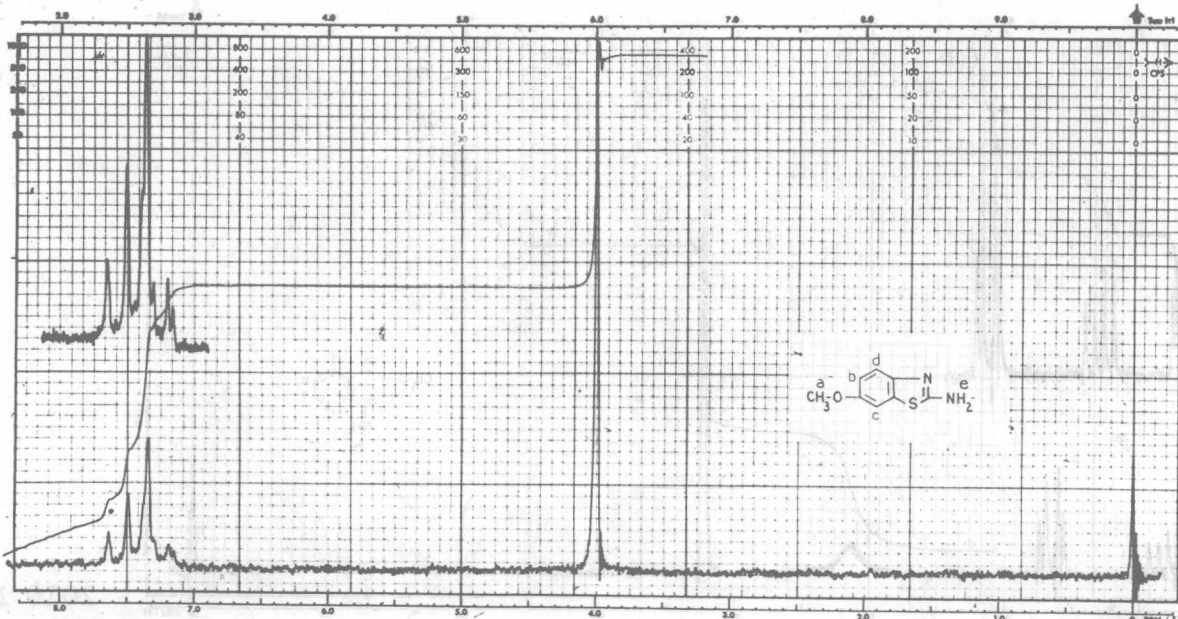


ASSIGNMENTS

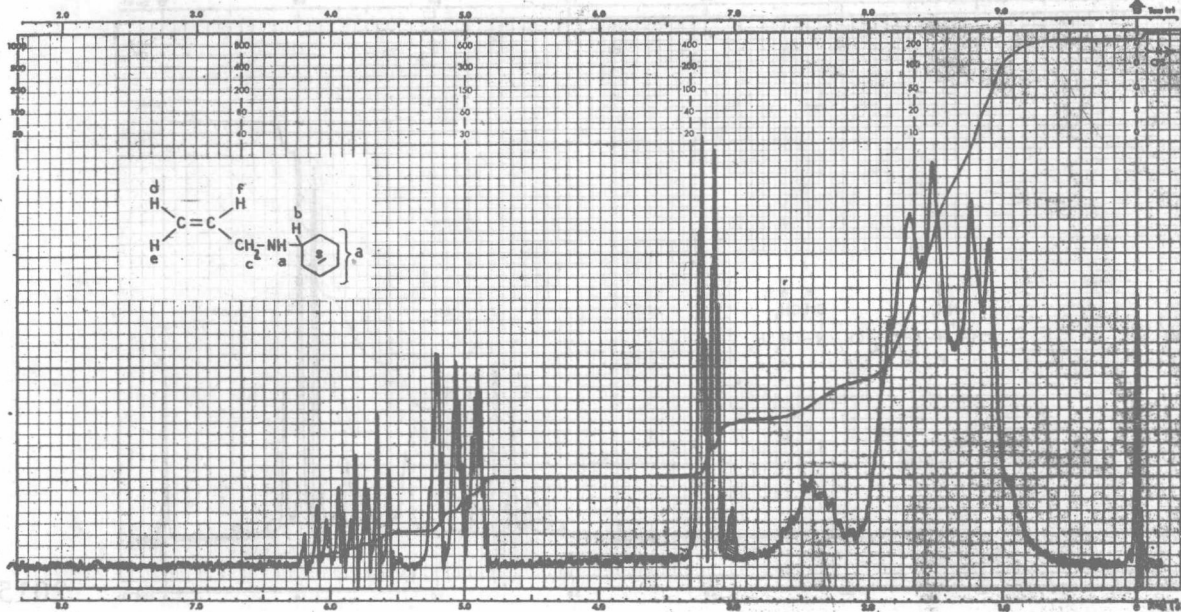
Filter Bandwidth: 2 cps
Sweep time: 250/500 sec
Sweep width: 500 cps
Sweep offset: - cps
Spectrum amp: 25/63
Integral amp: 80 (spec. amp. 8)
Conc. 100mg/0.5ml Trifluoroacetic acid

a	4.00	f	
b	7.25	g	
c	7.35	h	
d	7.56	i	
e	ca 8.00	j	

NH_2 is spread out



2012 M



2013 M

N-ALLYLCYCLOHEXYLAMINE

IR 18128

$C_9H_{17}N$

Mol. Wt. 139.24

Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 40
 Integral amp: 80 (spec. amp. 2)
 Conc. 100mg/0.5ml CCl_4

ASSIGNMENTS

a	<u>0.90-2.20</u>	f	<u>ca 5.75</u>
b	<u>ca 2.42</u>	g	<u> </u>
c	<u>3.20</u>	h	<u> </u>
d	<u>ca 5.00</u>	i	<u> </u>
e	<u>ca 5.05</u>	j	<u> </u>

5-CHLORO-2-PHENOXYANILINE

IR 18169

$C_{12}H_{10}ClNO$

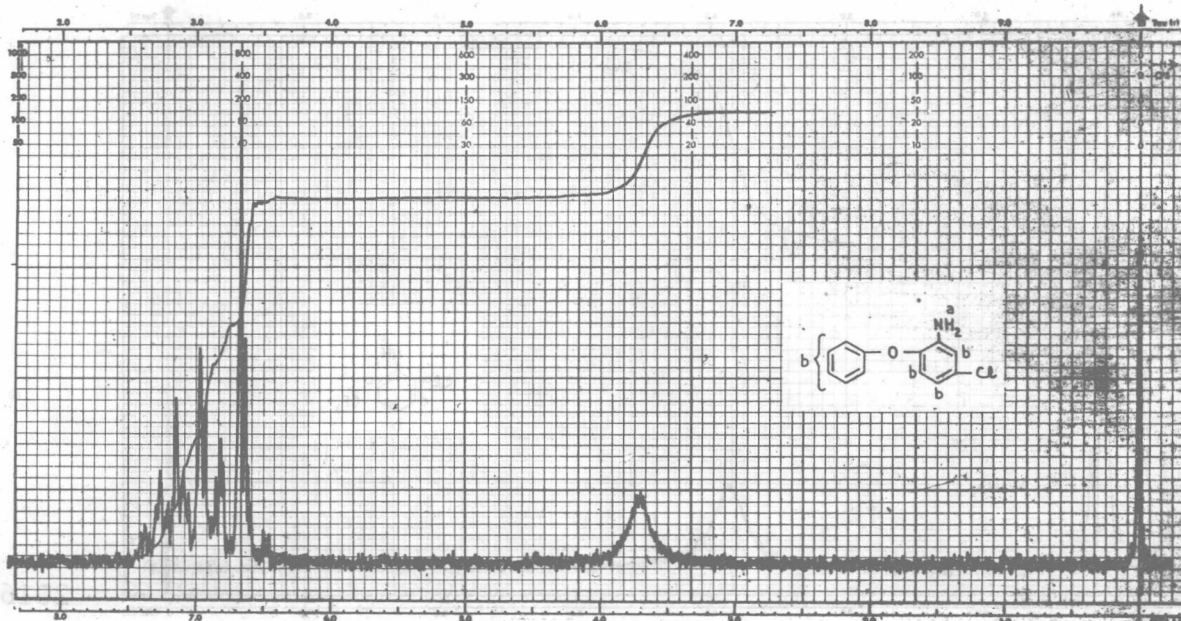
Mol. Wt. 219.68

Source: Aldrich Chemical Company, Milwaukee, Wis.

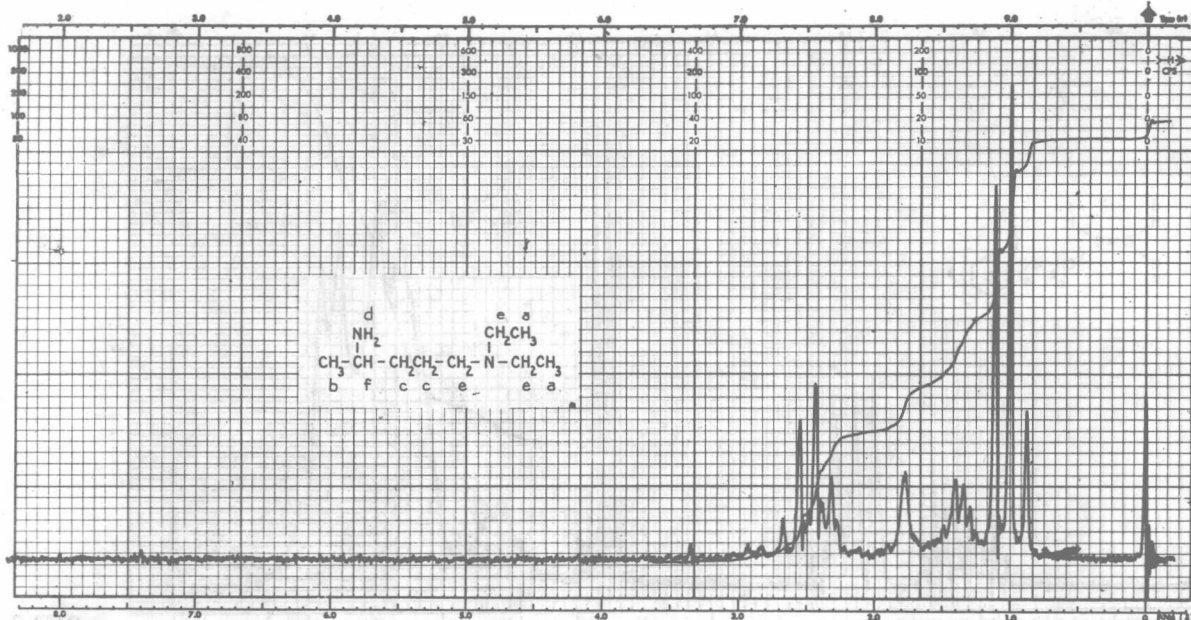
Filter Bandwidth: 4 cps
 Sweep time: 500 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 50
 Integral amp: 80 (spec. amp. 10)
 Conc. 100mg/0.5ml CCl_4

ASSIGNMENTS

a	<u>3.70</u>	f	<u> </u>
b	<u>6.40-7.45</u>	g	<u> </u>
c	<u> </u>	h	<u> </u>
d	<u> </u>	i	<u> </u>
e	<u> </u>	j	<u> </u>



2014 M



N',N'-DIETHYL-1,4-PENTANEDIAMINE

IR 18159

C₉H₂₂N₂

Mol. Wt. 158.29

Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 25
 Integral amp: 80 (spec. amp. 5)
 Conc. 100mg/0.5ml CDCl₃

ASSIGNMENTS

a	1.00	f	2.50
b	1.05	g	
c	1.36	h	
d	1.78	i	
e	2.43	i	

6-CHLORO- α,α,α -TRIFLUORO-m-TOLUIDINE

IR 18170

C₇H₅ClF₃N

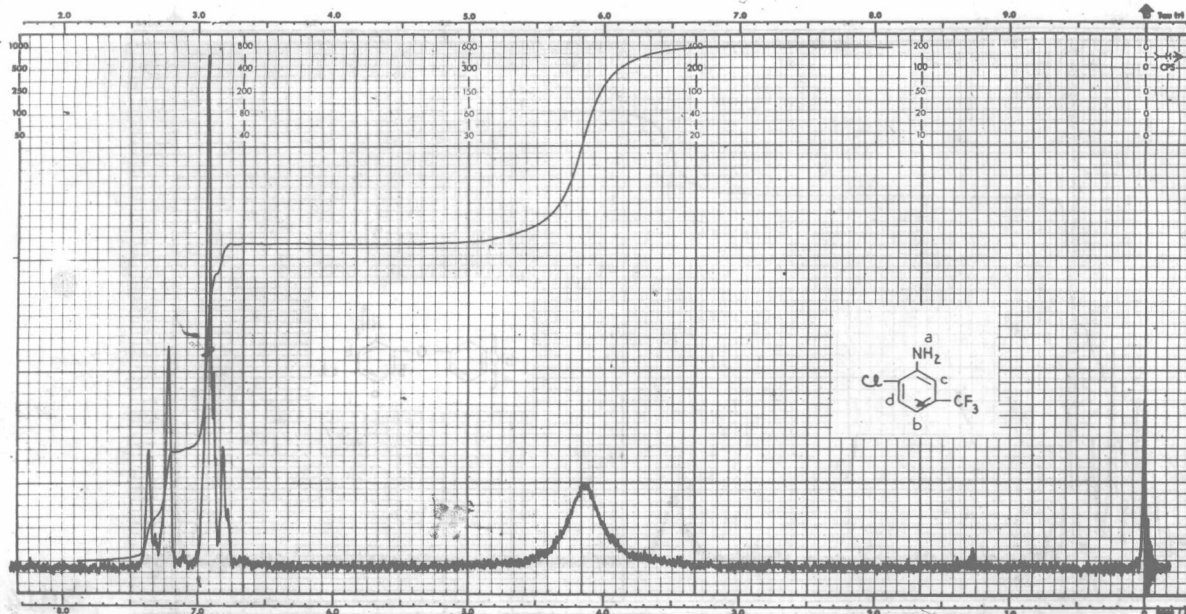
Mol. Wt. 195.57

Source: Aldrich Chemical Company, Milwaukee, Wis.

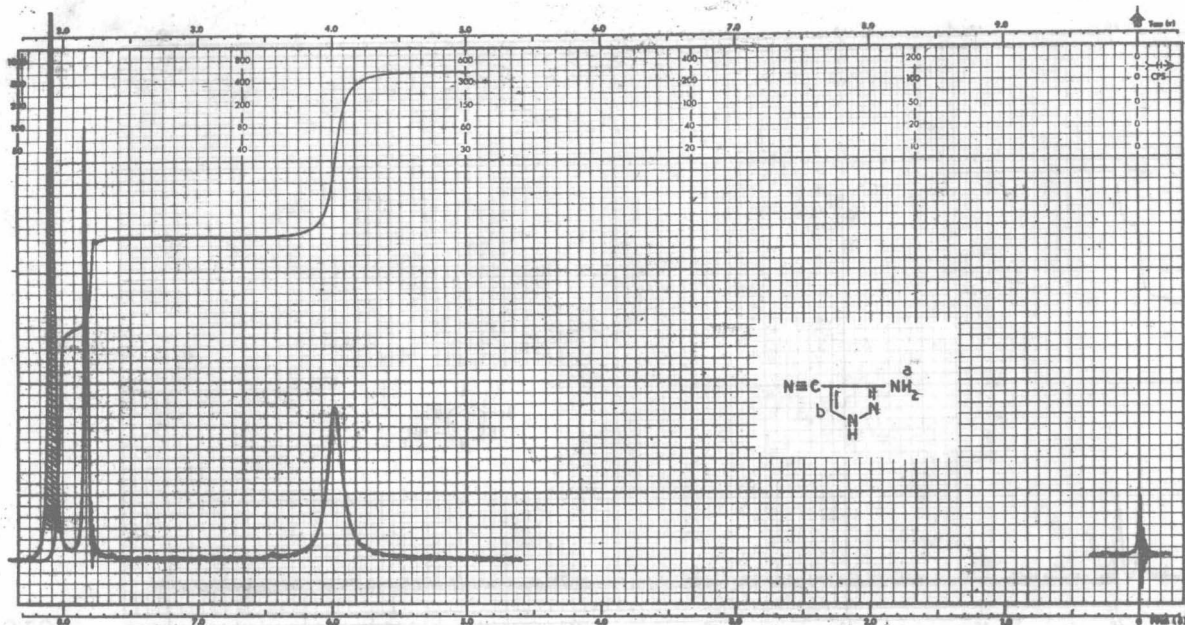
Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 32
 Integral amp: 80 (spec. amp. 8)
 Conc. 100mg/0.5ml CCl₄

ASSIGNMENTS

a	4.13	f	
b	6.85	g	
c	6.92	h	
d	7.29	i	
e		i	



2016 M



2017 M

3 (or 5)-AMINOPYRAZOLE-4-CARBONITRILE

IR 18172

$C_4H_4N_4$

Mol. Wt. 108.10

Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 10
 Integral amp: 80 (spec. amp. 2.5)
 Conc. Sat'd. sol'n./0.5ml Dimethylformamide

ASSIGNMENTS

a 5.99 f _____
 b 7.83 g _____
 c 8.08 DMF h _____
 d _____ i _____
 e _____ i _____
 NH is unobserved

4-AMINO-2,6-DICHLOROPHENOL

IR 18173

$C_6H_5Cl_2NO$

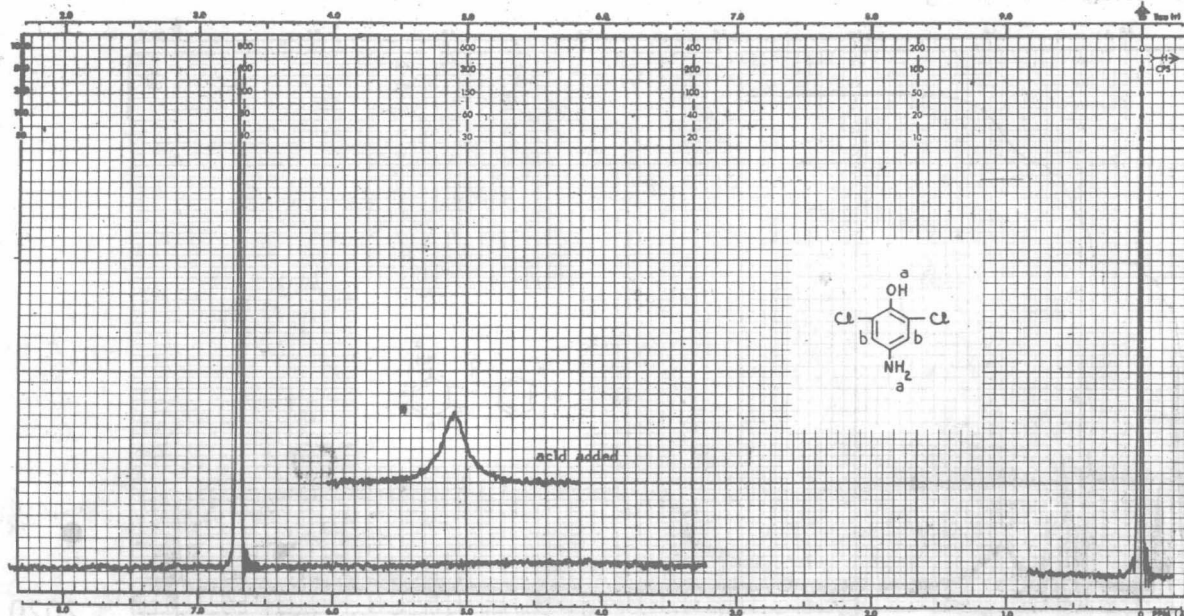
Mol. Wt. 178.02

Source: Aldrich Chemical Company, Milwaukee, Wis.

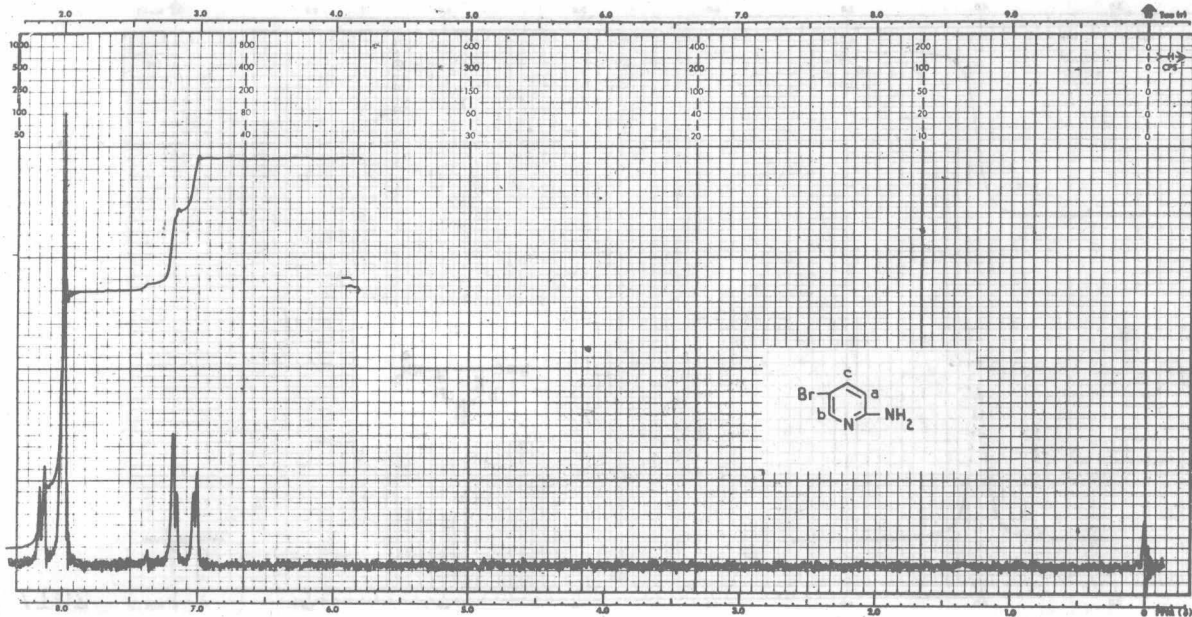
Filter Bandwidth: 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 50
 Integral amp: 80 (spec. amp. 12.5)
 Solvent Acetone

ASSIGNMENTS

a ca 4.20 f _____
 b 6.70 g _____
 c _____ h _____
 d _____ i _____
 e _____ i _____
 Trace of acid added for OH & NH₂



2018 M



2019 M

2-AMINO-5-BROMOPYRIDINE

IR 18347

$C_5H_5BrN_2$

Mol. Wt. 173.02

Source: Aldrich Chemical Company, Milwaukee, Wis.

ASSIGNMENTS

Filter Bandwidth: 4 cps

Sweep time: 500 sec

Sweep width: 500 cps

Sweep offset: - cps

Spectrum amp: 25

Integral amp: 80 (spec. amp. 12.5)

Conc. Sat'd. sol'n/0.5ml Trifluoroacetic acid

a 7.10 f

b 7.98 g

c 8.08 h

d i

e i

NH₂ is unobserved

2-AMINO BENZOPHENONE

IR 18349

$C_{13}H_{11}NO$

Mol. Wt. 197.24

Source: Aldrich Chemical Company, Milwaukee, Wis.



ASSIGNMENTS

Filter Bandwidth: 4 cps

Sweep time: 500 sec

Sweep width: 500 cps

Sweep offset: - cps

Spectrum amp: 20

Integral amp: 80 (spec. amp. 4)

Conc. 100mg/0.5ml CDCl₃

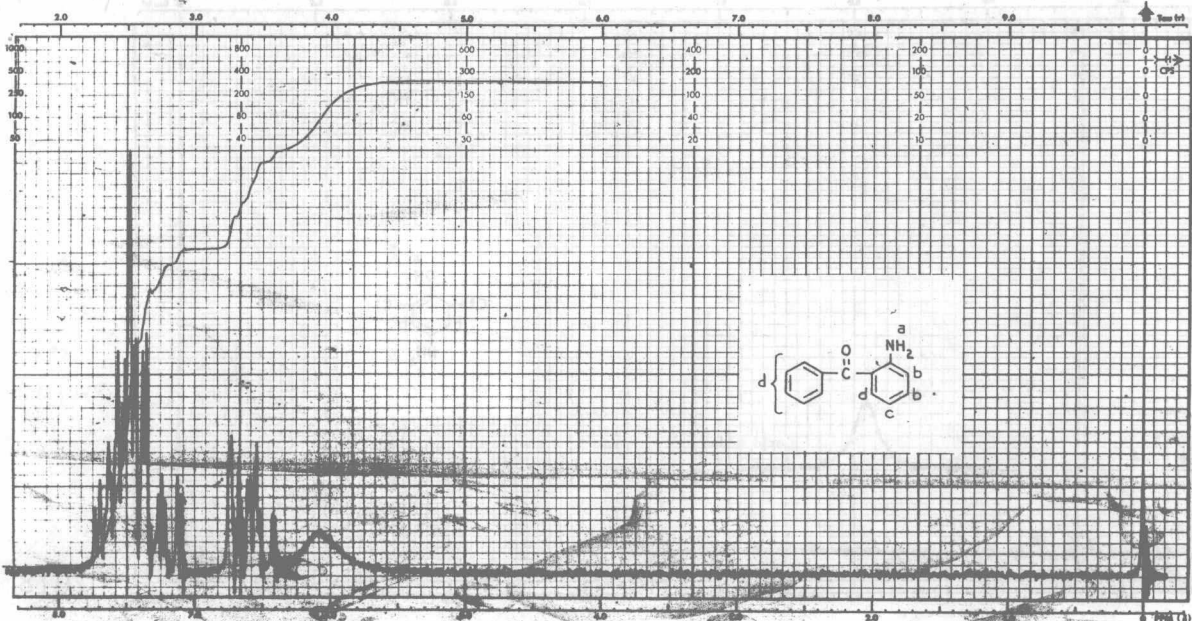
a 6.07 f

b 6.38-6.80 g

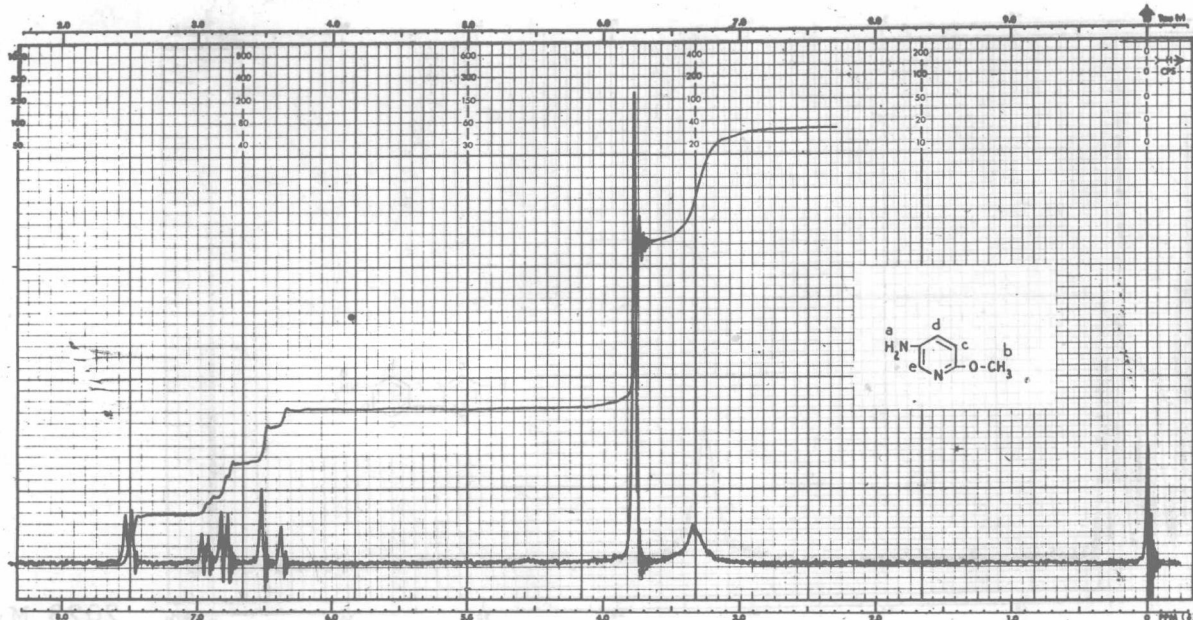
c 7.23 h

d ca 7.48 i

e i



2020 M



2021 M

5-AMINO-2-METHOXPYRIDINE

IR 18171

$C_6H_8N_2O$

Mol. Wt. 124.15

Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 12.5
 Integral amp: 80 (spec. amp. 8)
 Conc. 100mg/0.5ml CCl_4

ASSIGNMENTS

a	3.34	f	
b	3.78	g	
c	6.45	h	
d	6.87	i	
e	7.51	i	

6-AMINOHEXANONITRILE

IR 18352

$C_6H_{12}N_2$

Mol. Wt. 112.18

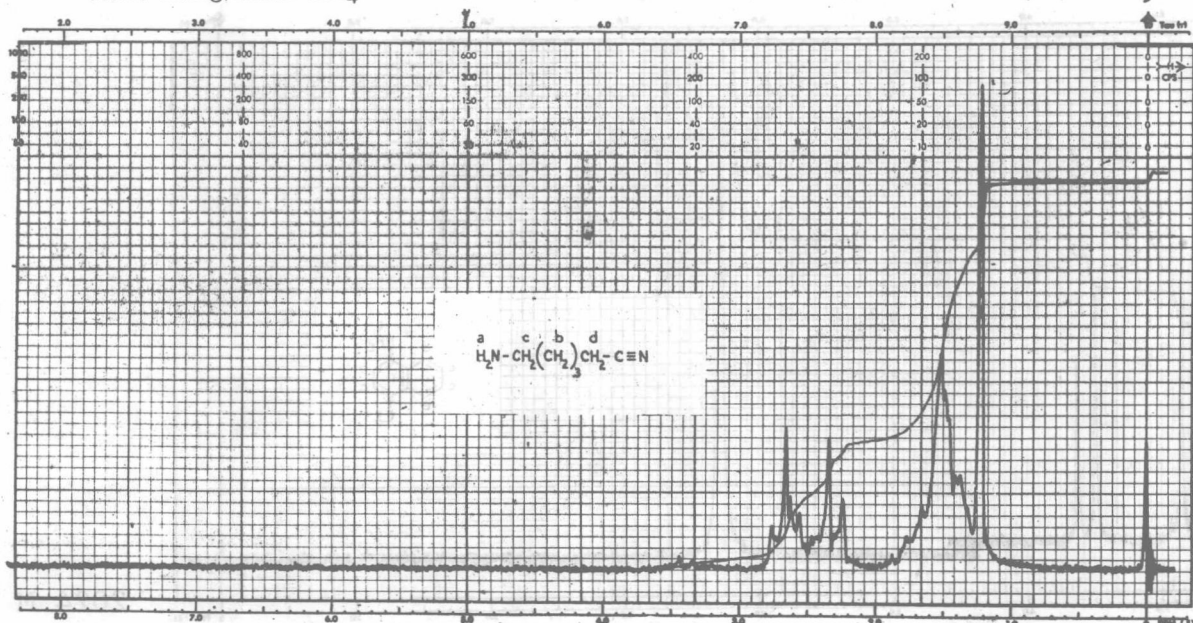
Source: Aldrich Chemical Company, Milwaukee, Wis.



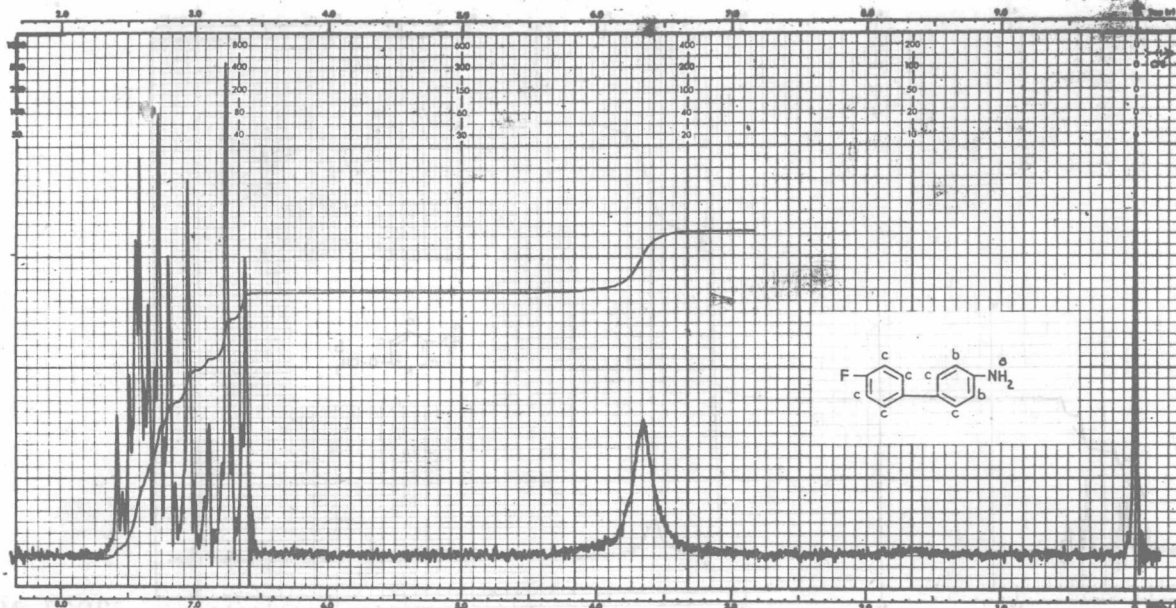
Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 16
 Integral amp: 80 (spec. amp. 2.5)
 Conc. 100mg/0.5ml CCl_4

ASSIGNMENTS

a	1.22	f	
b	ca 1.51	g	
c	2.34	h	
d	2.65	i	
e		i	



2022 M



2023 M

4'-FLUORO-4-BIPHENYLAMINE

IR 18353

$C_{12}H_{10}FN$

Mol. Wt. 187.22

Source: Aldrich Chemical Company, Milwaukee, Wis.

Filter Bandwidth: 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 80
 Integral amp: 80 (spec. amp. 6.3)
 Conc. 100mg/0.5ml $CDCl_3$

ASSIGNMENTS

a	<u>3.66</u>	f	_____
b	<u>6.70</u>	g	_____
c	<u>6.87-7.65</u>	h	_____
d	_____	i	_____
e	_____	j	_____

4-CHLORO-1-NAPHTHYLAMINE

IR 18361

$C_{10}H_8ClN$

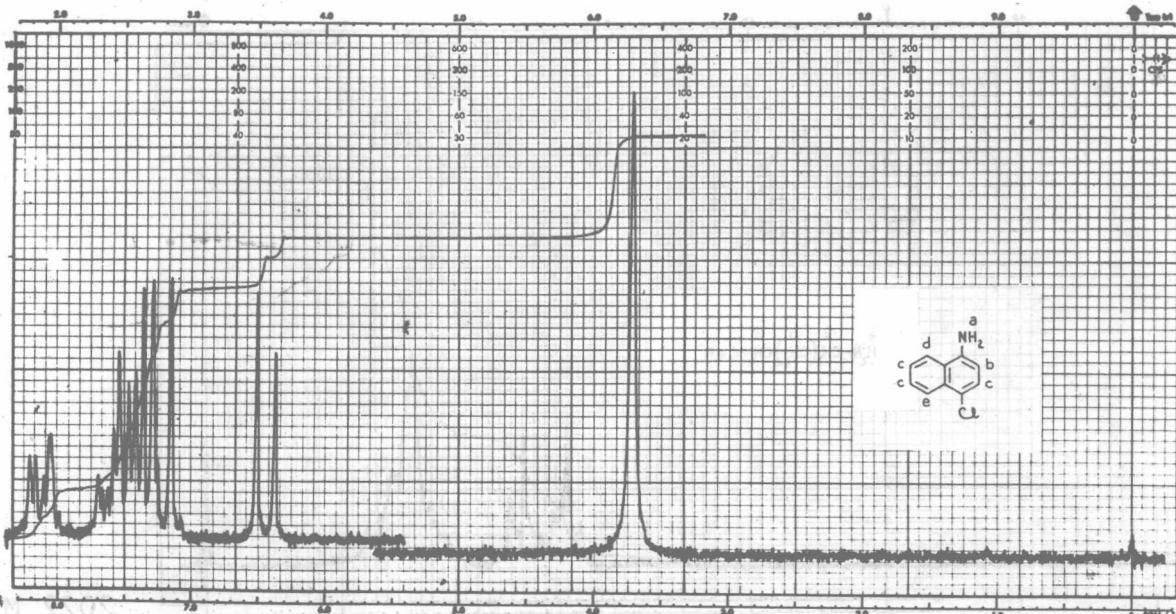
Mol. Wt. 177.63

Source: Aldrich Chemical Company, Milwaukee, Wis.

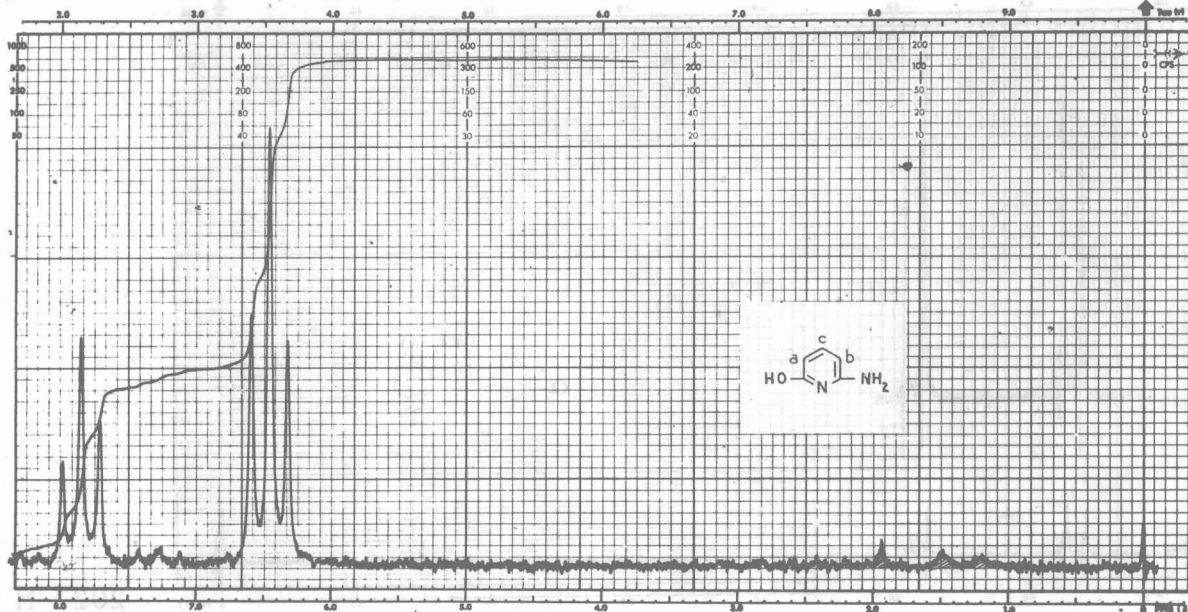
Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - /6 cps
 Spectrum amp: 40
 Integral amp: 80 (spec. amp. 5)
 Conc. Saturated solution/0.5ml $CDCl_3$

ASSIGNMENTS

a	<u>3.70</u>	f	_____
b	<u>6.54</u>	g	_____
c	<u>7.30</u>	h	_____
d	<u>7.32-7.60</u>	i	_____
e	<u>8.23</u>	j	_____



2024 M



2025 M

6-AMINO-2-PYRIDINOL

IR 18413

$C_5H_6N_2O$

Mol. Wt. 110.12

Source: Aldrich Chemical Company, Milwaukee, Wis.

ASSIGNMENTS

Filter Bandwidth: 2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 40
 Integral amp: 80 (spec. amp. 10)
 Conc.: 100mg/0.5ml Trifluoroacetic acid at 68°C

a 6.38 or b f _____
 b 6.52 or a g _____
 c 7.85 h _____
 d _____ i _____
 e _____ j _____
 OH, NH₂ unobserved

2-CHLOROMETHYL-5-(p-NITROPHENYL) OXAZOLE

IR 18416

$C_{10}H_7ClN_2O_3$

Mol. Wt. 238.63

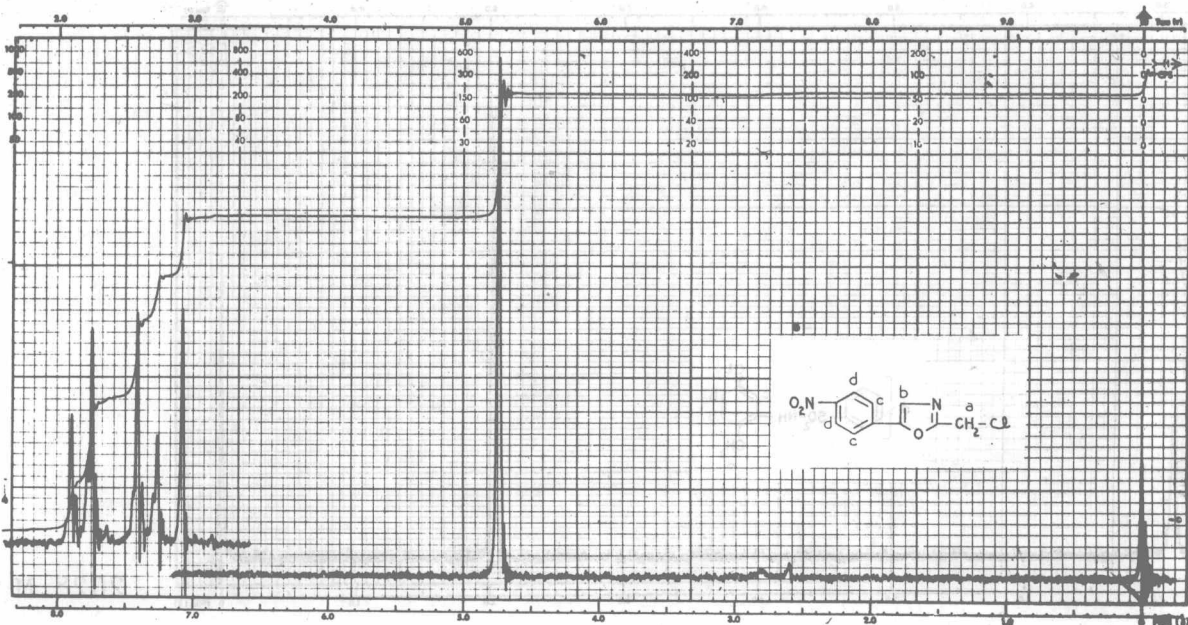
Source: Aldrich Chemical Company, Milwaukee, Wis.



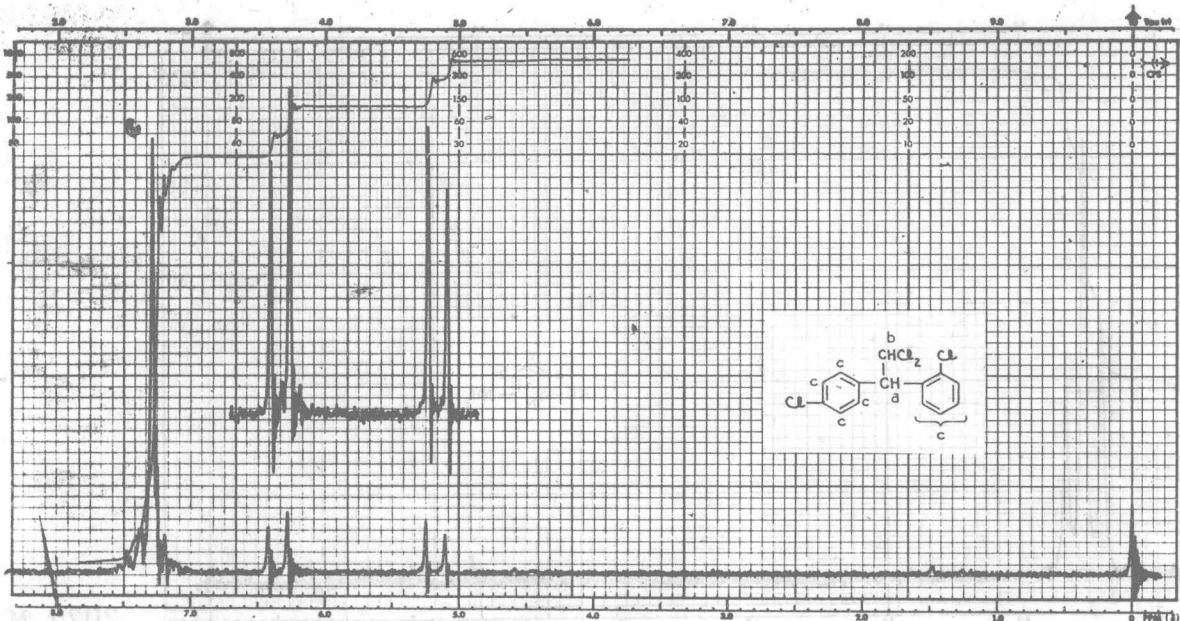
ASSIGNMENTS

Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - /30 cps
 Spectrum amp: 16
 Integral amp: 80 (spec. amp. 6.3)
 Conc.: Saturated solution/0.5ml $CDCl_3$

a 4.73 f _____
 b 7.58 g _____
 c 7.83 h _____
 d 8.32 i _____
 e _____ j _____



2026 M



2027 M

1,1-DICHLORO-2-(o-CHLOROPHENYL)-2-(p-CHLOROPHENYL) ETHANE

IR 18417

C₁₄H₁₀Cl₄

Mol. Wt. 320.06

Source: Aldrich Chemical Company, Milwaukee, Wis.

ASSIGNMENTS

Filter Bandwidth: 4/2 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 8/50
 Integral amp: 80 (spec. amp. 8)
 Conc. 100mg/0.5ml CDCl₃

a	<u>5.17</u>	f	
b	<u>6.35</u>	g	
c	<u>7.29</u>	h	
d		i	
e		j	

5'-CHLOROBENZENESULFONO-o-TOLUIDIDE

IR 18418

C₁₃H₁₂ClNO₂S

Mol. Wt. 281.76

Source: Aldrich Chemical Company, Milwaukee, Wis.

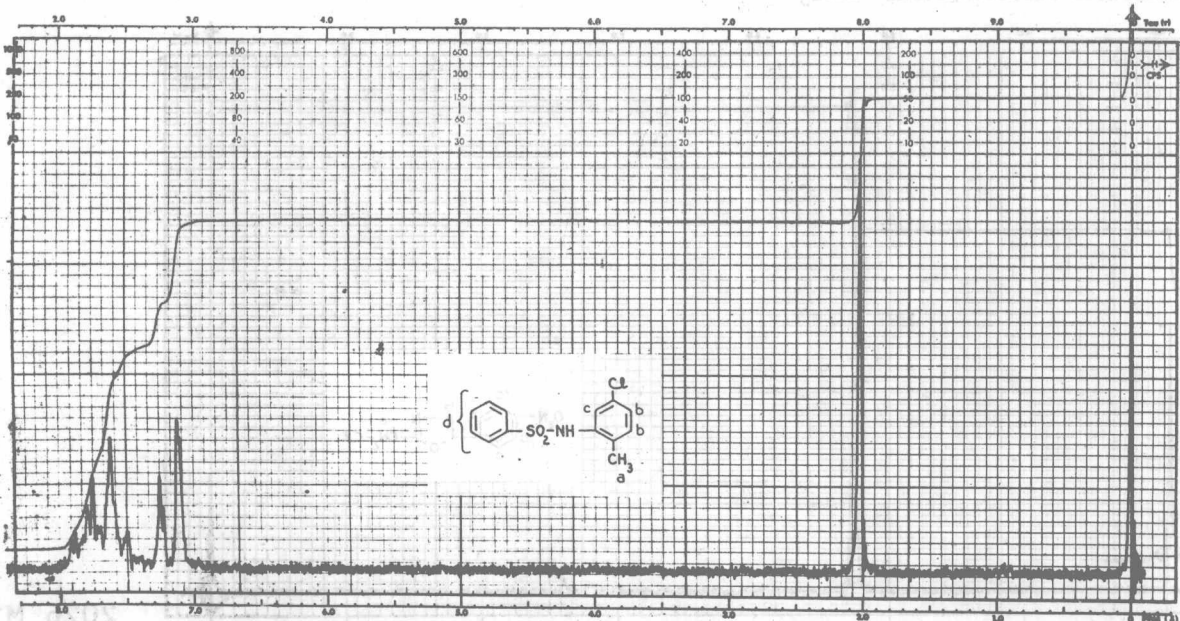


ASSIGNMENTS

Filter Bandwidth: 4 cps
 Sweep time: 250 sec
 Sweep width: 500 cps
 Sweep offset: - cps
 Spectrum amp: 20
 Integral amp: 80 (spec. amp. 8)
 Conc. Sat'd. sol'n./0.5ml Trifluoroacetic acid

a	<u>2.02</u>	f	
b	<u>7.11</u>	g	
c	<u>7.18</u>	h	
d	<u>7.38-7.97</u>	i	
e		j	

NH is unobserved



2028 M