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MASS SPECTRA OF N-NITROSO COMPOUNDS

W. Lijinsky
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ORNL-TM-4359

Contract No. W-7405-eng-26

ANALYTICAL CHEMISTRY AND BIOLOGY DIVISIONS

MASS SPECTRA OF N-NITROSO COMPOUNDS

W. Lijinsky, W. H. Christie, and W. T. Rainey, Jr.

OCTOBER 1973

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SUMMARY

The low-resolution electron impact mass spectra (70 eV) of 95 N-nitroso compounds are presented. Aliphatic, aromatic, and cyclic nitrosamines are represented, as are nitrosamino acids and nitrosamides. All but four of the compounds showed a molecular ion. Most of them gave a fragment ion at M-30 or M-31. Almost half of the compounds showed an ion at M-17, corresponding to loss of OH. It is expected that almost any N-nitroso compound can be characterized and identified from its mass spectrum.

1.0 INTRODUCTION

The N-nitroso compounds comprise the most broadly acting group of carcinogens. There seems to be no species nor any organ refractory to the tumorigenic action of one or more of them. Since man can come into contact with these compounds, either because they are present in the environment or because they can be formed by reaction of nitrite with secondary or tertiary amino compounds, especially in the acid conditions of the stomach, a means of identifying them is needed. Most methods are non-specific or require large quantities of sample, a serious disadvantage because these potent carcinogens would be expected to occur only in traces. The only method that is sufficiently sensitive and yet specific is mass spectrometry. Since most but not all N-nitroso compounds are carcinogens, it is essential to differentiate those that are from the inactive compounds.

We have examined a large number of N-nitroso compounds representing all classes and types, their mass spectra being measured under standard conditions and compared. We have looked for typical features of the mass spectra which would enable us to identify an unknown material as an N-nitroso compound and to assign a structure to it.

2.1 INDEX BY COMPOUND TYPE, INCLUDING PHYSICAL CONSTANTS

	MELTING POINT °C	BOILING POINT °C (TORR)	MOLAR ABSORP-TIVITY	λ MAX NM	SOL-VENT*	PAGE
ALIPHATIC NITROSAMINES						
N-NITROSO-						
DIMETHYLAMINE		148	100	332	W	12
HEXADEUTERODIMETHYLAMINE		148	99	331	W	13
DIETHYLAMINE		176	84	337	W	21
DI-N-PROPYLAMINE		103 (12)	86	351	E	51
DI-ISO-PROPYLAMINE	46-48		72	358	E	52
DI-N-BUTYLAMINE			89	350	E	74
1,1,1',1'-TETRADEUTERODI-N-BUTYLAMINE			86	342	W	87
DI-ISO-BUTYLAMINE		107-108 (12)	89	352	E	75
DICYCLOHEXYLAMINE	105					100
METHYLETHYLAMINE		57-58 (12)	78	333	W	16
METHYL-N-PROPYLAMINE		30-32 (0.7)	88	333	W	22
METHYL-ISO-PROPYLAMINE		28-30 (1)	79	333	W	23
METHYL-N-BUTYLAMINE		47-49 (1.5)	95	346	E	31
METHYL-ISO-BUTYLAMINE		40-42 (1.5)	95	348	E	32
METHYL-SEC-BUTYLAMINE		32-34 (0.5)	82	348	E	33
METHYL-TERT-BUTYLAMINE		38-40 (0.8)				34
METHYL-N-DODECYLAMINE		136-138 (0.9)	90	346	E	104
METHYLCYCLOHEXYLAMINE		128 (15)	79	332	W	61
TRIDEUTEROMETHYLCYCLOHEXYLAMINE						65
METHYL-2-HYDROXYETHYLAMINE		90-91 (0.2)	87	336	W	25
METHYL-2-CHLOROETHYLAMINE		75 (1)	45	337	W	41
ETHYL-N-PROPYLAMINE		35-37 (0.7)	86	350	E	35
ETHYL-ISO-PROPYLAMINE		29-31 (0.6)	77	352	E	36
METHYLVINYLAMINE						14
N-METHOXY-N-METHYLAMINE			95	331	W	17
AROMATIC NITROSAMINES						
N-NITROSO-						
METHYLPHENYLAMINE			210	370	E	58
METHYLBENZYLAMINE		68 (0.1)	82	350	E	69
PHENYLBENZYLAMINE	56-57					102
DIBENZYLAMINE	57.5-59		69	362	E	103
DIPHENYLAMINE	67					98
CARBAZOLE	79-80		280	417	E	97
NITROSAMIDES						
N-NITROSO-						
METHYLUREA	110-112 (DEC)		91	392	W	24
TRIDEUTEROMETHYLUREA	114-115 (DEC)		87	392	W	26
ETHYLUREA	98-98.5 (DEC)		74	395	W	37
PENTADEUTEROETHYLUREA	95.5-97 (DEC)		75	397	W	40
PHENYLUREA			159	403	E	88
METHYL-N'-NITROGUANIDINE	109 (DEC)		180	401	W	68
ETHYL-N'-NITROGUANIDINE	102 (DEC)		163	406	W	85
METHYL ETHYLCARBAMATE			131	400	W	56
ETHYL ETHYLCARBAMATE			127	405	W	67
1-NAPHTHYL-N-METHYLCARBAMATE	66-68		144	402	E	105
1,3,3-TRIMETHYLUREA		57 (3)	88	375	W	55
1,3,3-TRIETHYLUREA		69-70 (3)	80	371	W	94
1-METHYL-3,3-DIETHYLUREA		68 (4)	88	371	W	83
1,1-DIMETHYL-3-ETHYLUREA		67-69 (4)	77	375	W	66

	MELTING POINT °C	BOILING POINT °C (TORR)	MOLAR ABSORP-- TIVITY	λ MAX NM	SOL- VENT*	PAGE
NITROSAMINO ACIDS						
N-NITROSO-						
SARCOSINE	66-67		86	340	W	38
IMINODIACETIC ACID	145.5-146.5		84	350	W	86
AZETIDINE-2-CARBOXYLIC ACID	106-107		94	343	W	50
PROLINE	100-101		91	343	W	64
4-HYDROXYPROLINE	114-115		92	345	W	84
PIPECOLIC ACID	91-92		91	345	W	78
2-DEUTEROPIPECOLIC ACID						82
L-PIPECOLIC ACID						81
NIPECOTIC ACID	96-98		83	351	E	79
ISONIPECOTIC ACID	142-143		86	341	W	80
GUVACINE	174-174.5		89	340	W	73
GUVACOLINE		137-138 (3)	101	351	W	89
CYCLIC NITROSAMINES						
N-NITROSO-						
AZETIDINE		55-57 (0.5)	95	332	W	15
2,2,4,4-TETRADEUTEROAZETIDINE		52-54 (1.5)				18
PYRROLIDINE		78-79 (8)	104	333	W	20
PIPERIDINE		75-76 (6)	87	335	W	28
DECADEUTEROPIPERIDINE			85	338	W	42
HEXAMETHYLENEIMINE		120-121 (15)	93	334	W	48
HEPTAMETHYLENEIMINE	20-22		93	336	W	60
OCTAMETHYLENEIMINE	56-57		92	337	W	72
DODECAMETHYLENEIMINE	28-29		88	352	E	101
3-PYRROLINE	32.5-33					19
MORPHOLINE	27-29		93	340	W	30
3,3,5,5-TETRADEUTEROMORPHOLINE	28-30					39
THIOMORPHOLINE	50-51		99	347	W	57
PIPERAZINE		80-85 (0.1)	96	341	W	29
3-AZABICYCLO(3.2.2)NONANE	165-167		94	351	E	71
1,2,3,6-TETRAHYDROPYRIDINE			101	339	W	27
1-METHYL-PIPERAZINE		88 (8.5)	92	343	W	49
2,5-DIMETHYLPYRROLIDINE		86-88 (12)	86	342	W	47
2-METHYLPIPERIDINE		80 (7)	79	340	W	43
3-METHYLPIPERIDINE		88 (9)	92	340	W	44
4-METHYLPIPERIDINE		80-81 (7)	92	339	W	45
2,6-DIMETHYLPIPERIDINE	34-35		95	345	W	59
2,2,6,6-TETRAMETHYLPIPERIDINE		66-68 (4)	58	366	W	90
4-PIPERIDONE	65-67		95	341	W	46
3-PIPERIDINOL	40-42		78	353	E	53
4-PIPERIDINOL			101	357	W	54
2,2,6,6-TETRAMETHYL-4-PIPERIDONE	65-66		54	370	E	95
2,2,6,6-TETRAMETHYL-4-PIPERIDINOL	94-95		59	379	E	96
2,6-DIMETHYLMORPHOLINE		82-84 (8)	93	343	W	62
PHENMETRAZINE	63-64		84	344	W	99
METHYLPHENIDATE	105-106		97	345	W	106
N,N'-DINITROSO-						
PIPERAZINE	155-156		178	341	W	63
OCTADEUTEROPIPERAZINE			192	360	E	70
HOMOPIPERAZINE	91-91.5		172	347	E	76
1,5-DIAZACYCLOOCTANE	143-144		160	354	E	93
2-METHYL-PIPERAZINE	67-68		181	346	W	77
2,5-DIMETHYL-PIPERAZINE	169-170		163	362	W	91
2,6-DIMETHYL-PIPERAZINE	87-88		173	348	W	92

*W = WATER SOLUTION
E = ETHANOL SOLUTION

2.2 INDEX BY MOLECULAR WEIGHT

MW	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
74	12	N-NITROSODIMETHYLAMINE												
			42	100	74	88	30	52	43	51	44	21	32	13
80	13	N-NITROSOHEXADEUTERODIMETHYLAMINE												
			80	100	46	89	30	65	48	39	32	18	44	11
86	14	N-NITROSOMETHYLVINYLAMINE												
			30	100	42	94	57	28	56	25	41	19	86	15
86	15	N-NITROSOAZETIDINE												
			30	100	41	53	86	43	42	39	55	29	44	24
88	16	N-NITROSOMETHYLETHYLAMINE												
			42	100	88	68	43	66	30	42	56	21	57	14
90	17	N-NITROSO-N-METHOXY-N-METHYLAMINE												
			30	100	60	59	45	33	33	16	31	15	59	12
90	18	N-NITROSO-2,2,4,4-TETRADEUTEROAZETIDINE												
			90	100	30	77	32	41	43	39	46	39	33	35
98	19	N-NITROSO-3-PYRROLINE												
			41	100	32	68	39	64	44	62	98	49	67	32
100	20	N-NITROSOPYRROLIDINE												
			41	100	42	59	30	58	100	50	43	38	39	30
102	21	N-NITROSODIETHYLAMINE												
			44	100	42	99	102	58	56	54	57	48	30	26
102	22	N-NITROSOMETHYL-N-PROPYLAMINE												
			42	100	43	63	44	33	73	23	102	23	41	21
102	23	N-NITROSOMETHYLISOPROPYLAMINE												
			42	100	43	86	56	76	102	69	57	64	41	42
103	24	N-NITROSO-N-METHYLUREA												
			44	100	60	99	43	88	30	66	42	45	32	14
104	25	N-NITROSOMETHYL-2-HYDROXYETHYLAMINE												
			43	100	42	78	44	53	31	52	73	21	30	18
106	26	N-NITROSO-N-TRIDEUTEROMETHYLUREA												
			44	100	63	84	30	69	43	61	46	27	33	18
112	27	N-NITROSO-1,2,3,6-TETRAHYDROPYRIDINE												
			112	100	82	25	67	10	55	8	80	7	54	6
114	28	N-NITROSOPIPERIDINE												
			42	100	55	62	114	48	41	42	30	36	32	27
115	29	N-NITROSOPIPERAZINE												
			56	100	85	64	42	43	30	31	43	26	55	25
116	30	N-NITROSOMORPHOLINE												
			56	100	116	39	30	33	86	26	42	23	55	17
116	31	N-NITROSOMETHYL-N-BUTYLAMINE												
			43	100	42	99	44	97	73	66	74	42	41	39
116	32	N-NITROSOMETHYLISOBUTYLAMINE												
			42	100	43	70	41	51	30	36	44	36	39	29
116	33	N-NITROSOMETHYL-SEC-BUTYLAMINE												
			57	100	42	95	56	91	41	48	116	35	58	29
116	34	N-NITROSOMETHYL-TERT-BUTYLAMINE												
			57	100	56	83	41	63	39	27	32	25	116	22
116	35	N-NITROSOETHYL-N-PROPYLAMINE												
			42	100	116	88	56	84	57	73	32	55	43	50
116	36	N-NITROSOETHYLISOPROPYLAMINE												
			43	100	116	98	56	96	42	84	41	57	70	47
117	37	N-NITROSO-N-ETHYLUREA												
			44	100	43	98	74	64	30	62	42	44	59	31
118	38	N-NITROSOSARCOSINE												
			42	100	43	55	73	33	30	20	44	19	45	18
120	39	N-NITROSO-3,3,5,5-TETRADEUTEROMORPHOLINE												
			60	100	120	52	30	39	90	33	46	17	32	15
122	40	N-NITROSO-N-PENTADEUTEROETHYLUREA												
			30	100	43	84	34	79	44	78	32	51	79	48
122	41	N-NITROSOMETHYL-2-CHLOROETHYLAMINE												
			42	100	73	77	43	72	122	29	87	27	30	20
124	42	N-NITROSODECADEUTEROPIPERIDINE												
			46	100	62	49	124	49	30	44	44	31	34	30
128	43	N-NITROSO-2-METHYLPIPERIDINE												
			56	100	128	80	41	68	42	63	55	63	83	38

MW	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
128	44	N-NITROSO-3-METHYLPIPERIDINE												
			42	100	41	92	128	48	69	47	30	40	55	33
128	45	N-NITROSO-4-METHYLPIPERIDINE												
			42	100	41	76	128	56	56	44	30	31	55	31
128	46	N-NITROSO-4-PIPERIDONE												
			42	100	56	54	111	46	128	44	112	27	30	24
128	47	N-NITROSO-2,5-DIMETHYLPYRROLIDINE												
			42	100	41	63	55	63	128	63	56	38	39	33
128	48	N-NITROSOHEXAMETHYLENEIMINE												
			41	100	42	90	128	59	55	44	30	39	44	37
129	49	N-NITROSO-1-METHYLPIPERAZINE												
			99	100	57	56	70	10	58	6	100	5	45	5
130	50	N-NITROSOAZETIDINE-2-CARBOXYLIC ACID												
			45	100	55	96	30	89	54	57	41	48	85	48
130	51	N-NITROSODI-N-PROPYLAMINE												
			43	100	70	64	42	63	41	45	30	25	130	22
130	52	N-NITROSODIISOPROPYLAMINE												
			43	100	42	33	41	32	70	32	130	28	58	24
130	53	N-NITROSO-3-PIPERIDINOL												
			43	100	30	77	42	53	41	49	71	48	130	42
130	54	N-NITROSO-4-PIPERIDINOL												
			42	100	56	77	43	59	130	51	55	50	44	45
131	55	N-NITROSOTRIMETHYLUREA												
			72	100	42	32	43	20	30	13	44	13	73	9
132	56	N-NITROSO-N-METHYL ETHYL CARBAMATE												
			43	100	30	92	60	35	58	20	42	13	87	13
132	57	N-NITROSOTHIOMORPHOLINE												
			42	100	132	82	56	33	102	30	45	26	32	22
136	58	N-NITROSOMETHYLPHENYLAMINE												
			106	100	77	93	51	37	30	32	39	26	107	25
142	59	N-NITROSO-2,6-DIMETHYLPIPERIDINE												
			41	100	69	90	42	83	142	78	55	65	44	60
142	60	N-NITROSOHEPTAMETHYLENEIMINE												
			41	100	42	80	55	78	30	55	44	54	112	52
142	61	N-NITROSOMETHYLCYCLOHEXYLAMINE												
			42	100	83	100	55	95	142	80	61	48	41	44
144	62	N-NITROSO-2,6-DIMETHYLMORPHOLINE												
			42	100	41	76	70	54	114	34	43	18	39	16
144	63	1,4-DINITROSOPIPERAZINE												
			42	100	55	55	57	44	144	42	84	41	30	39
144	64	N-NITROSOPROLINE												
			41	100	99	89	69	58	68	41	42	36	30	33
145	65	N-NITROSOTRIDEUTEROMETHYLCYCLOHEXYLAMINE												
			45	100	55	57	83	41	41	39	64	27	73	27
145	66	N-NITROSO-1,1-DIMETHYL-3-ETHYLUREA												
			72	100	42	27	44	23	43	10	30	10	56	8
146	67	N-NITROSO-N-ETHYL ETHYL CARBAMATE												
			30	100	44	44	42	38	56	31	43	22	45	21
147	68	N-NITROSO-N-METHYL-N'-NITROGUANIDINE												
			43	100	72	100	42	98	57	87	101	35	46	26
150	69	N-NITROSOMETHYLBENZYLAMINE												
			91	100	42	55	51	24	39	23	77	20	30	16
152	70	1,4-DINITROSOOCTADEUTEROPIPERAZINE												
			46	100	60	50	30	49	64	37	32	32	152	28
154	71	N-NITROSO-3-AZABICYCLO(3.2.2)NONANE												
			44	100	42	60	41	56	154	56	95	41	30	35
156	72	N-NITROSOOCTAMETHYLENEIMINE												
			126	100	41	67	55	65	30	49	42	47	44	43
156	73	N-NITROSOGUVACINE												
			156	100	53	74	80	50	126	30	41	29	39	27
158	74	N-NITROSODI-N-BUTYLAMINE												
			57	100	41	80	84	80	42	71	43	64	30	57
158	75	N-NITROSODIISOBUTYLAMINE												
			57	100	43	98	42	75	84	75	115	62	41	60

MW	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
158	76	N,N'-DINITROSOHOMOPIPERAZINE												
			43	100	42	75	98	42	56	41	41	36	128	31
158	77	N,N'-DINITROSO-2-METHYLPIPERAZINE												
			56	100	98	53	42	52	69	26	41	20	30	20
158	78	N-NITROSOPIPECOLIC ACID												
			83	100	55	74	113	54	41	23	84	18	42	16
158	79	N-NITROSONIPECOTIC ACID												
			55	100	127	89	42	72	56	55	82	53	44	43
158	80	N-NITROSOISONIPECOTIC ACID												
			82	100	42	71	128	45	55	42	41	23	30	22
158	81	N-NITROSO-L-PIPECOLIC ACID												
			83	100	55	77	113	50	84	31	41	29	42	24
159	82	N-NITROSO-2-DEUTEROPIPECOLIC ACID												
			84	100	56	68	114	54	85	40	55	36	57	21
159	83	N-NITROSO-1-METHYL-3,3-DIETHYLUREA												
			72	100	100	85	44	43	42	38	56	24	30	19
160	84	N-NITROSO-4-HYDROXYPROLINE												
			56	100	41	86	30	72	42	53	44	53	115	46
161	85	N-NITROSO-N-ETHYL-N'-NITROGUANIDINE												
			43	100	30	34	72	33	42	31	56	20	115	19
162	86	N-NITROSOIMINODIACETIC ACID												
			42	100	30	53	88	48	117	29	43	27	44	26
162	87	N-NITROSO-1,1,1',1'-TETRADEUTERODI-N-BUTYLAMINE												
			59	100	46	88	30	81	87	72	43	68	47	59
165	88	N-NITROSO-N-PHENYLUREA												
			65	100	93	98	77	95	135	70	92	41	39	38
170	89	N-NITROSOGUVACOLINE												
			53	100	170	85	80	82	140	57	81	48	45	45
170	90	N-NITROSO-2,2,6,6-TETRAMETHYLPIPERIDINE												
			41	100	69	100	55	72	56	69	42	63	39	46
172	91	N,N'-DINITROSO-2,5-DIMETHYLPIPERAZINE												
			56	100	112	42	41	23	42	23	70	20	69	18
172	92	N,N'-DINITROSO-2,6-DIMETHYLPIPERAZINE												
			112	100	70	60	56	40	69	27	43	24	83	24
172	93	1,5-DINITROSO-1,5-DIAZACYCLOOCTANE												
			84	100	30	89	112	75	41	66	42	65	83	55
173	94	N-NITROSOTRIETHYLUREA												
			100	100	72	83	56	45	44	40	42	29	30	14
184	95	N-NITROSO-2,2,6,6-TETRAMETHYL-4-PIPERIDONE												
			56	100	41	35	42	27	39	17	83	15	97	15
186	96	N-NITROSO-2,2,6,6-TETRAMETHYL-4-PIPERIDINOL												
			71	100	57	99	86	81	41	58	56	55	42	44
196	97	N-NITROSOCARBAZOLE												
			167	100	166	73	140	16	139	13	168	11	30	5
198	98	N-NITROSODIPHENYLAMINE												
			169	100	168	52	167	33	30	32	51	32	39	21
206	99	N-NITROSOPHENMETRAZINE												
			70	100	176	48	42	19	105	10	77	9	56	6
210	100	N-NITROSODICYCLOHEXYLAMINE												
			83	100	55	81	41	75	67	31	138	31	54	30
212	101	N-NITROSODODECAMETHYLENEIMINE												
			41	100	55	97	44	71	43	70	182	60	30	59
212	102	N-NITROSOPHENYLBENZYLAMINE												
			182	100	77	81	91	62	105	33	183	30	51	28
226	103	N-NITROSODIBENZYLAMINE												
			91	100	65	14	226	11	92	9	39	6	51	5
228	104	N-NITROSOMETHYLDODECYLAMINE												
			211	100	44	67	43	63	74	39	73	33	42	32
230	105	N-NITROSO-1-NAPHTHYL-N-METHYLCARBAMATE												
			115	100	143	72	144	26	116	14	89	8	63	7
262	106	N-NITROSOMETHYLPHENIDATE												
			113	100	83	63	121	33	55	23	91	18	149	16

2.3 INDEX BY BASE PEAK

BASE	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30	67	N-NITROSO-N-ETHYL ETHYL CARBAMATE												
			30	100	44	44	42	38	56	31	43	22	45	21
30	40	N-NITROSO-N-PENTADEUTEROETHYLUREA												
			30	100	43	84	34	79	44	78	32	51	79	48
30	14	N-NITROSOMETHYLVINYLAMINE												
			30	100	42	94	57	28	56	25	41	19	86	15
30	15	N-NITROSOAZETIDINE												
			30	100	41	53	86	43	42	39	55	29	44	24
30	17	N-NITROSO-N-METHOXY-N-METHYLAMINE												
			30	100	60	59	45	33	33	16	31	15	59	12
41	64	N-NITROSOPROLINE												
			41	100	99	89	69	58	68	41	42	36	30	33
41	59	N-NITROSO-2,6-DIMETHYLPIPERIDINE												
			41	100	69	90	42	83	142	78	55	65	44	60
41	90	N-NITROSO-2,2,6,6-TETRAMETHYLPIPERIDINE												
			41	100	69	100	55	72	56	69	42	63	39	46
41	101	N-NITROSODODECAMETHYLENEIMINE												
			41	100	55	97	44	71	43	70	182	60	30	59
41	48	N-NITROSOHEXAMETHYLENEIMINE												
			41	100	42	90	128	59	55	44	30	39	44	37
41	60	N-NITROSOHEPTAMETHYLENEIMINE												
			41	100	42	80	55	78	30	55	44	54	112	52
41	19	N-NITROSO-3-PYRROLINE												
			41	100	32	68	39	64	44	62	98	49	67	32
41	20	N-NITROSOPYRROLIDINE												
			41	100	42	59	30	58	100	50	43	38	39	30
42	61	N-NITROSOMETHYLCYCLOHEXYLAMINE												
			42	100	83	100	55	95	142	80	61	48	41	44
42	62	N-NITROSO-2,6-DIMETHYLMORPHOLINE												
			42	100	41	76	70	54	114	34	43	18	39	16
42	63	1,4-DINITROSOPIPERAZINE												
			42	100	55	55	57	44	144	42	84	41	30	39
42	57	N-NITROSOTHIOMORPHOLINE												
			42	100	132	82	56	33	102	30	45	26	32	22
42	86	N-NITROSOIMINODIACETIC ACID												
			42	100	30	53	88	48	117	29	43	27	44	26
42	47	N-NITROSO-2,5-DIMETHYLPYRROLIDINE												
			42	100	41	63	55	63	128	63	56	38	39	33
42	44	N-NITROSO-3-METHYLPIPERIDINE												
			42	100	41	92	128	48	69	47	30	40	55	33
42	45	N-NITROSO-4-METHYLPIPERIDINE												
			42	100	41	76	128	56	56	44	30	31	55	31
42	54	N-NITROSO-4-PIPERIDINOL												
			42	100	56	77	43	59	130	51	55	50	44	45
42	46	N-NITROSO-4-PIPERIDONE												
			42	100	56	54	111	46	128	44	112	27	30	24
42	41	N-NITROSOMETHYL-2-CHLOROETHYLAMINE												
			42	100	73	77	43	72	122	29	87	27	30	20
42	38	N-NITROSOSARCOSINE												
			42	100	43	55	73	33	30	20	44	19	45	18
42	22	N-NITROSOMETHYL-N-PROPYLAMINE												
			42	100	43	63	44	33	73	23	102	23	41	21
42	23	N-NITROSOMETHYLISOPROPYLAMINE												
			42	100	43	86	56	76	102	69	57	64	41	42
42	35	N-NITROSOETHYL-N-PROPYLAMINE												
			42	100	116	88	56	84	57	73	32	55	43	50
42	32	N-NITROSOMETHYLISOBUTYLAMINE												
			42	100	43	70	41	51	30	36	44	36	39	29
42	28	N-NITROSOPIPERIDINE												
			42	100	55	62	114	48	41	42	30	36	32	27
42	12	N-NITROSODIMETHYLAMINE												
			42	100	74	88	30	52	43	51	44	21	32	13
42	16	N-NITROSOMETHYLETHYLAMINE												
			42	100	88	68	43	66	30	42	56	21	57	14

BASE	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
43	56	N-NITROSO-N-METHYL ETHYL CARBAMATE												
			43	100	30	92	60	35	58	20	42	13	87	13
43	76	N,N'-DINITROSOHOMOPIPERAZINE												
			43	100	42	75	98	42	56	41	41	36	128	31
43	68	N-NITROSO-N-METHYL-N'-NITROGUANIDINE												
			43	100	72	100	42	98	57	87	101	35	46	26
43	85	N-NITROSO-N-ETHYL-N'-NITROGUANIDINE												
			43	100	30	34	72	33	42	31	56	20	115	19
43	51	N-NITROSODI-N-PROPYLAMINE												
			43	100	70	64	42	63	41	45	30	25	130	22
43	52	N-NITROSODIISOPROPYLAMINE												
			43	100	42	33	41	32	70	32	130	28	58	24
43	53	N-NITROSO-3-PIPERIDINOL												
			43	100	30	77	42	53	41	49	71	48	130	42
43	36	N-NITROSOETHYLISOPROPYLAMINE												
			43	100	116	98	56	96	42	84	41	57	70	47
43	31	N-NITROSOMETHYL-N-BUTYLAMINE												
			43	100	42	99	44	97	73	66	74	42	41	39
43	25	N-NITROSOMETHYL-2-HYDROXYETHYLAMINE												
			43	100	42	78	44	53	31	52	73	21	30	18
44	71	N-NITROSO-3-AZABICYCLO(3.2.2)NONANE												
			44	100	42	60	41	56	154	56	95	41	30	35
44	21	N-NITROSODIETHYLAMINE												
			44	100	42	99	102	58	56	54	57	48	30	26
44	24	N-NITROSO-N-METHYLUREA												
			44	100	60	99	43	88	30	66	42	45	32	14
44	26	N-NITROSO-N-TRIDEUTEROMETHYLUREA												
			44	100	63	84	30	69	43	61	46	27	33	18
44	37	N-NITROSO-N-ETHYLUREA												
			44	100	43	98	74	64	30	62	42	44	59	31
45	65	N-NITROSOTRIDEUTEROMETHYLCYCLOHEXYLAMINE												
			45	100	55	57	83	41	41	39	64	27	73	27
45	50	N-NITROSOAZETIDINE-2-CARBOXYLIC ACID												
			45	100	55	96	30	89	54	57	41	48	85	48
46	42	N-NITROSODECADEUTEROPIPERIDINE												
			46	100	62	49	124	49	30	44	44	31	34	30
46	70	1,4-DINITROSOOCTADEUTEROPIPERAZINE												
			46	100	60	50	30	49	64	37	32	32	152	28
53	89	N-NITROSOGUVACOLINE												
			53	100	170	85	80	82	140	57	81	48	45	45
55	79	N-NITROSONIPECOTIC ACID												
			55	100	127	89	42	72	56	55	82	53	44	43
56	29	N-NITROSOPIPERAZINE												
			56	100	85	64	42	43	30	31	43	26	55	25
56	77	N,N'-DINITROSO-2-METHYLPIPERAZINE												
			56	100	98	53	42	52	69	26	41	20	30	20
56	91	N,N'-DINITROSO-2,5-DIMETHYLPIPERAZINE												
			56	100	112	42	41	23	42	23	70	20	69	18
56	95	N-NITROSO-2,2,6,6-TETRAMETHYL-4-PIPERIDONE												
			56	100	41	35	42	27	39	17	83	15	97	15
56	84	N-NITROSO-4-HYDROXYPROLINE												
			56	100	41	86	30	72	42	53	44	53	115	46
56	43	N-NITROSO-2-METHYLPIPERIDINE												
			56	100	128	80	41	68	42	63	55	63	83	38
56	30	N-NITROSOMORPHOLINE												
			56	100	116	39	30	33	86	26	42	23	55	17
57	74	N-NITROSODI-N-BUTYLAMINE												
			57	100	41	80	84	80	42	71	43	64	30	57
57	75	N-NITROSODIISOBUTYLAMINE												
			57	100	43	98	42	75	84	75	115	62	41	60
57	33	N-NITROSOMETHYL-SEC-BUTYLAMINE												
			57	100	42	95	56	91	41	48	116	35	58	29
57	34	N-NITROSOMETHYL-TERT-BUTYLAMINE												
			57	100	56	83	41	63	39	27	32	25	116	22

BASE	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
59	87	N-NITROSO-1,1,1',1'-TETRADEUTERODI-N-BUTYLAMINE												
			59	100	46	88	30	81	87	72	43	68	47	59
60	39	N-NITROSO-3,3,5,5-TETRADEUTEROMORPHOLINE												
			60	100	120	52	30	39	90	33	46	17	32	15
65	88	N-NITROSO-N-PHENYLUREA												
			65	100	93	98	77	95	135	70	92	41	39	38
70	99	N-NITROSOPHENMETRAZINE												
			70	100	176	48	42	19	105	10	77	9	56	6
71	96	N-NITROSO-2,2,6,6-TETRAMETHYL-4-PIPERIDINOL												
			71	100	57	99	86	81	41	58	56	55	42	44
72	55	N-NITROSOTRIMETHYLUREA												
			72	100	42	32	43	20	30	13	44	13	73	9
72	66	N-NITROSO-1,1-DIMETHYL-3-ETHYLUREA												
			72	100	42	27	44	23	43	10	30	10	56	8
72	83	N-NITROSO-1-METHYL-3,3-DIETHYLUREA												
			72	100	100	85	44	43	42	38	56	24	30	19
80	13	N-NITROSOHEXADEUTERODIMETHYLAMINE												
			80	100	46	89	30	65	48	39	32	18	44	11
82	80	N-NITROSOISONIPECOTIC ACID												
			82	100	42	71	128	45	55	42	41	23	30	22
83	78	N-NITROSOPIPECOLIC ACID												
			83	100	55	74	113	54	41	23	84	18	42	16
83	81	N-NITROSO-L-PIPECOLIC ACID												
			83	100	55	77	113	50	84	31	41	29	42	24
83	100	N-NITROSODICYCLOHEXYLAMINE												
			83	100	55	81	41	75	67	31	138	31	54	30
84	93	1,5-DINITROSO-1,5-DIAZACYCLOOCTANE												
			84	100	30	89	112	75	41	66	42	65	83	55
84	82	N-NITROSO-2-DEUTEROPIPECOLIC ACID												
			84	100	56	68	114	54	85	40	55	36	57	21
90	18	N-NITROSO-2,2,4,4-TETRADEUTEROAZETIDINE												
			90	100	30	77	32	41	43	39	46	39	33	35
91	69	N-NITROSOMETHYLBENZYLAMINE												
			91	100	42	55	51	24	39	23	77	20	30	16
91	103	N-NITROSODIBENZYLAMINE												
			91	100	65	14	226	11	92	9	39	6	51	5
99	49	N-NITROSO-1-METHYLPIPERAZINE												
			99	100	57	56	70	10	58	6	100	5	45	5
100	94	N-NITROSOTRIETHYLUREA												
			100	100	72	83	56	45	44	40	42	29	30	14
106	58	N-NITROSOMETHYLPHENYLAMINE												
			106	100	77	93	51	37	30	32	39	26	107	25
112	92	N,N'-DINITROSO-2,6-DIMETHYLPIPERAZINE												
			112	100	70	60	56	40	69	27	43	24	83	24
112	27	N-NITROSO-1,2,3,6-TETRAHYDROPYRIDINE												
			112	100	82	25	67	10	55	8	80	7	54	6
113	106	N-NITROSOMETHYLPHENIDATE												
			113	100	83	63	121	33	55	23	91	18	149	16
115	105	N-NITROSO-1-NAPHTHYL-N-METHYLCARBAMATE												
			115	100	143	72	144	26	116	14	89	8	63	7
126	72	N-NITROSOOCTAMETHYLENEIMINE												
			126	100	41	67	55	65	30	49	42	47	44	43
156	73	N-NITROSOGUVACINE												
			156	100	53	74	80	50	126	30	41	29	39	27
167	97	N-NITROSOCARBAZOLE												
			167	100	166	73	140	16	139	13	168	11	30	5
169	98	N-NITROSODIPHENYLAMINE												
			169	100	168	52	167	33	30	32	51	32	39	21
182	102	N-NITROSOPHENYLBENZYLAMINE												
			182	100	77	81	91	62	105	33	183	30	51	28
211	104	N-NITROSOMETHYLDODECYLAMINE												
			211	100	44	67	43	63	74	39	73	33	42	32

3.1 PREPARATION OF COMPOUNDS

All of the N-nitroso compounds were prepared by reaction of the secondary amino compound with a 2- to 3-fold molar ratio of sodium nitrite in acid solution, either hydrochloric acid at 0°C or, more usually, acetic acid at room temperature. The best yields were obtained, usually with acetic acid, and often approached 100% of theoretical; reaction times of 1 or 2 hours were adequate. Most of the amino compounds were from Aldrich Chemical Company, Milwaukee, Wisconsin, but some were from Eastman Organic Chemicals, Rochester, New York, and K and K Laboratories, New York.

At completion of the reaction the solutions were extracted twice with an equal volume of ether or, more usually, methylene chloride. In the case of the neutral nitroso compounds, other than nitrosamides, the extracts were shaken with anhydrous sodium carbonate, filtered and the solvent was evaporated in a stream of nitrogen at room temperature. The residual nitrosamine was distilled *in vacuo* if a liquid, or crystallized from methanol if a solid. The extraction of nitrosamino acids from the reaction mixtures was with ether, which was dried with anhydrous magnesium sulfate and the solution evaporated in nitrogen to a small volume, from which the nitrosamino acids crystallized.

The nitrosoalkylureas and nitrosoalkylguanidines crystallized from the nitrosation mixtures and were filtered off and recrystallized from methanol. Nitrosotrialkylureas and nitrosoalkylcarbamates were extracted with methylene chloride or ether, dried with magnesium sulfate and, after removal of the solvent, distilled *in vacuo*.

All nitrosamines were stored in the dark and nitrosamides in a subzero freezer.

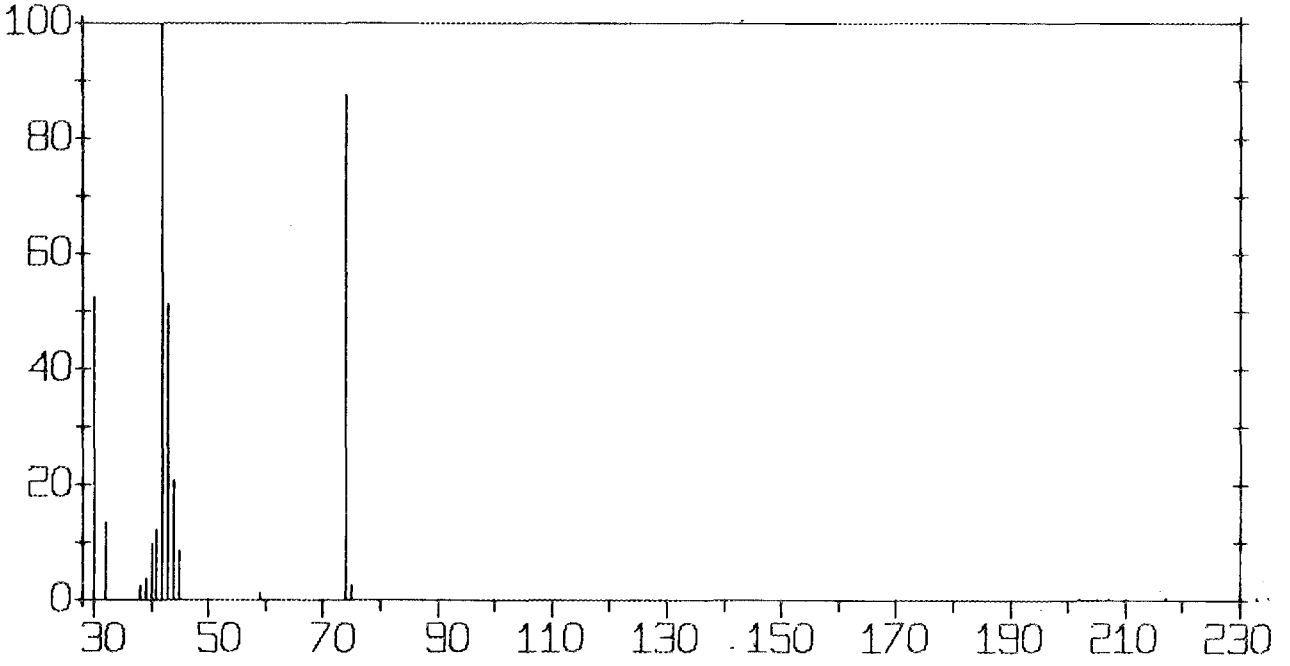
Purity of the compounds was established by sharpness of melting point or boiling point, molar absorptivity in water or ethanol and, occasionally, by thin layer chromatography and by elemental analysis.

3.2 MASS SPECTROMETRY

The mass spectra were obtained on a single-focusing mass spectrometer [30.5 cm (12 in) radius, 90° magnetic sector] constructed at this laboratory. The spectra are low resolution data ($M/\Delta M<1000$) recorded with a light pen oscillograph. The data were transferred manually to punched cards for computer reduction and plotting. Accelerating voltage was 4 kV, and ionizing voltage was 70 eV. The source can pressure was maintained at less than 5×10^{-6} torr uncorrected. The sample was introduced via a vacuum-lock direct-insertion probe operated at the lowest temperature required to give a suitable spectrum, generally below 100°C.

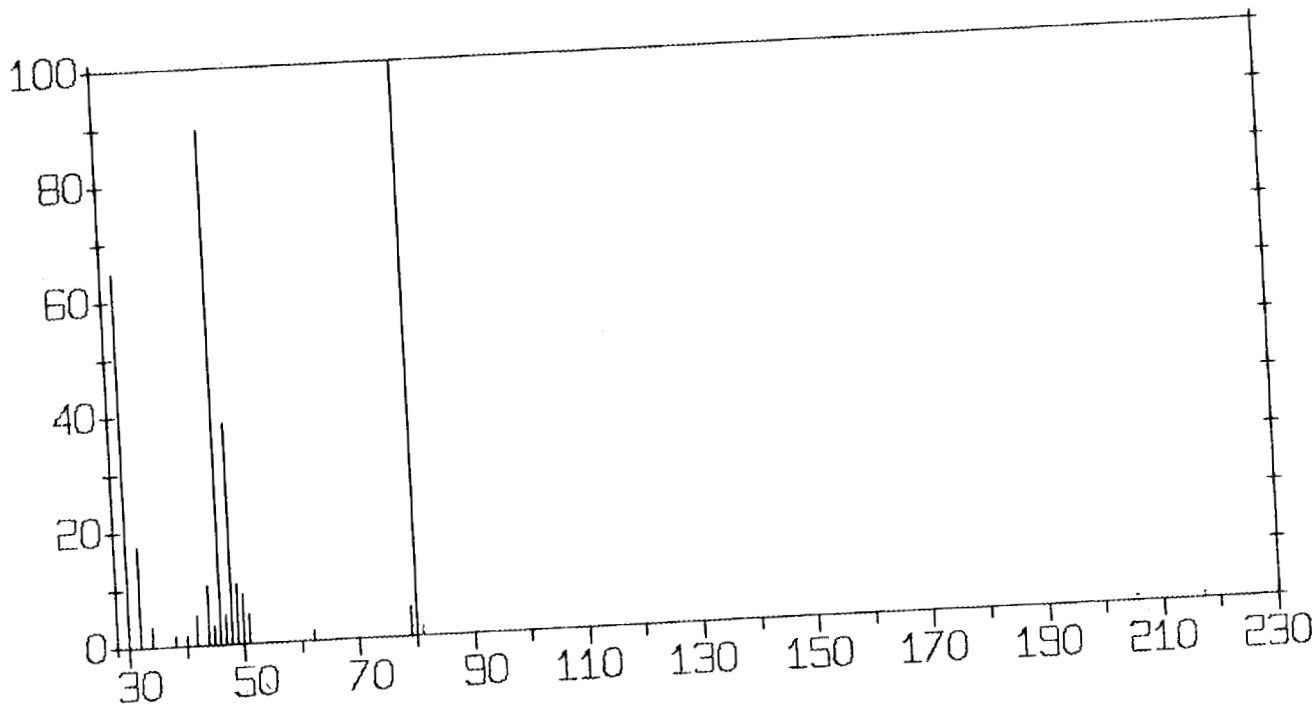
N-NITROSODIMETHYLAMINE
MW = 74 C2.H6.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	52.4	39.0	3.6	42.0	100.0	45.0	8.5	74.0	87.8
32.0	13.4	40.0	9.7	43.0	51.2	59.0	1.2	75.0	2.4
38.0	2.4	41.0	12.1	44.0	20.7				



N-NITROSOHEXADEUTERODIMETHYLAMINE
MW = 80 C2.D6.N2.O.

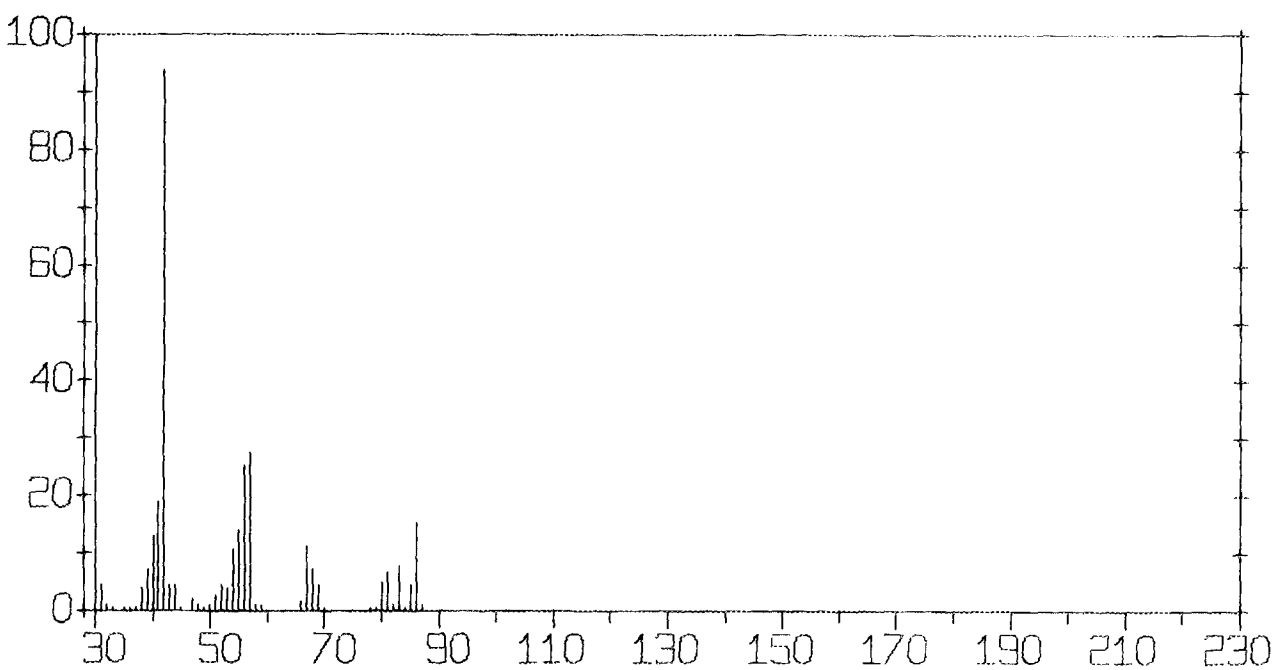
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	64.9	40.0	1.7	46.0	89.4	50.0	8.7	79.0	5.2
32.0	17.5	42.0	5.2	47.0	5.2	51.0	5.2	80.0	100.0
34.0	3.5	44.0	10.5	48.0	38.5	62.0	1.7	81.0	1.7
38.0	1.7	45.0	3.5	49.0	10.5				



N-NITROSOMETHYLVINYLAMINE
MW = 86 C3.H6.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	40.0	12.9	50.0	1.1	59.0	1.1	80.0	5.0
31.0	4.4	41.0	19.1	51.0	2.8	66.0	1.6	81.0	6.7
32.0	1.1	42.0	93.8	52.0	4.4	67.0	11.2	82.0	1.1
33.0	0.5	43.0	4.4	53.0	3.9	68.0	7.3	83.0	7.8
35.0	0.5	44.0	4.4	54.0	10.6	69.0	4.4	84.0	0.5
36.0	0.5	45.0	0.5	55.0	14.0	70.0	0.5	85.0	4.4
37.0	0.5	47.0	2.2	56.0	25.2	78.0	0.5	86.0	15.1
38.0	3.9	48.0	1.1	57.0	27.5	79.0	0.5	87.0	1.1
39.0	7.3	49.0	0.5	58.0	1.1				

OBSERVED METASTABLES
14.3, 20.5, 24.8, 76.2,



N-NITROSOAZETIDINE
MW = 86 C3.H6.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	40.0	14.2	51.0	4.0	56.0	14.2	69.0	10.2
31.0	2.0	41.0	53.0	52.0	6.1	57.0	12.2	70.0	2.0
32.0	12.2	42.0	38.7	53.0	4.0	58.0	2.0	71.0	2.0
37.0	4.0	43.0	8.1	54.0	22.4	67.0	2.0	86.0	42.8
38.0	6.1	44.0	24.4	55.0	28.5	68.0	2.0	87.0	2.0
39.0	22.4	50.0	2.0						

OBSERVED METASTABLES
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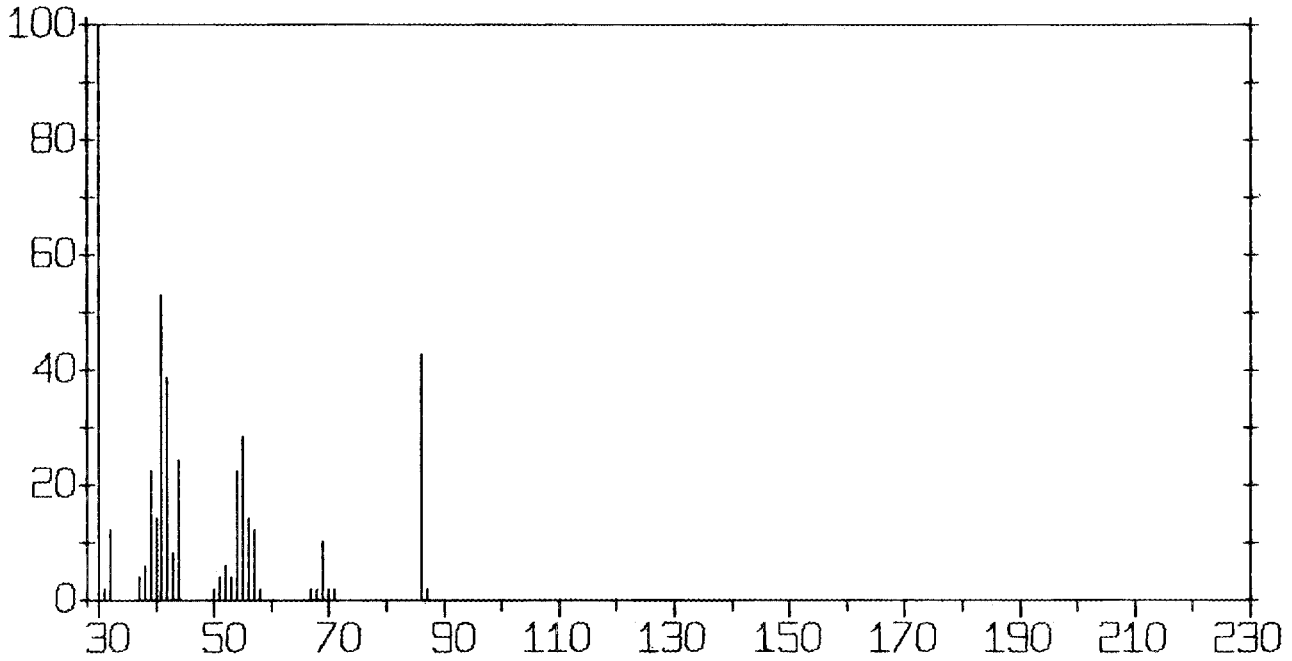

N-NITROSOMETHYLETHYLAMINE
Mw = 88 C3.H8.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	42.4	40.0	5.4	45.0	6.8	57.0	13.6	71.0	1.3
31.0	1.3	41.0	10.9	52.0	1.3	58.0	2.7	73.0	5.4
32.0	1.3	42.0	100.0	54.0	2.7	59.0	2.7	88.0	68.4
38.0	1.3	43.0	65.7	55.0	1.3	60.0	4.1	89.0	2.7
39.0	2.7	44.0	5.4	56.0	20.5				

OBSERVED METASTABLES
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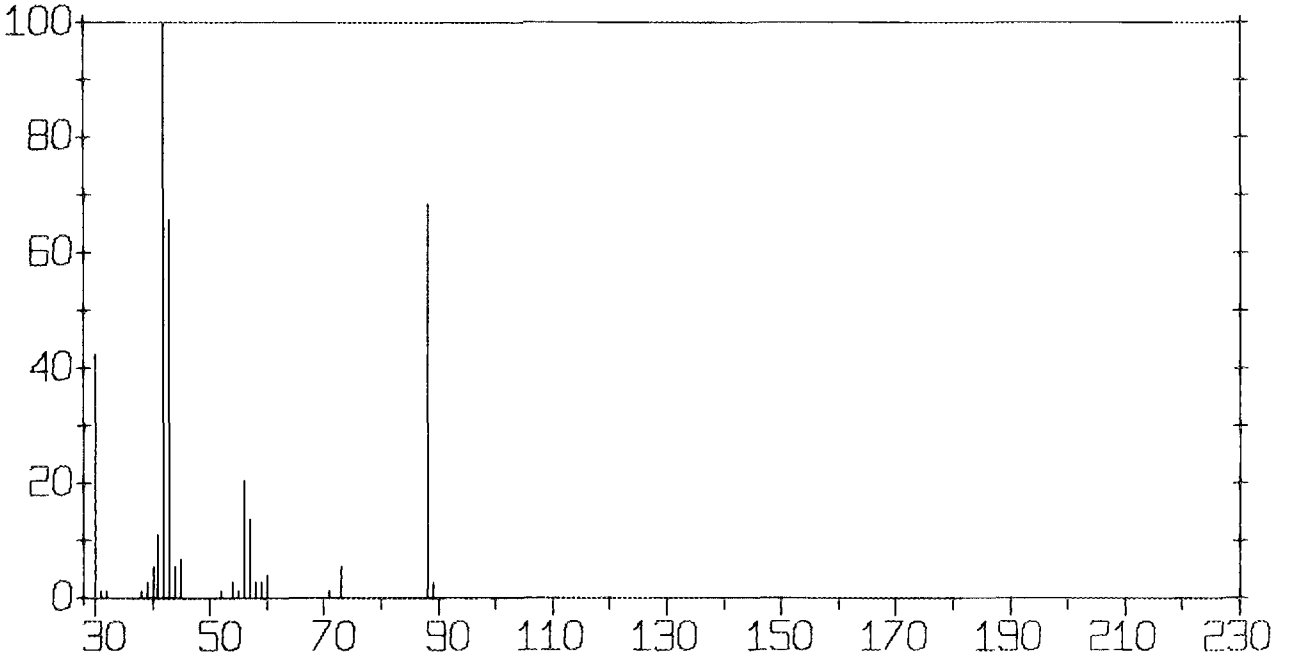
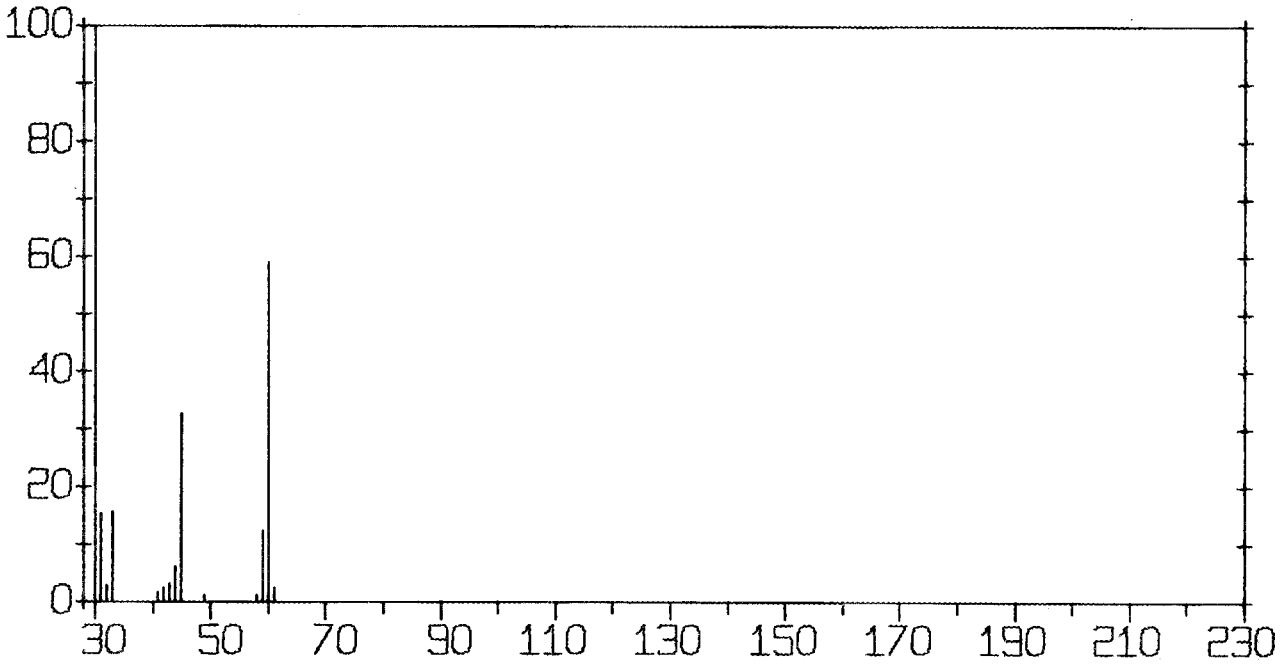


N-NITROSO-N-METHOXY-N-METHYLAMINE
MW = 90 C2.H6.N2.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	33.0	15.7	43.0	3.2	49.0	1.1	60.0	58.9
31.0	15.3	41.0	1.6	44.0	6.1	58.0	1.1	61.0	2.3
32.0	3.1	42.0	2.4	45.0	32.7	59.0	12.4		

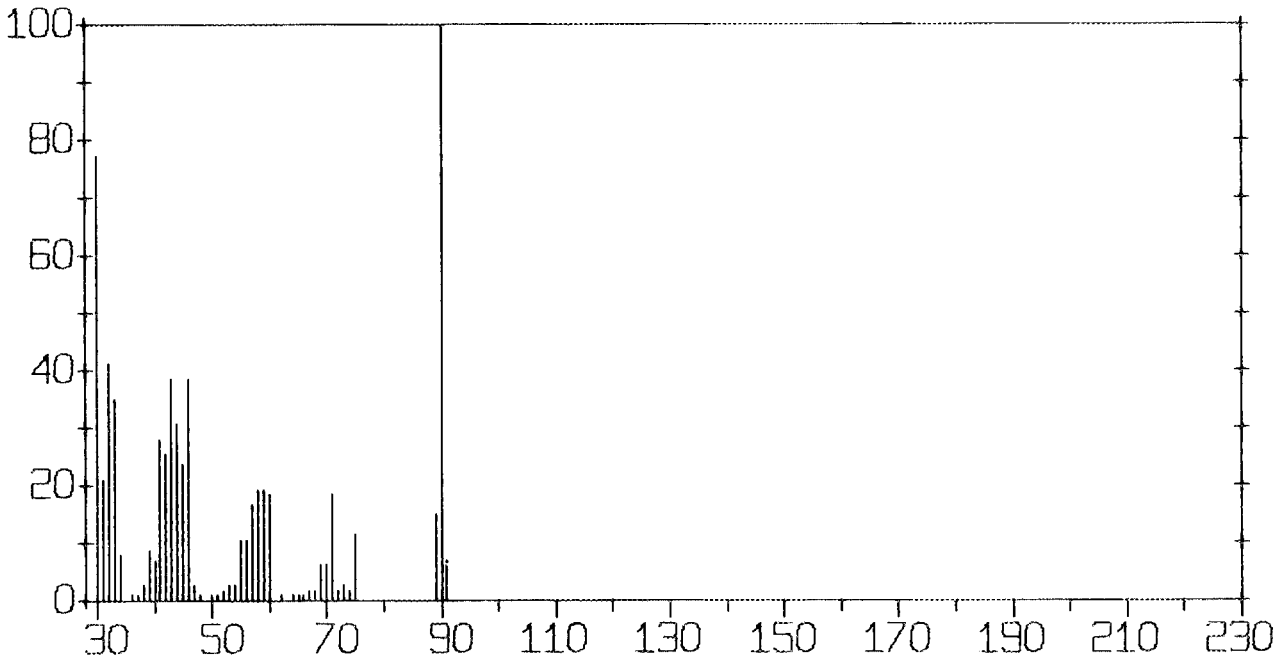
OBSERVED METASTABLES
18.1.



N-NITROSO-2,2,4,4-TETRADEUTEROAZETIDINE
MW = 90 C3,H2,D4,N2,O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	77.1	40.0	7.0	50.0	0.8	59.0	19.2	70.0	6.1
31.0	21.0	41.0	28.0	51.0	0.8	60.0	18.4	71.0	18.4
32.0	41.2	42.0	25.4	52.0	1.7	62.0	0.8	72.0	1.7
33.0	35.0	43.0	38.5	53.0	2.6	64.0	0.8	73.0	2.6
34.0	7.8	44.0	30.7	54.0	2.6	65.0	0.8	74.0	1.7
36.0	0.8	45.0	23.6	55.0	1[illegible].5	66.0	0.8	75.0	11.4
37.0	0.8	46.0	38.5	56.0	10.5	67.0	1.7	89.0	14.9
38.0	2.6	47.0	2.6	57.0	16.6	68.0	1.7	90.0	100.0
39.0	8.7	48.0	0.8	58.0	19.2	69.0	6.1	91.0	7.0

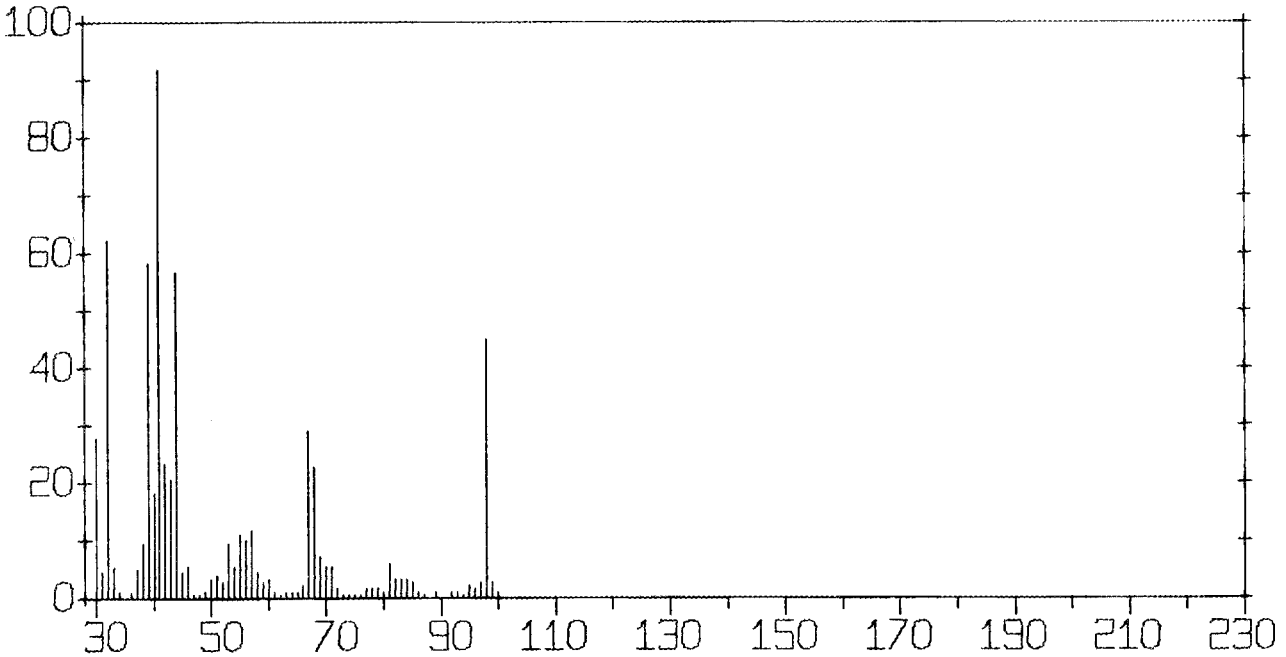
OBSERVED METASTABLES
23.5, 36.5,



N-NITROSO-3-PYRROLINE
MW = 98 C4.H6.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	27.7	45.0	4.4	59.0	2.7	72.0	1.6	85.0	2.7
31.0	4.4	46.0	5.5	60.0	3.3	73.0	0.5	86.0	1.1
32.0	62.2	47.0	0.5	61.0	1.1	74.0	0.5	87.0	0.5
33.0	5.5	48.0	0.5	62.0	0.5	75.0	0.5	89.0	1.1
34.0	1.1	49.0	1.1	63.0	1.1	76.0	0.5	92.0	1.1
36.0	1.1	50.0	3.3	64.0	1.1	77.0	1.6	93.0	1.1
37.0	5.0	51.0	3.8	65.0	1.1	78.0	1.6	94.0	0.5
38.0	9.4	52.0	2.7	66.0	2.2	79.0	1.6	95.0	2.2
39.0	58.3	53.0	9.4	67.0	28.8	80.0	1.1	96.0	1.6
40.0	18.3	54.0	5.5	68.0	22.7	81.0	6.1	97.0	2.7
41.0	91.6	55.0	11.1	69.0	7.2	82.0	3.3	98.0	45.0
42.0	23.3	56.0	10.0	70.0	5.5	83.0	3.3	99.0	2.7
43.0	20.5	57.0	11.6	71.0	5.5	84.0	3.3	100.0	1.1
44.0	56.6	58.0	4.4						

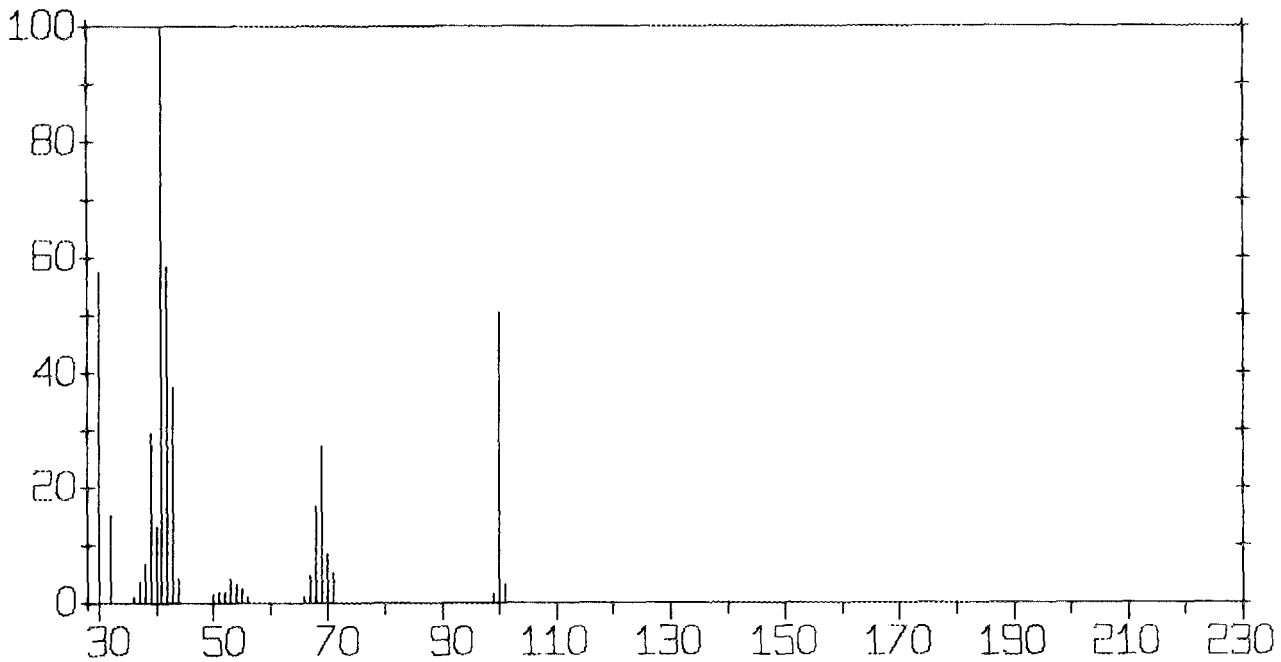
OBSERVED METASTABLES
24.8, 37.2, 67.0,



N-NITROSOPYRROLIDINE
MW = 100 C4.H8.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	57.6	40.0	13.3	51.0	1.9	56.0	0.9	70.0	8.5
32.0	15.2	41.0	100.0	52.0	1.9	66.0	0.9	71.0	5.2
36.0	0.9	42.0	58.5	53.0	4.2	67.0	4.7	99.0	1.4
37.0	3.8	43.0	37.6	54.0	3.3	68.0	16.6	100.0	50.4
38.0	6.6	44.0	4.2	55.0	2.3	69.0	27.1	101.0	3.3
39.0	29.5	50.0	1.4						

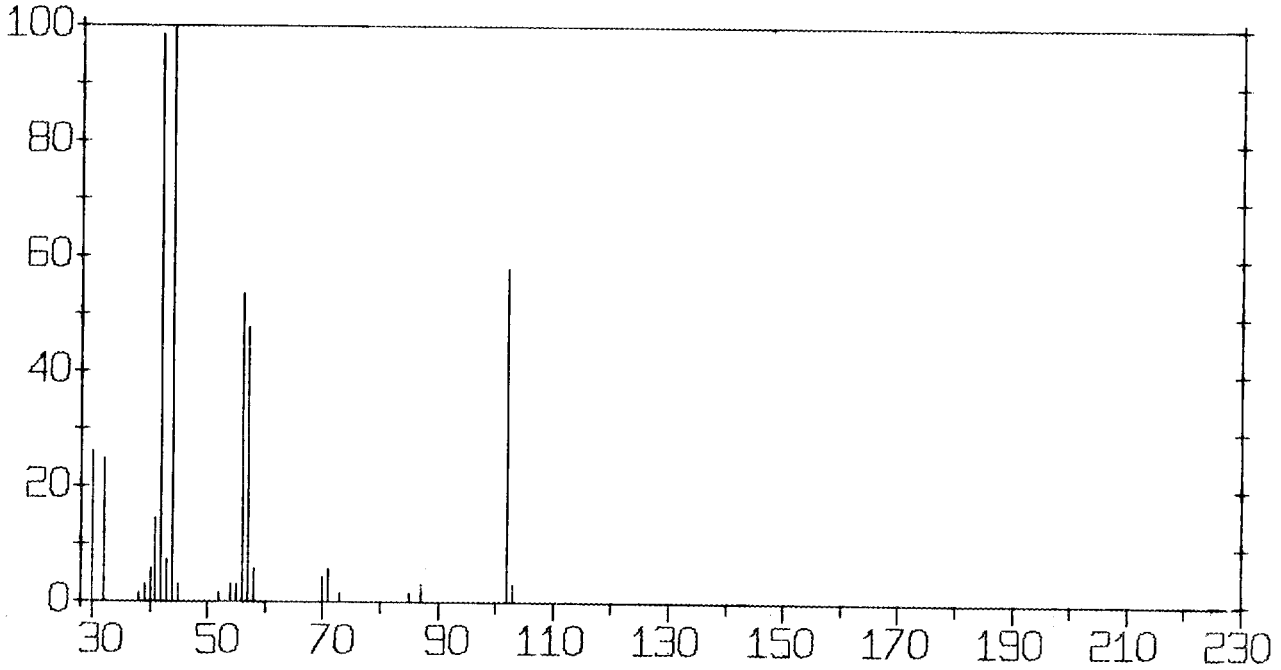
OBSERVED METASTABLES
24.8, 26.5, 37.2, 39.2, 67.2.



N-NITROSODIETHYLAMINE
MW = 102 C4.H10.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	26.0	41.0	14.4	52.0	1.4	58.0	5.7	85.0	1.4
32.0	24.6	42.0	98.5	54.0	2.8	70.0	4.3	87.0	2.8
38.0	1.4	43.0	7.2	55.0	2.8	71.0	5.7	102.0	57.9
39.0	2.8	44.0	100.0	56.0	53.6	73.0	1.4	103.0	2.8
40.0	5.7	45.0	2.8	57.0	47.8				

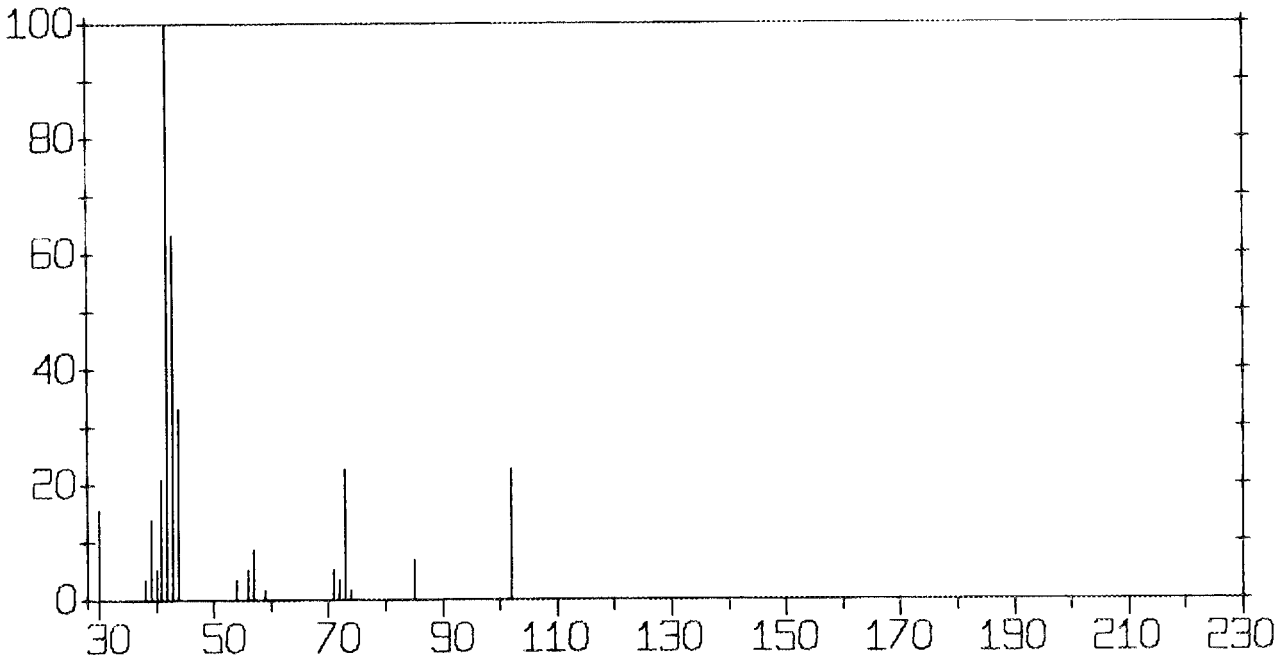
OBSERVED METASTABLES
25.2, 36.2, 7.0,



N-NITROSOMETHYL-N-PROPYLAMINE
MW = 102 C4.H10.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	15.7	41.0	21.0	54.0	3.5	71.0	5.2	74.0	1.7
38.0	3.5	42.0	100.0	56.0	5.2	72.0	3.5	85.0	7.0
39.0	14.0	43.0	63.1	57.0	8.7	73.0	22.8	102.0	22.8
40.0	5.2	44.0	33.3	59.0	1.7				

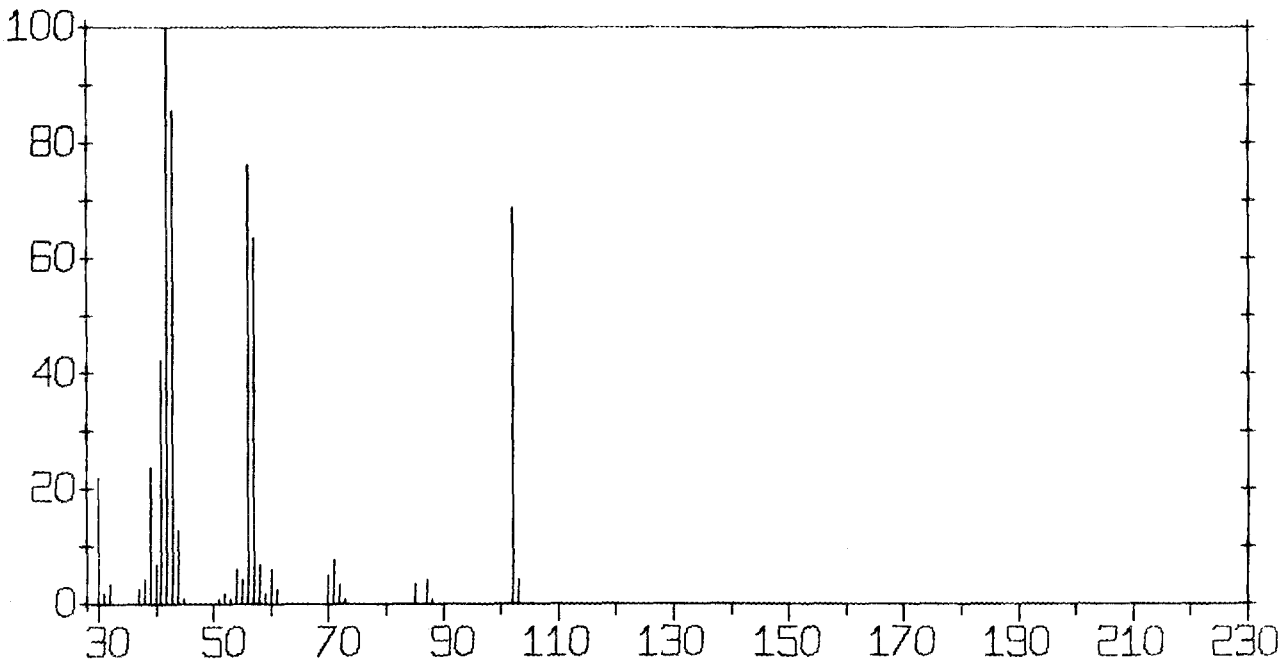
OBSERVED METASTABLES
24.2, 35.0, 37.1, 39.1, 55.2, 70.8,



N-NITROSOMETHYLISOPROPYLAMINE
MW = 102 C4.H10.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	22.0	41.0	42.3	53.0	0.8	59.0	1.6	73.0	0.8
31.0	1.6	42.0	100.0	54.0	5.9	60.0	5.9	85.0	3.3
32.0	3.3	43.0	85.5	55.0	4.2	61.0	2.5	87.0	4.2
37.0	2.5	44.0	12.7	56.0	76.2	70.0	5.0	88.0	0.8
38.0	4.2	45.0	0.8	57.0	63.5	71.0	7.6	102.0	68.6
39.0	23.7	51.0	0.8	58.0	6.7	72.0	3.3	103.0	4.2
40.0	6.7	52.0	1.6						

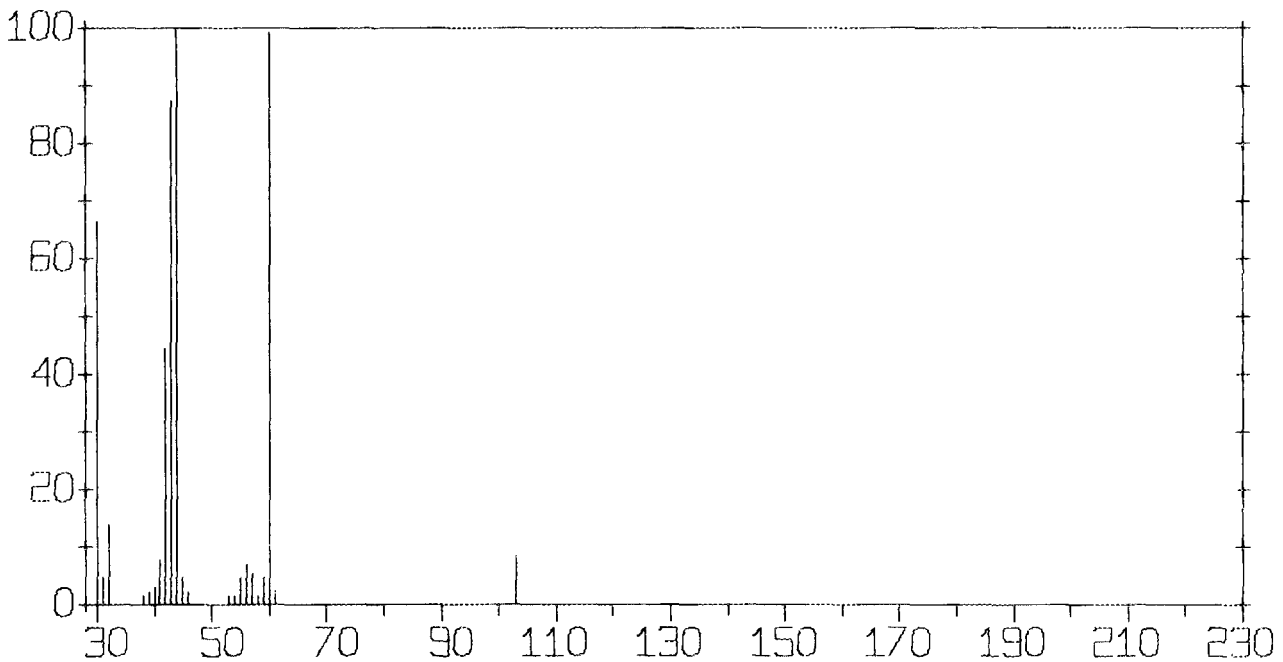
OBSERVED METASTABLES
37.1, 39.1, 55.2, 68.2, 71.0,



N-NITROSO-N-METHYLUREA
MW = 103 C2.H5.N3.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	66.4	40.0	3.1	45.0	4.6	55.0	4.6	59.0	4.6
31.0	4.6	41.0	7.8	46.0	2.3	56.0	7.0	60.0	99.2
32.0	14.0	42.0	44.5	53.0	1.5	57.0	5.4	61.0	3.1
38.0	1.5	43.0	87.5	54.0	1.5	58.0	1.5	103.0	8.5
39.0	2.3	44.0	100.0						

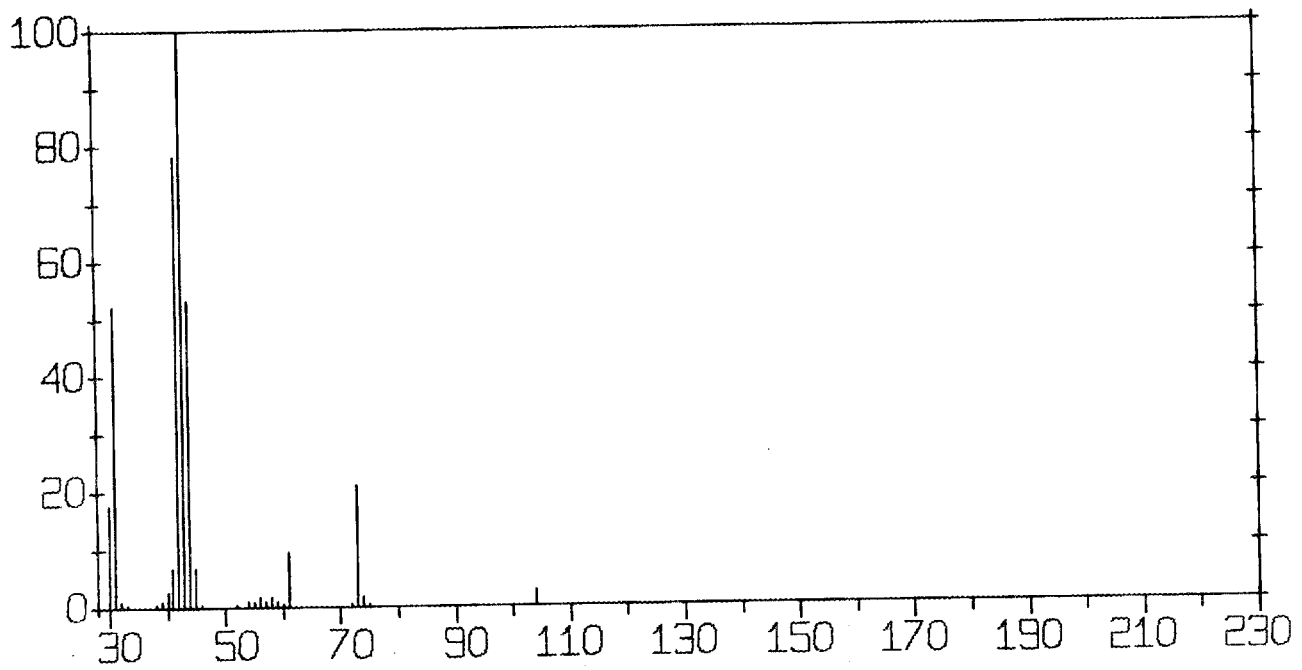
OBSERVED METASTABLES
26.2.



N-NITROSOMETHYL-2-HYDROXYETHYLAMINE
MW = 104 C3.H8.N2.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	17.7	40.0	2.7	46.0	0.5	57.0	1.1	72.0	0.5
31.0	52.2	41.0	6.6	52.0	0.5	58.0	1.6	73.0	21.1
32.0	1.1	42.0	78.3	54.0	1.1	59.0	1.1	74.0	1.6
33.0	0.5	43.0	100.0	55.0	1.1	60.0	0.5	75.0	0.5
38.0	0.5	44.0	53.3	56.0	1.6	61.0	9.4	104.0	2.7
39.0	1.1	45.0	6.6						

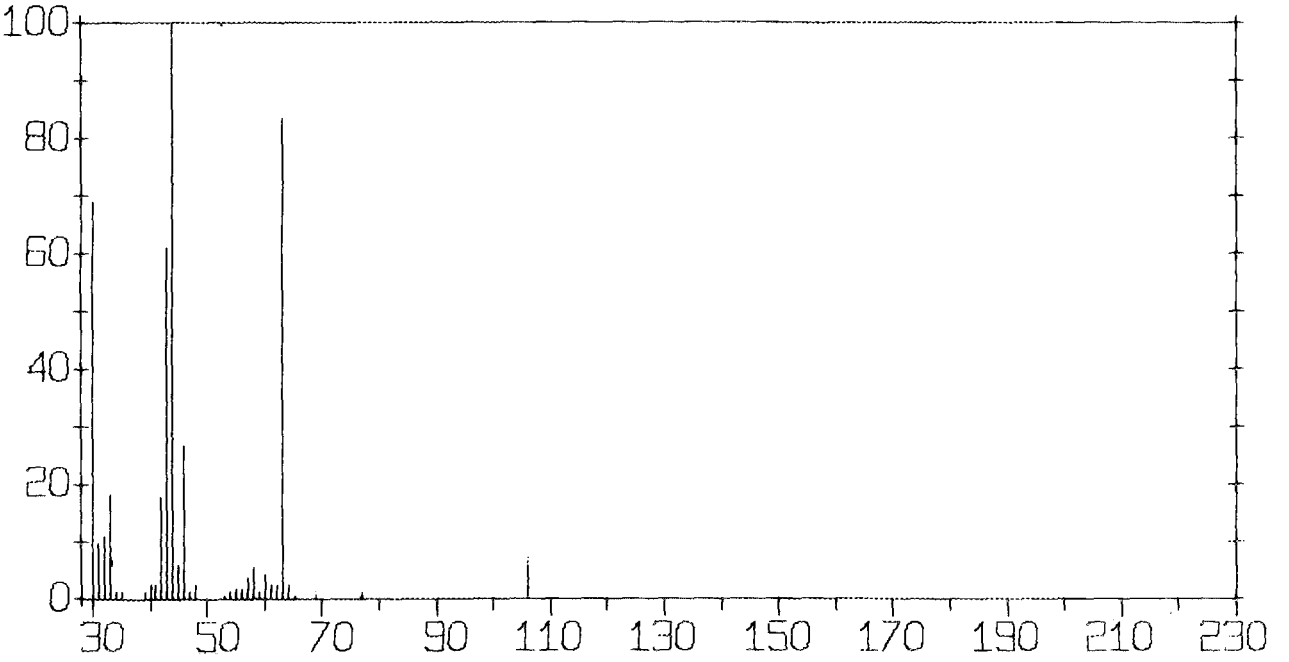
OBSERVED METASTABLES
24.2.



N-NITROSO-N-TRIDEUTEROMETHYLUREA
MW = 106 C2.H2.D3.N3.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	68.9	40.0	2.4	47.0	1.2	57.0	3.6	63.0	83.5
31.0	9.7	41.0	2.4	48.0	2.4	58.0	5.4	64.0	2.4
32.0	10.9	42.0	17.6	53.0	0.6	59.0	1.2	65.0	0.6
33.0	18.2	43.0	60.9	54.0	1.2	60.0	4.2	69.0	1.2
34.0	1.2	44.0	100.0	55.0	1.8	61.0	2.4	77.0	1.2
35.0	1.2	45.0	6.0	56.0	1.8	62.0	2.4	106.0	7.3
39.0	1.2	46.0	26.8						

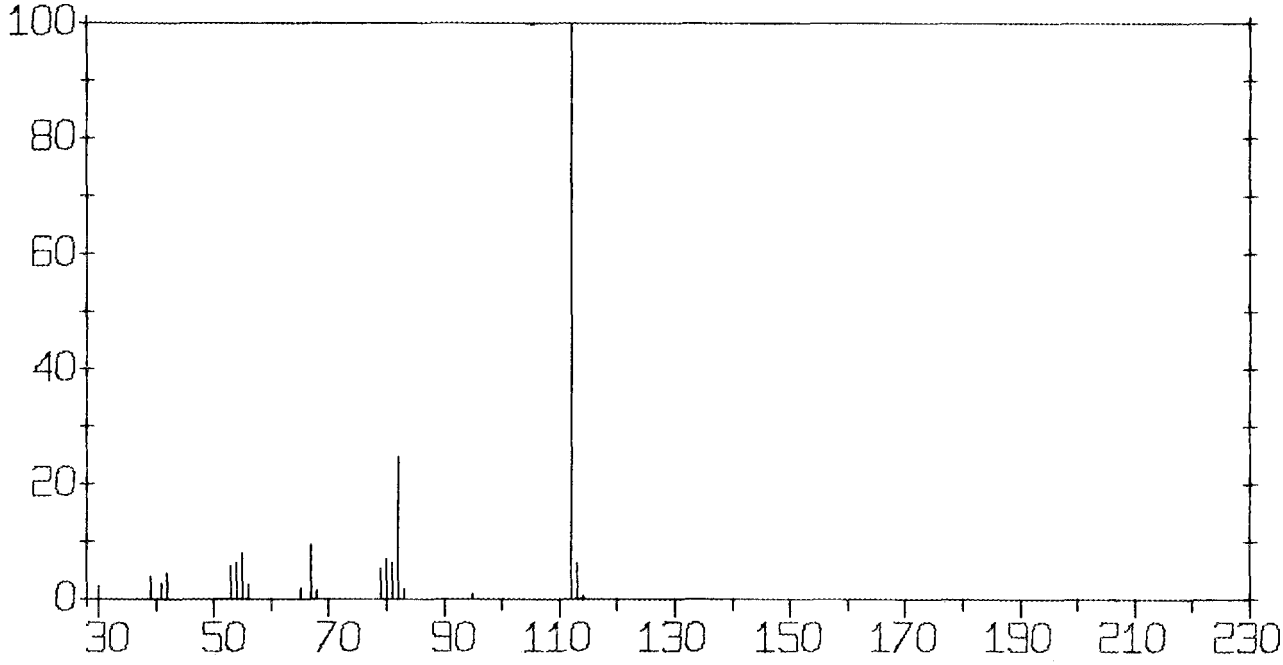
OBSERVED METASTABLES
28.2, 37.5,



N-NITROSO-1,2,3,6-TETRAHYDROPYRIDINE
MW = 112 C5,H8,N2,O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	2.2	53.0	5.8	65.0	2.0	80.0	7.0	95.0	0.8
39.0	4.0	54.0	6.2	67.0	9.5	81.0	6.1	112.0	100.0
41.0	2.6	55.0	8.0	68.0	1.5	82.0	24.6	113.0	6.2
42.0	4.5	56.0	2.4	79.0	5.2	83.0	1.8	114.0	0.4

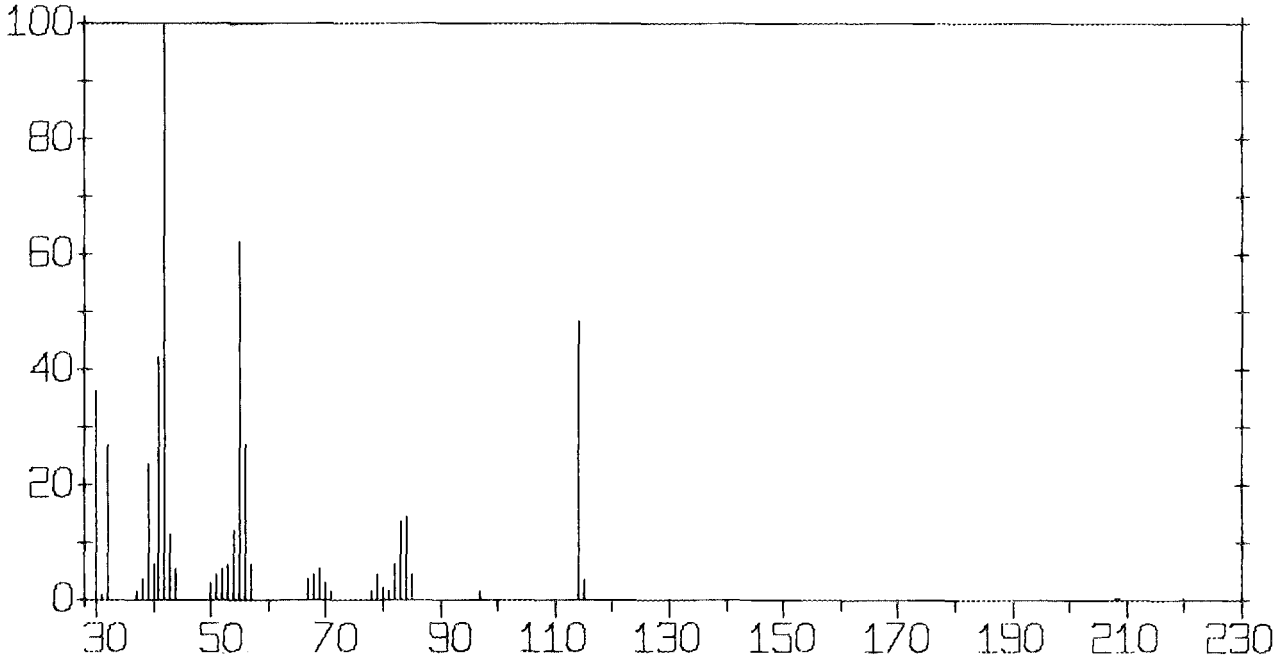
OBSERVED METASTABLES
36.8, 51.1, 60.1,



N-NITROSOPIPERIDINE
Mw = 114 C5.H10.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	36.1	41.0	42.3	53.0	6.1	69.0	5.3	82.0	6.1
31.0	0.7	42.0	100.0	54.0	12.3	70.0	3.0	83.0	13.8
32.0	26.9	43.0	11.5	55.0	62.3	71.0	1.5	84.0	14.6
37.0	1.5	44.0	5.3	56.0	26.9	78.0	1.5	85.0	4.6
38.0	3.8	50.0	3.0	57.0	6.1	79.0	4.6	97.0	1.5
39.0	23.8	51.0	4.6	67.0	3.8	80.0	2.3	114.0	48.4
40.0	6.1	52.0	5.3	68.0	4.6	81.0	1.5	115.0	3.8

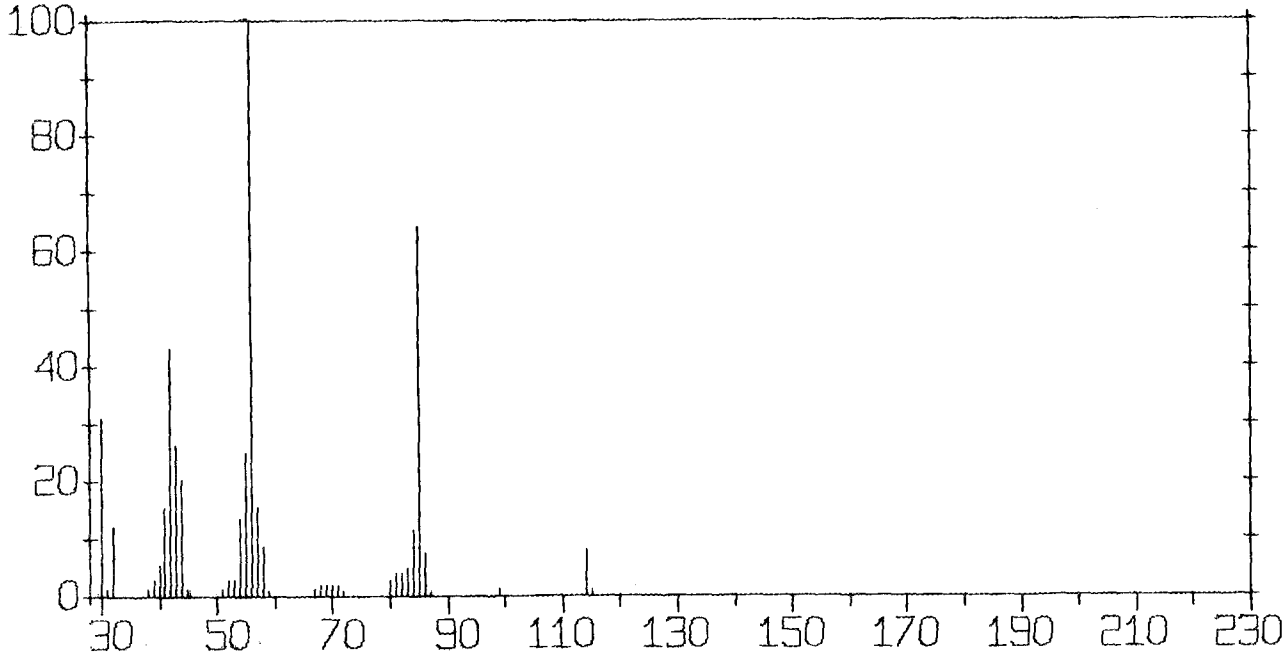
OBSERVED METASTABLES
15.0, 21.0, 36.0, 36.5, 37.2, 37.6,



N-NITROSOPIPERAZINE
MW = 115 C4.H9.N3.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	31.0	43.0	26.3	56.0	100.0	70.0	2.0	84.0	11.4
31.0	1.3	44.0	20.2	57.0	15.5	71.0	2.0	85.0	64.1
32.0	12.1	45.0	1.3	58.0	8.7	72.0	0.6	86.0	7.4
38.0	1.3	51.0	1.3	59.0	0.6	80.0	2.7	87.0	0.6
39.0	2.7	52.0	2.7	67.0	1.3	81.0	4.0	99.0	1.3
40.0	5.4	53.0	2.7	68.0	2.0	82.0	4.0	114.0	8.1
41.0	15.5	54.0	13.5	69.0	2.0	83.0	4.7	115.0	1.3
42.0	43.2	55.0	25.0						

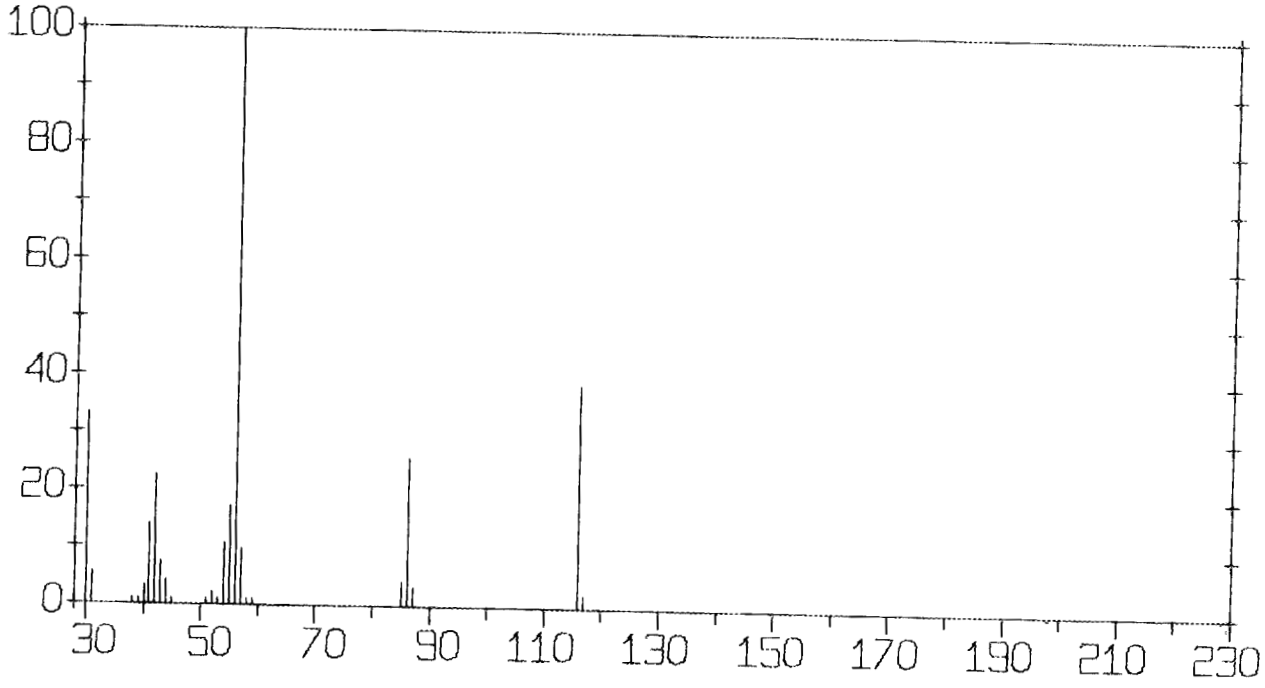
OBSERVED METASTABLES
15.5, 24.2, 25.2, 37.0, 62.5, 63.4, 80.2, 82.2,



N-NITROSOMORPHOLINE
MW = 116 C4.H8.N2.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	33.3	41.0	13.9	51.0	1.0	56.0	100.0	86.0	25.8
31.0	5.3	42.0	22.5	52.0	2.1	57.0	9.6	87.0	3.2
38.0	1.0	43.0	7.5	53.0	1.0	58.0	1.0	116.0	38.7
39.0	1.0	44.0	4.3	54.0	10.7	59.0	1.0	117.0	2.1
40.0	3.2	45.0	1.0	55.0	17.2	85.0	4.3		

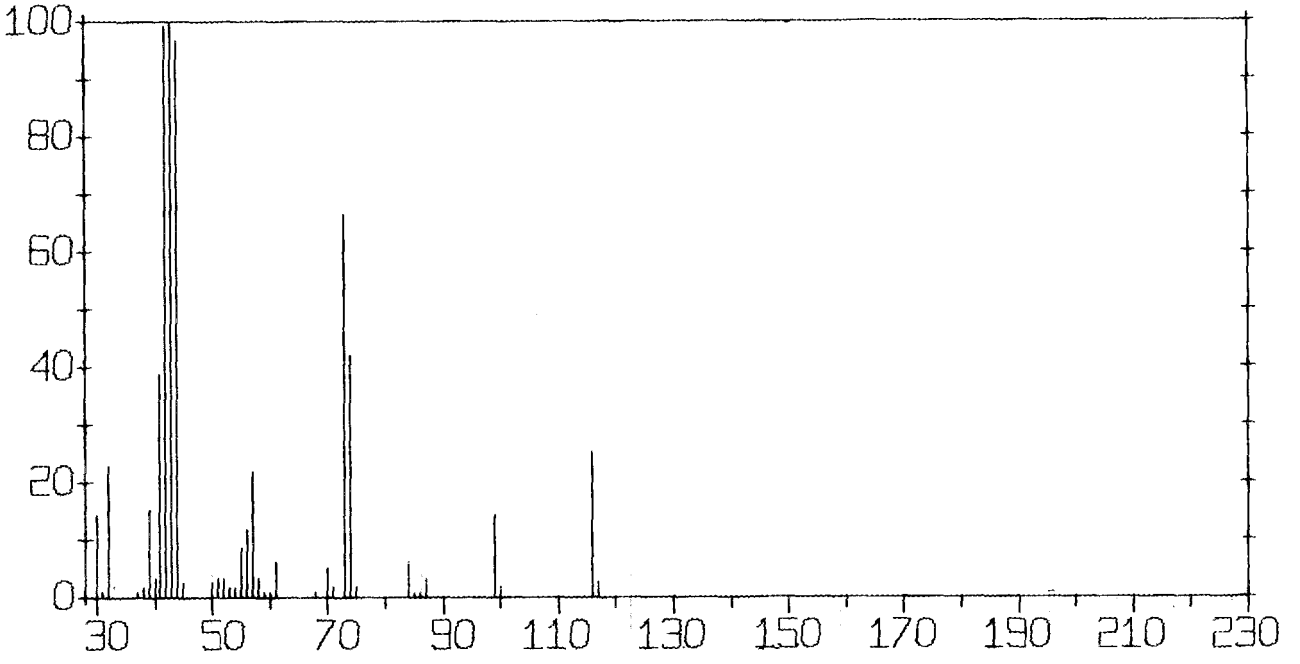
OBSERVED METASTABLES
14.3, 24.2, 25.2, 36.5, 63.8,



N-NITROSOMETHYL-N-BUTYLAMINE
MW = 116 C5.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	14.2	42.0	99.1	54.0	1.6	68.0	0.8	85.0	0.8
31.0	0.8	43.0	100.0	55.0	8.4	70.0	5.0	86.0	0.8
32.0	22.6	44.0	96.6	56.0	11.7	71.0	1.6	87.0	3.3
37.0	0.8	45.0	2.5	57.0	21.8	73.0	66.3	99.0	14.2
38.0	1.6	50.0	2.5	58.0	3.3	74.0	42.0	100.0	1.6
39.0	15.1	51.0	3.3	59.0	0.8	75.0	1.6	116.0	25.2
40.0	3.3	52.0	3.3	60.0	0.8	84.0	5.8	117.0	2.5
41.0	38.6	53.0	1.6	61.0	5.8				

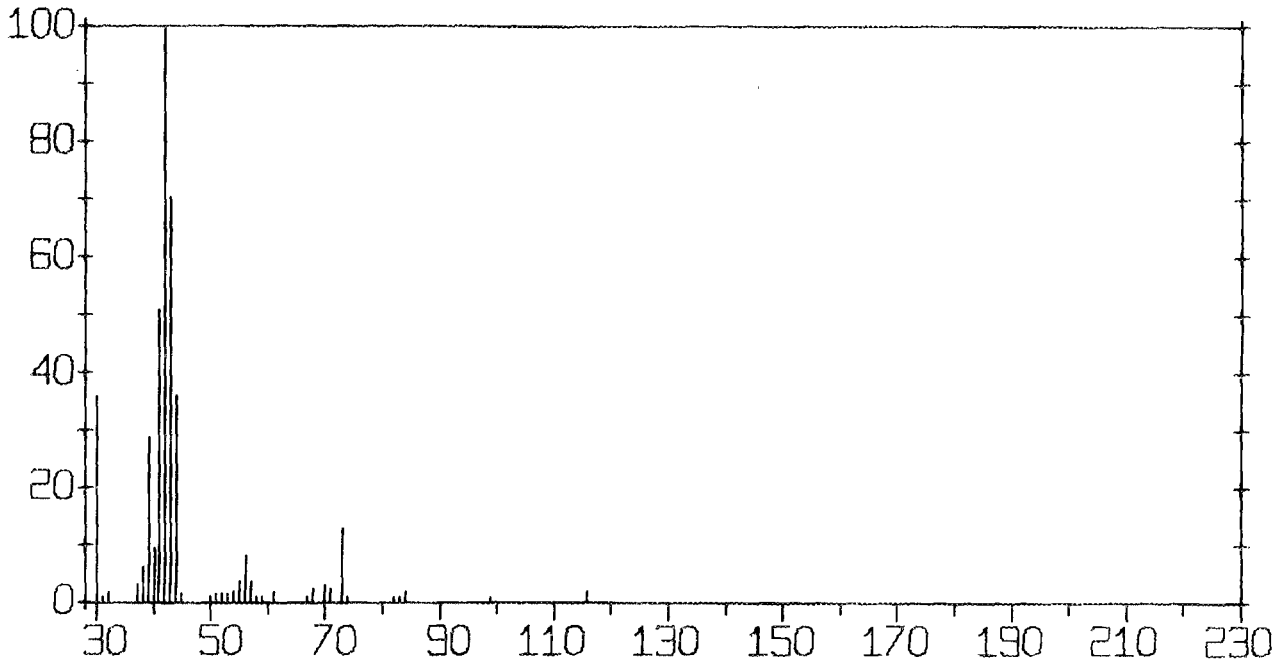
OBSERVED METASTABLES
24.2, 29.5, 37.1, 39.1, 47.2, 84.5,



N-NITROSOMETHYLISOBUTYLAMINE
MW = 116 C5.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	36.0	41.0	50.9	52.0	1.4	59.0	0.9	74.0	0.9
31.0	0.9	42.0	100.0	53.0	1.4	61.0	1.9	82.0	0.9
32.0	1.9	43.0	70.1	54.0	1.9	67.0	0.9	83.0	0.9
37.0	3.3	44.0	36.0	55.0	3.8	68.0	2.4	84.0	1.9
38.0	6.2	45.0	1.4	56.0	8.1	70.0	2.8	99.0	0.9
39.0	28.8	50.0	0.9	57.0	3.8	71.0	2.4	116.0	1.9
40.0	9.6	51.0	1.4	58.0	0.9	73.0	12.9		

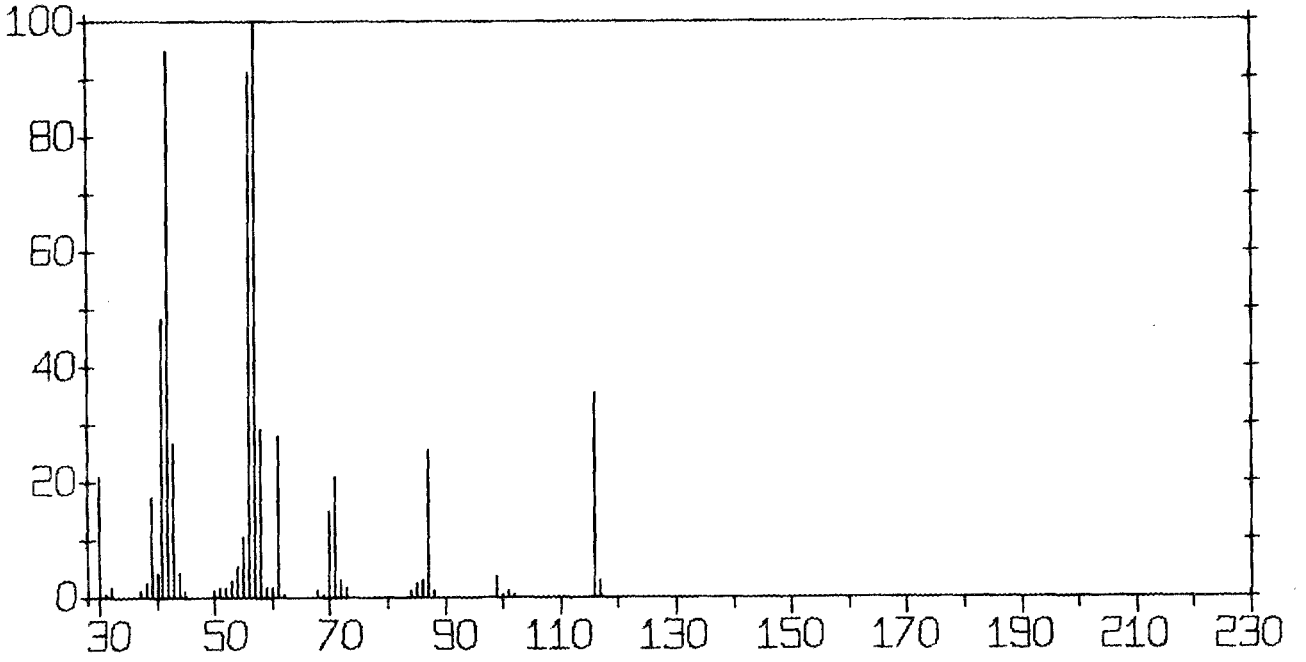
OBSERVED METASTABLES
24.2, 29.5, 35.1, 37.2, 39.2, 41.5,



N-NITROSOMETHYL-SEC-BUTYLAMINE
MW = 116 C5.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	21.1	43.0	26.7	56.0	91.3	69.0	0.6	87.0	25.4
31.0	0.6	44.0	4.3	57.0	100.0	70.0	14.9	88.0	1.2
32.0	1.8	45.0	1.2	58.0	29.1	71.0	21.1	99.0	3.7
37.0	1.2	50.0	1.2	59.0	1.8	72.0	3.1	100.0	0.6
38.0	2.4	51.0	1.8	60.0	1.8	73.0	1.8	101.0	1.2
39.0	17.3	52.0	1.8	61.0	27.9	84.0	1.2	102.0	0.6
40.0	4.3	53.0	3.1	62.0	0.6	85.0	2.4	116.0	35.4
41.0	48.4	54.0	5.5	68.0	1.2	86.0	3.1	117.0	3.1
42.0	95.0	55.0	10.5						

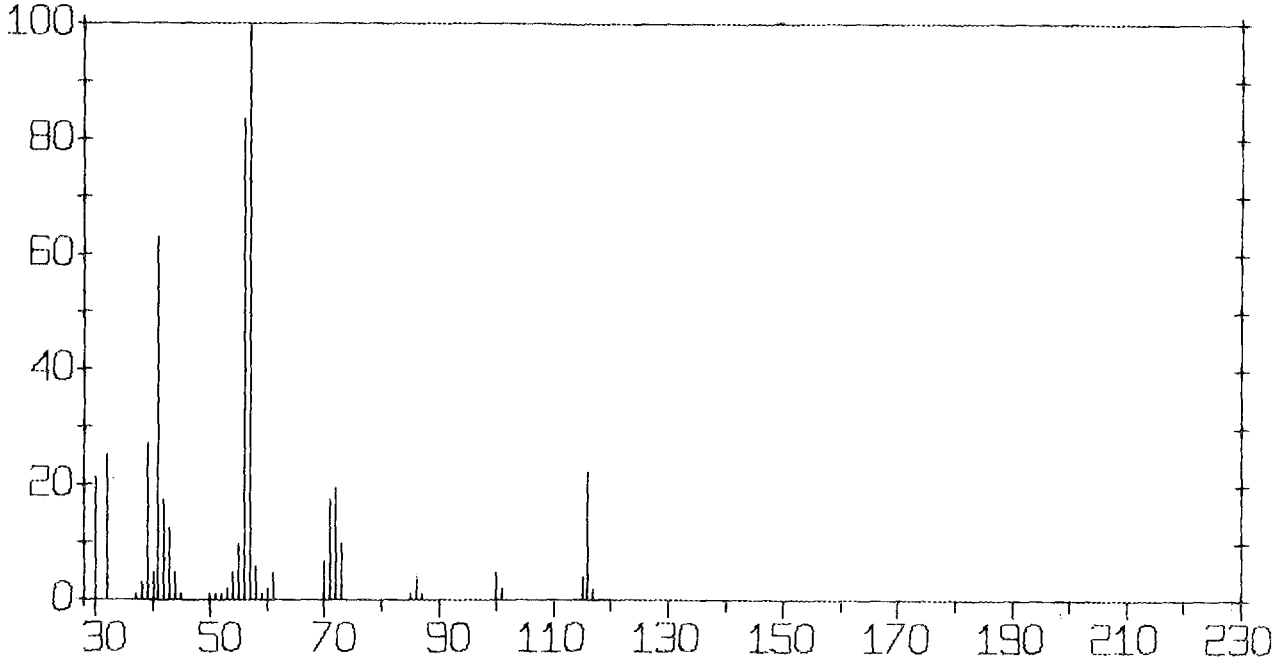
OBSERVED METASTABLES
15.5, 25.2, 29.5, 36.2, 44.2, 54.2, 69.2, 84.5,



N-NITROSOMETHYL-TERT-BUTYLAMINE
MW = 116 C5.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	21.3	42.0	17.4	53.0	1.9	60.0	1.9	86.0	4.8
32.0	25.2	43.0	12.6	54.0	4.8	61.0	4.8	87.0	0.9
37.0	0.9	44.0	4.8	55.0	9.7	70.0	6.7	100.0	4.8
38.0	2.9	45.0	0.9	56.0	83.4	71.0	17.4	101.0	1.9
39.0	27.1	50.0	0.9	57.0	100.0	72.0	19.4	115.0	3.8
40.0	4.8	51.0	0.9	58.0	5.8	73.0	9.7	116.0	22.3
41.0	63.1	52.0	0.9	59.0	0.9	85.0	0.9	117.0	1.9

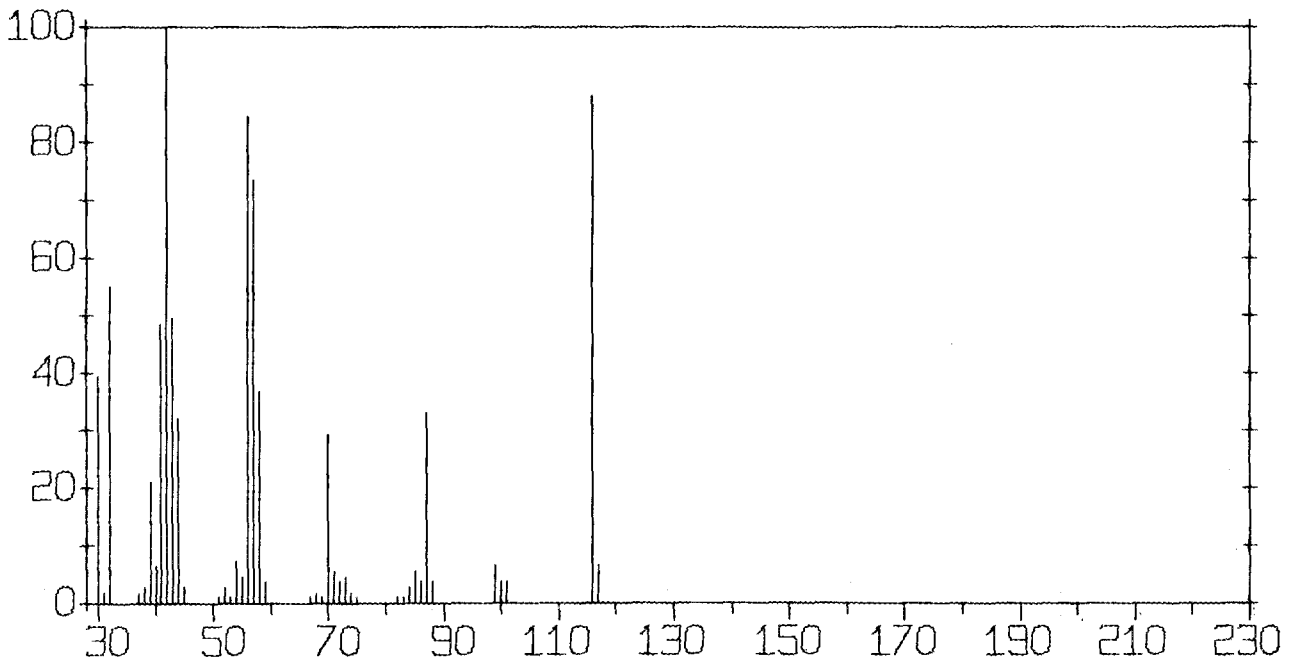
OBSERVED METASTABLES
25.2, 29.5, 35.0, 37.2, 44.2, 58.6, 68.1, 82.2,



N-NITROSOETHYL-N-PROPYLAMINE
MW = 116 C5.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	39.4	43.0	49.5	57.0	73.3	72.0	3.6	86.0	3.6
31.0	1.8	44.0	32.1	58.0	36.6	73.0	4.5	87.0	33.0
32.0	55.0	45.0	2.7	59.0	3.6	74.0	1.8	88.0	3.6
37.0	1.8	51.0	0.9	67.0	0.9	75.0	0.9	99.0	6.4
38.0	2.7	52.0	2.7	68.0	1.8	82.0	0.9	100.0	3.6
39.0	21.1	53.0	0.9	69.0	0.9	83.0	0.9	101.0	3.6
40.0	6.4	54.0	7.3	70.0	29.3	84.0	2.7	116.0	88.0
41.0	48.6	55.0	4.5	71.0	5.5	85.0	5.5	117.0	6.4
42.0	100.0	56.0	84.4						

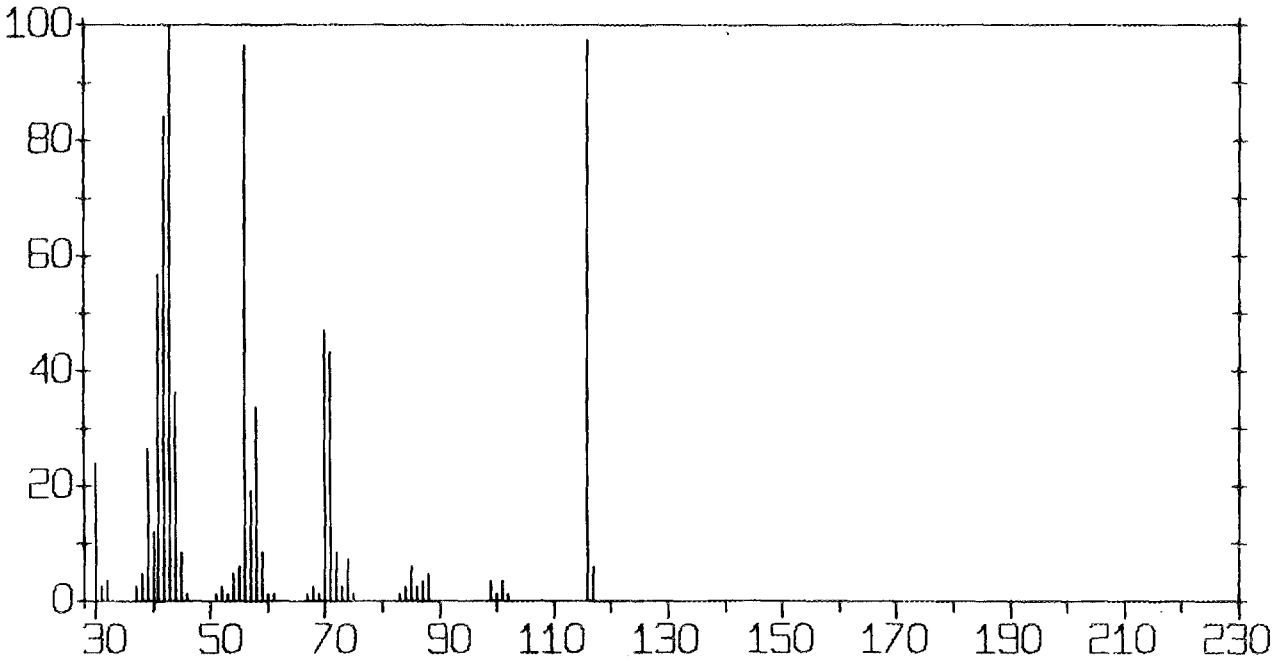
OBSERVED METASTABLES
15.5, 25.2, 36.2, 39.2, 84.5,



N-NITROSOETHYLISOPROPYLAMINE
MW = 116 C5.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	24.0	43.0	100.0	56.0	96.3	70.0	46.9	86.0	2.4
31.0	2.4	44.0	36.1	57.0	19.2	71.0	43.3	87.0	3.6
32.0	3.6	45.0	8.4	58.0	33.7	72.0	8.4	88.0	4.8
37.0	2.4	46.0	1.2	59.0	8.4	73.0	2.4	99.0	3.6
38.0	4.8	51.0	1.2	60.0	1.2	74.0	7.2	100.0	1.2
39.0	26.5	52.0	2.4	61.0	1.2	75.0	1.2	101.0	3.6
40.0	12.0	53.0	1.2	67.0	1.2	83.0	1.2	102.0	1.2
41.0	56.6	54.0	4.8	68.0	2.4	84.0	2.4	116.0	97.5
42.0	84.3	55.0	6.0	69.0	1.2	85.0	6.0	117.0	6.0

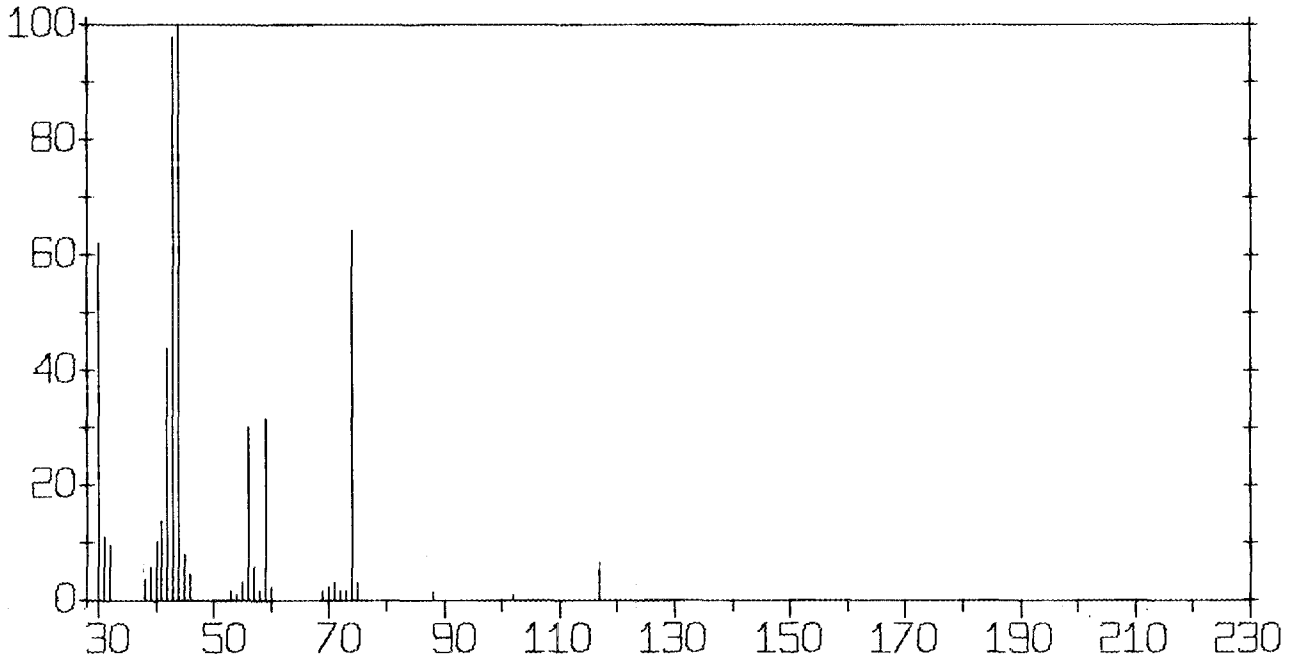
OBSERVED METASTABLES
15.5, 25.2, 39.2, 44.2, 47.2, 48.5, 54.3, 57.8, 84.5, 85.5,



N-NITROSO-N-ETHYLUREA
MW = 117 C3.H8.N3.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	62.0	41.0	13.8	53.0	1.4	59.0	31.3	73.0	1.4
31.0	10.9	42.0	43.7	54.0	0.7	60.0	2.1	74.0	64.2
32.0	9.4	43.0	97.8	55.0	2.9	69.0	1.4	75.0	2.9
38.0	3.6	44.0	100.0	56.0	29.9	70.0	2.1	88.0	1.4
39.0	5.8	45.0	8.0	57.0	5.8	71.0	2.9	102.0	0.7
40.0	10.2	46.0	4.3	58.0	1.4	72.0	1.4	117.0	6.5

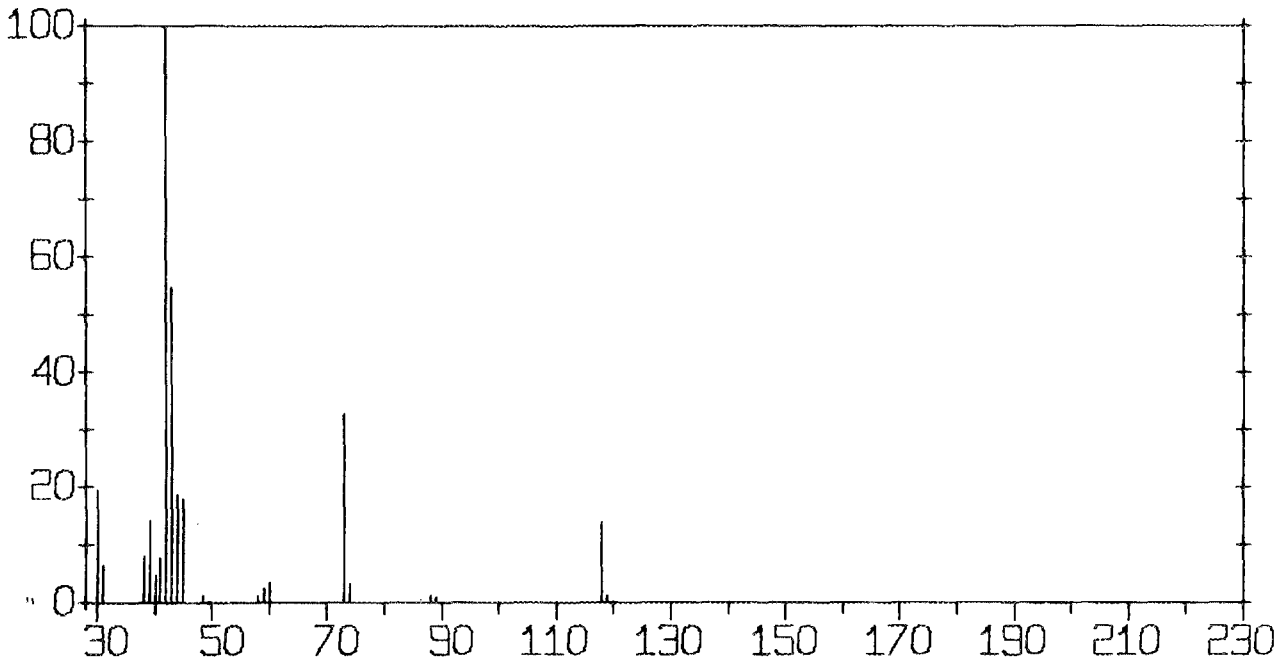
OBSERVED METASTABLES
24.2, 25.2, 28.2, 46.8,



N-NITROSOSARCOSINE
MW = 118 C3.H6.N2.O3.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	19.5	40.0	4.6	44.0	18.7	60.0	3.5	89.0	0.8
31.0	6.5	41.0	7.8	45.0	17.9	73.0	32.8	118.0	14.0
38.0	7.9	42.0	100.0	58.0	1.2	74.0	3.2	119.0	1.2
39.0	14.3	43.0	54.6	59.0	2.4	88.0	1.2	120.0	0.1

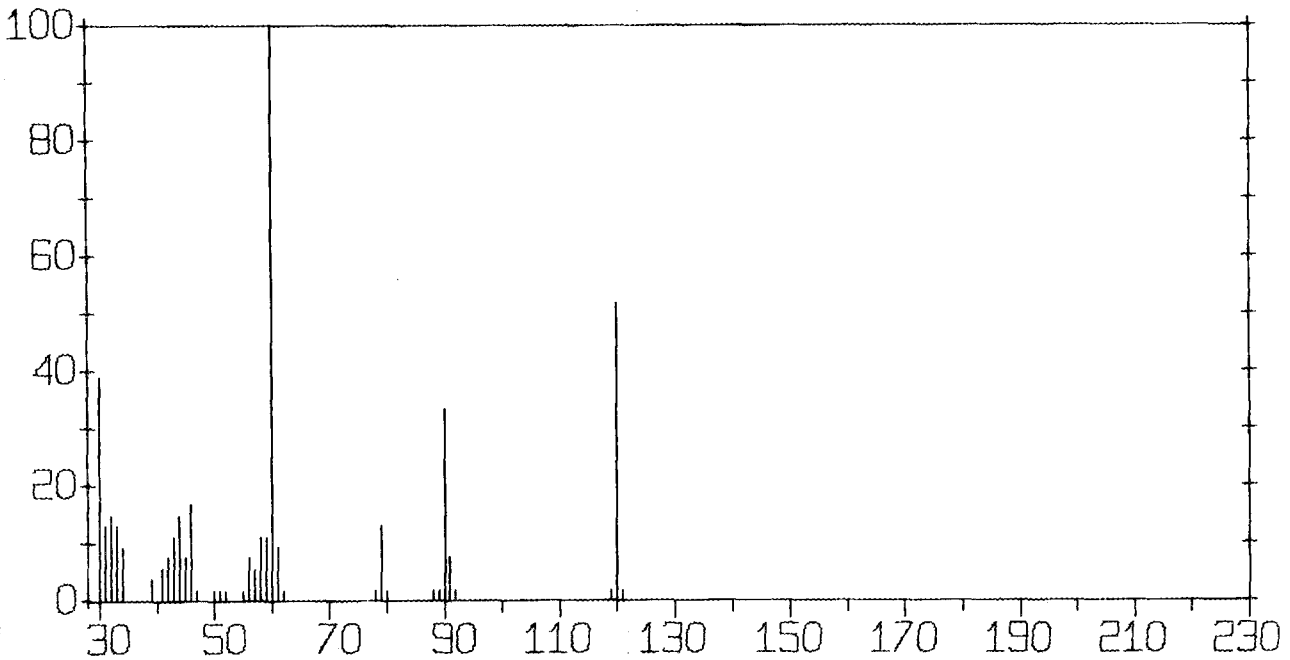
OBSERVED METASTABLES
24.3, 41.2, 65.6,



N-NITROSO-3,3,5,5-TETRADEUTEROMORPHOLINE
MW = 120 C4,H4,D4,N2,O2,

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	38.8	42.0	7.4	51.0	1.8	60.0	100.0	89.0	1.8
31.0	12.9	43.0	11.1	52.0	1.8	61.0	9.2	90.0	33.3
32.0	14.8	44.0	14.8	55.0	1.8	62.0	1.8	91.0	7.4
33.0	12.9	45.0	7.4	56.0	7.4	78.0	1.8	92.0	1.8
34.0	9.2	46.0	16.6	57.0	5.5	79.0	12.9	119.0	1.8
39.0	3.7	47.0	1.8	58.0	11.1	80.0	1.8	120.0	51.8
41.0	5.5	50.0	1.8	59.0	11.1	88.0	1.8	121.0	1.8

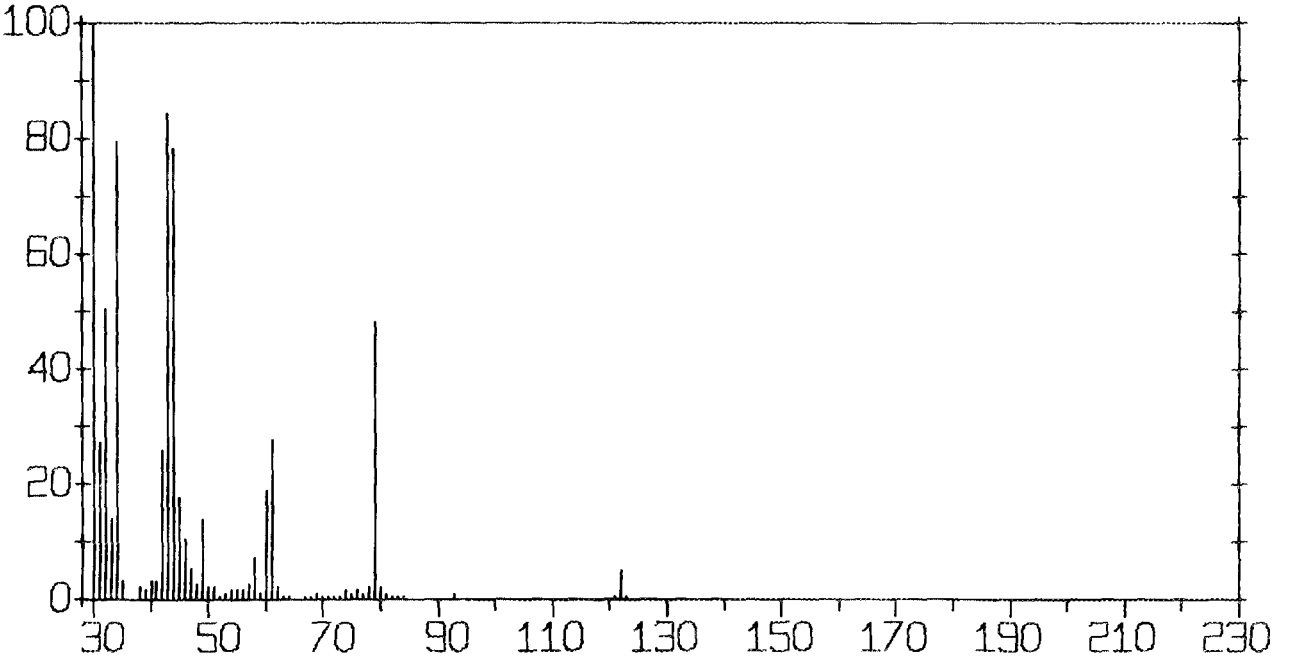
OBSERVED METASTABLES
40.2, 67.8,



N-NITROSO-N-PENTADEUTEROETHYLUREA
MW = 122 C3.H3.D5.N3.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	43.0	84.4	54.0	1.6	67.0	0.5	78.0	2.2
31.0	27.2	44.0	78.3	55.0	1.6	68.0	0.5	79.0	48.3
32.0	50.5	45.0	17.7	56.0	1.6	69.0	1.1	80.0	2.2
33.0	13.8	46.0	10.5	57.0	2.7	70.0	0.5	81.0	1.1
34.0	79.4	47.0	5.5	58.0	7.2	71.0	0.5	82.0	0.5
35.0	3.3	48.0	2.7	59.0	1.1	72.0	0.5	83.0	0.5
38.0	2.2	49.0	13.8	60.0	18.8	73.0	0.5	84.0	0.5
39.0	1.6	50.0	2.2	61.0	27.7	74.0	1.6	93.0	1.1
40.0	3.3	51.0	2.2	62.0	2.2	75.0	1.1	121.0	0.5
41.0	3.3	52.0	0.5	63.0	0.5	76.0	1.6	122.0	5.0
42.0	26.1	53.0	1.1	64.0	0.5	77.0	1.1	123.0	0.5

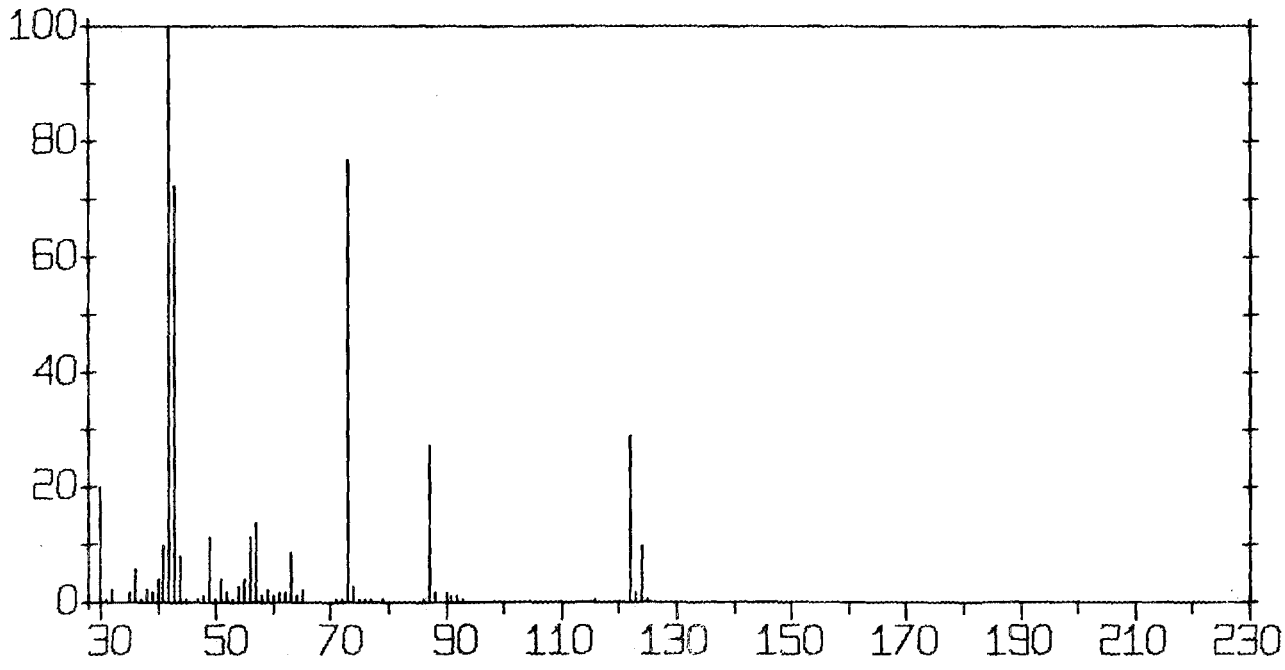
OBSERVED METASTABLES
26.2, 51.2,



N-NITROSOMETHYL-2-CHLOROETHYLAMINE
MW = 122 C3.H7.N2.O.CL.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	19.8	43.0	72.1	55.0	3.9	71.0	0.5	88.0	1.7
31.0	0.5	44.0	7.9	56.0	11.3	72.0	0.5	90.0	1.7
32.0	2.2	45.0	0.5	57.0	13.6	73.0	76.7	91.0	1.1
35.0	1.7	47.0	0.5	58.0	1.1	74.0	2.8	92.0	1.1
36.0	5.6	48.0	1.1	59.0	2.2	75.0	0.5	93.0	0.5
37.0	0.5	49.0	11.3	60.0	1.1	76.0	0.5	116.0	0.5
38.0	2.2	50.0	0.5	61.0	1.7	77.0	0.5	122.0	28.9
39.0	1.7	51.0	3.9	62.0	1.7	79.0	0.5	123.0	1.7
40.0	3.9	52.0	1.7	63.0	8.5	86.0	0.5	124.0	9.6
41.0	9.6	53.0	0.5	64.0	1.1	87.0	27.2	125.0	0.5
42.0	100.0	54.0	2.8	65.0	2.2				

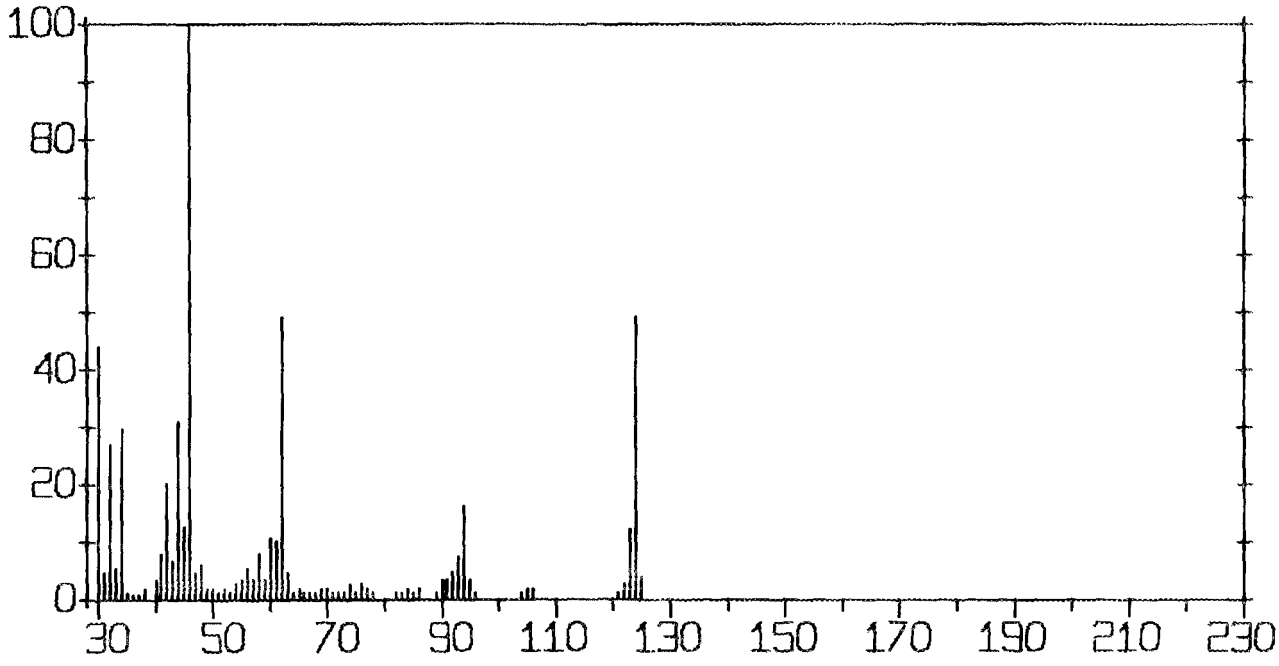
OBSERVED METASTABLES
24.2, 55.2, 61.2, 62.2,



N-NITROSODECADEUTEROPIPERIDINE
MW = 124 C5.D10.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	43.9	45.0	12.8	59.0	3.3	73.0	1.3	92.0	4.7
31.0	4.7	46.0	100.0	60.0	10.8	74.0	2.7	93.0	7.4
32.0	27.0	47.0	4.7	61.0	10.1	75.0	1.3	94.0	16.2
33.0	5.4	48.0	6.0	62.0	49.3	76.0	2.7	95.0	3.3
34.0	29.7	49.0	2.0	63.0	4.7	77.0	2.0	96.0	1.3
35.0	1.3	50.0	2.0	64.0	1.3	78.0	1.3	104.0	1.3
36.0	0.6	51.0	1.3	65.0	2.0	82.0	1.3	105.0	2.0
37.0	0.6	52.0	2.0	66.0	1.3	83.0	1.3	106.0	2.0
38.0	2.0	53.0	1.3	67.0	1.3	84.0	2.0	121.0	1.3
40.0	3.3	54.0	2.7	68.0	1.3	85.0	1.3	122.0	2.7
41.0	3.1	55.0	3.3	69.0	2.0	86.0	2.0	123.0	12.1
42.0	20.2	56.0	5.4	70.0	2.0	89.0	1.3	124.0	49.3
43.0	6.7	57.0	3.3	71.0	1.3	90.0	3.3	125.0	4.0
44.0	31.0	58.0	8.1	72.0	1.3	91.0	3.3		

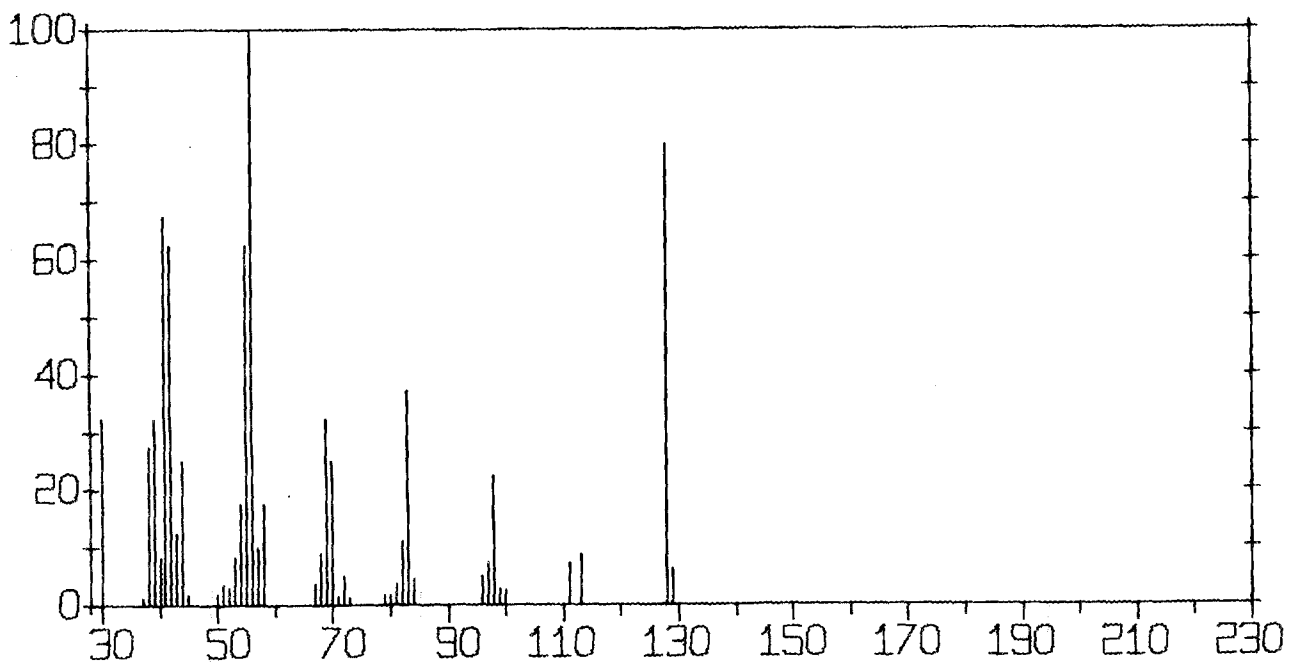
OBSERVED METASTABLES
14.5, 18.7, 22.5, 28.4, 38.5,



N-NITROSO-2-METHYLPIPERIDINE
MW = 128 C6.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	32.5	45.0	1.7	57.0	10.0	73.0	1.2	97.0	7.5
37.0	1.2	50.0	2.0	58.0	17.5	79.0	1.7	98.0	22.5
38.0	27.5	51.0	3.5	67.0	3.7	80.0	1.7	99.0	2.7
39.0	32.5	52.0	3.0	68.0	9.0	81.0	3.7	100.0	2.5
40.0	8.2	53.0	8.2	69.0	32.5	82.0	11.2	111.0	7.2
41.0	67.5	54.0	17.5	70.0	25.0	83.0	37.5	113.0	8.7
42.0	62.5	55.0	62.5	71.0	1.5	84.0	4.5	128.0	80.0
43.0	12.5	56.0	100.0	72.0	5.0	96.0	5.0	129.0	6.2
44.0	25.0								

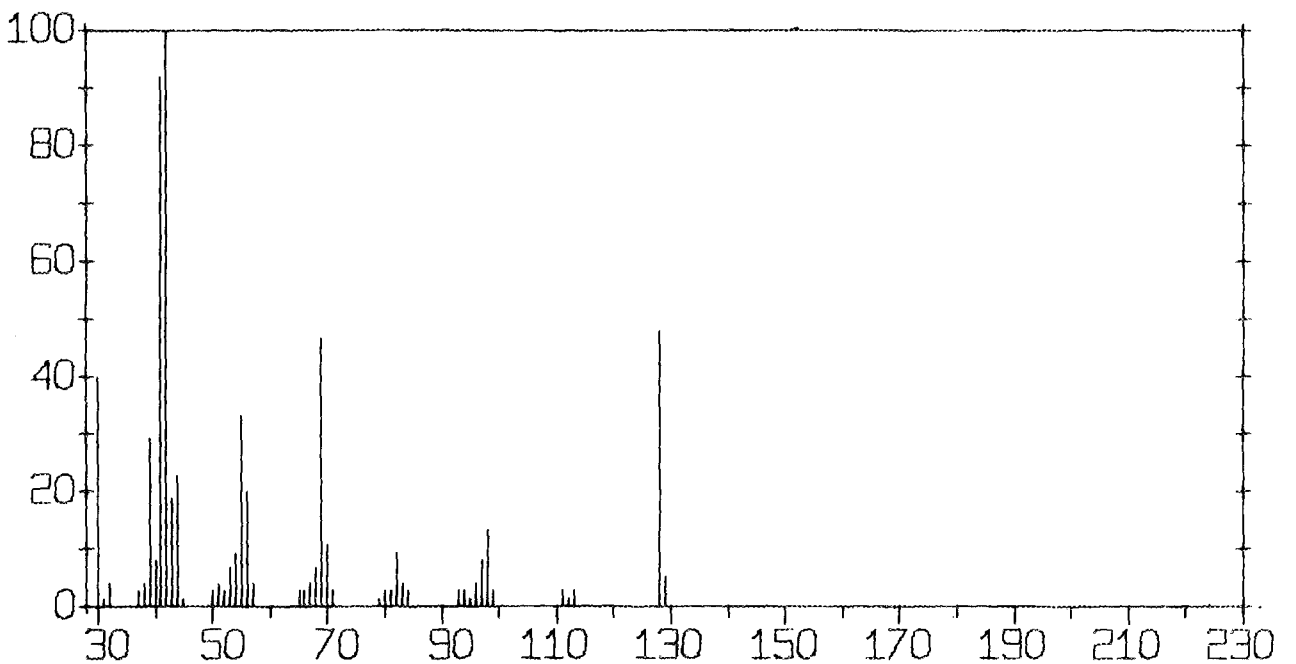
OBSERVED METASTABLES
31.9, 48.3, 49.0, 55.1, 60.9, 77.1, 96.3,



N-NITROSO-3-METHYLPIPERIDINE
MW = 128 C6.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	40.0	43.0	18.6	56.0	20.0	79.0	1.3	96.0	4.0
31.0	1.3	44.0	22.6	57.0	4.0	80.0	2.6	97.0	8.0
32.0	4.0	45.0	1.3	65.0	2.6	81.0	2.6	98.0	13.3
37.0	2.6	50.0	2.6	66.0	2.6	82.0	9.3	99.0	2.6
38.0	4.0	51.0	4.0	67.0	4.0	83.0	4.0	111.0	2.6
39.0	29.3	52.0	2.6	68.0	6.6	84.0	2.6	112.0	1.3
40.0	8.0	53.0	6.6	69.0	46.6	93.0	2.6	113.0	2.6
41.0	92.0	54.0	9.3	70.0	10.6	94.0	2.6	128.0	48.0
42.0	100.0	55.0	33.3	71.0	2.6	95.0	1.3	129.0	5.3

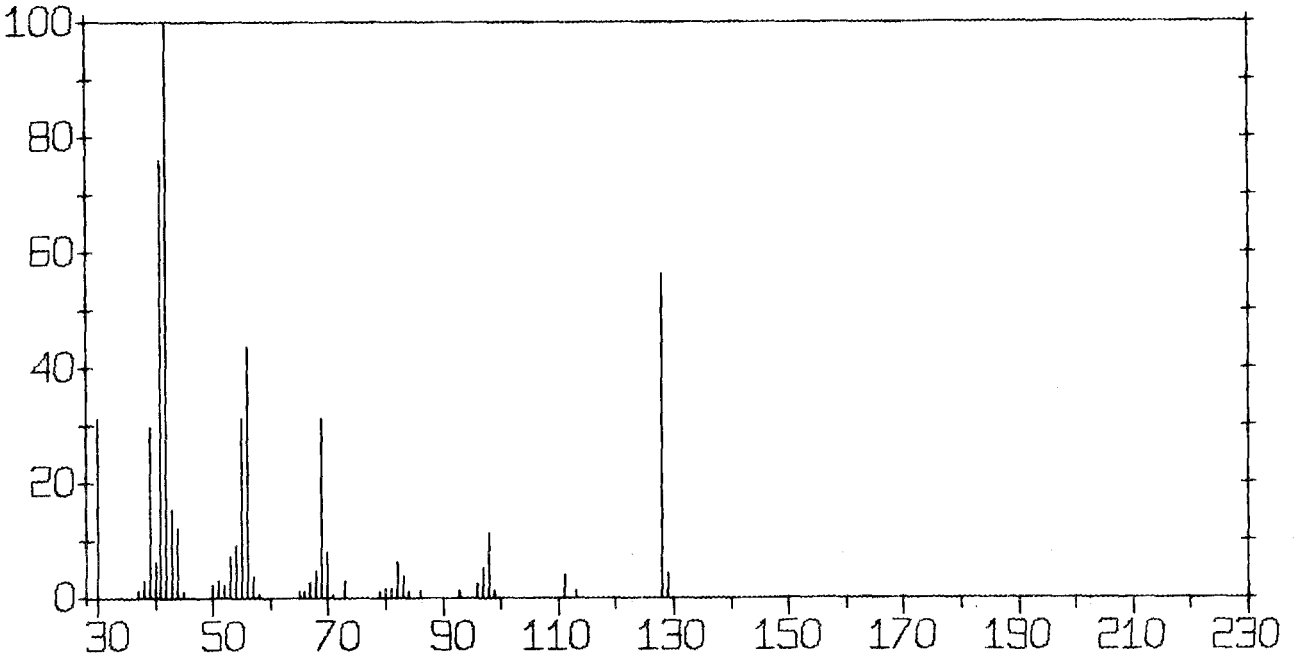
OBSERVED METASTABLES
24.4, 35.2, 37.2, 48.6, 65.2, 77.2,



N-NITROSO-4-METHYLPIPERIDINE
MW = 128 C6.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	31.2	45.0	0.9	58.0	0.6	79.0	0.9	96.0	2.5
37.0	1.2	50.0	2.1	65.0	1.2	80.0	1.5	97.0	5.3
38.0	3.1	51.0	3.1	66.0	1.2	81.0	1.5	98.0	11.2
39.0	29.6	52.0	2.1	67.0	2.8	82.0	6.2	99.0	1.2
40.0	6.2	53.0	7.1	68.0	4.6	83.0	3.7	111.0	4.0
41.0	75.9	54.0	9.3	69.0	31.2	84.0	0.9	113.0	1.2
42.0	100.0	55.0	31.2	70.0	8.1	86.0	1.2	128.0	56.2
43.0	15.6	56.0	43.7	71.0	0.6	93.0	1.2	129.0	4.3
44.0	12.1	57.0	3.7	73.0	3.1				

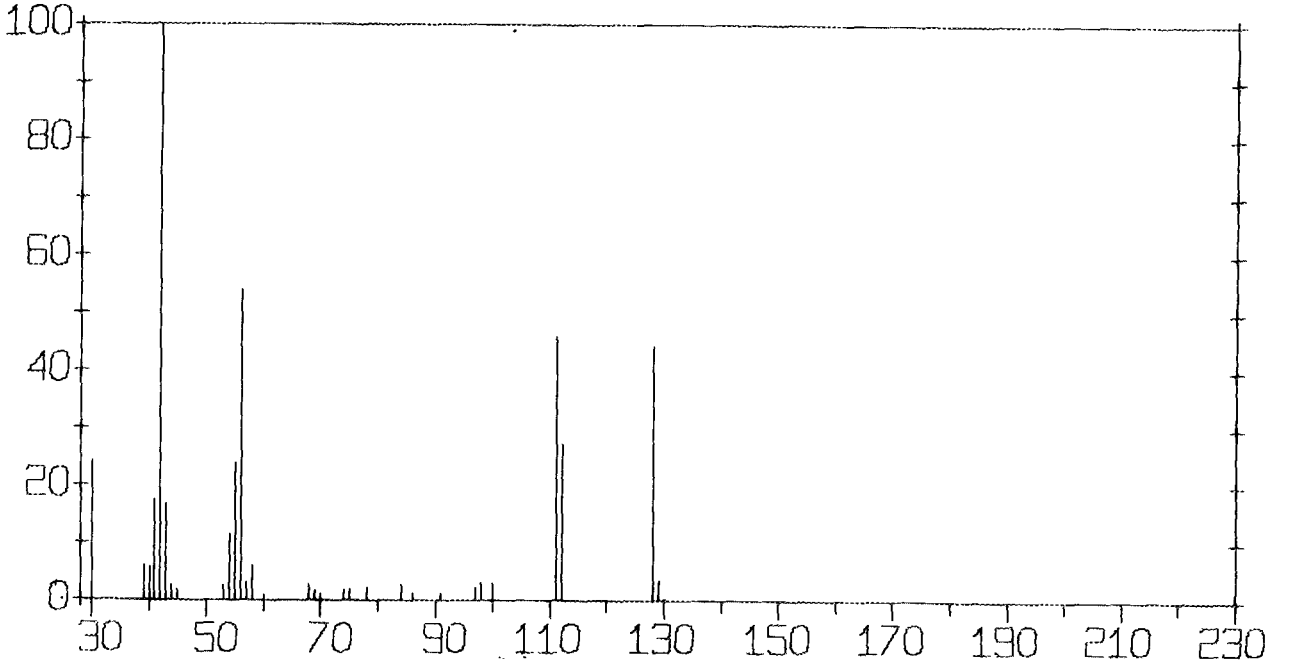
OBSERVED METASTABLES
27.9, 32.0, 37.1, 40.8, 41.9, 48.7, 55.5, 68.7,



N-NITROSO-4-PIPERIDONE
MW = 128 C4.H8.N2.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	24.2	45.0	1.6	60.0	0.8	78.0	2.2	100.0	2.9
39.0	6.0	53.0	2.6	68.0	2.8	84.0	2.7	111.0	45.9
40.0	5.7	54.0	11.4	69.0	1.8	86.0	1.2	112.0	27.2
41.0	17.3	55.0	23.9	70.0	0.9	91.0	1.3	128.0	44.2
42.0	100.0	56.0	54.0	74.0	1.8	97.0	2.2	129.0	3.5
43.0	16.7	57.0	3.0	75.0	1.9	98.0	2.9	130.0	0.2
44.0	2.6	58.0	5.9						

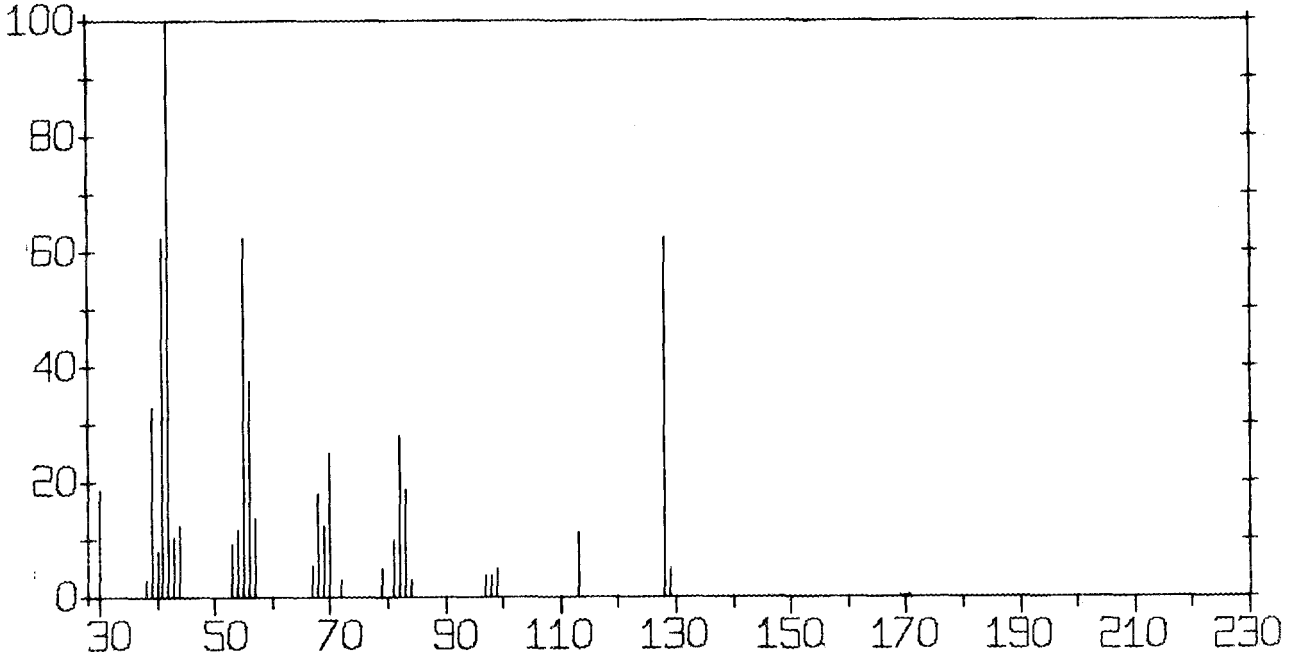
OBSERVED METASTABLES
96.2,



N-NITROSO-2,5-DIMETHYLPYRROLIDINE
MW = 128 C6.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	18.7	43.0	10.6	57.0	13.7	79.0	5.0	98.0	3.7
38.0	3.1	44.0	12.5	67.0	5.6	81.0	10.0	99.0	5.0
39.0	33.1	53.0	9.3	68.0	18.1	82.0	28.1	113.0	11.2
40.0	8.1	54.0	11.8	69.0	12.5	83.0	18.7	128.0	62.5
41.0	62.5	55.0	62.5	70.0	25.0	84.0	3.1	129.0	5.0
42.0	100.0	56.0	37.5	72.0	3.1	97.0	3.7		

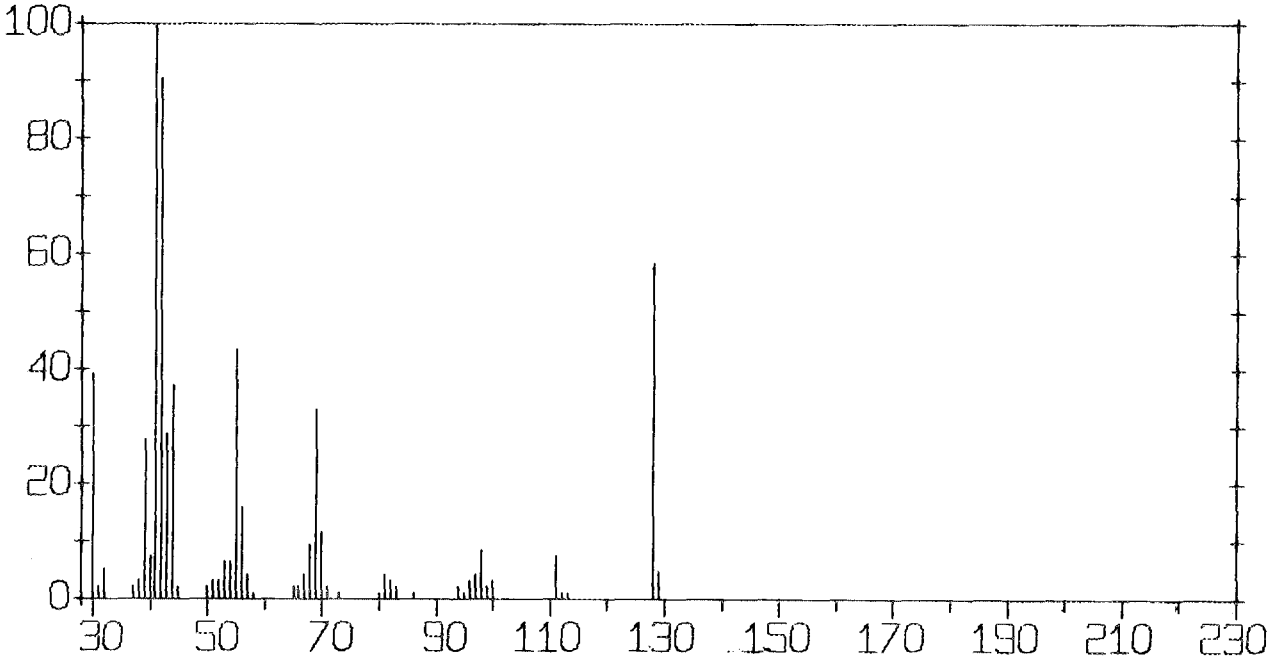
OBSERVED METASTABLES
59.7, 77.1, 96.2,



N-NITROSOHEXAMETHYLENEIMINE
MW = 128 C6.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	39.3	44.0	37.2	57.0	4.2	73.0	1.0	97.0	4.2
31.0	2.1	45.0	2.1	58.0	1.0	80.0	1.0	98.0	8.5
32.0	5.3	50.0	2.1	65.0	2.1	81.0	4.2	99.0	2.1
37.0	2.1	51.0	3.1	66.0	2.1	82.0	3.1	100.0	3.1
38.0	3.1	52.0	3.1	67.0	4.2	83.0	2.1	111.0	7.4
39.0	27.6	53.0	6.3	68.0	9.5	86.0	1.0	112.0	1.0
40.0	7.4	54.0	6.3	69.0	32.9	94.0	2.1	113.0	1.0
41.0	100.0	55.0	43.6	70.0	11.7	95.0	1.0	128.0	58.5
42.0	90.4	56.0	15.9	71.0	2.1	96.0	3.1	129.0	5.3
43.0	28.7								

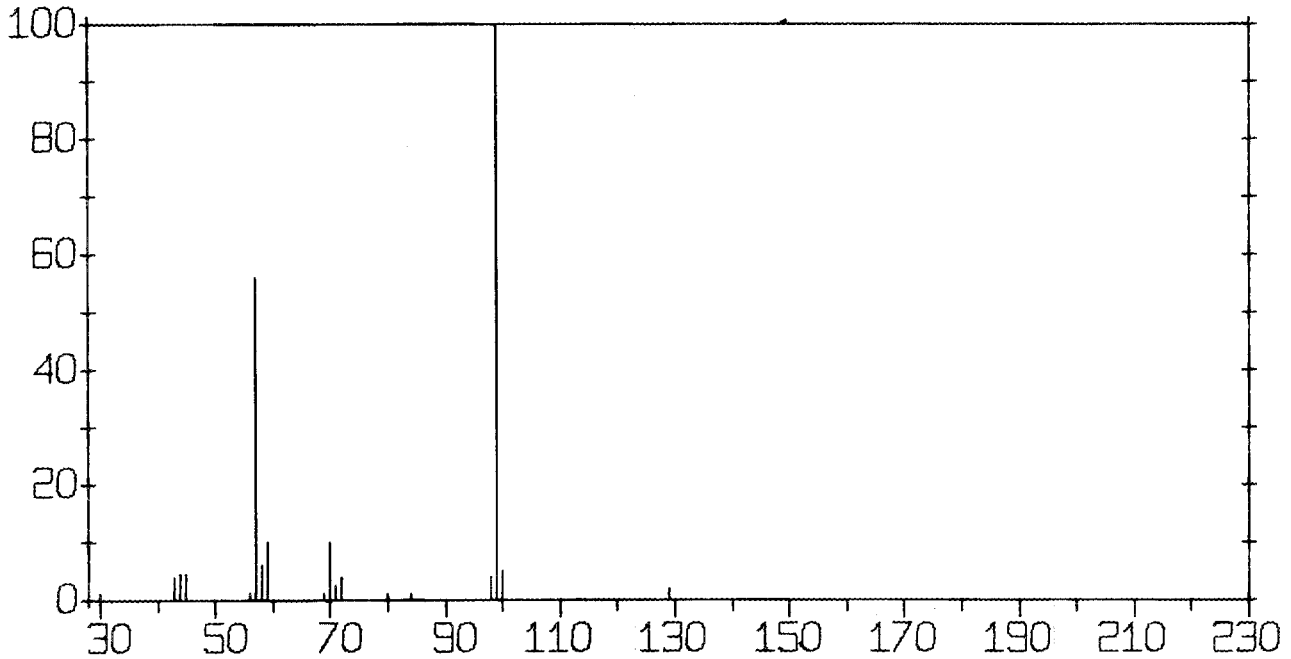
OBSERVED METASTABLES
24.4, 37.2, 50.0, 96.2,



1-NITROSO-4-METHYLPIPERAZINE
MW = 129 C5.H11.N3.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	1.0	56.0	1.2	69.0	1.0	80.0	1.0	99.0	100.0
43.0	4.0	57.0	56.0	70.0	10.0	84.0	1.0	100.0	5.0
44.0	4.4	58.0	6.0	71.0	2.6	98.0	4.0	129.0	2.0
45.0	4.6	59.0	10.0	72.0	4.0				

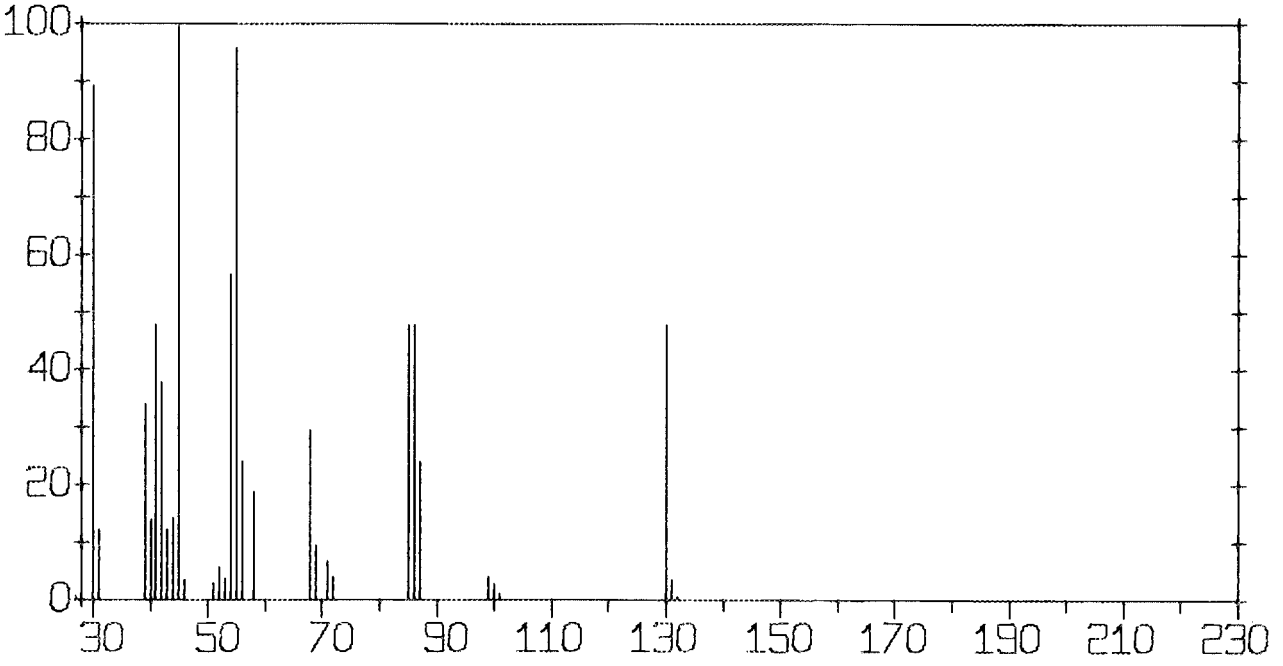
OBSERVED METASTABLES
31.6, 51.0, 76.0,



N-NITROSOAZETIDINE-2-CARBOXYLIC ACID
MW = 130 C4.H6.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	89.1	43.0	12.1	53.0	3.6	69.0	9.5	99.0	3.9
31.0	12.1	44.0	14.3	54.0	56.5	71.0	6.7	100.0	2.8
39.0	33.9	45.0	100.0	55.0	95.6	72.0	3.9	101.0	1.0
40.0	13.9	46.0	3.4	56.0	23.9	85.0	47.8	130.0	47.8
41.0	47.8	51.0	3.0	58.0	18.6	86.0	47.8	131.0	3.5
42.0	37.8	52.0	5.6	68.0	29.5	87.0	23.9	132.0	0.4

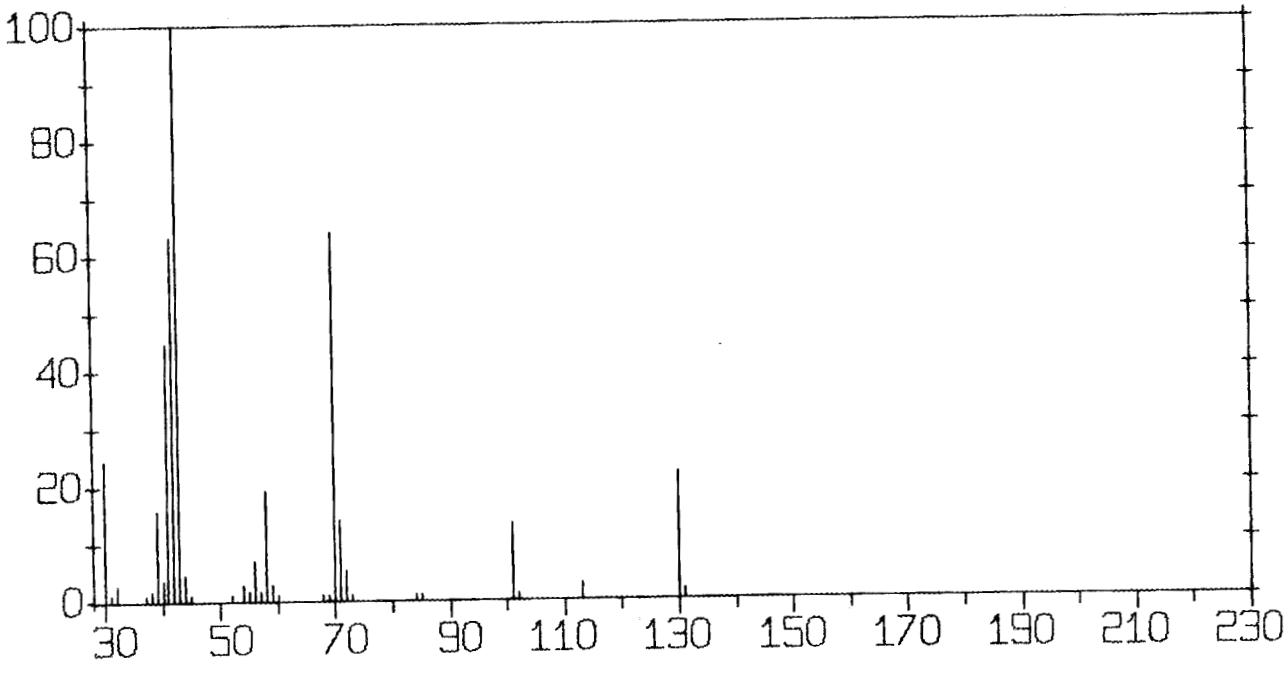
OBSERVED METASTABLES
35.7, 39.1, 53.8, 56.9,



N-NITROSODI-N-PROPYLAMINE
MW = 130 C6.H14.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	24.5	41.0	44.7	55.0	1.7	69.0	0.8	85.0	0.8
31.0	0.8	42.0	63.1	56.0	7.0	70.0	64.0	101.0	13.1
32.0	2.6	43.0	100.0	57.0	1.7	71.0	14.0	102.0	0.8
37.0	0.8	44.0	4.3	58.0	19.2	72.0	5.2	113.0	2.6
38.0	1.7	45.0	0.8	59.0	2.6	73.0	0.8	130.0	21.9
39.0	15.7	52.0	0.8	60.0	0.8	84.0	0.8	131.0	1.7
40.0	3.5	54.0	2.6	68.0	0.8				

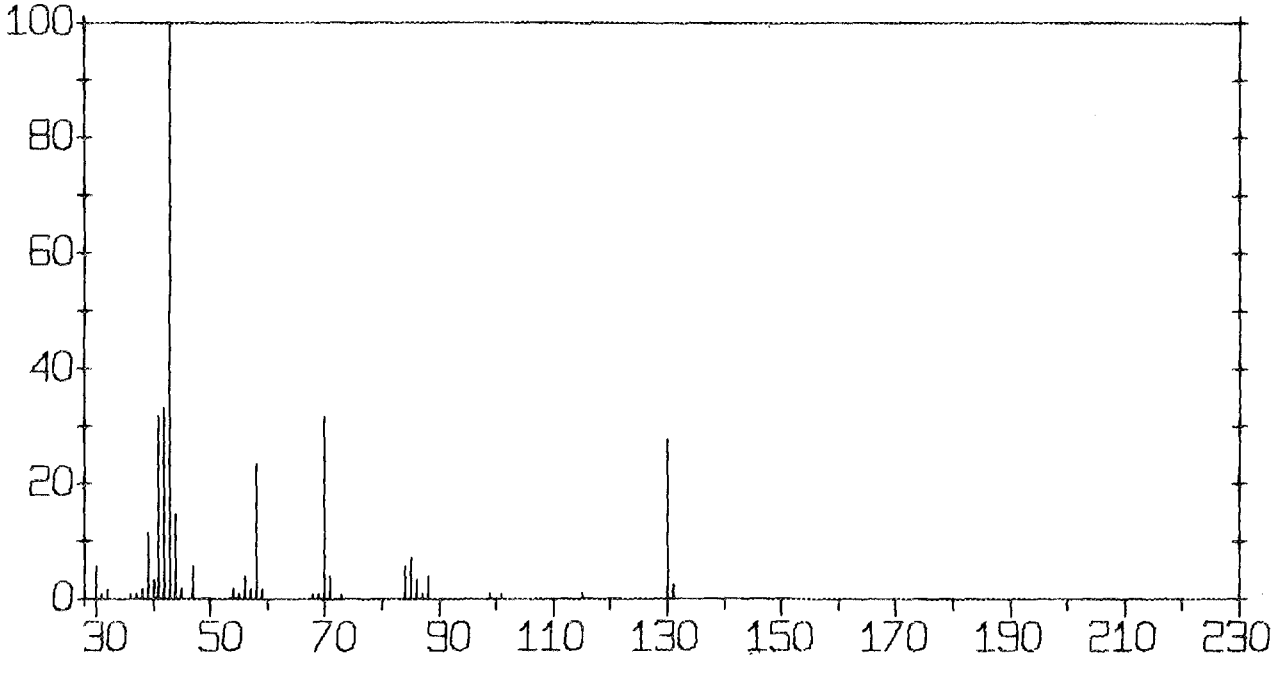
OBSERVED METASTABLES
37.2, 39.2, 48.5, 49.5, 59.5, 98.2,



N-NITROSODIISOPROPYLAMINE
MW = 130 C6.H14.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	5.6	40.0	3.2	54.0	1.6	69.0	0.8	87.0	0.8
31.0	0.8	41.0	31.7	55.0	0.8	70.0	31.7	88.0	4.0
32.0	1.6	42.0	33.3	56.0	4.0	71.0	4.0	99.0	0.8
36.0	0.8	43.0	100.0	57.0	1.6	73.0	0.8	101.0	0.8
37.0	0.8	44.0	14.6	58.0	23.5	84.0	5.6	115.0	0.8
38.0	1.6	45.0	1.6	59.0	1.6	85.0	7.3	130.0	27.6
39.0	11.3	47.0	5.6	68.0	0.8	86.0	3.2	131.0	2.4

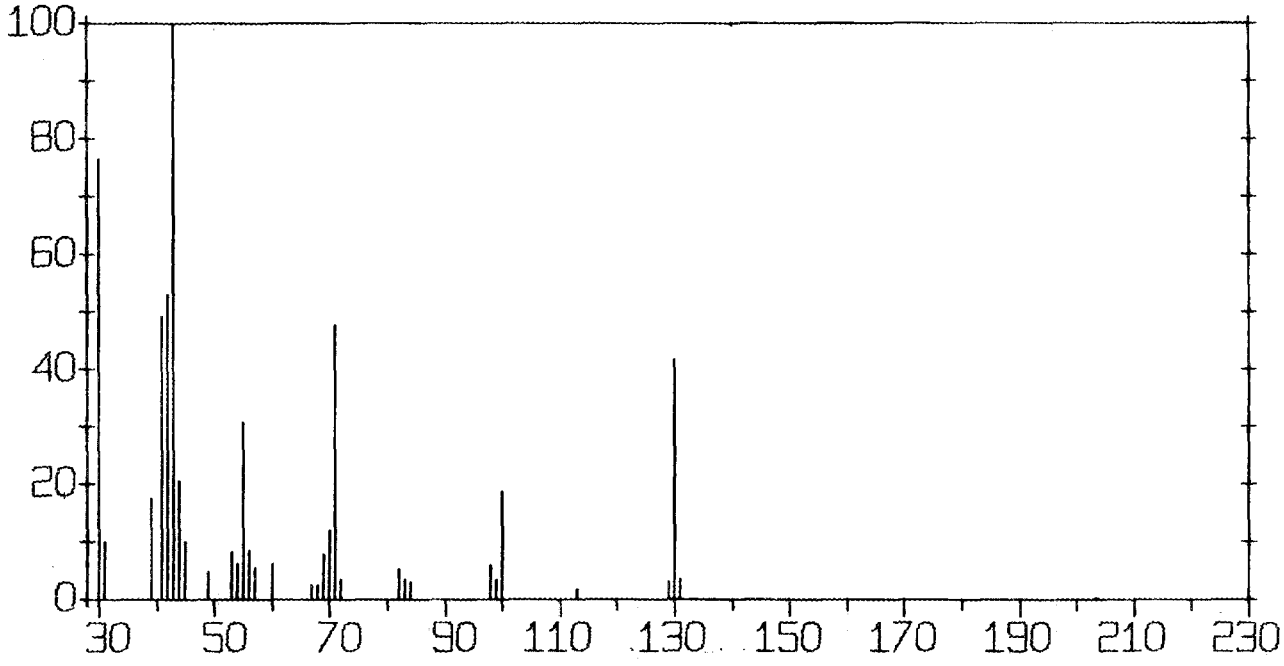
OBSERVED METASTABLES
15.5, 21.0, 22.5, 25.2, 26.5, 35.4, 37.2, 39.2, 54.2, 57.8, 59.6, 73.1,
98.2,



N-NITROSO-3-PIPERIDINOL
MW = 130 C5.H10.N2.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	76.5	45.0	10.0	57.0	5.4	71.0	47.8	99.0	3.3
31.0	10.0	49.0	4.7	60.0	6.3	72.0	3.3	100.0	18.6
39.0	17.3	53.0	8.2	67.0	2.6	82.0	5.3	113.0	1.8
41.0	49.1	54.0	6.3	68.0	2.6	83.0	3.4	129.0	3.0
42.0	53.0	55.0	30.8	69.0	7.8	84.0	3.0	130.0	41.7
43.0	100.0	56.0	8.6	70.0	11.9	98.0	6.0	131.0	3.4
44.0	20.4								

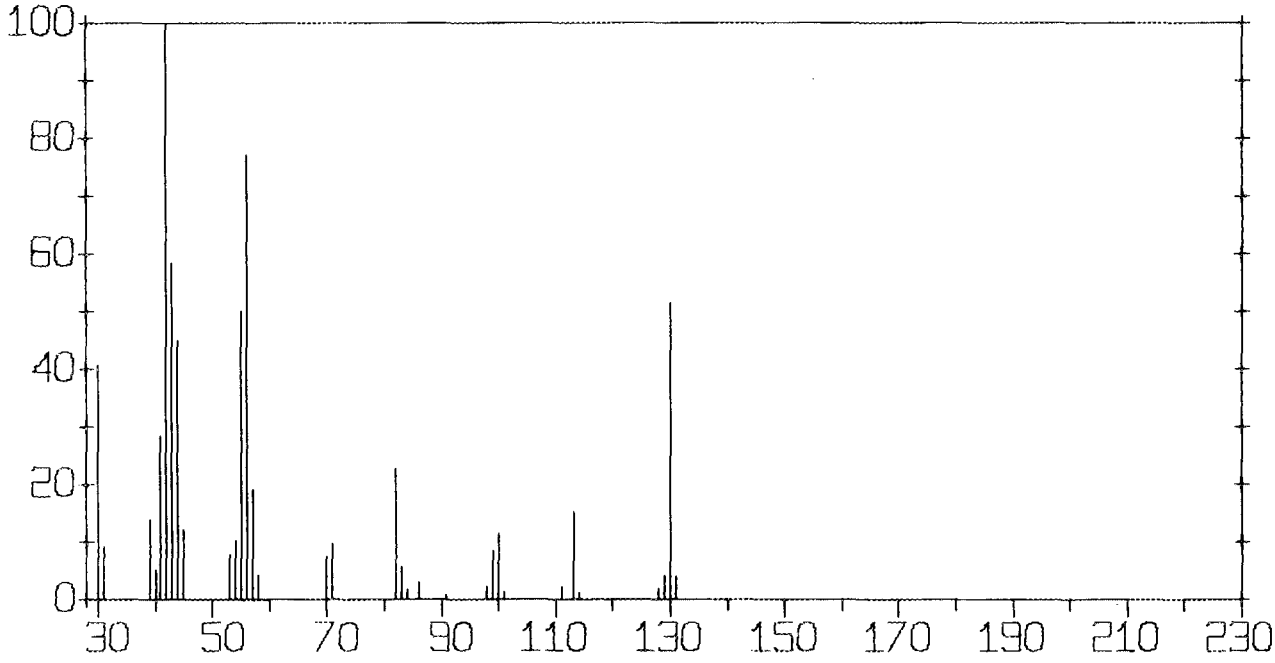
OBSERVED METASTABLES
26.1, 39.1, 47.7, 50.4, 51.6, 74.6, 77.1,



N-NITROSO-4-PIPERIDINOL
MW = 130 C5.H10.N2.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	40.7	44.0	45.0	58.0	4.2	91.0	0.7	113.0	15.1
31.0	9.2	45.0	12.1	70.0	7.5	98.0	2.1	114.0	0.9
39.0	13.9	53.0	7.8	71.0	9.6	99.0	8.4	128.0	2.0
40.0	5.3	54.0	10.3	82.0	22.8	100.0	11.4	129.0	4.2
41.0	28.5	55.0	50.0	83.0	5.7	101.0	1.1	130.0	51.4
42.0	100.0	56.0	77.1	84.0	1.7	111.0	2.1	131.0	3.9
43.0	58.5	57.0	19.2	86.0	3.0				

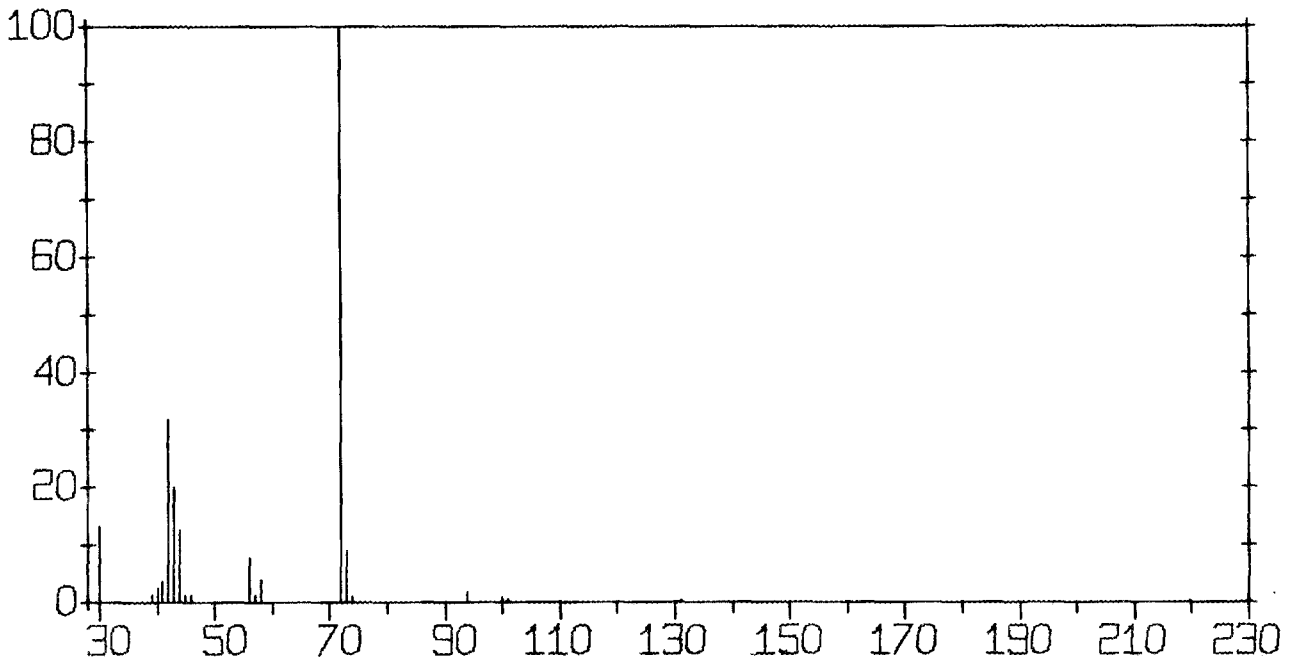
OBSERVED METASTABLES
51.8, 76.0, 78.0, 98.2,



N-NITROSOTRIMETHYL UREA
MW = 131 C4.H9.N3.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	13.3	42.0	31.6	46.0	1.1	72.0	100.0	100.0	0.6
39.0	1.3	43.0	20.0	56.0	7.6	73.0	9.0	101.0	0.5
40.0	2.5	44.0	12.5	57.0	1.1	74.0	1.0	131.0	0.3
41.0	3.8	45.0	1.1	58.0	4.0	94.0	1.6		

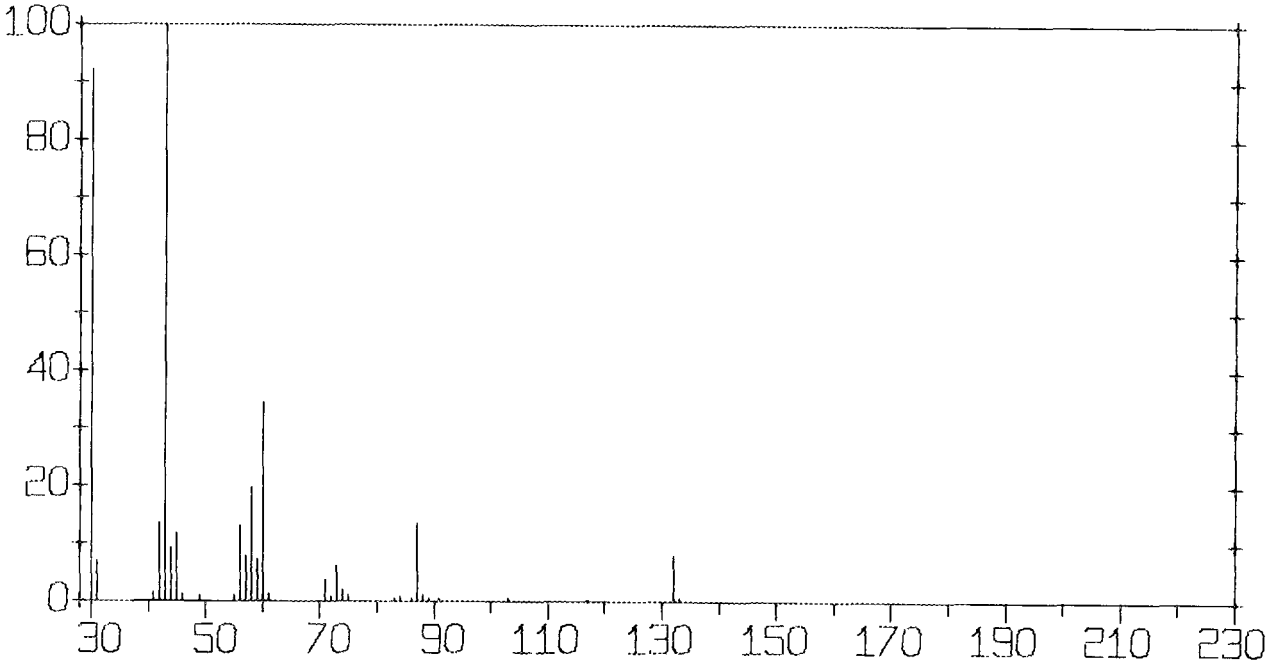
OBSERVED METASTABLES
26.7, 43.6, 71.6,



N-NITROSO-N-METHYL ETHYL CARBAMATE
MW = 132 C4.H8.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	92.3	46.0	1.3	60.0	34.6	75.0	0.9	89.0	0.4
31.0	6.9	49.0	1.0	61.0	1.3	83.0	0.4	91.0	0.4
41.0	1.4	55.0	1.0	71.0	3.6	84.0	0.7	103.0	0.4
42.0	13.4	56.0	12.8	72.0	0.6	86.0	0.4	117.0	0.3
43.0	100.0	57.0	7.6	73.0	6.1	87.0	13.4	132.0	7.8
44.0	9.2	58.0	19.8	74.0	1.9	88.0	1.1	133.0	0.5
45.0	11.7	59.0	7.3						

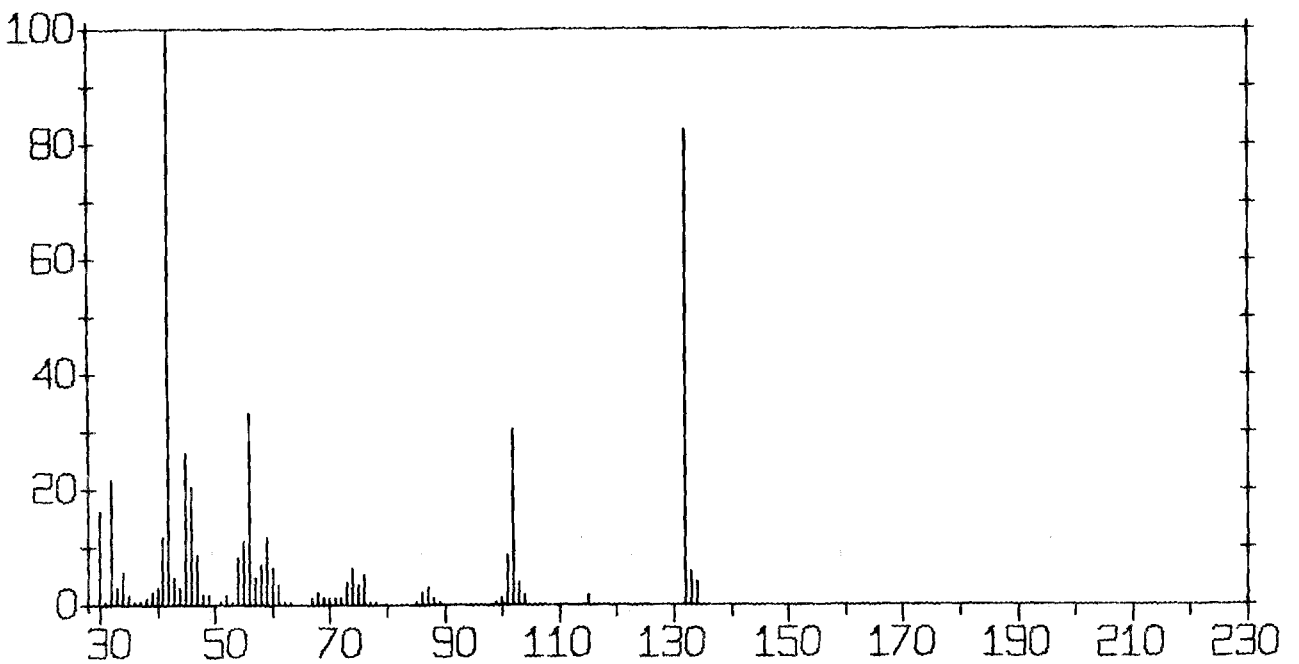
OBSERVED METASTABLES
24.2, 38.2, 54.1, 57.1, 67.9,



N-NITROSOTHIOMORPHOLINE
MW = 132 C4.H8.N2.O.S.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	16.3	42.0	100.0	55.0	11.1	70.0	1.1	88.0	1.1
31.0	0.5	43.0	4.6	56.0	33.3	71.0	1.1	89.0	0.5
32.0	21.6	44.0	2.9	57.0	4.6	72.0	1.1	99.0	0.5
33.0	2.9	45.0	26.3	58.0	7.0	73.0	4.0	100.0	1.1
34.0	5.8	46.0	20.4	59.0	11.6	74.0	6.4	101.0	8.7
35.0	1.7	47.0	8.7	60.0	6.4	75.0	3.5	102.0	30.4
36.0	0.5	48.0	1.7	61.0	3.5	76.0	5.2	103.0	4.0
37.0	0.5	49.0	1.7	62.0	0.5	77.0	0.5	104.0	1.7
38.0	1.1	51.0	0.5	63.0	0.5	78.0	0.5	115.0	1.7
39.0	2.3	52.0	1.7	67.0	1.1	85.0	0.5	132.0	82.4
40.0	2.9	53.0	0.5	68.0	2.3	86.0	2.3	133.0	5.8
41.0	11.6	54.0	8.1	69.0	1.1	87.0	2.9	134.0	4.0

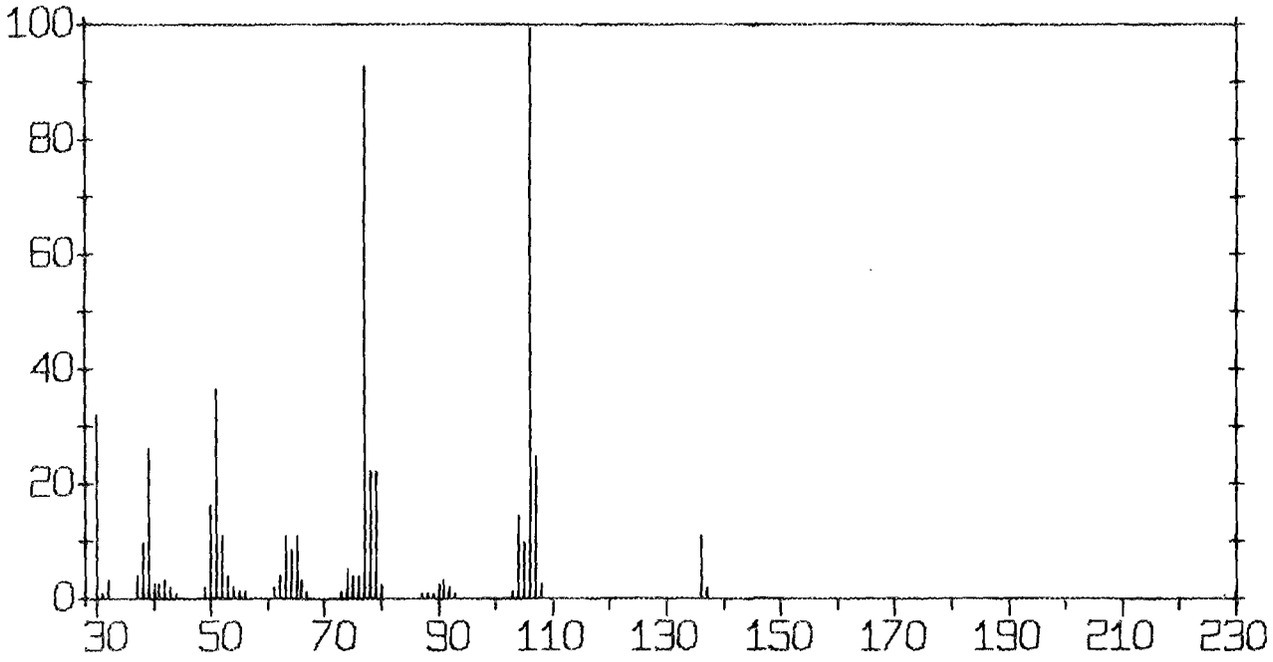
OBSERVED METASTABLES
17.4, 29.5, 78.8, 100.2,



N-NITROSOMETHYLPHENYLAMINE
MW = 136 C7.H8.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	32.0	44.0	0.6	62.0	3.9	77.0	92.8	93.0	0.6
31.0	0.6	49.0	1.9	63.0	11.1	78.0	22.2	103.0	1.3
32.0	3.2	50.0	16.3	64.0	8.4	79.0	22.2	104.0	14.3
37.0	3.9	51.0	36.6	65.0	11.1	80.0	2.6	105.0	9.8
38.0	9.8	52.0	11.1	66.0	3.2	87.0	0.6	106.0	100.0
39.0	26.1	53.0	3.9	67.0	1.3	88.0	0.6	107.0	24.8
40.0	2.6	54.0	1.9	73.0	1.3	89.0	0.6	108.0	2.6
41.0	2.6	55.0	1.3	74.0	5.2	90.0	2.6	136.0	11.1
42.0	3.2	56.0	1.3	75.0	3.9	91.0	3.2	137.0	1.9
43.0	1.9	61.0	1.9	76.0	3.9	92.0	1.9		

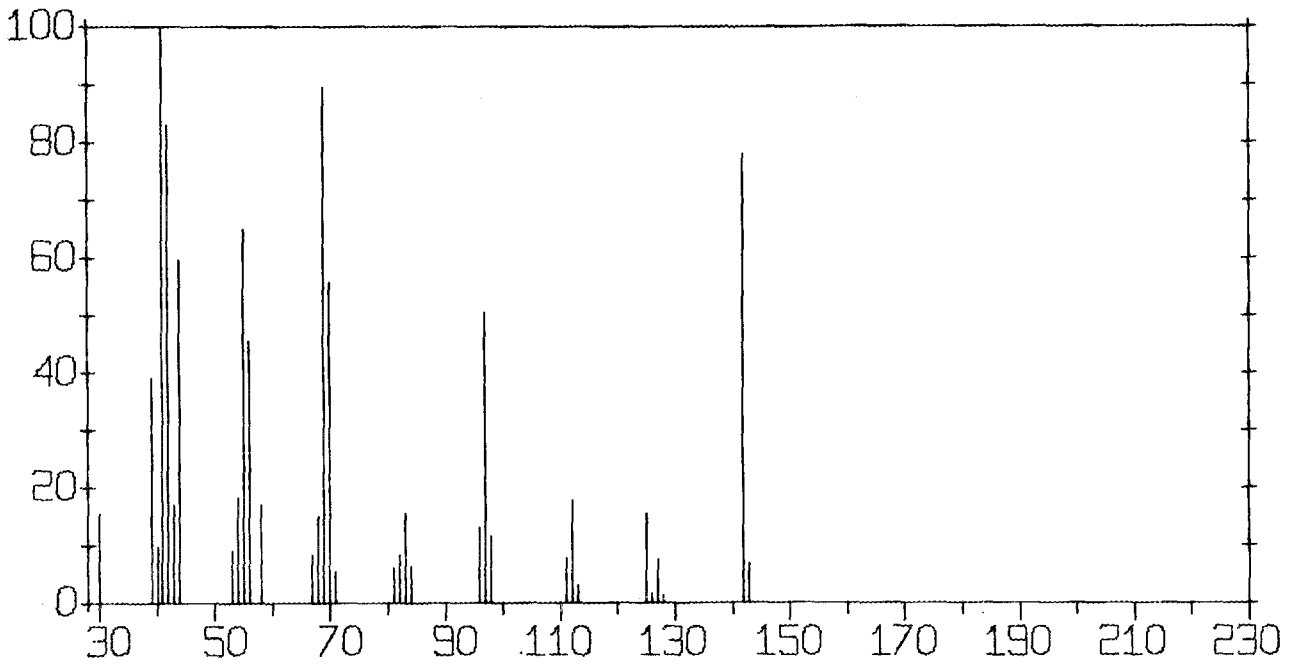
OBSERVED METASTABLES
33.8, 55.9, 57.2, 59.0, 75.2, 82.6, 102.2, 103.2,



N-NITROSO-2,6-DIMETHYLPIPERIDINE
MW = 142 C7,H14,N2,O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	15.5	53.0	9.0	69.0	89.6	96.0	12.9	125.0	15.5
39.0	38.9	54.0	18.1	70.0	55.8	97.0	50.5	126.0	1.5
40.0	9.7	55.0	64.9	71.0	5.4	98.0	11.4	127.0	7.4
41.0	100.0	56.0	45.4	81.0	6.1	111.0	7.7	128.0	1.1
42.0	83.1	58.0	16.8	82.0	8.3	112.0	17.6	142.0	77.9
43.0	16.8	67.0	8.1	83.0	15.5	113.0	2.9	143.0	6.7
44.0	59.7	68.0	14.9	84.0	6.2				

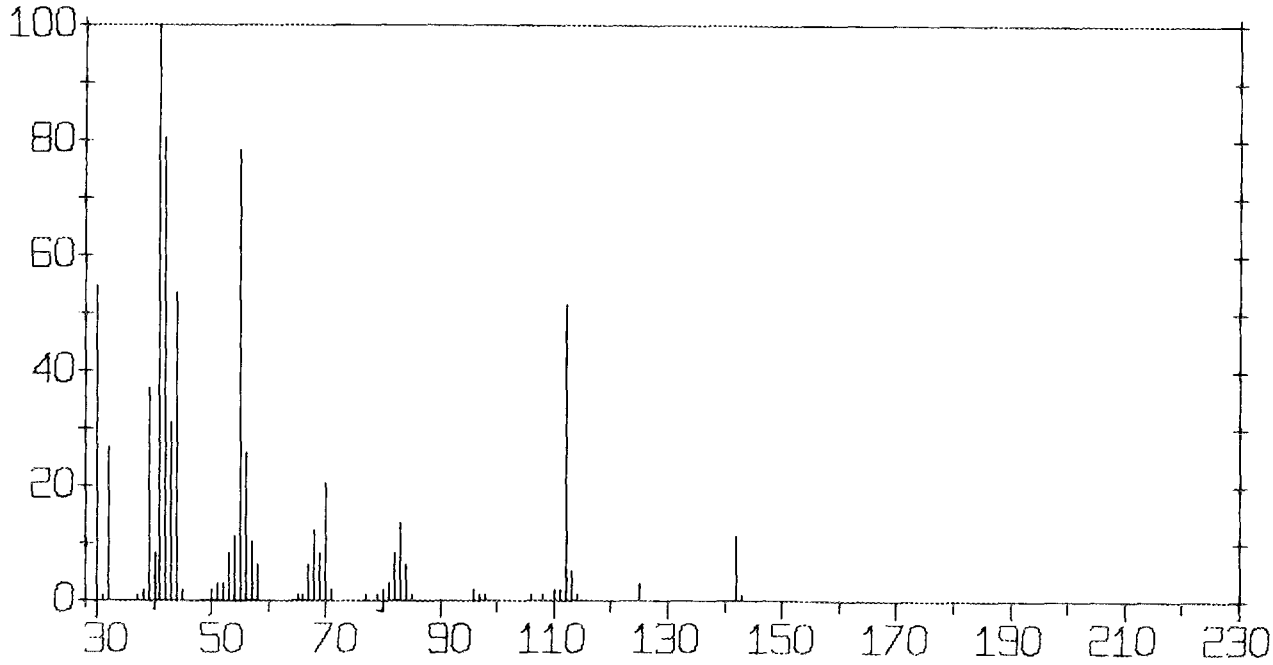
OBSERVED METASTABLES
42.3, 49.0, 74.1, 110.1,



N-NITROSOHEPTAMETHYLENEIMINE
MW = 142 C7.H14.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	54.6	44.0	53.6	58.0	6.1	80.0	2.0	108.0	1.0
31.0	1.0	45.0	2.0	65.0	1.0	81.0	3.0	110.0	2.0
32.0	26.8	50.0	2.0	66.0	1.0	82.0	8.2	111.0	2.0
37.0	1.0	51.0	3.0	67.0	6.1	83.0	13.4	112.0	51.5
38.0	2.0	52.0	3.0	68.0	12.3	84.0	6.1	113.0	5.1
39.0	37.1	53.0	8.2	69.0	8.2	85.0	1.0	114.0	1.0
40.0	8.2	54.0	11.3	70.0	20.6	96.0	2.0	125.0	3.0
41.0	100.0	55.0	78.3	71.0	2.0	97.0	1.0	142.0	11.3
42.0	80.4	56.0	25.7	77.0	1.0	98.0	1.0	143.0	1.0
43.0	30.9	57.0	10.3	79.0	1.0	106.0	1.0		

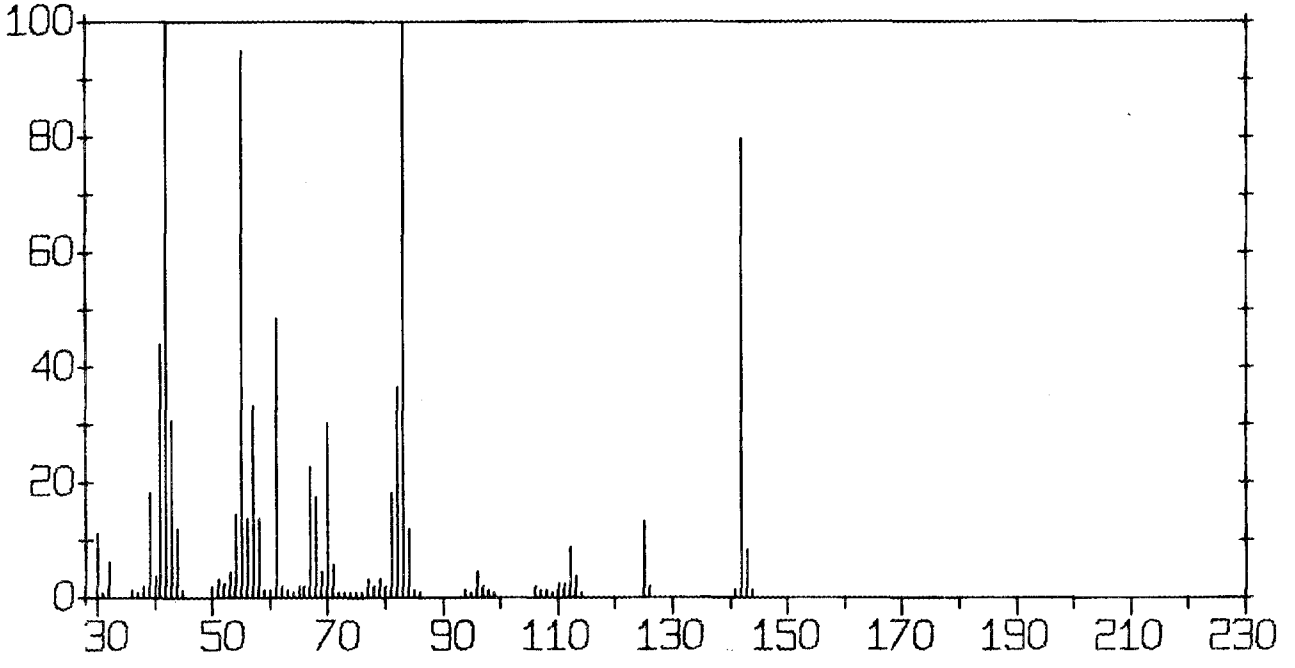
OBSERVED METASTABLES
17.3, 36.5, 37.2, 60.6, 61.6, 88.8,



N-NITROSOMETHYLCYCLOHEXYLAMINE
MW = 142 C7.H14.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	11.3	52.0	2.5	66.0	1.8	80.0	1.8	107.0	1.2
31.0	0.6	53.0	4.4	67.0	22.6	81.0	18.2	108.0	1.2
32.0	6.2	54.0	0.0	68.0	17.6	82.0	36.4	109.0	0.6
36.0	1.2	54.0	14.4	69.0	4.4	83.0	100.0	110.0	2.5
37.0	0.6	55.0	94.9	70.0	30.1	84.0	11.9	111.0	2.5
38.0	1.8	56.0	13.8	71.0	5.6	85.0	1.2	112.0	8.8
39.0	13.2	57.0	33.3	72.0	0.6	86.0	0.6	113.0	3.7
40.0	3.7	58.0	13.8	73.0	0.6	94.0	1.2	114.0	0.6
41.0	44.0	59.0	1.2	74.0	0.6	95.0	0.6	125.0	13.2
42.0	100.0	60.0	1.2	75.0	0.6	96.0	4.4	126.0	1.8
43.0	30.8	61.0	48.4	76.0	0.6	97.0	1.8	141.0	1.2
44.0	11.9	62.0	1.8	77.0	3.1	98.0	1.2	142.0	79.8
45.0	1.2	63.0	1.2	78.0	1.8	99.0	0.6	143.0	8.1
50.0	1.8	64.0	0.6	79.0	3.1	106.0	1.8	144.0	1.2
51.0	3.1	65.0	1.8						

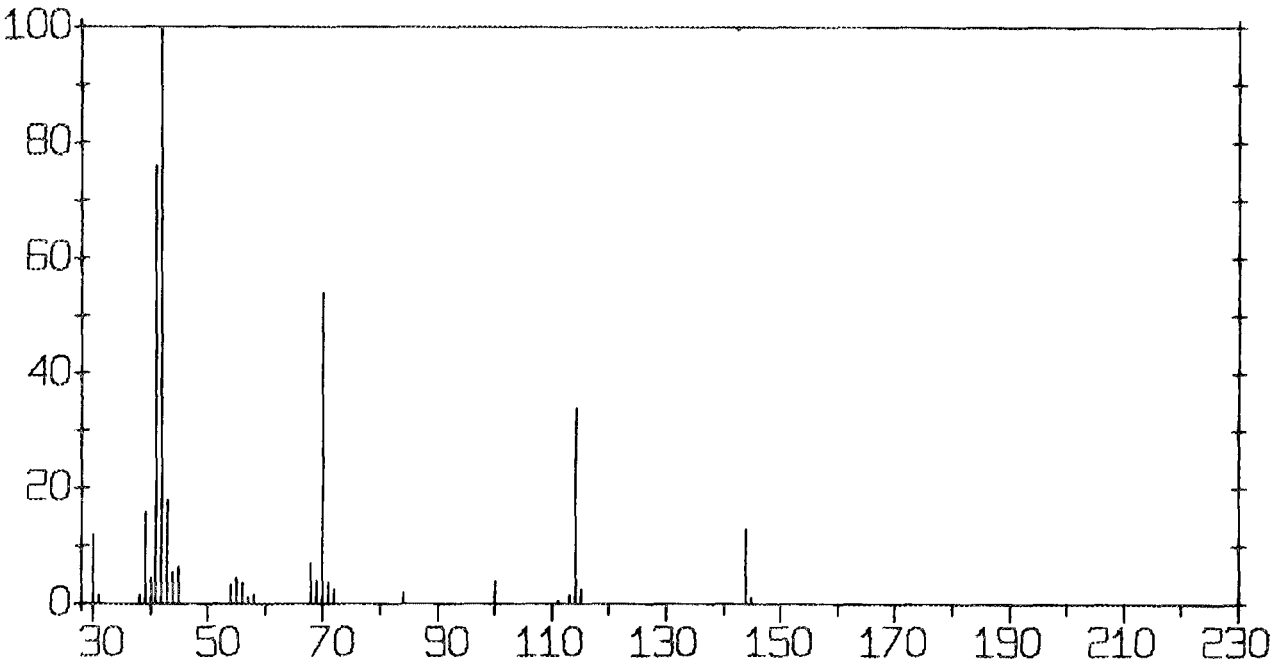
OBSERVED METASTABLES
26.2, 27.8, 28.2, 36.5, 37.2, 37.4, 39.2, 54.8, 77.2, 110.2,



N-NITROSO-2,6-DIMETHYLMORPHOLINE
MW = 144 C6.H12.N2.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	12.0	42.0	100.0	56.0	3.8	71.0	3.8	113.0	1.4
31.0	1.6	43.0	18.0	57.0	1.0	72.0	2.6	114.0	34.0
38.0	1.6	44.0	5.4	58.0	1.6	84.0	2.0	115.0	2.6
39.0	16.0	45.0	6.6	68.0	7.0	100.0	4.0	144.0	13.0
40.0	4.6	54.0	3.2	69.0	4.0	111.0	0.6	145.0	1.0
41.0	76.0	55.0	4.6	70.0	54.0				

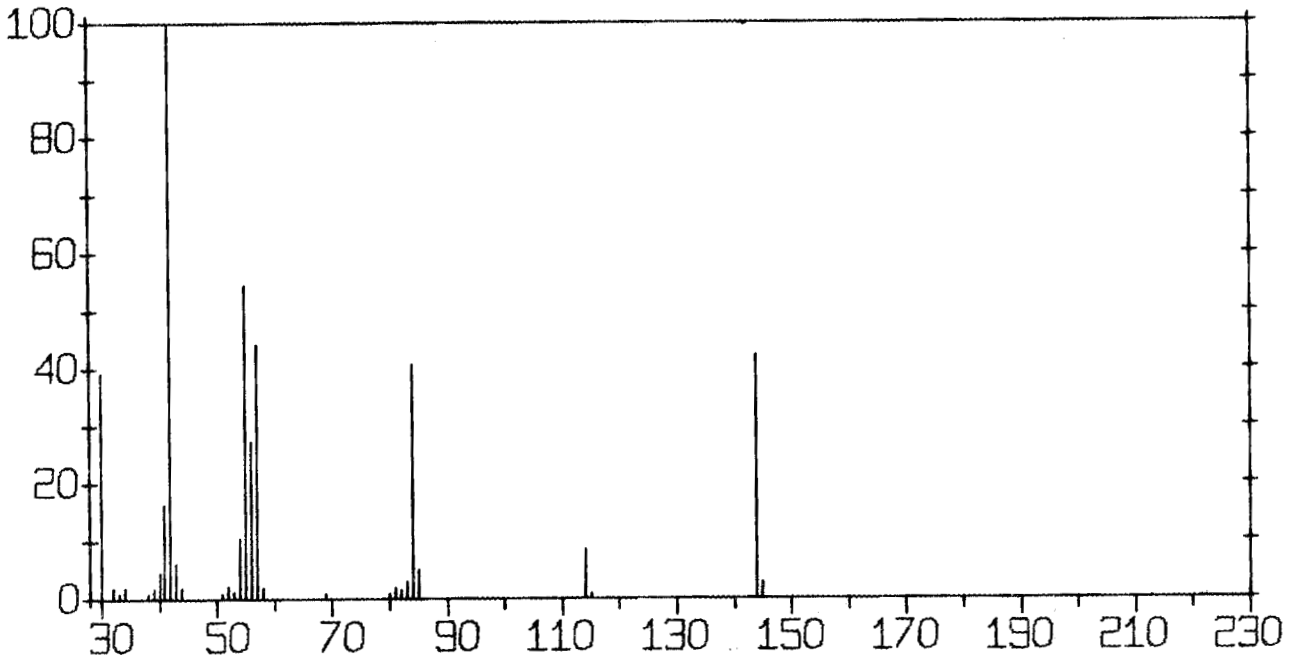
OBSERVED METASTABLES
25.4, 26.4, 45.9, 90.0,



1,4-DINITROSOPIPERAZINE
MW = 144 C4.H8.N4.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	39.2	40.0	4.6	52.0	2.3	58.0	1.9	84.0	40.7
32.0	1.9	41.0	16.5	53.0	1.1	69.0	0.7	85.0	5.0
33.0	0.7	42.0	100.0	54.0	10.3	80.0	0.7	114.0	8.4
34.0	1.9	43.0	6.1	55.0	54.6	81.0	1.9	115.0	0.7
38.0	0.7	44.0	1.9	56.0	27.3	82.0	1.5	144.0	42.3
39.0	1.9	51.0	0.7	57.0	44.2	83.0	3.0	145.0	2.6

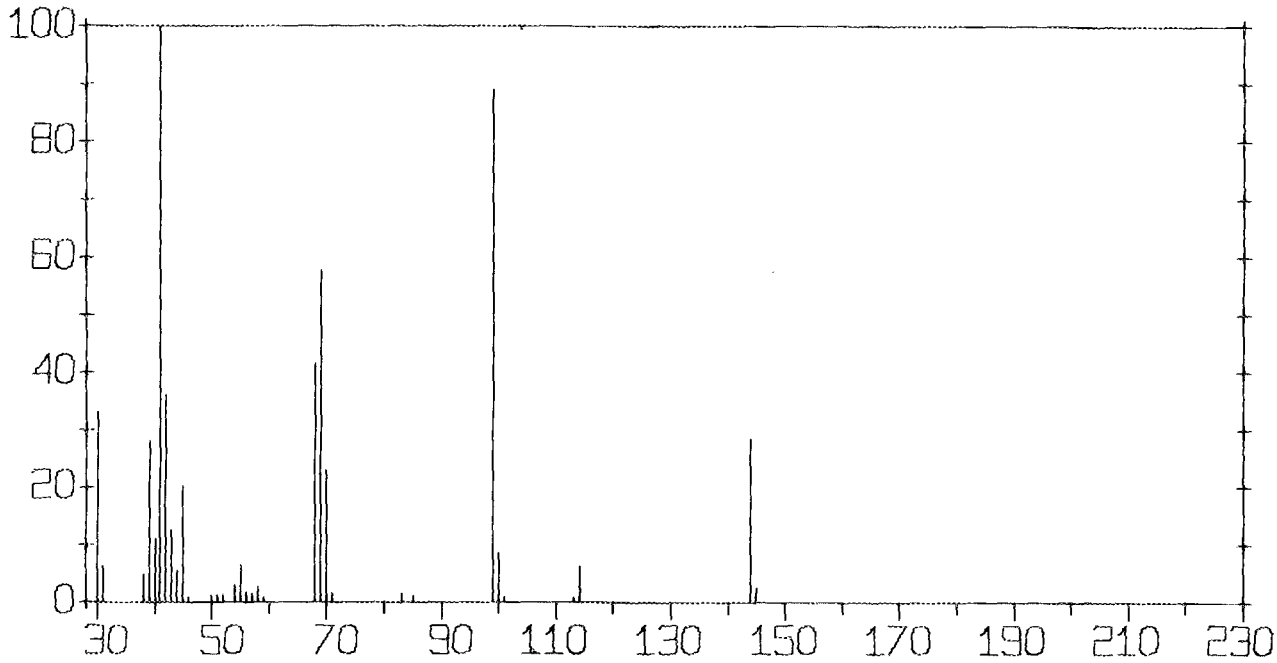
OBSERVED METASTABLES
24.3, 25.2, 36.2, 37.5, 37.8, 49.1, 53.2, 55.2, 62.0, 80.4, 90.4,



N-NITROSOPROLINE
MW = 144 C5.H8.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	33.1	43.0	12.5	54.0	3.1	69.0	57.8	101.0	0.7
31.0	6.2	44.0	5.4	55.0	6.5	70.0	23.1	113.0	0.7
38.0	4.6	45.0	20.3	56.0	1.8	71.0	1.5	114.0	6.2
39.0	28.1	46.0	0.8	57.0	1.4	83.0	1.5	144.0	28.5
40.0	10.9	50.0	1.0	58.0	2.7	85.0	0.9	145.0	2.3
41.0	100.0	51.0	1.1	59.0	0.7	99.0	89.0	146.0	0.3
42.0	35.9	52.0	1.2	68.0	41.4	100.0	8.5		

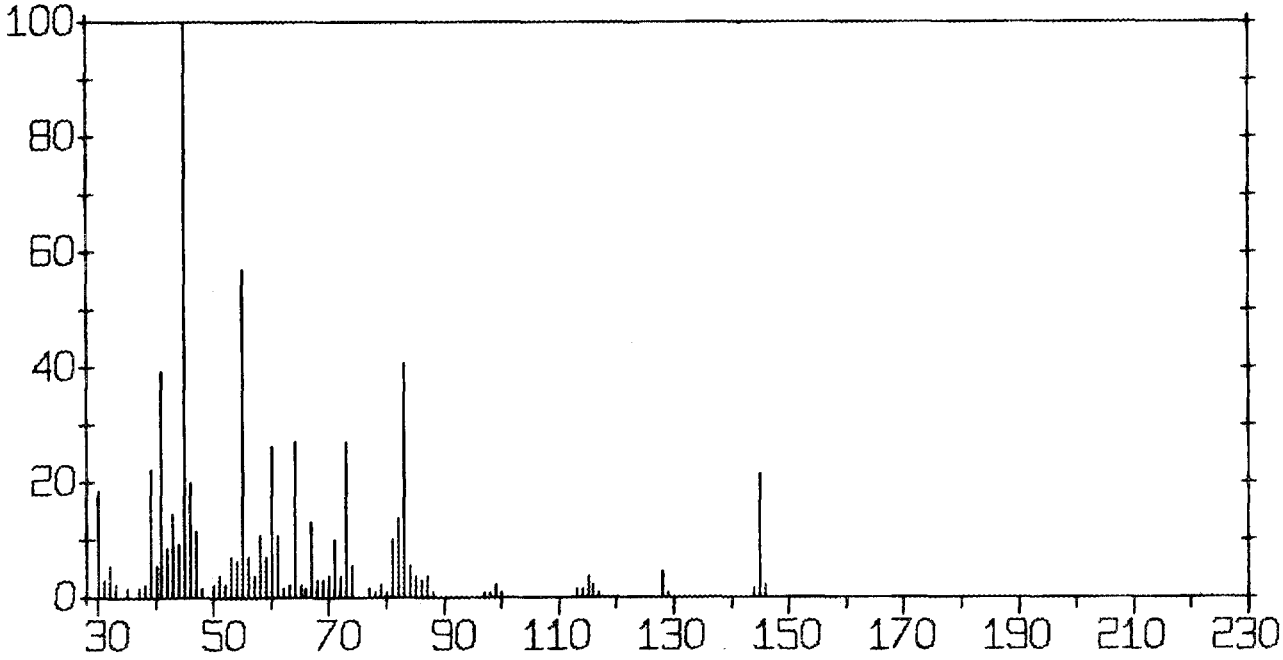
OBSERVED METASTABLES
24.8, 26.4, 46.7, 48.2, 90.3,



N-NITROSOTRIDEUTEROMETHYLCYCLOHEXYLAMINE
MW = 145 C7.H11.D3.N2.O.

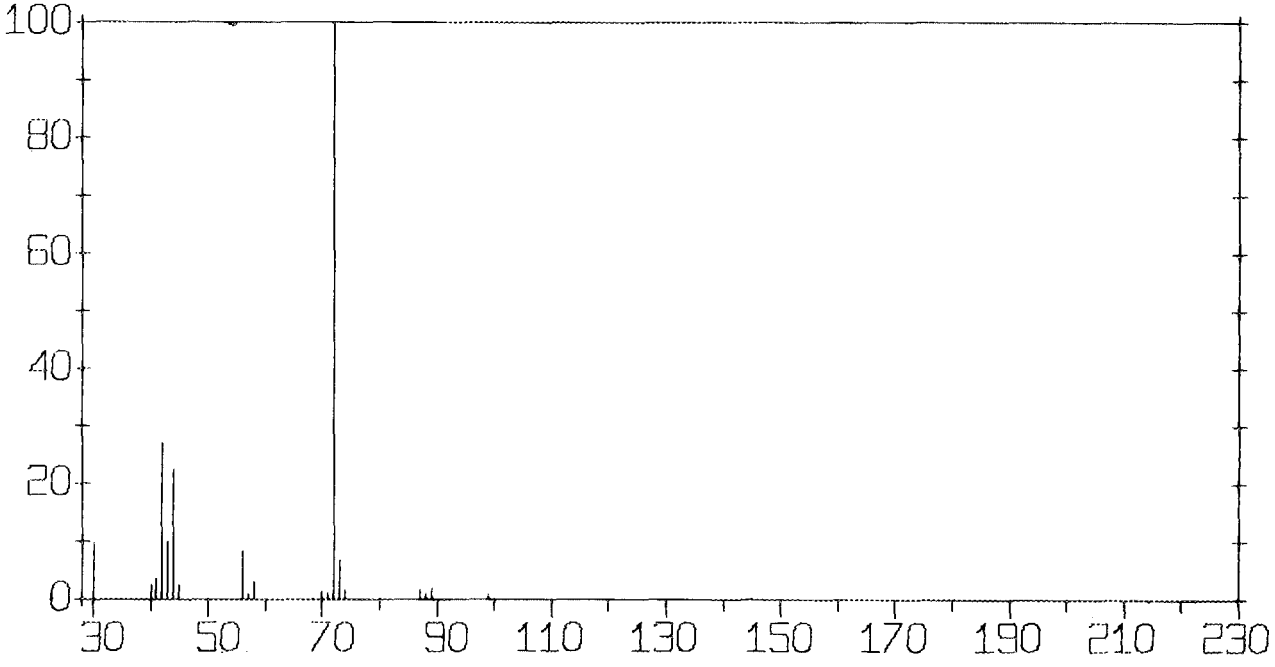
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	18.4	46.0	20.0	61.0	10.7	77.0	1.5	98.0	0.7
31.0	3.0	47.0	11.5	62.0	1.5	78.0	0.7	99.0	2.3
32.0	5.3	48.0	1.5	63.0	2.3	79.0	2.3	100.0	0.7
33.0	2.3	50.0	2.3	64.0	26.9	80.0	0.7	113.0	1.5
35.0	1.5	51.0	3.8	65.0	2.3	81.0	10.0	114.0	1.5
37.0	1.5	52.0	2.3	66.0	1.5	82.0	13.8	115.0	3.8
38.0	2.3	53.0	6.9	67.0	13.0	83.0	40.7	116.0	2.3
39.0	22.3	54.0	6.1	68.0	3.0	84.0	5.3	117.0	0.7
40.0	5.3	55.0	56.9	69.0	3.0	85.0	3.8	128.0	4.6
41.0	39.2	56.0	6.9	70.0	3.8	86.0	3.0	129.0	0.7
42.0	8.4	57.0	3.8	71.0	10.0	87.0	3.8	144.0	1.5
43.0	14.6	58.0	10.7	72.0	3.8	88.0	0.7	145.0	21.5
44.0	9.2	59.0	6.9	73.0	26.9	97.0	0.7	146.0	2.3
45.0	100.0	60.0	26.1	74.0	5.3				

OBSERVED METASTABLES
28.3, 32.4, 36.5, 37.4, 54.8, 77.2, 113.2,



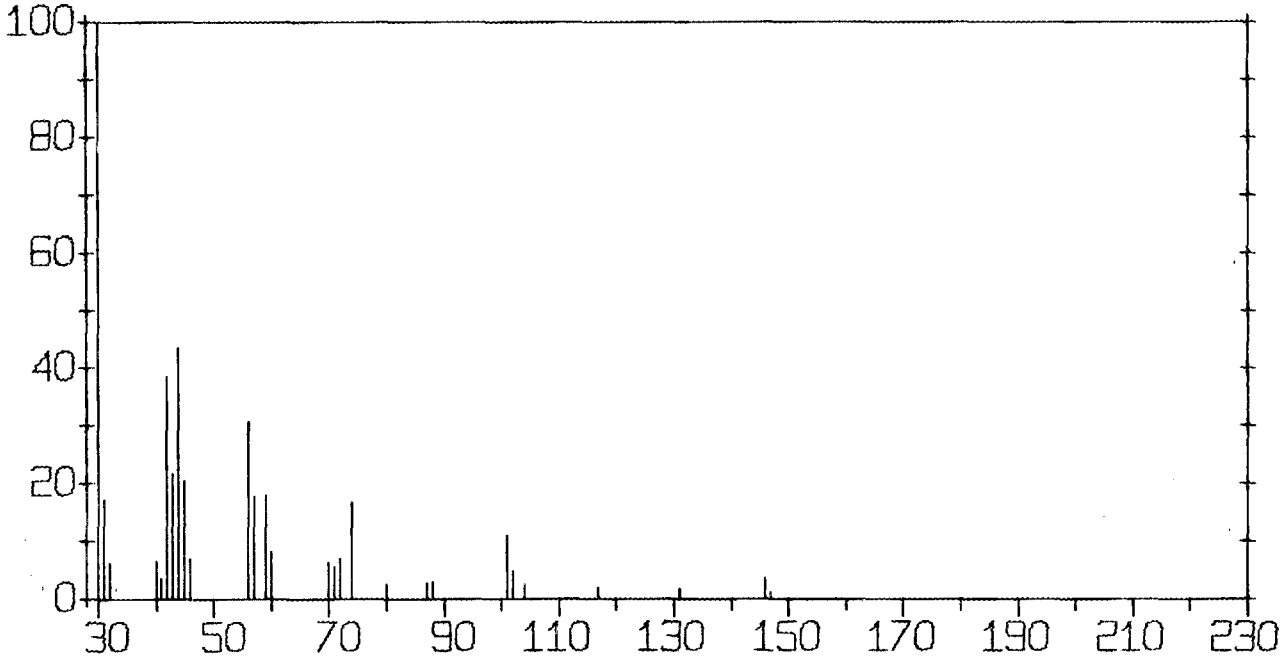
N-NITROSO-1,1-DIMETHYL-3-ETHYLUREA
MW = 145 C5.H11.N3.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	9.7	43.0	10.1	57.0	0.7	72.0	100.0	88.0	1.0
40.0	2.4	44.0	22.5	58.0	2.9	73.0	6.7	89.0	2.0
41.0	3.4	45.0	2.5	70.0	1.1	74.0	1.4	99.0	0.6
42.0	26.9	56.0	8.1	71.0	1.0	87.0	1.7	145.0	0.3



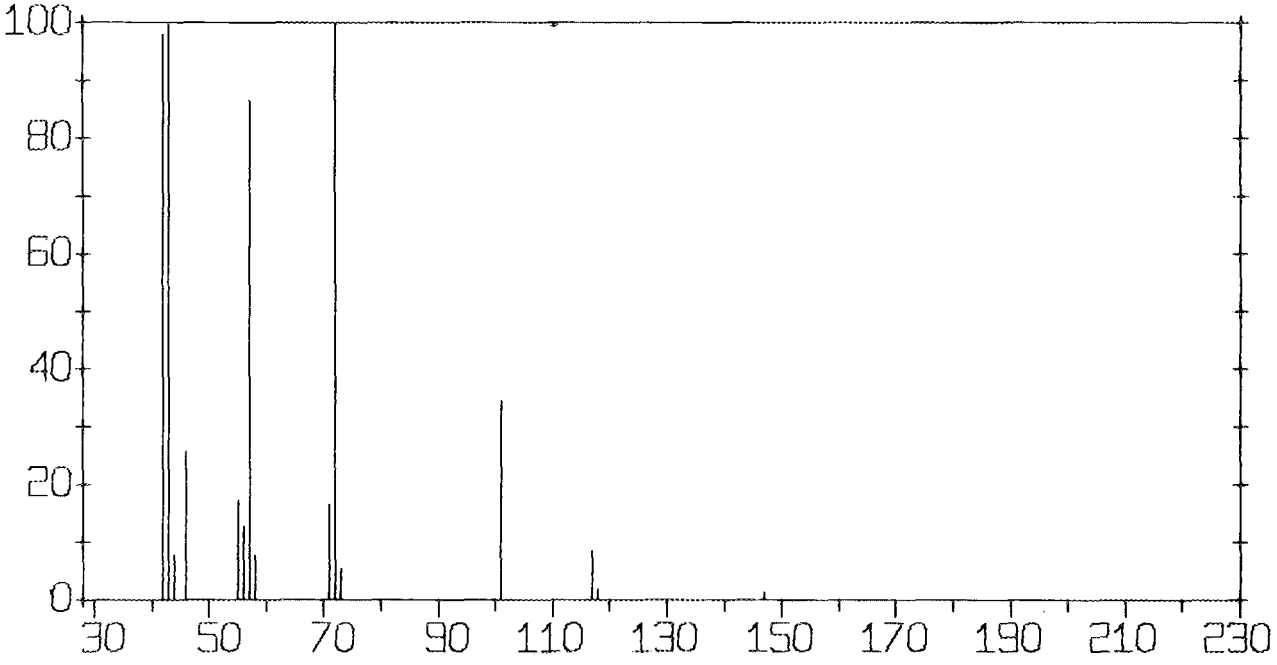
N-NITROSO-N-ETHYL ETHYL CARBAMATE
MW = 146 C5.H10.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	43.0	21.7	59.0	17.9	80.0	2.5	104.0	2.5
31.0	17.3	44.0	43.5	60.0	8.2	87.0	2.6	117.0	1.9
32.0	6.1	45.0	20.5	70.0	6.1	88.0	2.9	131.0	1.7
40.0	6.4	46.0	7.0	71.0	5.5	101.0	10.8	146.0	3.4
41.0	3.4	56.0	30.7	72.0	6.9	102.0	4.8	147.0	0.8
42.0	38.4	57.0	17.6	74.0	16.6				



N-NITROSO-N-METHYL-N'-NITROGUANIDINE
MW = 147 C2.H5.N5.O3

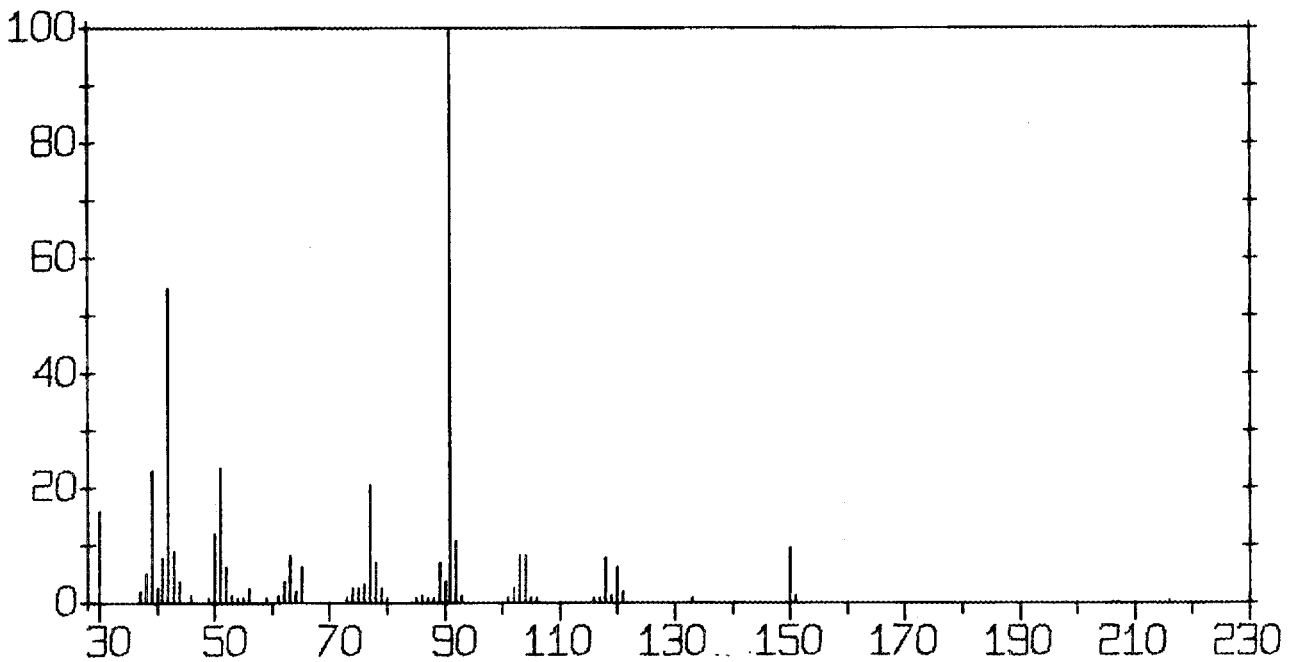
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
42.0	98.0	46.0	25.7	57.0	86.5	72.0	100.0	117.0	8.4
43.0	100.0	55.0	17.3	58.0	7.6	73.0	5.3	118.0	1.9
44.0	7.6	56.0	12.6	71.0	16.5	101.0	34.6	147.0	1.1



N-NITROSOMETHYLBENZYLAMINE
MW = 150 C8.H10.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	15.9	51.0	23.5	65.0	6.3	87.0	0.6	105.0	0.6
37.0	1.9	52.0	6.3	73.0	0.6	88.0	0.6	106.0	0.6
38.0	5.0	53.0	1.2	74.0	2.5	89.0	7.0	116.0	0.6
39.0	22.9	54.0	0.6	75.0	2.5	90.0	3.8	117.0	0.6
40.0	2.5	55.0	0.6	76.0	3.1	91.0	100.0	118.0	7.6
41.0	7.6	56.0	2.5	77.0	20.3	92.0	10.8	119.0	1.2
42.0	54.7	59.0	0.6	78.0	7.0	93.0	1.2	120.0	6.3
43.0	8.9	61.0	1.2	79.0	2.5	101.0	0.6	121.0	1.9
44.0	3.8	62.0	3.8	80.0	0.6	102.0	2.5	133.0	0.6
46.0	1.2	63.0	8.2	85.0	0.6	103.0	8.2	150.0	9.5
49.0	0.6	64.0	1.9	86.0	1.2	104.0	8.2	151.0	1.2
50.0	12.1								

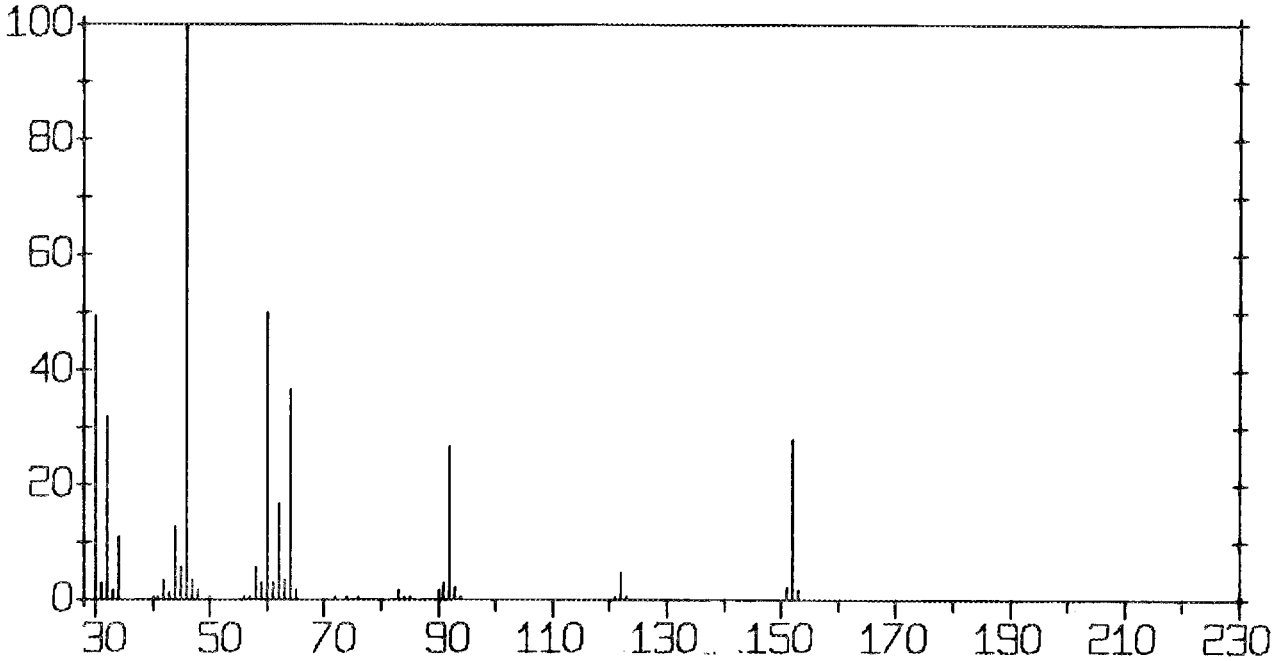
OBSERVED METASTABLES
23.5, 32.8, 33.8, 35.0, 37.2, 46.5, 55.2, 56.5, 70.2, 72.2, 88.2, 96.0, 103.2, 116.2,



1,4-DINITROSOOCTADEUTEROPIPERAZINE
MW = 152 C4.D8.N4.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	49.4	44.0	12.7	59.C	2.9	74.0	0.5	93.0	2.3
31.0	2.9	45.0	5.8	60.0	50.0	76.0	0.5	94.0	0.5
32.0	31.9	46.0	100.0	61.0	2.9	83.0	1.7	121.0	0.5
33.0	1.7	47.0	3.4	62.0	16.8	84.0	0.5	122.0	4.6
34.0	11.0	48.0	1.7	63.0	3.4	85.0	0.5	123.0	0.5
40.0	0.5	50.0	0.5	64.0	36.6	90.0	1.7	151.0	2.3
41.0	0.5	56.0	0.5	65.0	1.7	91.0	2.9	152.0	27.9
42.0	3.4	57.0	0.5	72.0	0.5	92.0	26.7	153.0	1.7
43.0	1.1	58.0	5.8						

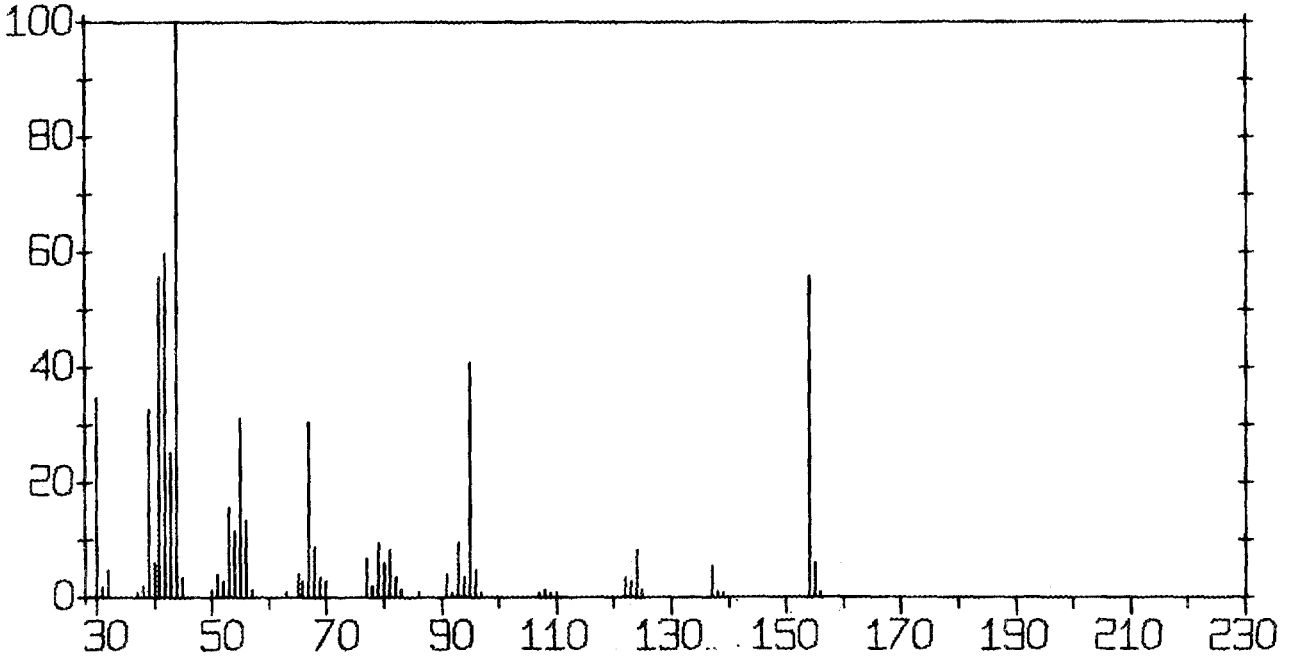
OBSERVED METASTABLES
24.5, 55.8, 68.5, 69.5, 70.5, 98.0,



N-NITROSO-3-AZABICYCLO(3.2.2)NONANE
MW = 154 C8.H14.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	34.6	50.0	1.3	67.0	30.6	86.0	0.6	110.0	0.6
31.0	2.0	51.0	4.0	68.0	8.8	91.0	4.0	122.0	3.4
32.0	4.7	52.0	2.7	69.0	3.4	92.0	0.6	123.0	2.7
37.0	0.6	53.0	15.6	70.0	2.7	93.0	9.5	124.0	8.1
38.0	2.0	54.0	11.5	77.0	6.8	94.0	3.4	125.0	1.3
39.0	32.6	55.0	31.2	78.0	2.0	95.0	40.8	137.0	5.4
40.0	6.1	56.0	13.6	79.0	9.5	96.0	4.7	138.0	0.6
41.0	55.7	57.0	1.3	80.0	6.1	97.0	0.6	139.0	0.6
42.0	59.8	63.0	0.6	81.0	8.1	107.0	0.6	154.0	55.7
43.0	25.1	65.0	4.0	82.0	3.4	108.0	1.3	155.0	6.1
44.0	100.0	66.0	2.7	83.0	1.3	109.0	0.6	156.0	0.6
45.0	3.4								

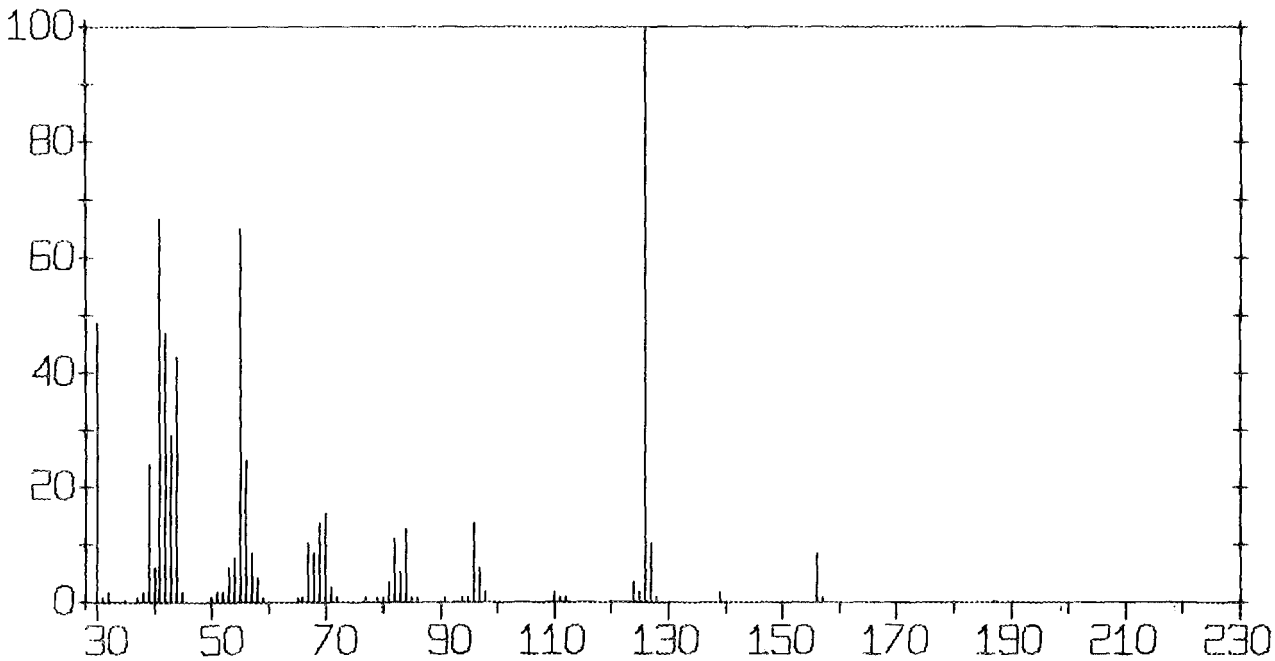
OBSERVED METASTABLES
15.7, 25.2, 27.6, 28.2, 35.2, 37.2, 47.4, 49.2, 51.1, 63.8, 66.4, 69.8,
71.8, 74.2, 77.2, 89.2, 91.2, 100.0,



N-NITROSOOCTAMETHYLENEIMINE
MW = 156 C8.H16.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	48.7	50.0	0.8	66.0	0.8	82.0	11.1	110.0	1.7
31.0	0.8	51.0	1.7	67.0	10.2	83.0	5.1	111.0	0.8
32.0	1.7	52.0	1.7	68.0	8.5	84.0	12.8	112.0	0.8
37.0	0.8	53.0	5.9	69.0	13.6	85.0	0.8	124.0	3.4
38.0	1.7	54.0	7.6	70.0	15.3	86.0	0.8	125.0	1.7
39.0	23.9	55.0	64.9	71.0	2.5	91.0	0.8	126.0	100.0
40.0	5.9	56.0	24.7	72.0	0.8	94.0	0.8	127.0	10.2
41.0	66.6	57.0	8.5	77.0	0.8	95.0	0.8	128.0	0.8
42.0	47.0	58.0	4.2	79.0	0.8	96.0	13.6	139.0	1.7
43.0	29.0	59.0	0.8	80.0	0.8	97.0	5.9	156.0	8.5
44.0	42.7	65.0	0.8	81.0	3.4	98.0	1.7	157.0	0.8
45.0	1.7								

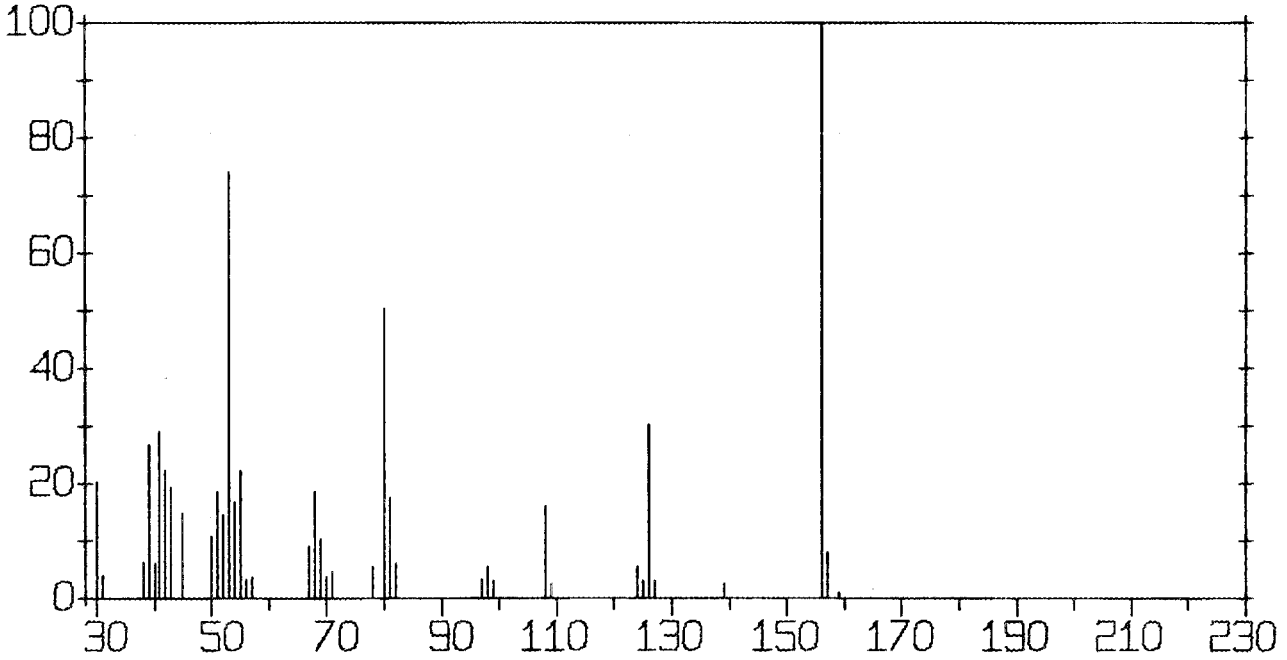
OBSERVED METASTABLES
15.4, 24.4, 35.8, 37.2, 39.2, 51.2, 63.2, 71.6, 74.8, 77.2, 94.2, 102.0,



N-NITROSOGUVACINE
MW = 156 C6.H8.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	20.3	45.0	14.8	57.0	3.7	81.0	17.4	125.0	2.9
31.0	3.9	50.0	10.7	67.0	8.8	82.0	5.9	126.0	30.3
38.0	6.2	51.0	18.5	68.0	18.5	97.0	3.3	127.0	2.9
39.0	26.6	52.0	14.4	69.0	10.3	98.0	5.4	139.0	2.4
40.0	5.9	53.0	74.0	70.0	3.7	99.0	2.9	156.0	100.0
41.0	28.8	54.0	16.6	71.0	4.4	108.0	15.9	157.0	8.0
42.0	22.2	55.0	22.2	78.0	5.5	109.0	2.4	159.0	0.8
43.0	19.2	56.0	3.3	80.0	50.3	124.0	5.5		

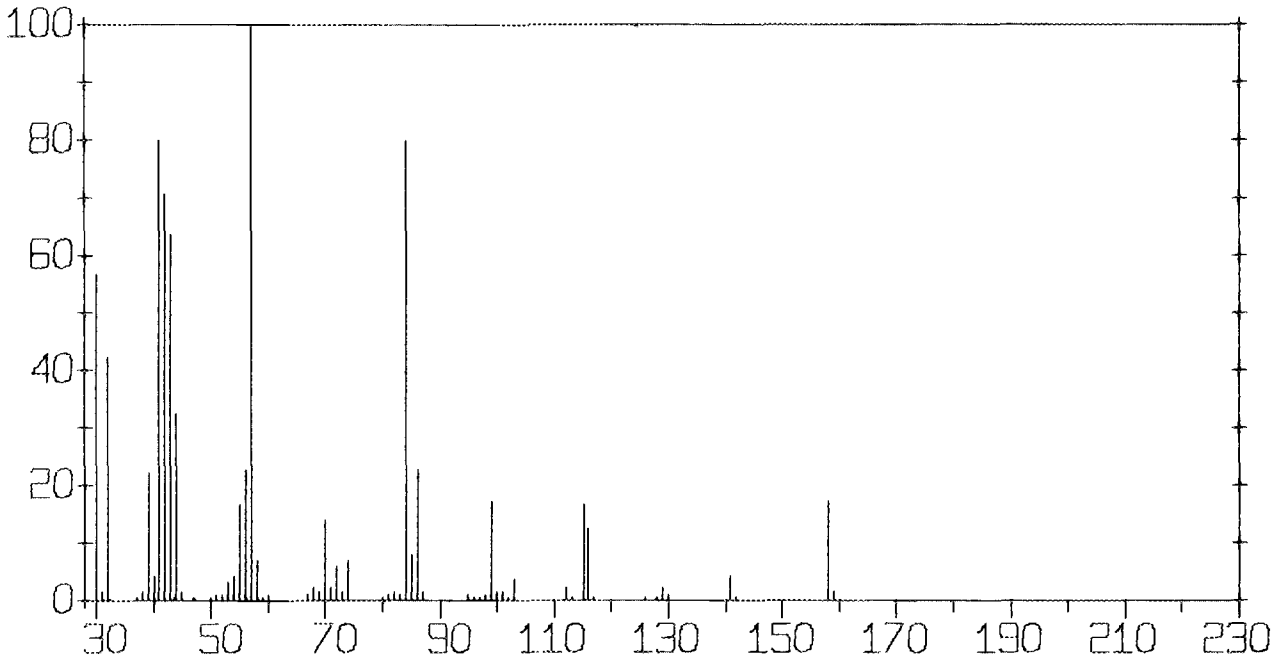
OBSERVED METASTABLES
35.2, 92.7, 102.0,



N-NITROSODI-N-BUTYLAMINE
MW = 158 C8.H18.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	56.7	50.0	0.5	69.0	1.6	86.0	22.7	113.0	0.5
31.0	1.6	51.0	1.0	70.0	14.0	87.0	1.6	115.0	16.7
32.0	42.1	52.0	1.0	71.0	2.1	95.0	1.0	116.0	12.4
37.0	0.5	53.0	3.2	72.0	5.9	96.0	0.5	117.0	0.5
38.0	1.6	54.0	4.3	73.0	1.6	97.0	0.5	126.0	0.5
39.0	22.1	55.0	16.7	74.0	7.0	98.0	1.0	128.0	0.5
40.0	4.3	56.0	22.7	80.0	0.5	99.0	17.2	129.0	2.1
41.0	80.0	57.0	100.0	81.0	1.0	100.0	1.6	130.0	1.0
42.0	70.8	58.0	7.0	82.0	1.6	101.0	1.6	141.0	4.3
43.0	63.7	59.0	0.5	83.0	1.0	102.0	0.5	142.0	0.5
44.0	32.4	60.0	1.0	84.0	80.0	103.0	3.7	158.0	17.2
45.0	1.6	67.0	1.0	85.0	8.1	112.0	2.1	159.0	1.6
47.0	0.5	68.0	2.1						

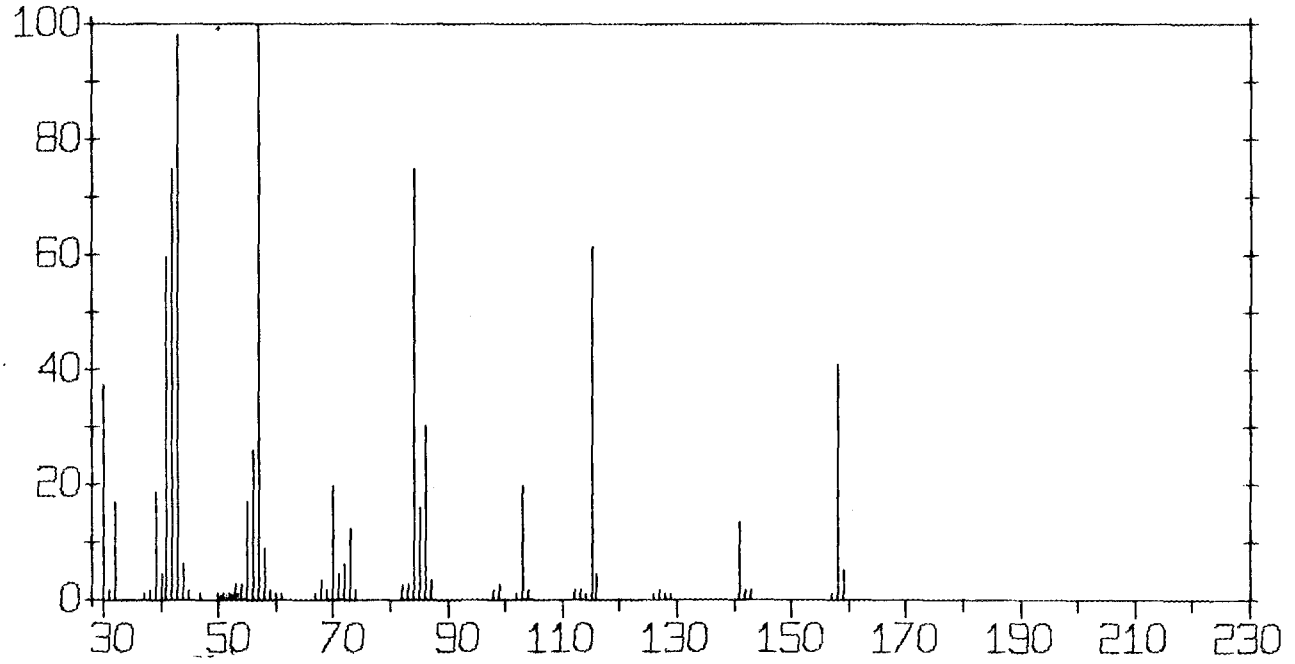
OBSERVED METASTABLES
22.5, 29.5, 37.2, 38.8, 39.2, 61.4, 125.8,



N-NITROSODIISOBUTYLAMINE
MW = 158 C8.H18.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	37.5	47.0	0.8	61.0	0.8	85.0	16.0	116.0	4.4
31.0	1.7	50.0	0.8	67.0	0.8	86.0	30.3	126.0	0.8
32.0	16.9	51.0	0.8	68.0	3.5	87.0	3.5	127.0	1.7
37.0	0.8	52.0	0.8	69.0	1.7	98.0	1.7	128.0	0.8
38.0	1.7	53.0	2.6	70.0	19.6	99.0	2.6	129.0	0.8
39.0	18.7	54.0	2.6	71.0	4.4	102.0	0.8	141.0	13.3
40.0	4.4	55.0	16.9	72.0	6.2	103.0	19.6	142.0	1.7
41.0	59.8	56.0	25.8	73.0	12.5	104.0	1.7	143.0	1.7
42.0	75.0	57.0	100.0	74.0	1.7	112.0	1.7	157.0	0.8
43.0	98.2	58.0	8.9	82.0	2.6	113.0	1.7	158.0	41.0
44.0	6.2	59.0	1.7	83.0	2.6	114.0	0.8	159.0	5.3
45.0	1.7	60.0	0.8	84.0	75.0	115.0	61.6		

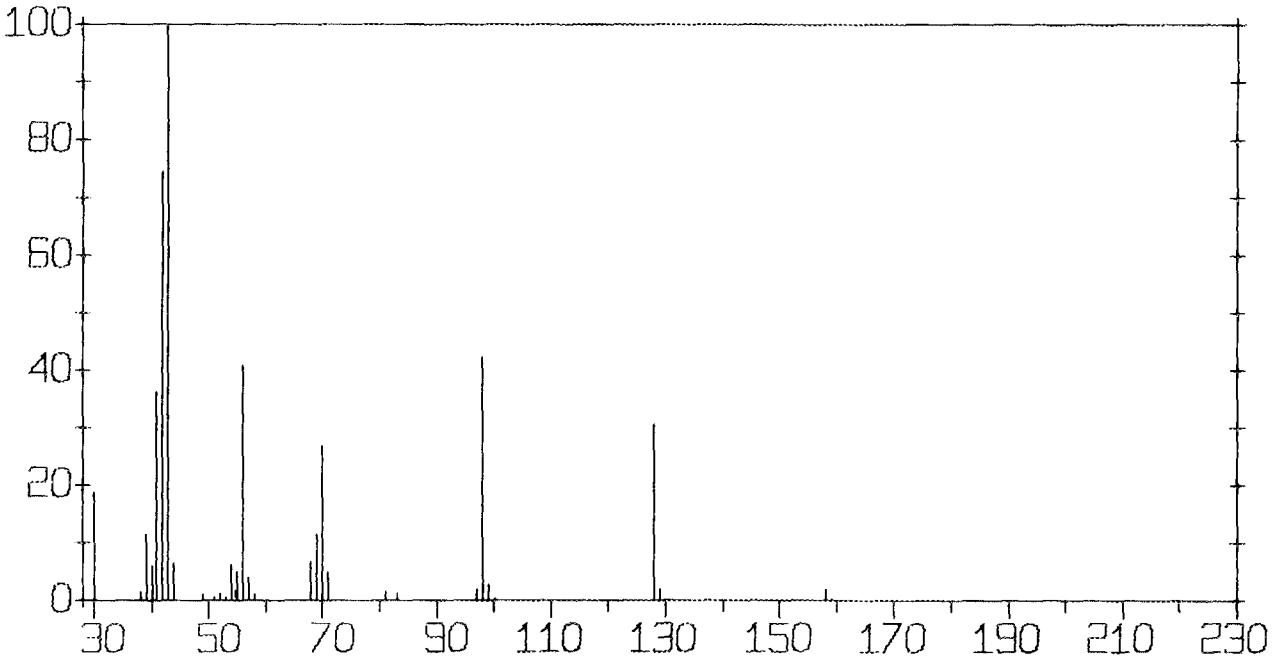
OBSERVED METASTABLES
29.5, 37.2, 38.8, 39.2, 41.5, 61.4, 126.0,



N,N'-DINITROSOHOMOPIPERAZINE
MW = 158 C5.H10.N4.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	18.6	44.0	6.5	55.0	4.9	70.0	26.7	99.0	2.7
38.0	1.5	49.0	0.9	56.0	40.6	71.0	5.0	100.0	0.3
39.0	11.5	51.0	0.5	57.0	3.8	81.0	1.5	128.0	30.5
40.0	6.1	52.0	1.2	58.0	1.0	83.0	1.1	129.0	2.0
41.0	36.2	53.0	0.6	68.0	6.7	97.0	2.0	158.0	2.0
42.0	74.5	54.0	6.1	69.0	11.5	98.0	42.3	159.0	0.2
43.0	100.0								

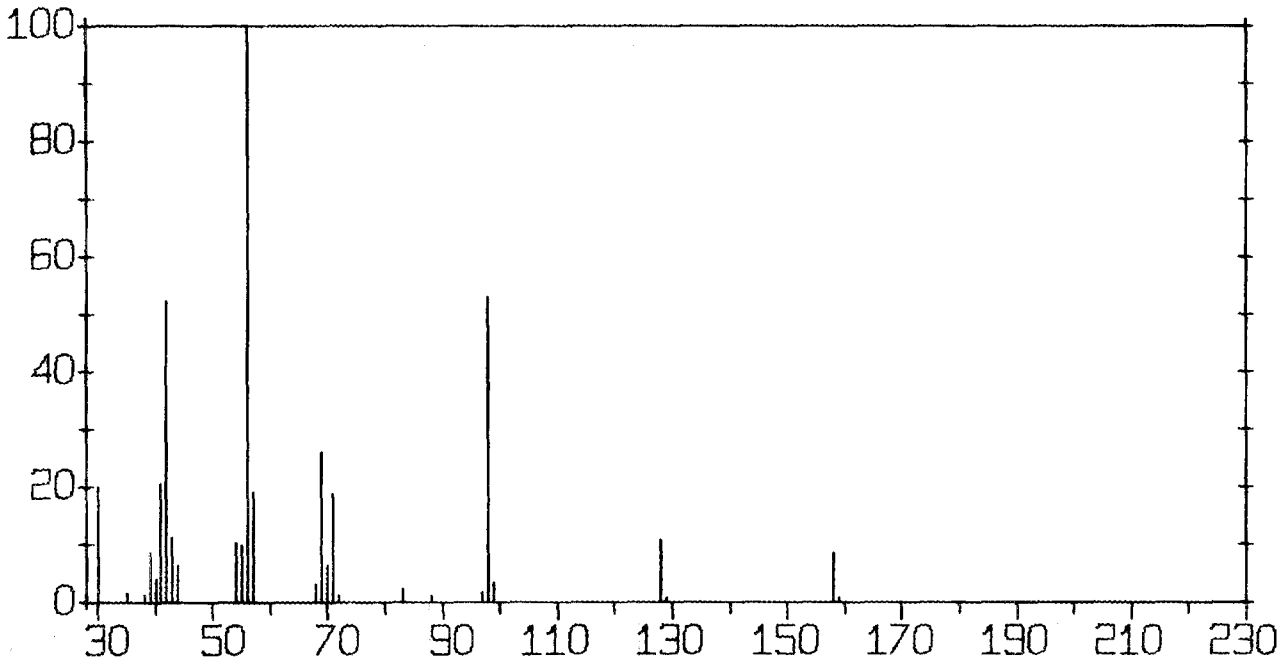
OBSERVED METASTABLES
75.2, 103.9,



N,N'-DINITROSO-2-METHYLPIPERAZINE
MW = 158 C5.H10.N4.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	20.0	42.0	52.2	57.0	19.0	72.0	1.0	99.0	3.2
35.0	1.4	43.0	11.3	68.0	3.0	83.0	2.2	128.0	10.6
38.0	1.1	44.0	6.3	69.0	25.9	88.0	1.0	129.0	0.7
39.0	8.4	54.0	10.2	70.0	6.1	97.0	1.7	158.0	8.4
40.0	4.0	55.0	9.7	71.0	18.8	98.0	52.9	159.0	0.6
41.0	20.4	56.0	100.0						

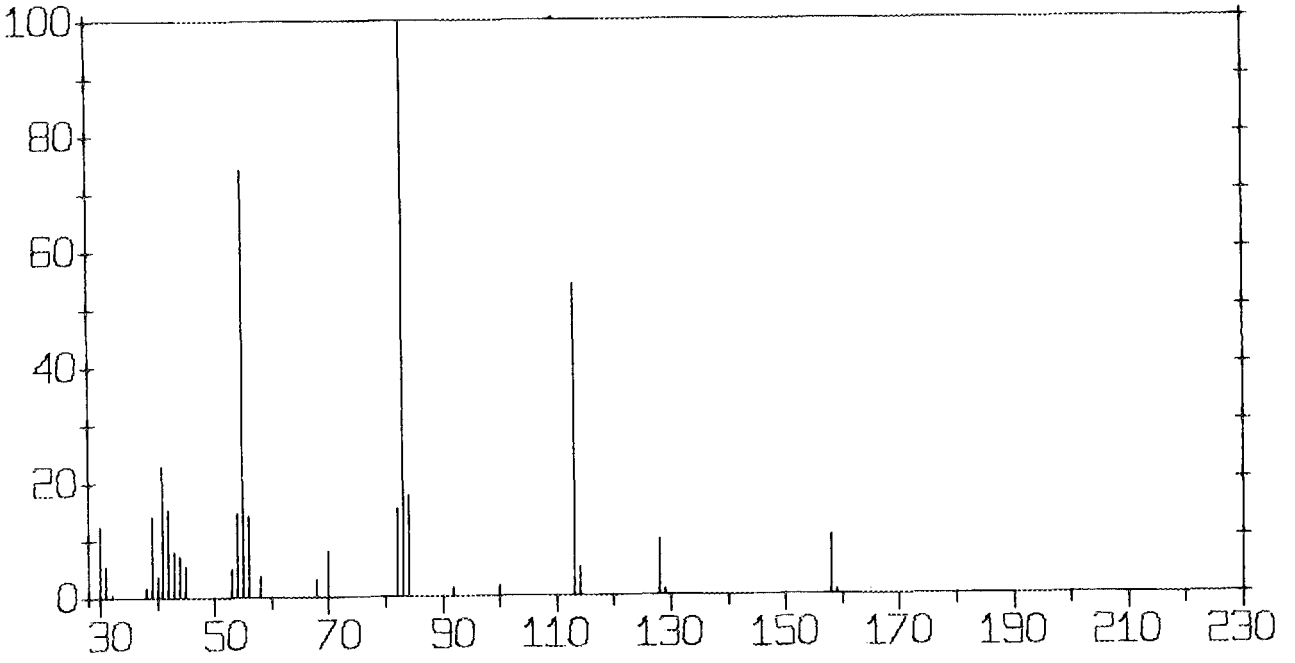
OBSERVED METASTABLES
44.1, 52.4, 55.8, 60.9, 75.1, 75.9, 103.5,



N-NITROSOPIPECOLIC ACID
MW = 158 C6.H10.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	12.4	42.0	15.5	55.0	74.2	83.0	100.0	114.0	4.8
31.0	5.5	43.0	8.0	56.0	14.2	84.0	17.7	128.0	9.7
38.0	1.7	44.0	7.3	58.0	3.8	92.0	1.5	129.0	0.8
39.0	14.2	45.0	5.5	68.0	3.0	100.0	2.0	158.0	10.5
40.0	3.7	53.0	5.1	70.0	8.0	113.0	54.2	159.0	0.8
41.0	23.1	54.0	14.6	82.0	15.5				

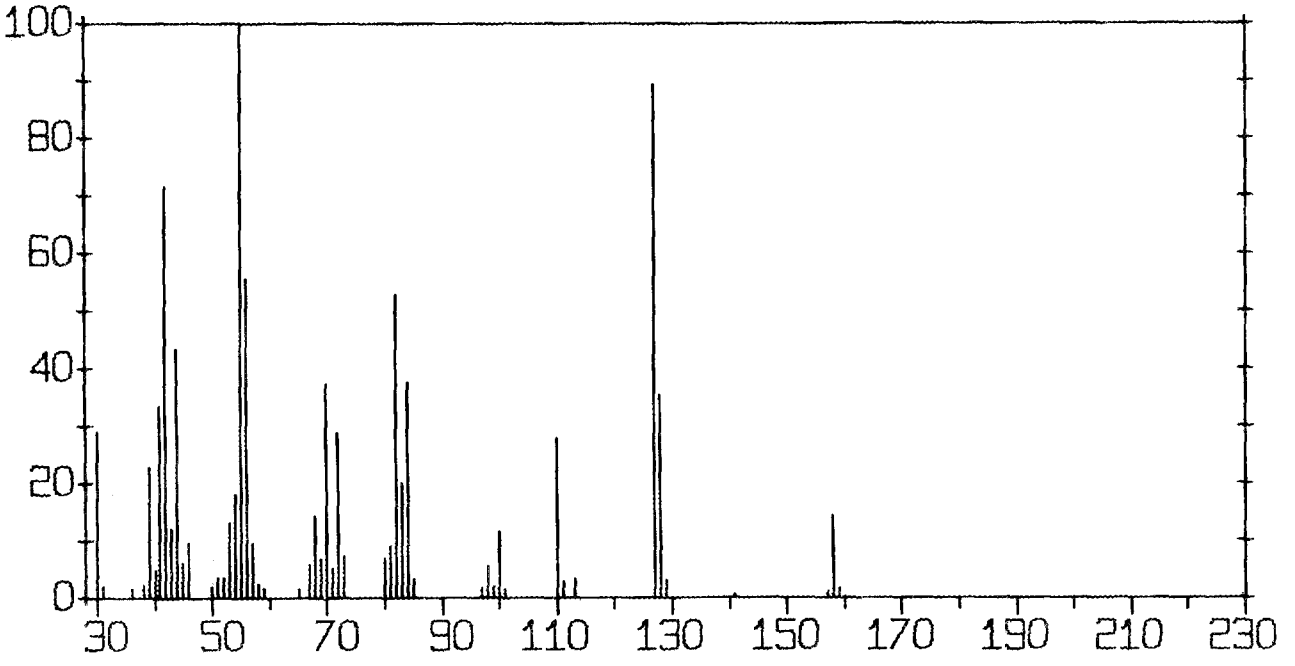
OBSERVED METASTABLES
61.0, 113.7,



N-NITROSONIPECOTIC ACID
MW = 158 C6.H10.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	28.9	46.0	9.4	65.0	1.6	82.0	52.7	111.0	2.7
31.0	2.0	50.0	2.0	67.0	5.8	83.0	20.0	113.0	3.2
36.0	1.6	51.0	3.4	68.0	14.1	84.0	37.5	127.0	89.1
38.0	2.3	52.0	3.5	69.0	6.7	85.0	3.2	128.0	35.1
39.0	22.7	53.0	13.1	70.0	37.1	97.0	1.8	129.0	3.0
40.0	4.8	54.0	17.9	71.0	5.0	98.0	5.5	141.0	0.4
41.0	33.5	55.0	100.0	72.0	28.7	99.0	2.0	157.0	1.1
42.0	71.6	56.0	55.4	73.0	7.1	100.0	11.6	158.0	14.3
43.0	11.8	57.0	9.4	80.0	6.7	101.0	1.6	159.0	1.5
44.0	43.2	58.0	2.1	81.0	8.9	110.0	27.7	160.0	0.1
45.0	6.0	59.0	1.4						

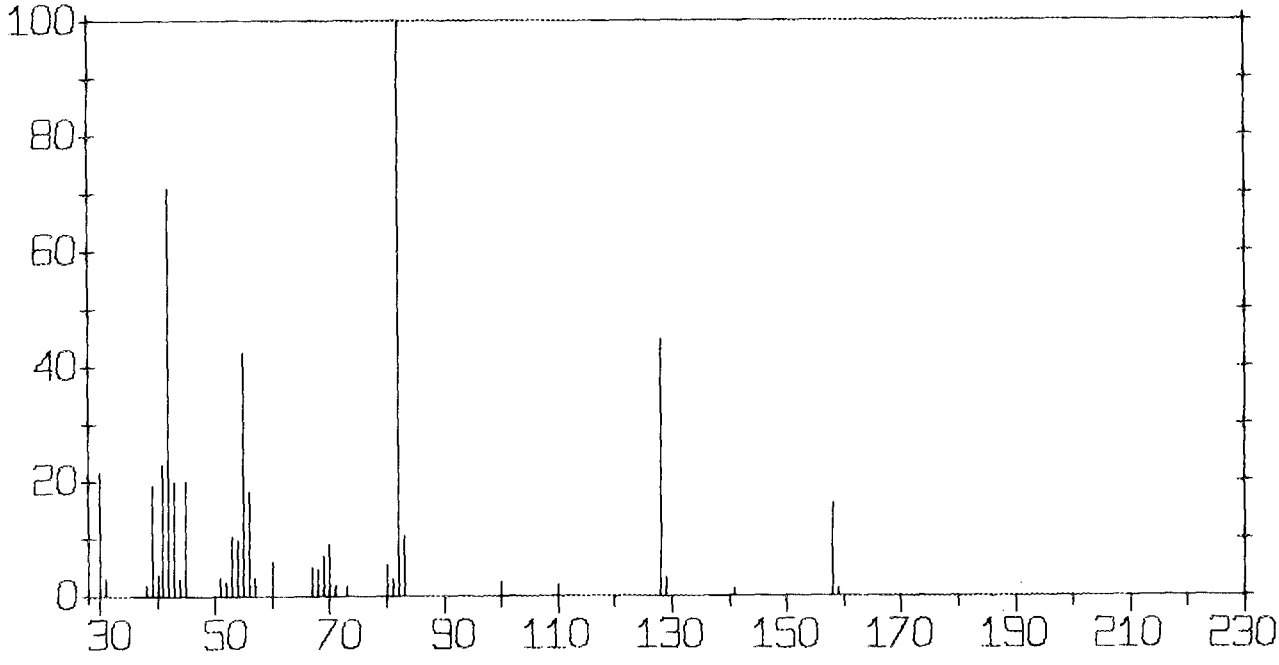
OBSERVED METASTABLES
37.2, 49.1, 55.7, 61.2, 78.2, 78.9, 94.7, 95.3, 103.9,



N-NITROSOISONIPECOTIC ACID
MW = 158 C6.H10.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	21.8	43.0	20.0	55.0	42.4	70.0	8.9	100.0	2.4
31.0	3.0	44.0	3.0	56.0	18.1	71.0	2.1	110.0	2.0
38.0	2.1	45.0	20.0	57.0	3.3	73.0	1.8	128.0	44.8
39.0	19.3	51.0	3.3	60.0	6.0	80.0	5.4	129.0	3.2
40.0	3.6	52.0	2.4	67.0	5.0	81.0	3.0	141.0	1.2
41.0	23.0	53.0	10.6	68.0	4.8	82.0	100.0	158.0	16.3
42.0	70.9	54.0	9.6	69.0	6.9	83.0	10.6	159.0	1.2

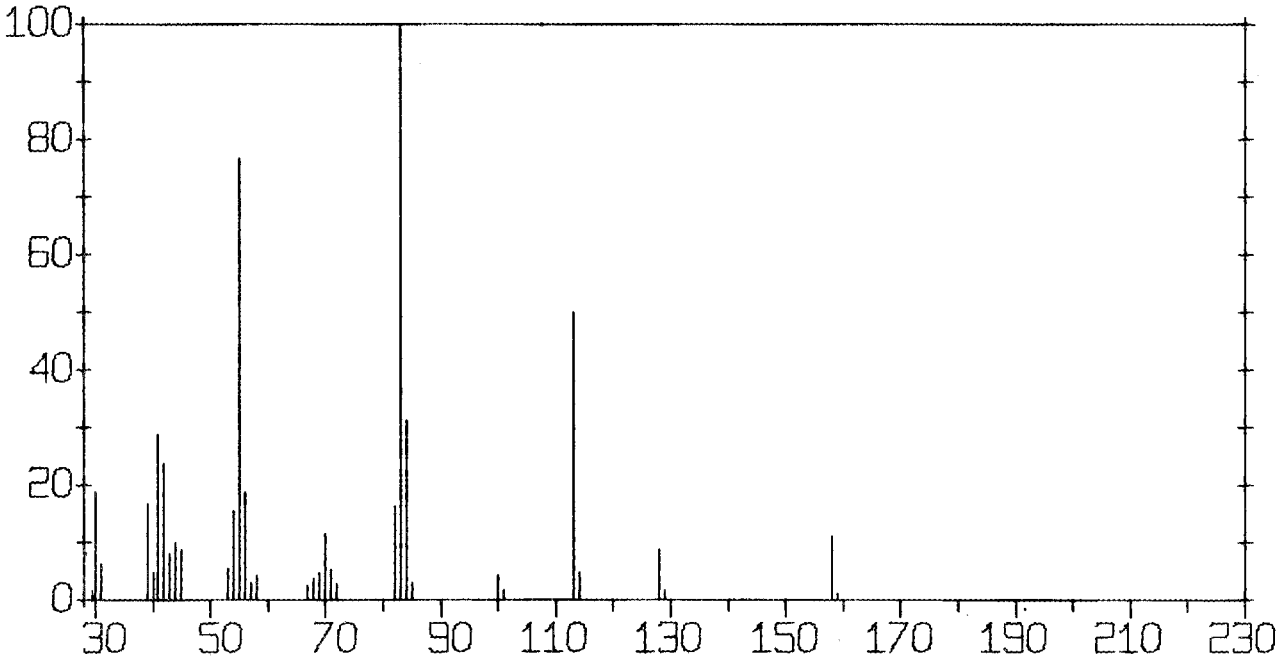
OBSERVED METASTABLES
62.7, 78.1, 94.6, 104.0,



N-NITROSO-L-PIPECOLIC ACID
MW = 158 C6.H10.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	18.7	44.0	10.0	58.0	4.3	82.0	16.2	113.0	50.0
31.0	6.2	45.0	8.7	67.0	2.5	83.0	100.0	114.0	4.6
39.0	16.8	53.0	5.6	68.0	3.8	84.0	31.2	128.0	8.7
40.0	4.8	54.0	15.6	69.0	4.6	85.0	3.0	129.0	1.4
41.0	28.7	55.0	76.8	70.0	11.5	100.0	4.3	158.0	11.1
42.0	23.7	56.0	18.7	71.0	5.3	101.0	1.8	159.0	1.0
43.0	8.1	57.0	3.1	72.0	2.8				

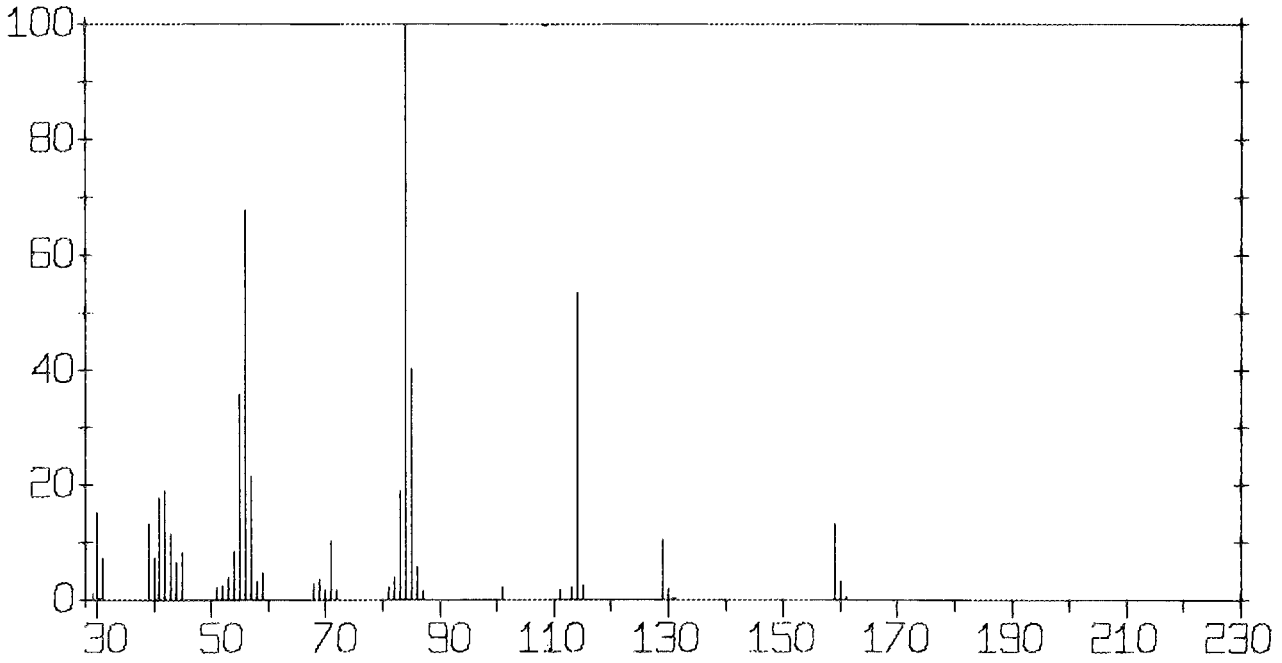
OBSERVED METASTABLES
36.4, 61.1, 103.8,



N-NITROSO-2-DEUTEROPIPECOLIC ACID
MW = 159 C6.H9.D.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	15.1	51.0	2.1	59.0	4.6	83.0	18.9	114.0	53.5
31.0	7.1	52.0	2.4	68.0	2.6	84.0	100.0	115.0	2.5
39.0	13.2	53.0	3.9	69.0	3.5	85.0	40.3	129.0	10.5
40.0	7.1	54.0	8.3	70.0	1.7	86.0	5.7	130.0	2.0
41.0	17.8	55.0	35.7	71.0	10.3	87.0	1.4	131.0	0.2
42.0	18.9	56.0	67.8	72.0	1.7	101.0	2.1	159.0	13.1
43.0	11.4	57.0	21.4	81.0	2.1	111.0	1.6	160.0	3.2
44.0	6.4	58.0	3.2	82.0	3.9	113.0	2.2	161.0	0.3
45.0	8.2								

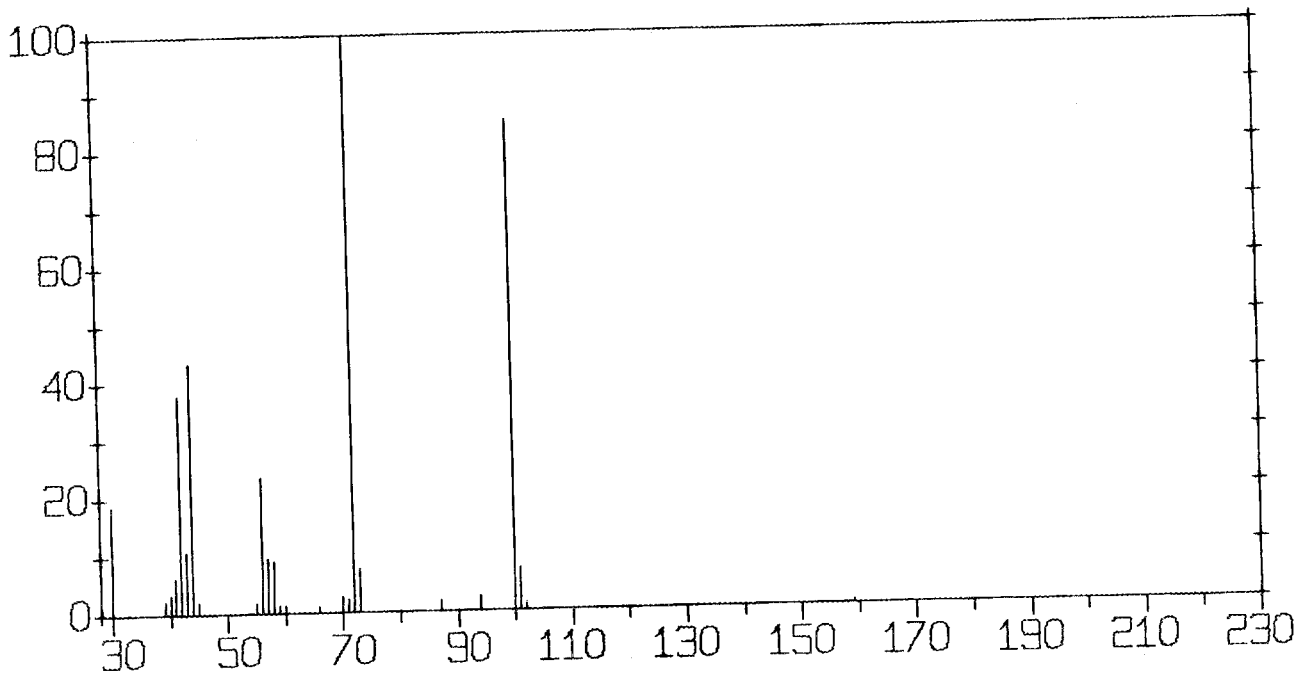
OBSERVED METASTABLES
61.9, 104.5,



N-NITROSO-1-METHYL-3,3-DIETHYL UREA
MW = 159 C6.H13.N3.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	18.8	43.0	10.7	57.0	9.4	70.0	2.8	94.0	2.4
39.0	2.2	44.0	43.3	58.0	9.0	71.0	2.2	100.0	84.9
40.0	3.2	45.0	1.8	59.0	1.1	72.0	100.0	101.0	7.1
41.0	6.2	55.0	1.6	60.0	1.1	73.0	7.5	102.0	1.1
42.0	37.7	56.0	23.5	66.0	0.9	87.0	1.6	159.0	0.5

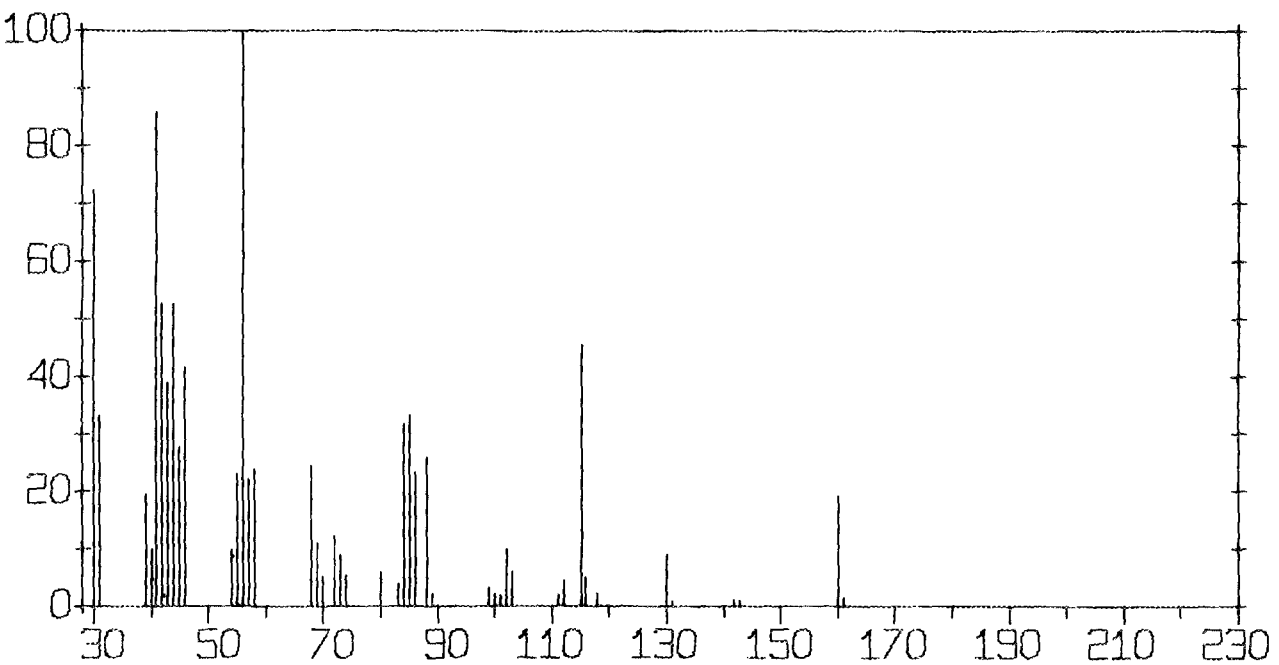
OBSERVED METASTABLES
27.8, 43.7, 51.8, 71.8,



N-NITROSO-4-HYDROXYPROLINE
MW = 160 C5.H8.N2.O4

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	72.2	46.0	41.6	72.0	12.2	89.0	2.2	116.0	5.0
31.0	33.3	54.0	10.0	73.0	8.8	99.0	3.3	118.0	2.2
39.0	19.4	55.0	23.3	74.0	5.5	100.0	2.2	130.0	8.8
40.0	10.0	56.0	100.0	80.0	6.1	101.0	2.1	131.0	0.6
41.0	86.1	57.0	22.2	83.0	3.8	102.0	10.0	142.0	0.8
42.0	52.7	58.0	23.8	84.0	31.6	103.0	6.1	143.0	0.9
43.0	38.8	68.0	24.4	85.0	33.3	111.0	2.1	160.0	19.3
44.0	52.7	69.0	11.1	86.0	23.3	112.0	4.6	161.0	1.5
45.0	27.7	70.0	5.2	88.0	26.1	115.0	45.5		

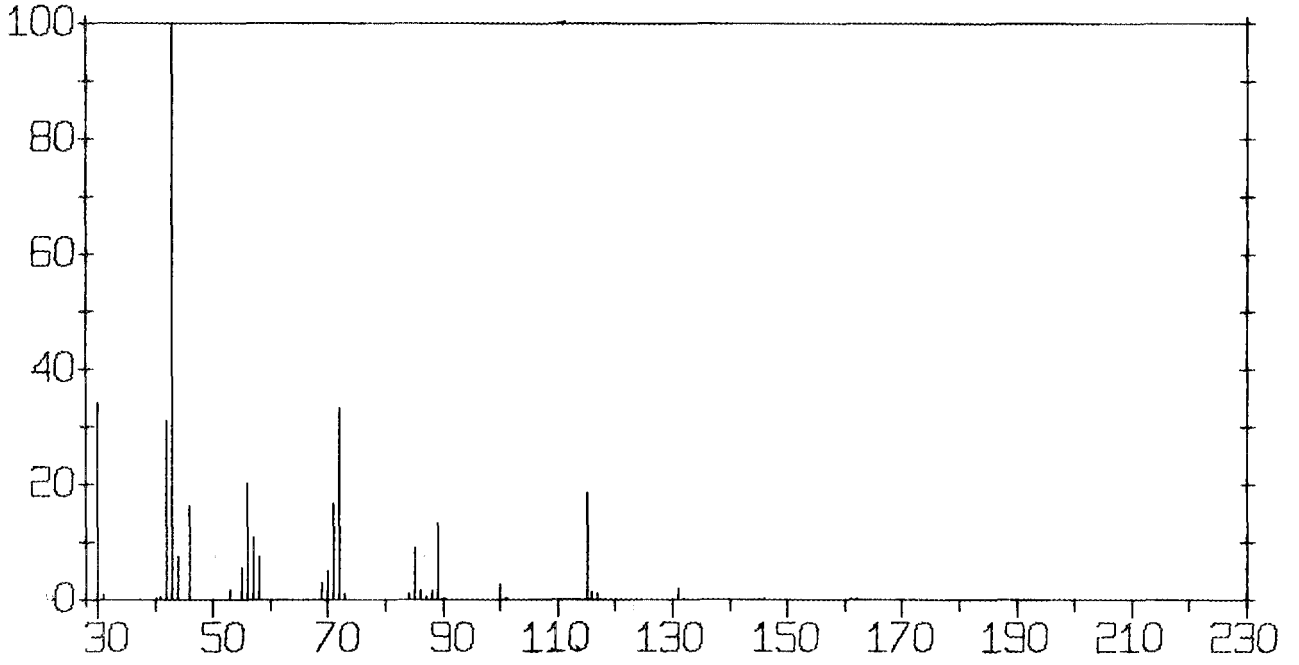
OBSERVED METASTABLES
21.1, 24.8, 59.5, 62.9, 96.6, 105.5,



N-NITROSO-N-ETHYL-N'-NITROGUANIDINE
MW = 161 C3.H7.N5.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	34.2	53.0	1.8	71.0	16.6	88.0	1.5	117.0	0.8
31.0	0.7	55.0	5.5	72.0	33.3	89.0	13.3	131.0	2.0
40.0	0.2	56.0	20.3	73.0	0.9	90.0	0.3	132.0	0.3
41.0	0.5	57.0	10.7	84.0	1.0	100.0	2.6	145.0	0.1
42.0	30.9	58.0	7.4	85.0	9.0	101.0	0.2	146.0	0.3
43.0	100.0	69.0	2.9	86.0	1.4	115.0	18.5	161.0	0.3
44.0	7.4	70.0	5.0	87.0	0.5	116.0	1.2	162.0	0.1
46.0	16.2								

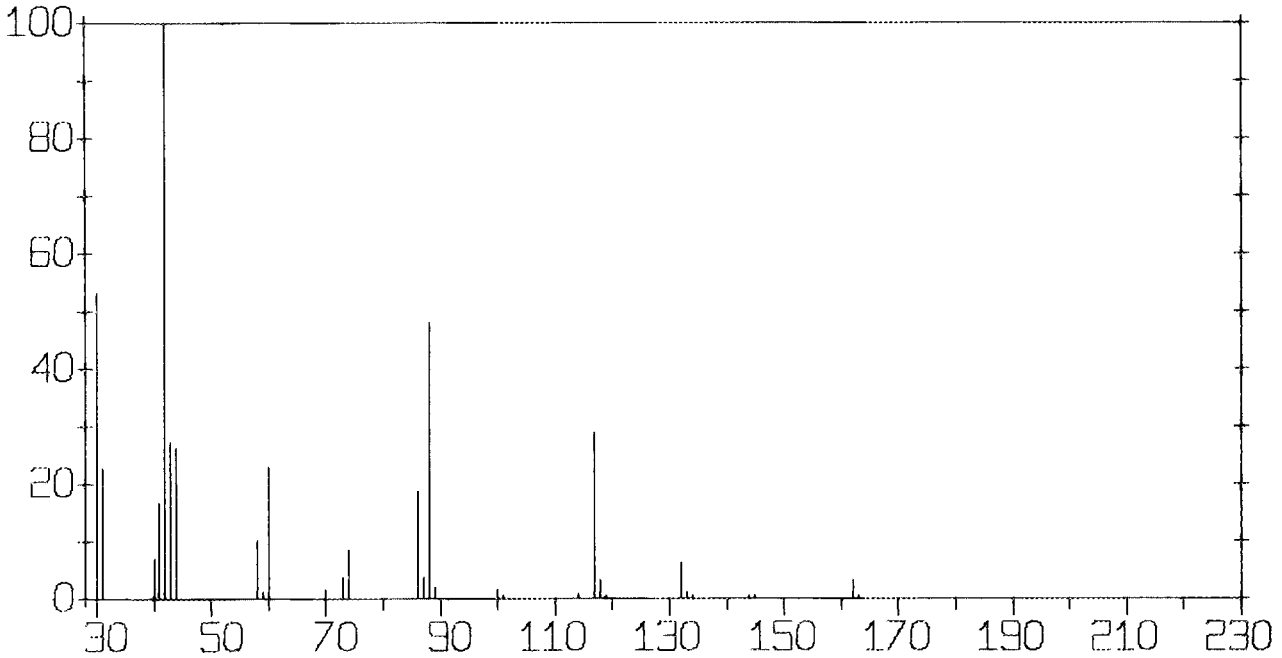
OBSERVED METASTABLES
37.2, 60.4, 83.0,



N-NITROSOIMINODIACETIC ACID
MW = 162 C4.H6.N2.O5

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	53.3	44.0	26.2	74.0	8.3	101.0	0.4	133.0	1.0
31.0	22.8	58.0	10.2	86.0	18.6	114.0	0.8	134.0	0.5
40.0	7.0	59.0	1.1	87.0	3.8	117.0	28.9	144.0	0.3
41.0	13.7	60.0	23.0	88.0	48.0	118.0	3.1	145.0	0.4
42.0	100.0	70.0	1.4	89.0	2.0	119.0	0.4	162.0	3.1
43.0	27.2	73.0	3.8	100.0	1.4	132.0	6.2	163.0	0.4

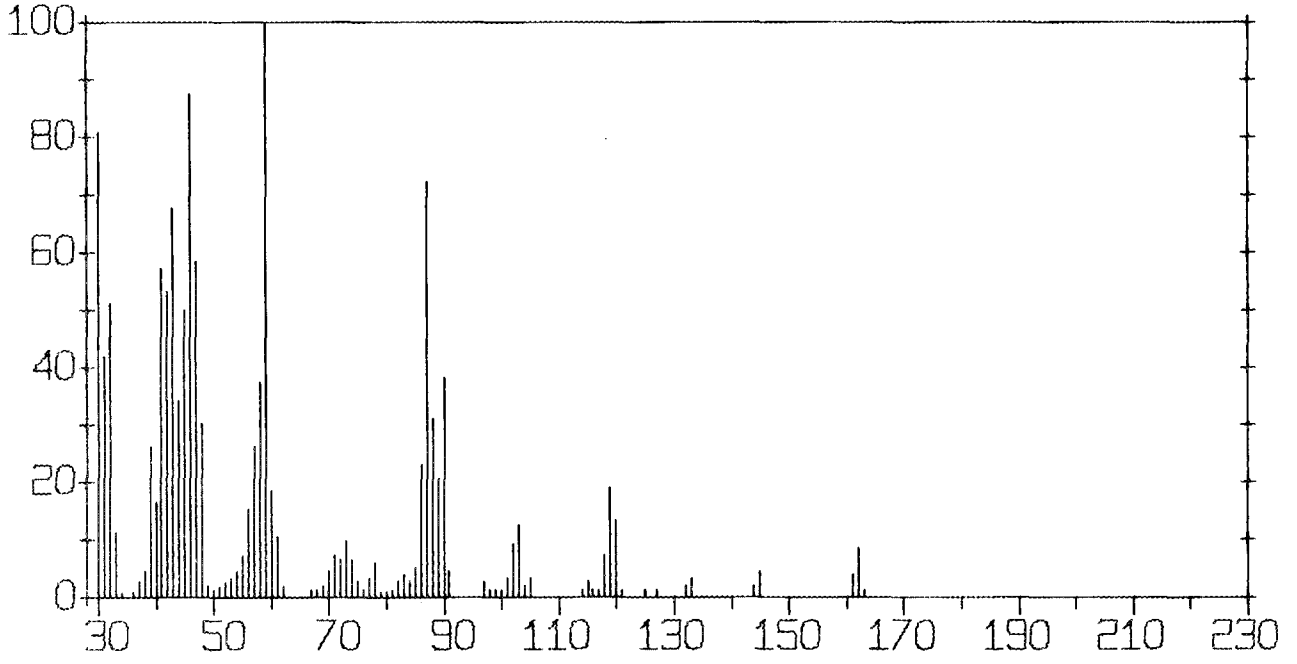
OBSERVED METASTABLES
47.6, 55.7, 63.2, 82.0, 98.5, 107.5,



N-NITROSO-1,1,1',1'-TETRADEUTERODI-N-BUTYLAMINE
MW=162 C8,H14,D4,N2,O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	80.9	48.0	30.2	69.0	1.9	86.0	23.0	115.0	2.6
31.0	42.1	49.0	1.9	70.0	4.6	87.0	72.3	116.0	1.3
32.0	51.3	50.0	1.3	71.0	7.2	88.0	30.9	117.0	1.3
33.0	11.1	51.0	1.9	72.0	6.5	89.0	20.3	118.0	7.2
34.0	0.6	52.0	2.6	73.0	9.8	90.0	38.1	119.0	19.0
36.0	0.6	53.0	3.2	74.0	6.5	91.0	4.6	120.0	13.1
37.0	2.6	54.0	4.6	75.0	2.6	97.0	2.6	121.0	1.3
38.0	4.6	55.0	7.2	76.0	1.3	98.0	1.3	125.0	1.3
39.0	26.3	56.0	15.1	77.0	3.2	99.0	1.3	127.0	1.3
40.0	16.4	57.0	26.3	78.0	5.9	100.0	1.3	132.0	1.9
41.0	57.2	58.0	37.5	79.0	0.6	101.0	3.2	133.0	3.2
42.0	53.2	59.0	100.0	80.0	0.6	102.0	9.2	144.0	1.9
43.0	67.7	60.0	18.4	81.0	1.3	103.0	12.5	145.0	4.6
44.0	34.2	61.0	10.5	82.0	2.6	104.0	1.9	161.0	3.9
45.0	50.0	62.0	1.9	83.0	3.9	105.0	3.2	162.0	8.5
46.0	87.5	67.0	1.3	84.0	2.6	114.0	1.3	163.0	1.3
47.0	58.5	68.0	1.3	85.0	5.2				

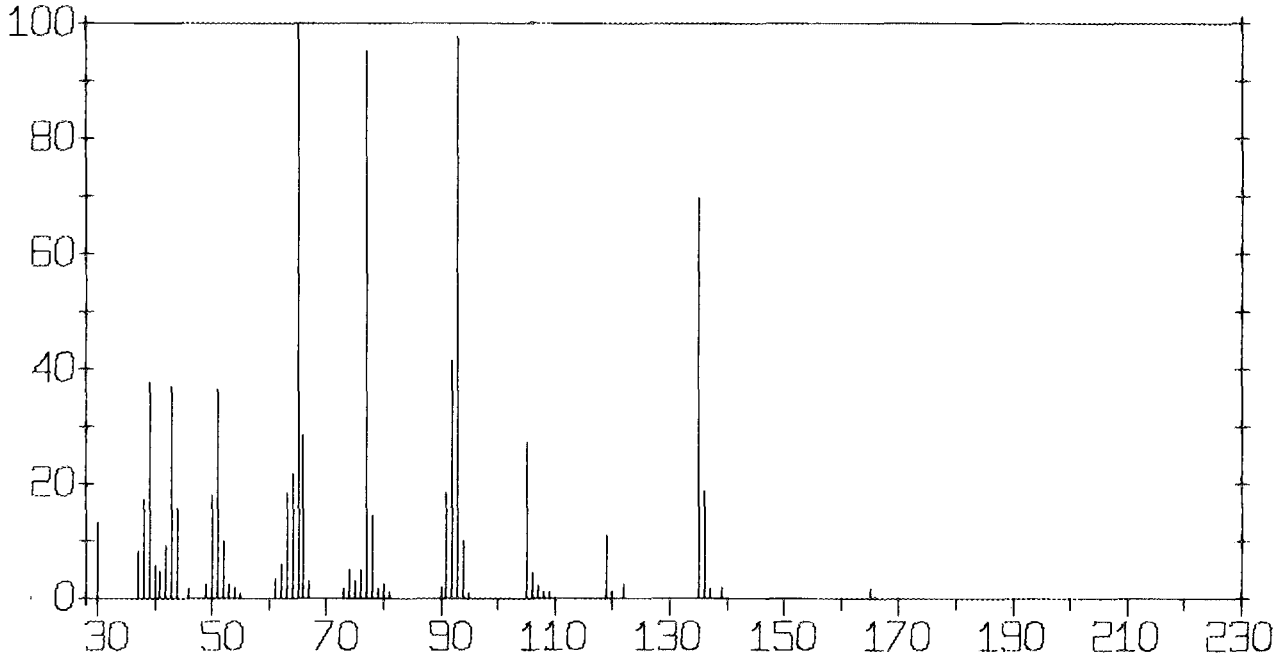
OBSERVED METASTABLES
25.8, 28.5, 29.8, 30.4, 31.4, 36.2, 37.2, 38.2, 39.2, 62.8, 63.6, 65.8,
66.7, 87.2,



N-NITROSO-N-PHENYLUREA
MW = 165 C7.H7.N3.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	13.2	50.0	17.9	66.0	28.6	90.0	1.9	109.0	0.9
37.0	8.1	51.0	36.5	67.0	3.0	91.0	18.6	119.0	10.9
38.0	17.2	52.0	10.0	73.0	1.6	92.0	41.3	120.0	1.3
39.0	37.6	53.0	2.4	74.0	5.1	93.0	97.6	122.0	2.5
40.0	5.8	54.0	2.0	75.0	3.0	94.0	10.0	135.0	69.7
41.0	4.6	55.0	0.6	76.0	4.8	95.0	0.6	136.0	18.8
42.0	9.3	61.0	3.4	77.0	95.3	105.0	27.2	137.0	1.7
43.0	36.9	62.0	5.9	78.0	14.4	106.0	4.5	139.0	1.9
44.0	15.7	63.0	18.6	79.0	1.6	107.0	2.3	165.0	1.6
46.0	1.6	64.0	21.6	80.0	2.5	108.0	0.9	166.0	0.2
49.0	2.6	65.0	100.0	81.0	1.0				

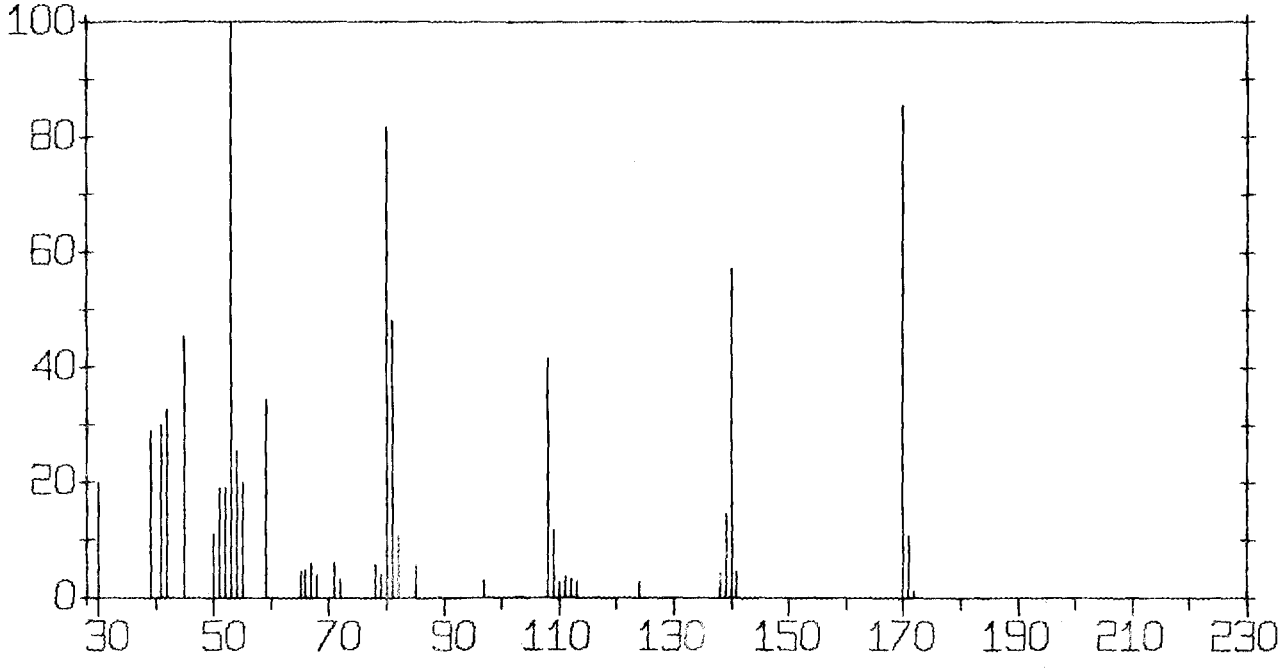
OBSERVED METASTABLES
23.4, 33.8, 46.9, 69.5,



N-NITROSOGUVACOLINE
MW = 170 C7.H11.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	20.0	53.0	100.0	71.0	5.9	97.0	2.9	138.0	4.2
39.0	29.0	54.0	25.4	72.0	3.1	108.0	41.8	139.0	14.5
41.0	30.0	55.0	20.0	78.0	5.7	109.0	11.8	140.0	57.2
42.0	32.7	59.0	34.5	79.0	4.0	110.0	2.7	141.0	4.5
43.0	45.4	65.0	4.5	80.0	81.8	111.0	3.6	170.0	85.4
50.0	10.9	66.0	4.7	81.0	48.1	112.0	3.1	171.0	10.7
51.0	19.0	67.0	5.9	82.0	10.7	113.0	2.9	172.0	1.0
52.0	19.0	68.0	4.0	85.0	5.7	124.0	2.7		

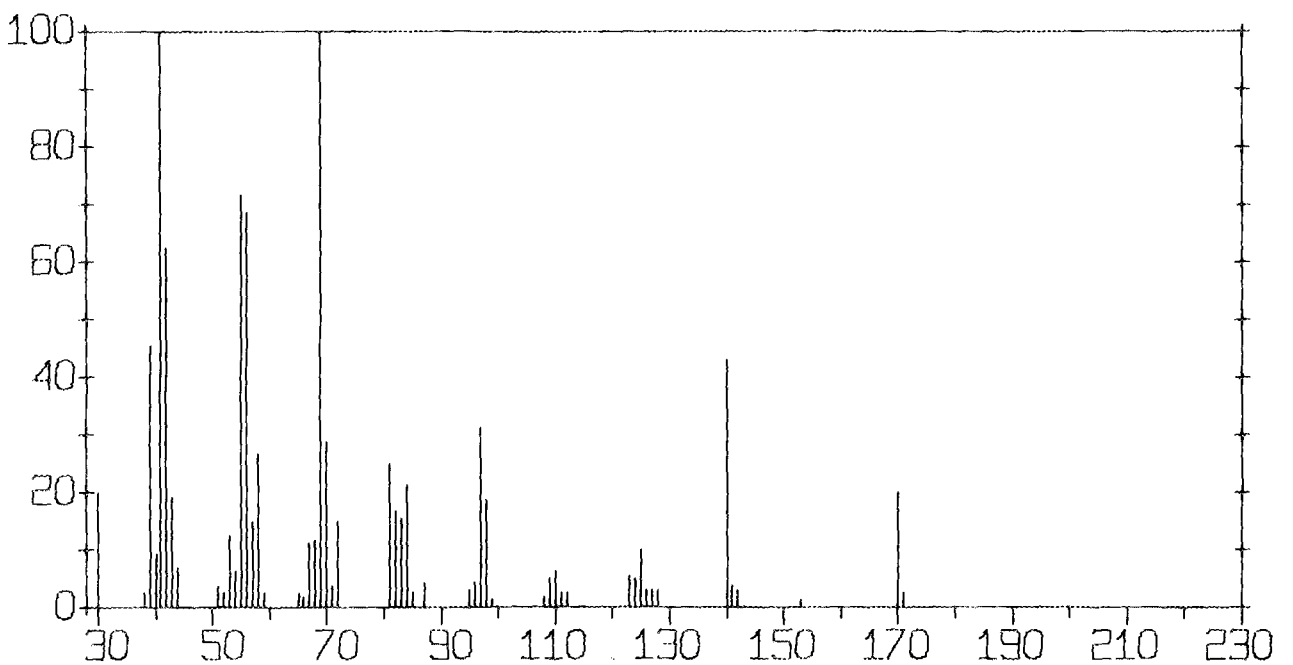
OBSERVED METASTABLES
34.9, 44.9, 66.8, 83.2, 115.2,



N-NITROSO-2,2,6,6-TETRAMETHYLPIPERIDINE
MW = 170 C9.H18.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	20.0	54.0	6.2	70.0	28.7	97.0	31.2	125.0	10.0
38.0	2.5	55.0	71.8	71.0	3.7	98.0	18.7	126.0	3.1
39.0	45.6	56.0	68.7	72.0	15.0	99.0	1.2	127.0	3.1
40.0	9.3	57.0	15.0	81.0	25.0	108.0	1.8	128.0	3.1
41.0	100.0	58.0	26.8	82.0	16.8	109.0	5.0	140.0	43.1
42.0	62.5	59.0	2.5	83.0	15.6	110.0	6.2	141.0	3.7
43.0	19.3	65.0	2.5	84.0	21.2	111.0	2.5	142.0	3.1
44.0	6.8	66.0	1.8	85.0	2.5	112.0	2.5	153.0	1.2
51.0	3.7	67.0	11.2	87.0	4.3	123.0	5.6	170.0	20.0
52.0	2.5	68.0	11.8	95.0	3.1	124.0	5.0	171.0	2.5
53.0	12.5	69.0	100.0	96.0	4.3				

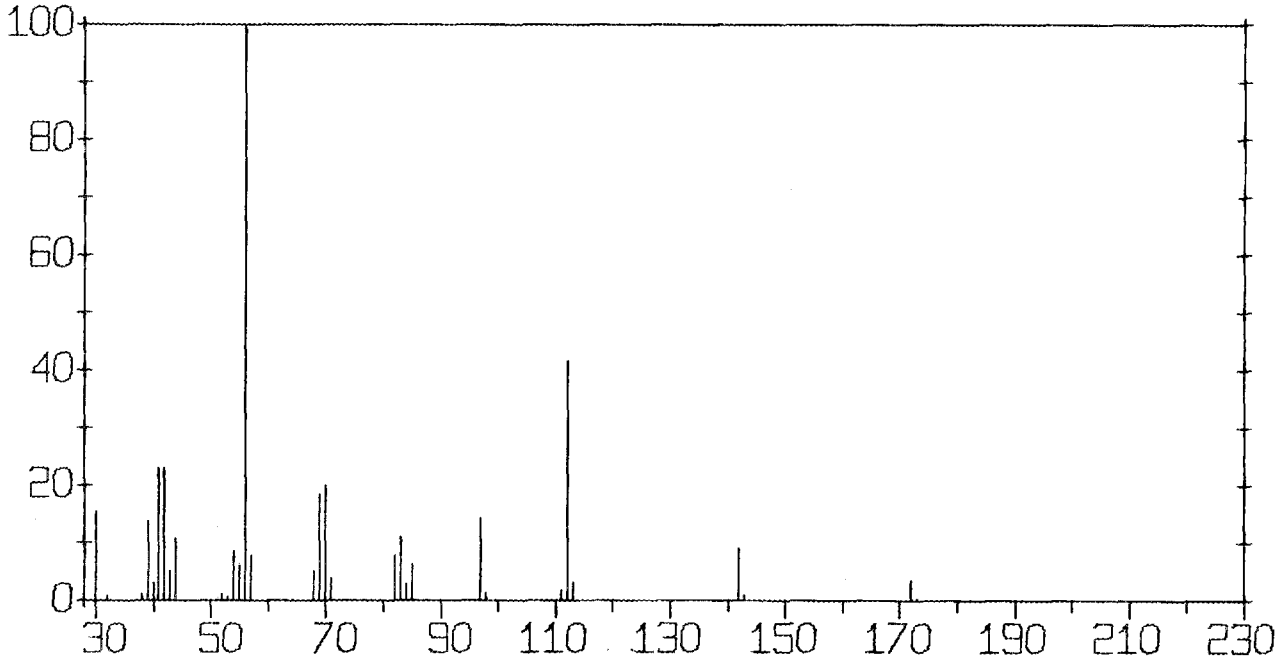
OBSERVED METASTABLES
24.5, 36.5, 37.2, 50.5, 53.5, 74.3, 75.5, 80.9, 107.9, 115.1, 115.8, 122.9, 139.9,



N,N'-DINITROSO-2,5-DIMETHYLPIPERAZINE
MW = 172 C6.H12.N4.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	15.3	43.0	5.0	57.0	7.6	83.0	11.0	112.0	41.5
32.0	0.7	44.0	10.7	68.0	5.0	84.0	2.7	113.0	3.0
38.0	1.0	52.0	1.0	69.0	18.4	85.0	6.1	142.0	8.9
39.0	13.8	53.0	0.6	70.0	20.0	97.0	14.1	143.0	0.7
40.0	3.0	54.0	8.4	71.0	3.6	98.0	1.2	172.0	3.5
41.0	23.0	55.0	6.3	82.0	7.6	111.0	1.6	173.0	0.3
42.0	23.0	56.0	100.0						

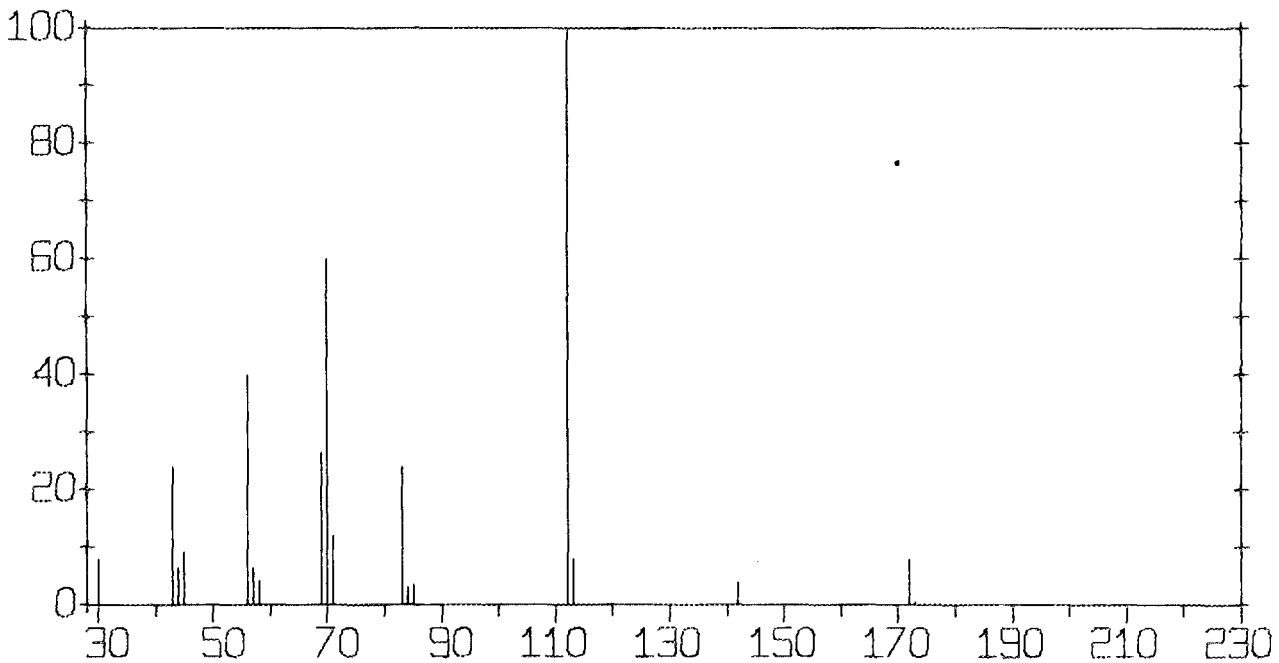
OBSERVED METASTABLES
27.6, 37.1, 55.8, 57.6, 61.5, 69.7, 88.2, 99.5, 117.5, 141.5,



N,N'-DINITROSO-2,6-DIMETHYLPIPERAZINE
MW = 172 C6,H12,N4,O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	8.0	56.0	40.0	70.0	60.0	85.0	3.6	142.0	4.0
43.0	24.0	57.0	6.6	71.0	12.0	112.0	100.0	172.0	8.0
44.0	6.6	58.0	4.3	83.0	24.0	113.0	8.0	173.0	0.6
45.0	9.3	69.0	26.6	84.0	3.0				

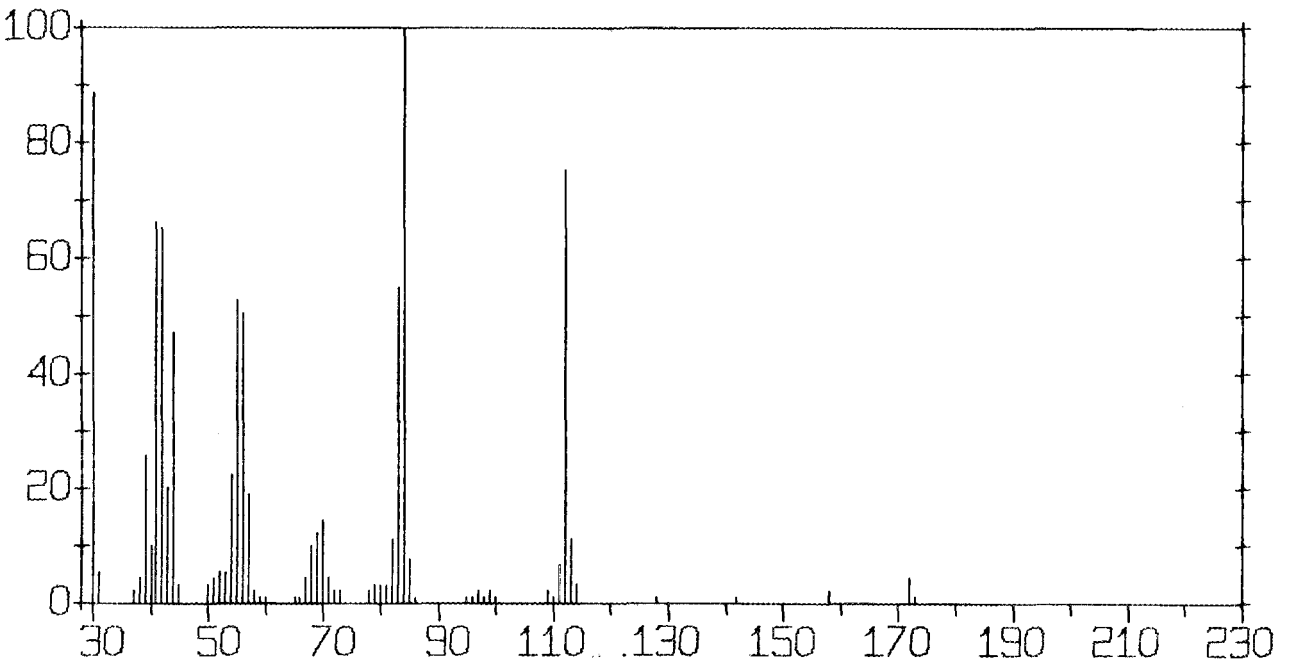
OBSERVED METASTABLES
31.6, 42.1, 66.0, 98.5,



1,5-DINITROSO-1,5-DIAZACYCLOOCTANE
MW = 172 C6,H12,N4,O2,

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	88.7	51.0	4.4	67.0	4.4	82.0	11.2	109.0	2.2
31.0	5.6	52.0	5.6	68.0	10.1	83.0	55.0	110.0	1.1
37.0	2.2	53.0	5.6	69.0	12.3	84.0	100.0	111.0	6.7
38.0	4.4	54.0	22.4	70.0	14.6	85.0	7.8	112.0	75.2
39.0	25.8	55.0	52.8	71.0	4.4	86.0	1.1	113.0	11.2
40.0	10.1	56.0	50.5	72.0	2.2	95.0	1.1	114.0	3.3
41.0	66.2	57.0	19.1	73.0	2.2	96.0	1.1	128.0	1.1
42.0	65.1	58.0	2.2	78.0	2.2	97.0	2.2	142.0	1.1
43.0	20.2	59.0	1.1	79.0	3.3	98.0	1.1	158.0	2.2
44.0	47.1	60.0	1.1	80.0	3.3	99.0	2.2	172.0	4.4
45.0	3.3	65.0	1.1	81.0	3.3	100.0	1.1	173.0	1.1
50.0	3.3	66.0	1.1						

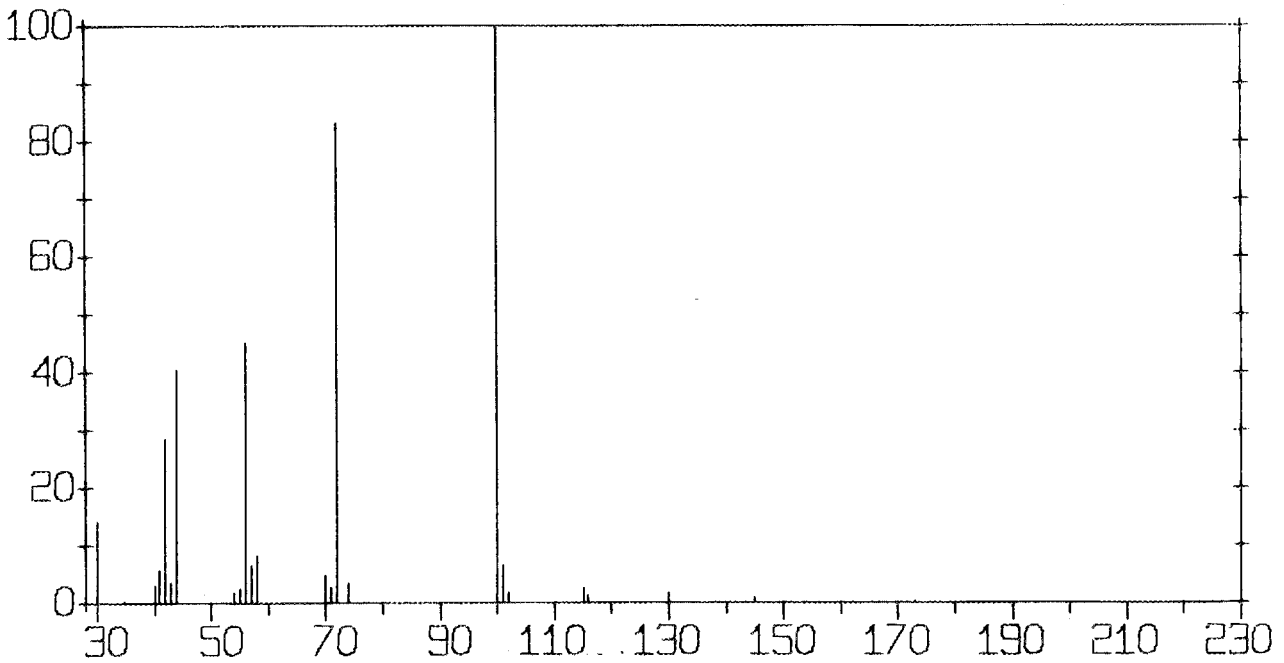
OBSERVED METASTABLES
63.0, 82.2,



N-NITROSOTRIETHYL UREA
MW = 173 C7.H15.N3.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	14.2	44.0	40.4	58.0	8.3	100.0	100.0	116.0	1.1
40.0	3.0	54.0	1.6	70.0	4.7	101.0	6.4	130.0	1.6
41.0	5.7	55.0	2.3	71.0	2.8	102.0	1.6	145.0	0.7
42.0	28.5	56.0	45.2	72.0	33.3	115.0	2.6	173.0	0.2
43.0	3.5	57.0	6.4	74.0	3.5				

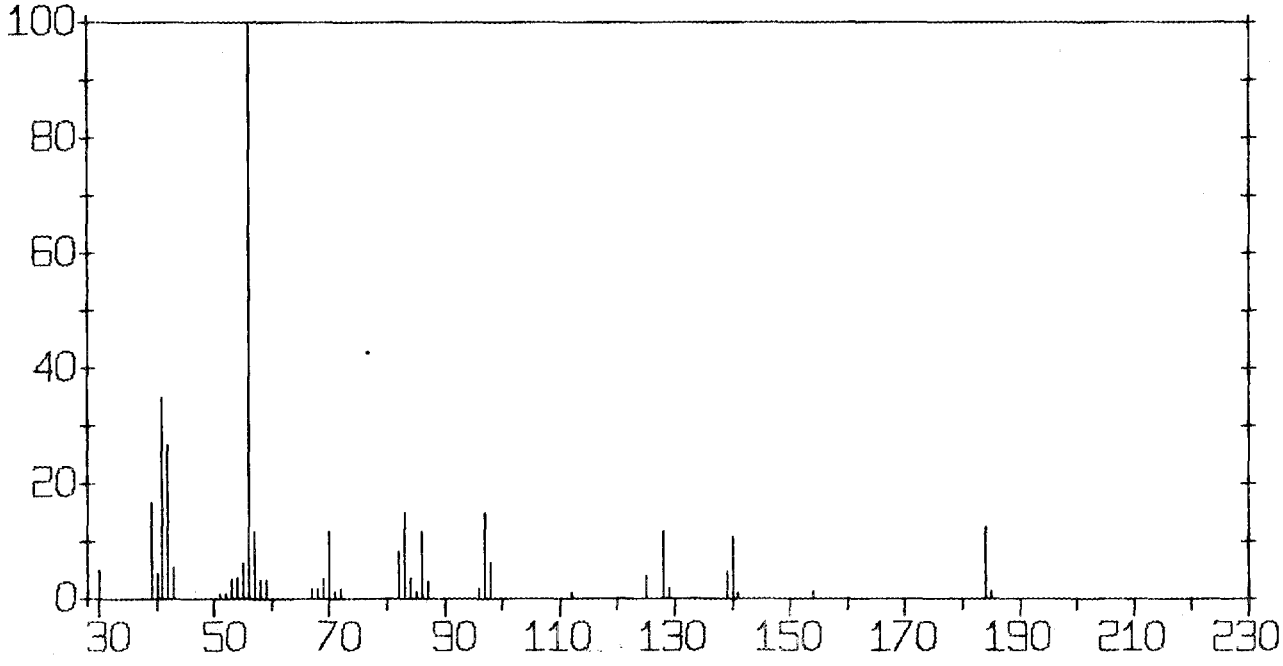
OBSERVED METASTABLES
44.7, 51.8, 71.8,



N-NITROSO-2,2,6,6-TETRAMETHYL-4-PIPERIDONE
MW = 184 C9.H16.N2.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	5.0	53.0	3.5	68.0	1.8	85.0	1.3	128.0	11.6
39.0	16.6	54.0	3.6	69.0	3.5	86.0	11.6	129.0	1.6
40.0	4.5	55.0	6.3	70.0	11.6	87.0	3.0	139.0	4.6
41.0	35.0	56.0	100.0	71.0	1.3	96.0	1.6	140.0	10.8
42.0	26.6	57.0	11.6	72.0	1.6	97.0	15.0	141.0	1.0
43.0	5.5	58.0	3.3	82.0	8.3	98.0	6.1	154.0	1.1
51.0	0.8	59.0	3.3	83.0	15.0	112.0	1.0	184.0	12.5
52.0	0.8	67.0	1.6	84.0	3.6	125.0	4.0	185.0	1.3

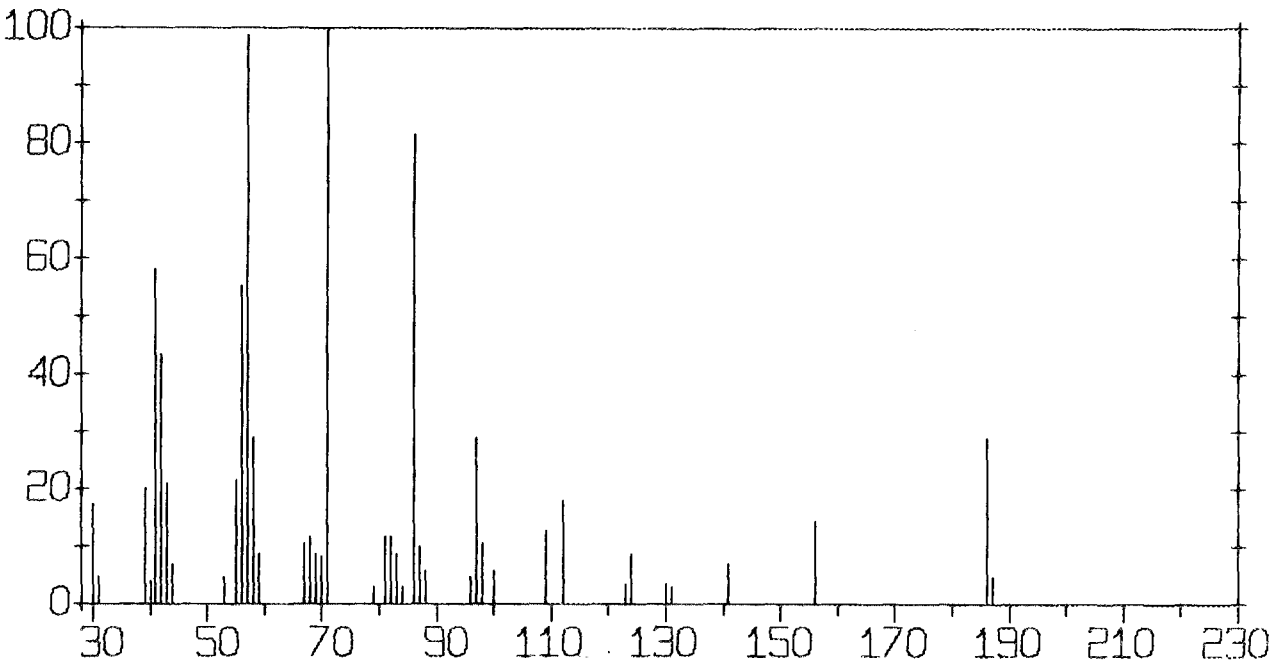
OBSERVED METASTABLES
31.9, 36.5, 49.5, 106.6, 116.6, 124.7, 135.9,



N-NITROSO-2,2,6,6-TETRAMETHYL-4-PIPERIDINOL
MW = 186 C9.H18.N2.O2.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	17.4	55.0	21.5	70.0	8.1	87.0	9.8	123.0	3.4
31.0	4.6	56.0	55.2	71.0	100.0	88.0	5.8	124.0	8.7
39.0	20.3	57.0	98.8	79.0	2.9	96.0	4.6	130.0	3.4
40.0	4.0	58.0	29.0	81.0	11.6	97.0	29.0	131.0	2.9
41.0	58.1	59.0	8.7	82.0	11.6	98.0	10.4	141.0	6.9
42.0	43.6	67.0	10.4	83.0	8.7	100.0	5.8	156.0	14.5
43.0	20.9	68.0	11.6	84.0	2.9	109.0	12.7	186.0	29.0
44.0	6.9	69.0	8.7	86.0	81.3	112.0	18.0	187.0	4.6
53.0	4.6								

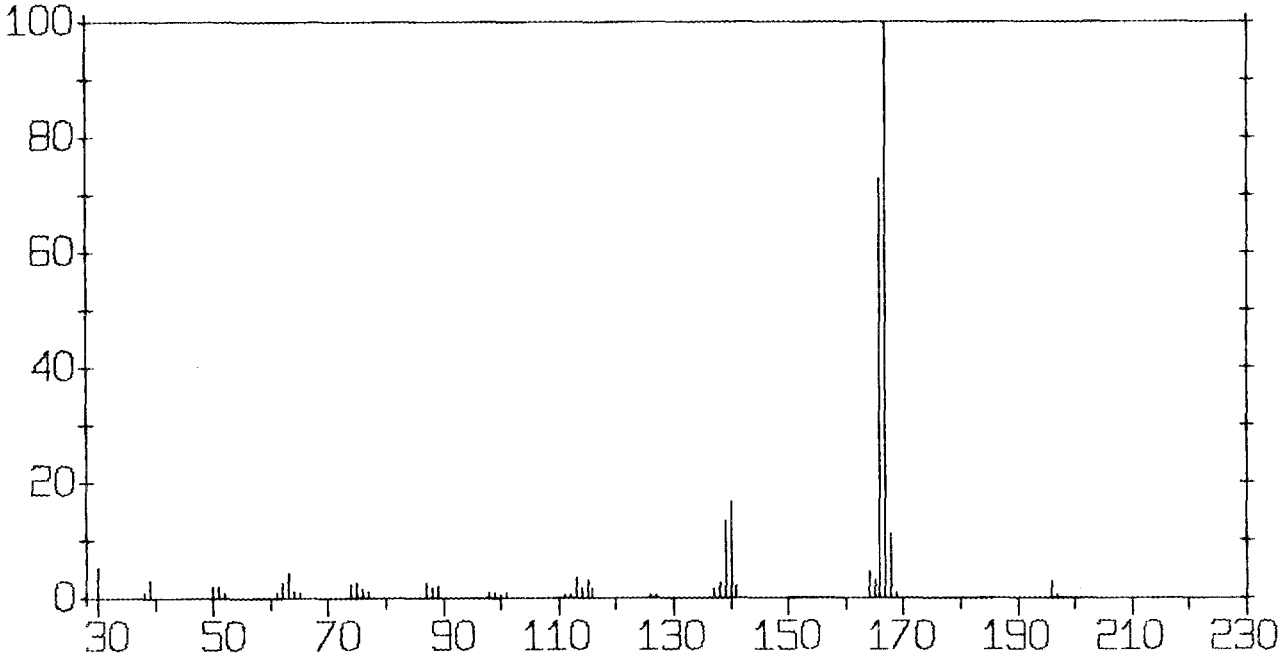
OBSERVED METASTABLES
38.2, 52.9, 64.5, 95.9, 131.1, 155.5,



N-NITROSOCARBAZOLE
MW = 196 C12.H8.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	5.2	64.0	0.9	98.0	0.8	116.0	1.4	164.0	4.5
38.0	0.7	65.0	0.6	99.0	0.6	126.0	0.5	165.0	2.8
39.0	2.9	74.0	2.1	100.0	0.6	127.0	0.5	166.0	72.8
50.0	1.8	75.0	2.5	101.0	0.6	137.0	1.4	167.0	100.0
51.0	2.0	76.0	1.3	111.0	0.5	138.0	2.4	168.0	11.1
52.0	0.7	77.0	0.8	112.0	0.5	139.0	13.3	169.0	0.7
61.0	0.8	87.0	2.5	113.0	3.4	140.0	16.4	196.0	2.6
62.0	2.4	88.0	1.7	114.0	1.7	141.0	1.9	197.0	0.4
63.0	4.3	89.0	2.0	115.0	3.0				

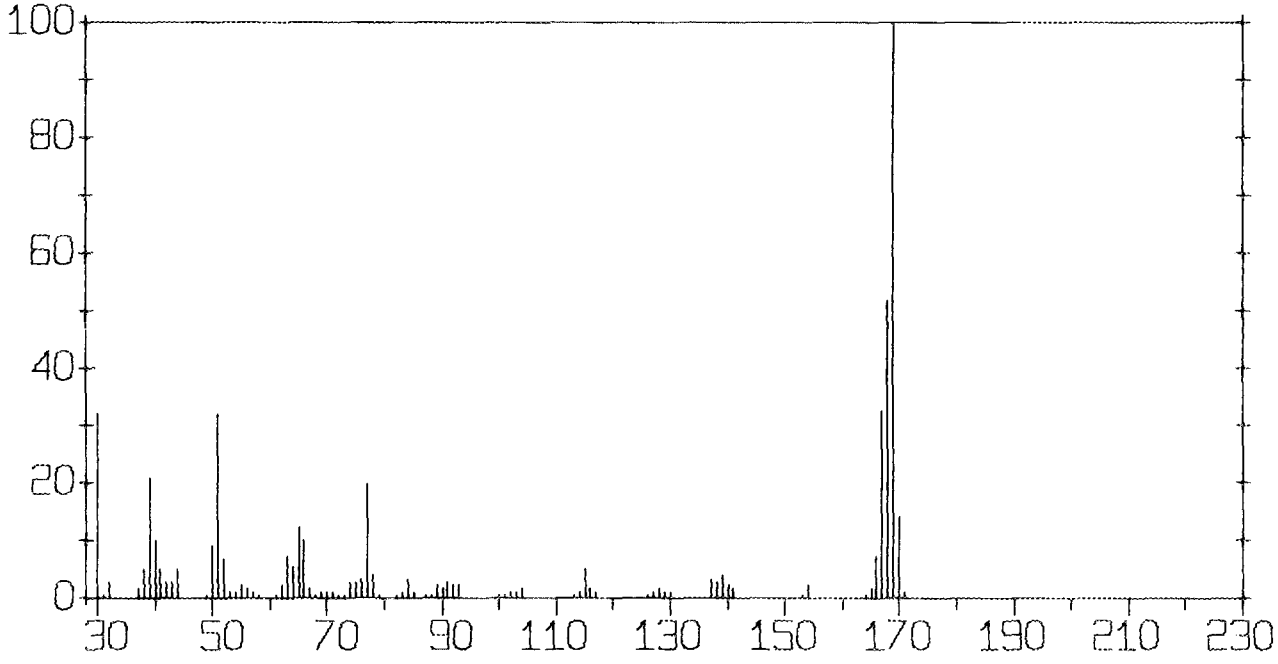
OBSERVED METASTABLES
91.4, 116.2, 117.6, 165.0.



N-NITROSODIPHENYLAMINE
MW = 198 C12.H10.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	32.0	55.0	2.2	73.0	0.5	92.0	2.2	130.0	1.1
31.0	0.5	56.0	1.6	74.0	2.8	93.0	2.2	137.0	3.3
32.0	2.8	57.0	1.1	75.0	2.8	100.0	0.5	138.0	2.8
37.0	1.6	58.0	0.5	76.0	3.3	101.0	0.5	139.0	3.9
38.0	5.0	61.0	0.5	77.0	19.6	102.0	1.1	140.0	2.2
39.0	20.7	62.0	2.2	78.0	3.9	103.0	1.1	141.0	1.6
40.0	10.1	63.0	7.3	79.0	0.5	104.0	1.6	153.0	0.5
41.0	5.0	64.0	5.6	82.0	0.5	113.0	0.5	154.0	2.2
42.0	2.8	65.0	12.3	83.0	1.1	114.0	1.1	164.0	0.5
43.0	2.8	66.0	10.1	84.0	3.3	115.0	5.0	165.0	1.6
44.0	5.0	67.0	1.6	85.0	1.1	116.0	1.6	166.0	7.3
49.0	0.5	68.0	0.5	87.0	0.5	117.0	1.1	167.0	32.5
50.0	8.9	69.0	1.1	88.0	0.5	126.0	0.5	168.0	51.6
51.0	32.0	70.0	1.1	89.0	2.2	127.0	1.1	169.0	100.0
52.0	6.7	71.0	1.1	90.0	1.6	128.0	1.6	170.0	14.0
53.0	1.1	72.0	0.5	91.0	2.8	129.0	1.1	171.0	1.1
54.0	1.1								

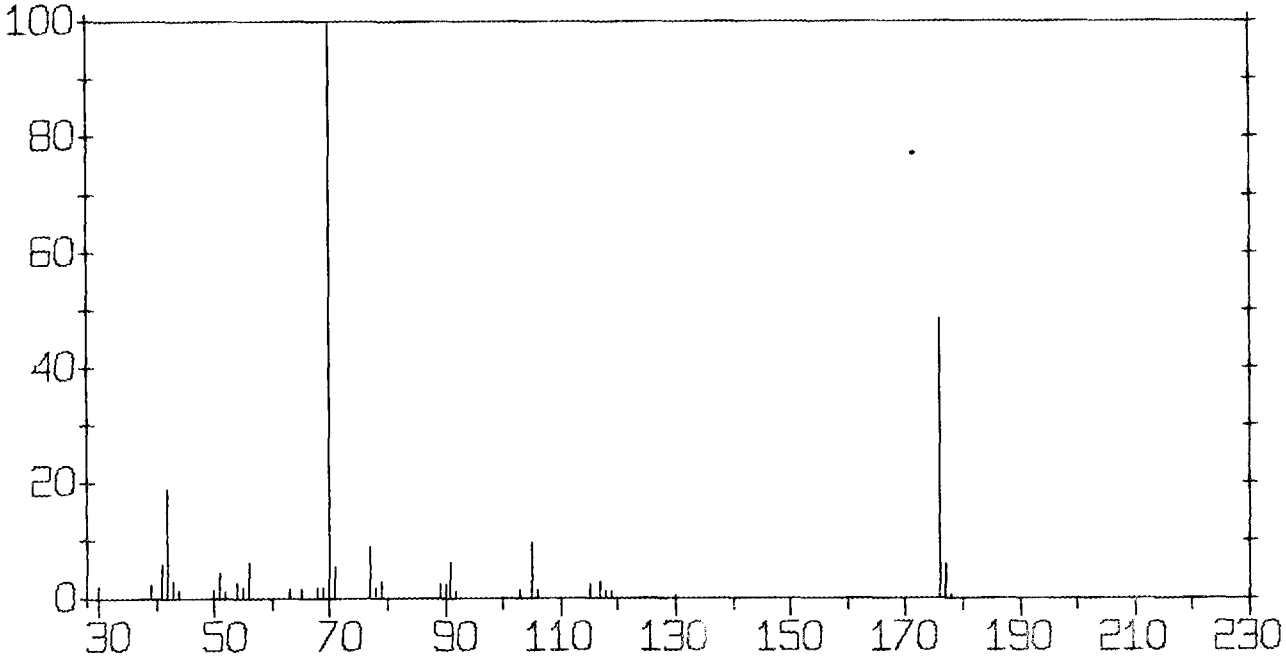
OBSERVED METASTABLES
33.8.



N-NITROSOPHENMETRAZINE
MW = 206 C11.H14.N2.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	2.1	52.0	1.2	69.0	2.0	90.0	2.4	117.0	2.9
39.0	2.4	54.0	2.8	70.0	100.0	91.0	6.2	118.0	1.2
41.0	6.1	55.0	1.9	71.0	5.4	92.0	1.3	119.0	1.3
42.0	19.0	56.0	6.2	77.0	8.9	103.0	1.4	130.0	0.5
43.0	3.0	63.0	1.7	78.0	2.0	105.0	9.6	176.0	48.4
44.0	1.5	65.0	1.6	79.0	3.0	106.0	1.5	177.0	5.9
50.0	1.5	68.0	2.0	89.0	2.5	115.0	2.4	178.0	0.4
51.0	4.4								

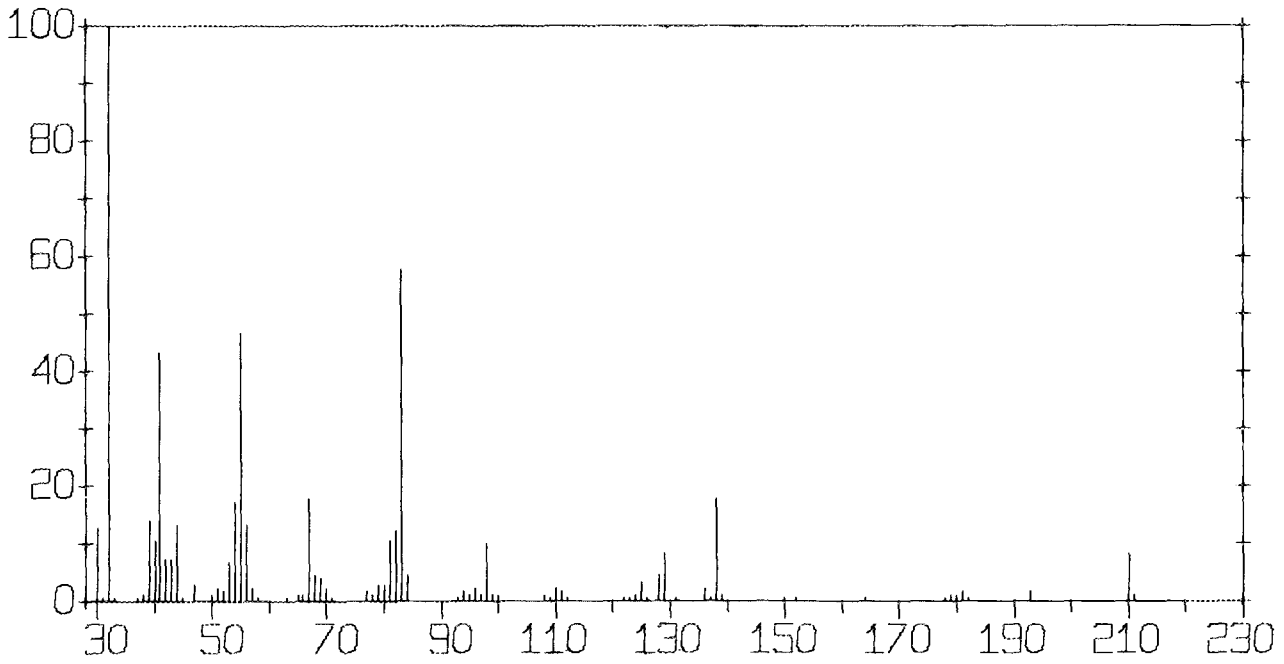
OBSERVED METASTABLES
25.0, 27.9, 56.1, 101.0, 113.0,



N-NITROSODICYCLOHEXYLAMINE
MW = 210 C12.H22.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	22.1	51.0	3.8	71.0	0.9	99.0	1.9	136.0	3.8
31.0	0.9	52.0	2.8	77.0	2.8	100.0	1.9	137.0	0.9
32.0	4.8	53.0	11.5	78.0	1.9	108.0	1.9	138.0	30.7
33.0	0.9	54.0	29.8	79.0	4.8	109.0	0.9	139.0	1.9
37.0	0.9	55.0	80.7	80.0	4.8	110.0	3.8	150.0	0.9
38.0	1.9	56.0	23.0	81.0	18.2	111.0	2.8	152.0	0.9
39.0	24.0	57.0	3.8	82.0	21.1	112.0	0.9	164.0	0.9
40.0	18.2	58.0	0.9	83.0	100.0	122.0	0.9	178.0	0.9
41.0	75.0	63.0	0.9	84.0	7.6	123.0	0.9	179.0	1.9
42.0	12.5	65.0	1.9	93.0	0.9	124.0	1.9	180.0	1.9
43.0	12.5	66.0	1.9	94.0	2.8	125.0	5.7	181.0	2.8
44.0	23.0	67.0	30.7	95.0	1.9	126.0	0.9	182.0	0.9
45.0	0.9	68.0	7.6	96.0	3.8	128.0	7.6	193.0	2.8
47.0	4.8	69.0	6.7	97.0	1.9	129.0	14.4	210.0	14.4
50.0	1.9	70.0	3.8	98.0	17.3	131.0	0.9	211.0	1.9

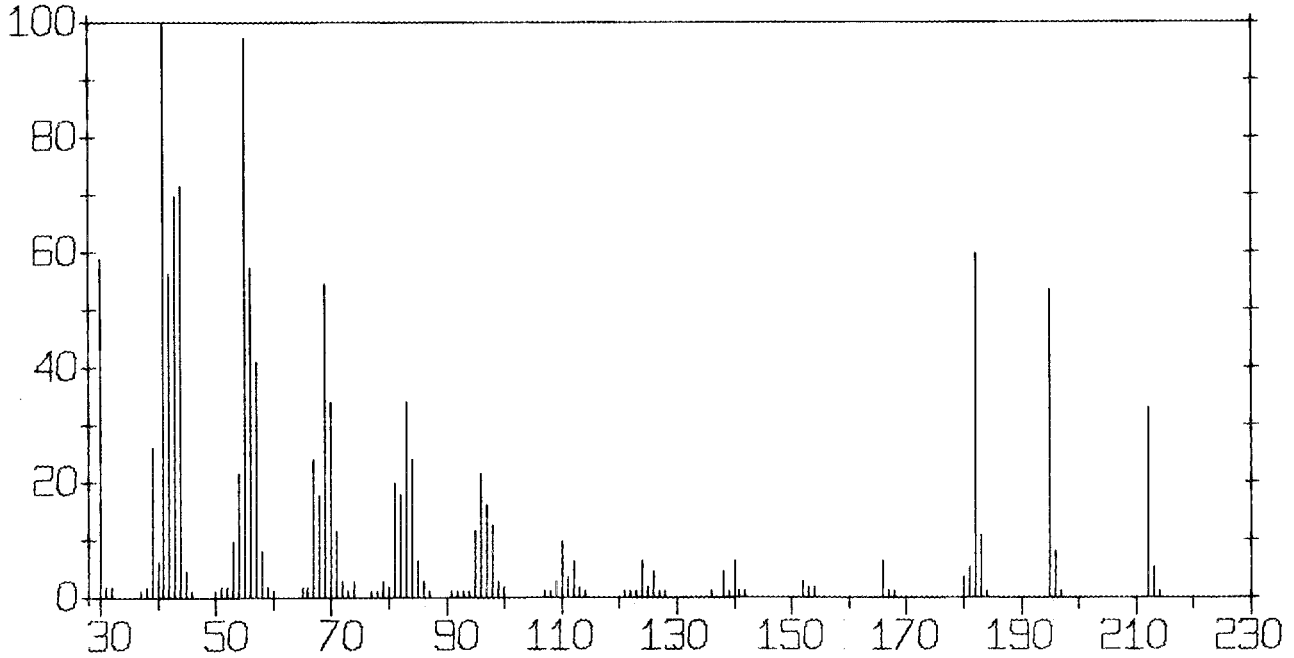
OBSERVED METASTABLES
36.5, 37.4, 54.8, 77.2, 96.2, 104.2,



N-NITROSODODECAMETHYLENEIMINE
MW = 212 C12.H24.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	58.9	56.0	57.1	81.0	19.6	109.0	2.6	142.0	0.8
31.0	1.7	57.0	41.0	82.0	17.8	110.0	9.8	152.0	2.6
32.0	1.7	58.0	8.0	83.0	33.9	111.0	3.5	153.0	1.7
37.0	0.8	59.0	1.7	84.0	24.1	112.0	6.2	154.0	1.7
38.0	1.7	60.0	0.8	85.0	6.2	113.0	1.7	166.0	6.2
39.0	25.8	65.0	1.7	86.0	2.6	114.0	0.8	167.0	0.8
40.0	6.2	66.0	1.7	87.0	0.8	121.0	0.8	168.0	0.8
41.0	100.0	67.0	24.1	91.0	0.8	122.0	0.8	180.0	3.5
42.0	56.2	68.0	17.8	92.0	0.8	123.0	0.8	181.0	5.3
43.0	69.6	69.0	54.4	93.0	0.8	124.0	6.2	182.0	59.8
44.0	71.4	70.0	33.9	94.0	0.8	125.0	1.7	183.0	10.7
45.0	4.4	71.0	11.6	95.0	11.6	126.0	4.4	184.0	0.8
46.0	0.8	72.0	2.6	96.0	21.4	127.0	0.8	195.0	53.5
50.0	0.8	73.0	0.8	97.0	16.0	128.0	0.8	196.0	8.0
51.0	1.7	74.0	2.6	98.0	12.5	136.0	0.8	197.0	0.8
52.0	1.7	77.0	0.8	99.0	2.6	138.0	4.4	212.0	33.0
53.0	9.8	78.0	0.8	100.0	1.7	139.0	0.8	213.0	5.3
54.0	21.4	79.0	2.6	107.0	0.8	140.0	6.2	214.0	0.8
55.0	97.3	80.0	1.7	108.0	0.8	141.0	0.8		

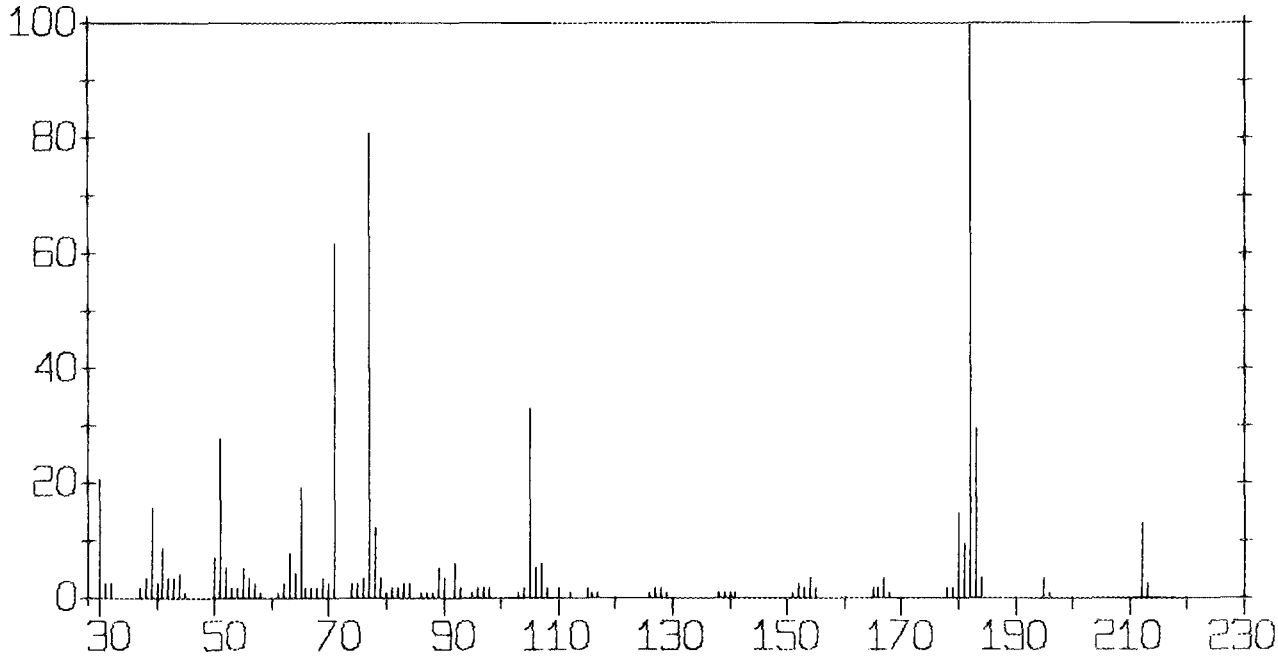
OBSERVED METASTABLES
24.4, 36.5, 37.2, 38.2, 39.2, 49.7, 51.2, 82.2, 118.5, 163.5, 179.5,



N-NITROSOPHENYLBENZYLAMINE
MW = 212 C13.H12.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	20.8	57.0	2.6	80.0	0.8	105.0	33.0	153.0	1.7
31.0	2.6	58.0	0.8	81.0	1.7	106.0	5.2	154.0	3.4
32.0	2.6	61.0	0.8	82.0	1.7	107.0	6.0	155.0	1.7
37.0	1.7	62.0	2.6	83.0	2.6	108.0	1.7	165.0	1.7
38.0	3.4	63.0	7.8	84.0	2.6	110.0	1.7	166.0	1.7
39.0	15.6	64.0	4.3	86.0	0.8	112.0	0.8	167.0	3.4
40.0	2.6	65.0	19.1	87.0	0.8	115.0	1.7	168.0	0.8
41.0	8.6	66.0	1.7	88.0	0.8	116.0	0.8	178.0	1.7
42.0	3.4	67.0	1.7	89.0	5.2	117.0	0.8	179.0	1.7
43.0	3.4	68.0	1.7	90.0	3.4	126.0	0.8	180.0	14.7
44.0	4.3	69.0	3.4	71.0	61.7	127.0	1.7	181.0	9.5
45.0	0.8	70.0	2.6	92.0	6.0	128.0	1.7	182.0	100.0
50.0	6.9	71.0	0.8	93.0	1.7	129.0	0.8	183.0	29.5
51.0	27.8	74.0	2.6	95.0	0.8	138.0	0.8	184.0	3.4
52.0	5.2	75.0	2.6	96.0	1.7	139.0	0.8	195.0	3.4
53.0	1.7	76.0	3.4	97.0	1.7	140.0	0.8	196.0	0.8
54.0	1.7	77.0	80.8	98.0	1.7	141.0	0.8	212.0	13.0
55.0	5.2	78.0	12.1	103.0	0.8	151.0	0.8	213.0	2.6
56.0	3.4	79.0	3.4	104.0	1.7	152.0	2.6		

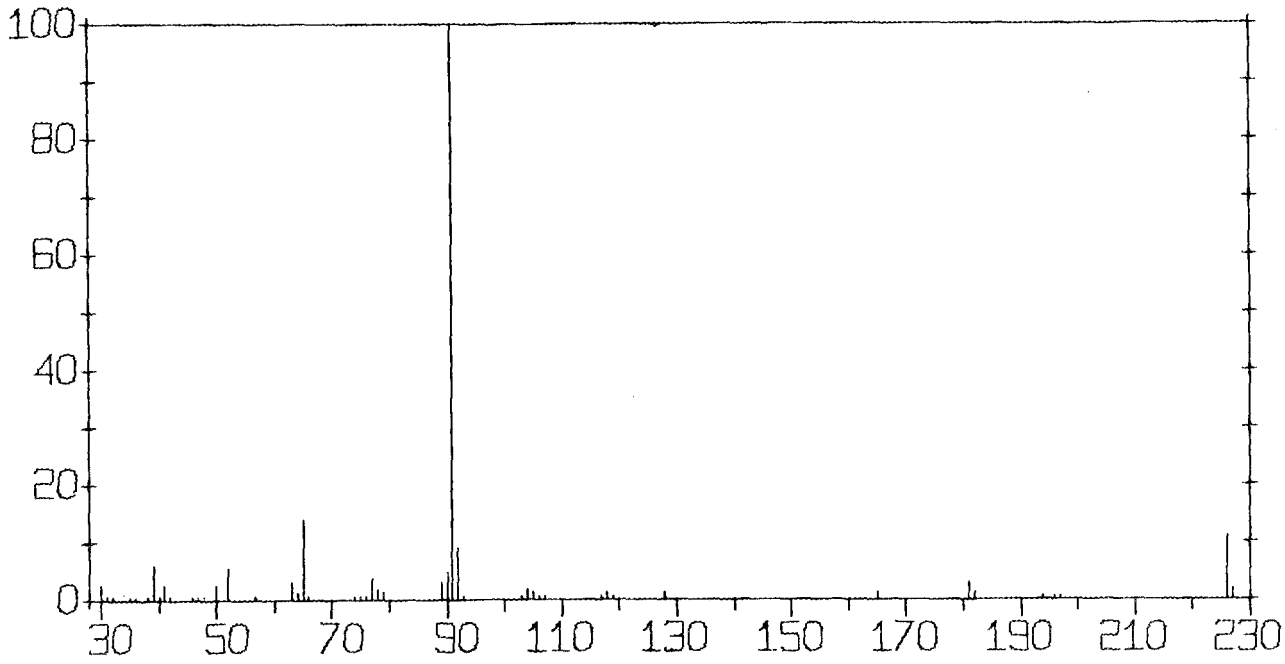
OBSERVED METASTABLES
32.5, 33.8, 36.5, 37.1, 43.2, 46.4, 59.4, 66.4, 130.2, 149.8, 156.2, 157.0,



N-NITROSODIBENZYLAMINE
MW = 226 C14.H14.N2.O.

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	2.4	52.0	5.4	77.0	3.6	104.0	1.8	165.0	1.2
31.0	0.6	52.0	1.8	78.0	1.8	105.0	1.2	181.0	3.0
32.0	0.6	63.0	3.0	79.0	1.2	106.0	0.6	182.0	1.2
38.0	0.6	64.0	1.2	89.0	3.0	107.0	0.6	194.0	0.6
39.0	6.0	65.0	13.9	90.0	4.8	117.0	0.6	196.0	0.6
40.0	0.6	66.0	0.6	91.0	100.0	118.0	1.2	197.0	0.6
41.0	2.4	74.0	0.6	92.0	9.0	119.0	0.6	226.0	10.9
42.0	0.6	75.0	0.6	93.0	0.6	128.0	1.2	227.0	1.8
50.0	2.4	76.0	0.6	103.0	0.6				

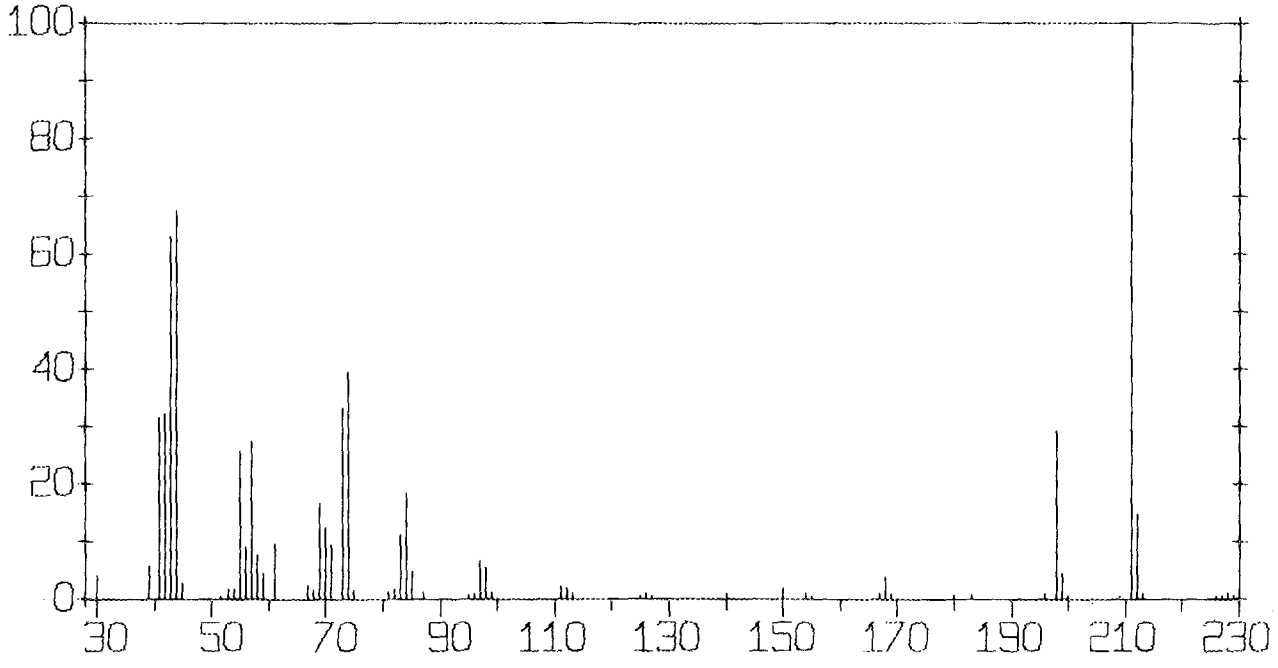
OBSERVED METASTABLES
23.5, 33.8, 45.5, 46.5, 60.8,



N-NITROSOMETHYLDODECYLAMINE
MW = 228 C13.H28.N2.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	4.1	59.0	4.6	83.0	11.3	125.0	0.6	196.0	1.1
39.0	5.8	61.0	9.6	84.0	18.4	126.0	1.0	198.0	29.1
41.0	31.4	67.0	2.4	85.0	5.0	127.0	0.4	199.0	4.4
42.0	32.2	68.0	1.8	87.0	1.3	140.0	0.7	200.0	0.3
43.0	62.8	69.0	16.8	95.0	0.6	150.0	2.0	209.0	0.5
44.0	67.4	70.0	12.4	96.0	0.9	154.0	0.9	211.0	100.0
45.0	2.7	71.0	9.5	97.0	6.7	155.0	0.4	212.0	14.7
53.0	1.8	73.0	33.2	98.0	5.5	167.0	0.9	213.0	1.1
54.0	1.8	74.0	39.4	99.0	1.3	168.0	3.9	226.0	0.4
55.0	25.7	75.0	1.4	111.0	2.1	169.0	0.8	227.0	0.5
56.0	8.8	81.0	1.2	112.0	1.9	180.0	0.6	228.0	0.9
57.0	27.6	82.0	1.6	113.0	0.9	183.0	0.6	229.0	0.5
58.0	7.8								

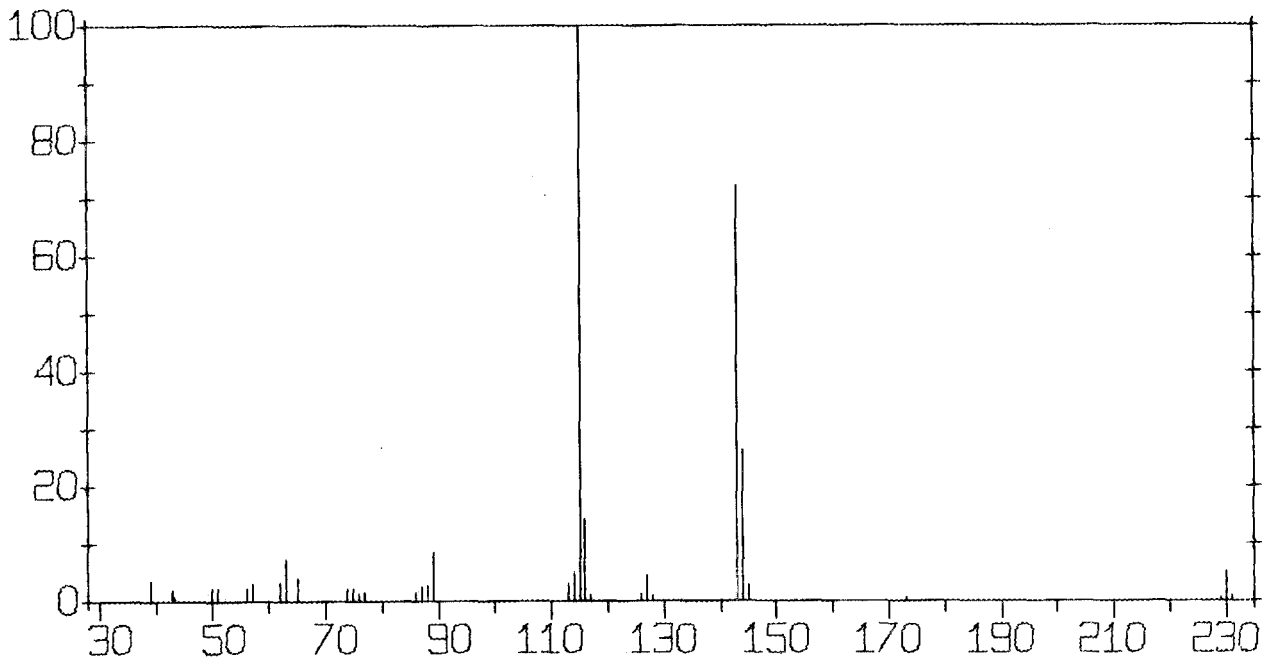
OBSERVED METASTABLES
34.8, 35.5, 36.3, 134.0, 153.8, 195.2,



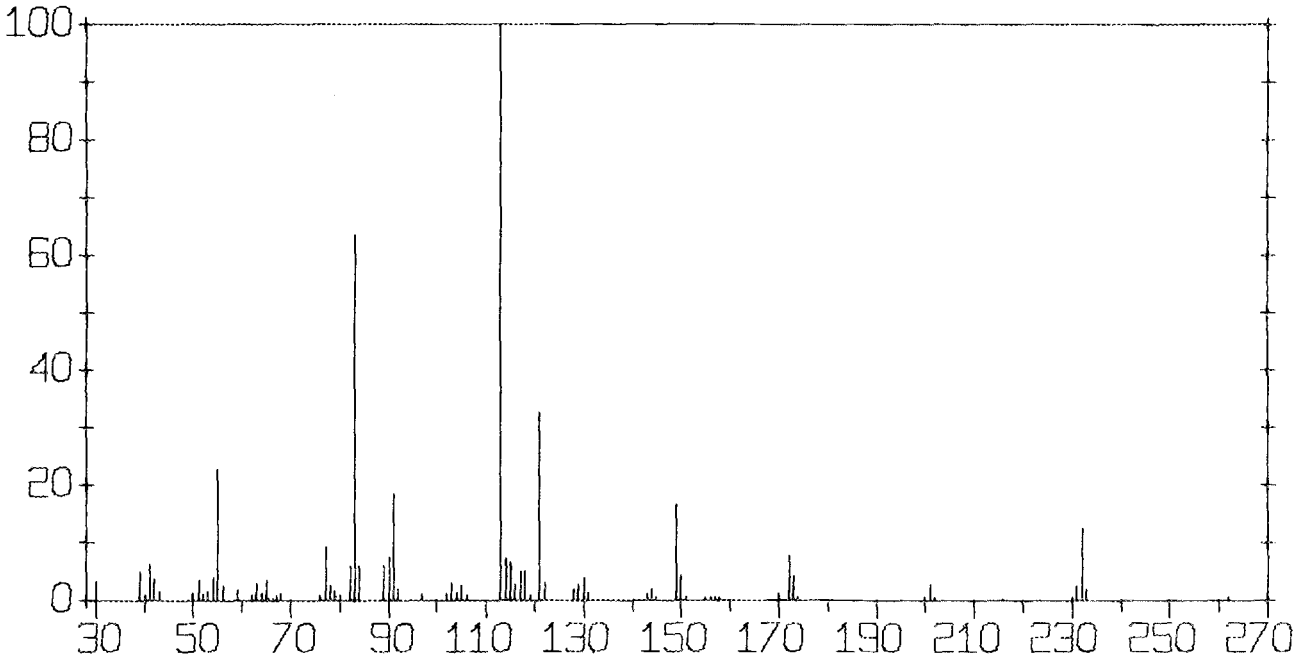
N-NITROSO-1-NAPHTHYL-N-METHYLCARBAMATE
MW = 230 C12.H10.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
39.0	3.4	63.0	7.2	87.0	2.4	116.0	14.1	144.0	26.3
43.0	2.0	65.0	4.0	88.0	2.7	117.0	0.9	145.0	2.7
50.0	2.3	74.0	2.1	89.0	8.3	126.0	1.2	173.0	0.4
51.0	2.1	75.0	2.3	113.0	3.0	127.0	4.5	229.0	0.5
56.0	2.3	76.0	1.3	114.0	5.0	128.0	0.7	230.0	5.0
57.0	2.8	77.0	1.4	115.0	100.0	143.0	72.2	231.0	0.6
62.0	3.1	86.0	1.6						

OBSERVED METASTABLES
68.9, 88.8, 92.7,



N-NITROSOMETHYLPHENIDATE
MW = 262 C14.H18.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	3.2	63.0	3.0	91.0	18.3	121.0	32.6	158.0	0.4
39.0	5.0	64.0	1.1	92.0	1.8	122.0	2.8	170.0	0.9
40.0	0.9	65.0	3.5	97.0	0.9	128.0	1.8	172.0	7.7
41.0	6.2	67.0	0.7	102.0	1.2	129.0	2.7	173.0	4.2
42.0	3.8	68.0	0.9	103.0	3.0	130.0	4.0	174.0	0.5
43.0	1.5	76.0	0.7	104.0	1.1	131.0	1.3	200.0	0.5
50.0	1.3	77.0	9.3	105.0	2.4	143.0	0.9	201.0	2.7
51.0	3.5	78.0	2.6	106.0	0.7	144.0	2.0	202.0	0.4
52.0	1.1	79.0	1.4	113.0	100.0	145.0	0.5	216.0	0.2
53.0	1.5	80.0	0.6	114.0	7.2	149.0	16.3	230.0	0.3
54.0	4.1	82.0	5.9	115.0	6.4	150.0	4.1	231.0	2.5
55.0	22.7	83.0	63.4	116.0	2.7	151.0	0.4	232.0	12.6
56.0	2.5	84.0	6.0	117.0	5.0	155.0	0.4	233.0	1.9
59.0	1.8	89.0	5.9	118.0	4.9	156.0	0.5	262.0	0.4
62.0	0.8	90.0	7.5	119.0	0.8	157.0	0.5		

OBSERVED METASTABLES
21.2, 33.9, 36.6, 46.4, 48.8, 61.0, 95.8, 127.7, 168.1,