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Mass Spectra of N-Nitroso Compounds

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ANALYTICAL CHEMISTRY AND BIOLOGY DIVISIONS

MASS SPECTRA OF N-NITROSO COMPOUNDS

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CONTENTS

Page

SUMMARY v

1.0 Introduction 1

2.0 Indices 2

2.1 Index by Compound Type, Including Physical Constants . . 2

2.2 Index by Molecular Weight 4

2.3 Index by Base Peak 6

3.0 Experimental 8

3.1 Compound Preparation 8

3.2 Mass Spectrometry 9

4.0 Mass Spectra 10

SUMMARY

The low-resolution electron impact mass spectra (70 eV) of 52 N-nitroso compounds are presented. Aliphatic, aromatic, and cyclic nitrosamines are represented, as are nitrosamino acids and nitrosamides. Most of the compounds showed a molecular ion. Many of them gave a fragment ion at M-30 or M-31 and an ion of m/e 30 of variable intensity. A large number 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, and this publication, with the previously published ORNL-TM-4359, serves as a source of useful comparative spectra of a diverse list of nitrosamines.

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 samples, 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. The mass spectra of 95 of these compounds were published in ORNL-TM-4359 in October, 1973. This publication of an additional 52 spectra brings the mass spectral information to date. The interpretation and generalizations concerning mass spectra of nitrosamines will be published in the open literature in the near future.

2.1 INDEX BY COMPOUND TYPE, INCLUDING PHYSICAL CONSTANTS

	MOL WT	MP OR BP (TORR)	U V ABS	SOL	PAGE
ALIPHATIC NITROSAMINES					
N-NITROSO-					
METHYL-D3-ETHYLAMINE	91		82 332	W	10
DIETHYL-D10-AMINE	112				11
DIALLYLAMINE	126		82 343	W	14
DISECBUTYLAMINE	158		73 359	E	28
METHYLUNDECYLAMINE	214		73 359	E	46
DIOCTYLAMINE	270		103 358	E	55
METHYLOCTADECYLAMINE	312	M 43-45	101 345	E	59
DIDECYLAMINE	326		90 350	E	60
DIDODECYLAMINE	382	M 31-32	81 351	E	61
POLYFUNCTIONAL ALIPHATIC NITROSAMINES					
N-NITROSO-					
ETHYL-2-HYDROXYETHYLAMINE	118		77 341	W	12
BIS(2-HYDROXYETHYL)AMINE	134		78 252	E	16
BIS(2-HYDROXYPROPYL)AMINE	162		84 353	E	29
BIS(2-OXOPROPYL)AMINE	158	53-54	90 348	W	27
BIS(2-CHLOROETHYL)AMINE	170		78 362	E	33
BIS-(2-CHLOROPROPYL)AMINE	198		92 364	E	43
BIS(CYANOMETHYL)AMINE	124	M 39-41	84 368	E	13
BIS(2-CYANOETHYL)AMINE	152	M 47-49	80 354	W	26
BIS(2-METHOXYETHYL)AMINE	162		87 353	E	30
BIS(2-ETHOXYETHYL)AMINE	190		86 345	W	39
BIS(2,2-DIETHOXYETHYL)AMINE	278		97 352	E	58
AROMATIC SUBSTITUTED NITROSAMINES					
N-NITROSO-					
ATRAZINE	244	89-91	81 412	E	51
SUBSTITUTED ALICYCLIC NITROSAMINES					
N-NITROSO-					
3,5-DIMETHYLPIPERIDINE	142		75 350	E	19
4-TERTBUTYLPIPERIDINE	170	M 51-54	97 350	E	34
4-PHENYLPIPERIDINE	190	M 66-68	103 351	E	40
NORNICOTINE	177		64 346	W	35
3-CHLOROPIPERIDINE	148		93 350	E	21
4-CHLOROPIPERIDINE	148		88 355	E	22
3,4-DICHLOROPYRROLIDINE	168	M 54-55	91 345	W	32
3,4-DIBROMOPYRROLIDINE	256	M 110-12	97 357	E	54
3,4-DICHLOROPIPERIDINE	182	M 81-82	88 345	W	38
3,4-DIBROMOPIPERIDINE	270	M 86-87.5	92 344	W	56
2,6-DICYANOPIPERIDINE	164	M 141-142	85 382	E	31

2.1 INDEX BY COMPOUND TYPE, INCLUDING PHYSICAL CONSTANTS

	MOL WT	MP OR BP (TORR)	U V ABS	SOL	PAGE
DINITROSO ALICYCLIC NITROSAMINES					
N,N-DINITROSO- 2,3,5,6-TETRAMETHYLPIPERAZINE	200	M 107-109	149 363	E	44
NITROSAMIDES					
N-NITROSO- NORBUTYLUREA	145	M 183			20
2-FLUOROETHYLUREA	135	M 81-3(D)	105 397	E	17
2-CHLOROETHYL UREA	151	M 45-47	156 402	E	25
1,1-DIMETHYL-3(2-CHLOROETHYL)UREA	179		79 388	E	36
1-METHYL-3,3-BIS(2-CHLOROETHYL)UREA	227		80 400	E	49
1,1-DIETHYL-3(2-CHLOROETHYL)UREA	207		80 388	E	45
1,1,3-TRIS(2-CHLOROETHYL)UREA	275		80 403	E	57
2-BROMOETHYLUREA	195	M 45-46	213 402	E	42
2-HYDROXYETHYLUREA	133	M 51-55	155 401	E	15
NITROSOGUANIDINES					
N-NITROSO- N-METHYL-D3-N'-NITROGUANIDINE	150				23
NITROSOCARBAMATES					
N-NITROSO- ETHYL N-METHYL-D3-CARBAMATE	135		132 401	W	18
ETHYL N-ETHYL-D5-CARBAMATE	151		124 406	E	24
METHYL N-PHENYLCARBAMATE	180	78-79	100 402	E	37
METHOMYL	191	63-65	122 402	E	41
ALDICARB	219	44-46	137 400	E	47
LANDRIN	222		107 401	E	48
BAYGON	238		117 400	E	50
CARBOFURAN	250	44-46	130 401	E	53
BUXTEN	250		121 401	E	52

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	M/E	INT
91	10	N-NITROSOMETHYL-D3-ETHYLAMINE														
			45	100	91	92	46	78	33	24	30	21	43	21	59	20
112	11	N-NITROSODIETHYL-D10-AMINE														
			50	100	112	88	62	77	44	67	70	60	64	52	71	46
118	12	N-NITROSOETHYL-2-HYDROXYETHYLAMINE														
			42	100	57	58	56	53	43	50	31	36	58	32	87	23
124	13	N-NITROSO-BIS(CYANOMETHYL)AMINE														
			124	100	40	75	67	33	41	21	39	10	53	7	38	7
126	14	N-NITROSODIALLYLAMINE														
			41	100	39	39	42	23	109	18	54	10	68	9	81	8
133	15	N-NITROSO-2-HYDROXYETHYLUREA														
			30	100	42	70	57	38	41	7	117	7	89	7	58	5
134	16	N-NITROSO-BIS(2-HYDROXYETHYL)AMINE														
			43	100	42	46	74	29	55	27	56	25	87	25	72	24
135	17	N-NITROSO-2-FLUOROETHYLUREA														
			44	100	92	71	59	47	47	35	102	29	93	28	46	26
135	18	N-NITROSO-ETHYL N-METHYL-D3-CARBAMATE														
			61	100	78	34	46	24	45	22	76	16	60	14	63	14
142	19	N-NITROSO-3,5-DIMETHYLPIPERIDINE														
			55	100	42	95	41	74	142	66	39	33	83	29	56	26
145	20	N-NITROSONORBUTYLUREA														
			30	100	41	97	44	82	56	50	59	48	57	42	39	38
148	21	N-NITROSO-3-CHLOROPIPERIDINE														
			42	100	55	70	56	39	43	38	30	36	40	36	82	36
148	22	N-NITROSO-4-CHLOROPIPERIDINE														
			42	100	148	70	55	43	82	30	43	25	56	23	150	23
150	23	N-NITROSO-N-METHYL-D3-N'-NITROGUANIDINE														
			30	100	44	91	42	44	72	42	46	39	60	34	57	29
151	24	N-NITROSO-ETHYL N-ETHYL-D5-CARBAMATE														
			34	100	30	70	58	33	45	27	44	20	61	17	46	16
151	25	N-NITROSO-2-CHLOROETHYL UREA														
			56	100	42	96	41	21	116	17	57	11	40	9	44	7
152	26	N-NITROSO-BIS(2-CYANOETHYL)AMINE														
			30	100	40	94	54	85	42	76	43	42	81	39	52	15
158	27	N-NITROSO-BIS(2-OXOPROPYL)AMINE														
			43	100	86	78	42	55	85	11	84	10	30	10	58	8
158	28	N-NITROSODISECBUTYLAMINE														
			57	100	41	56	70	48	84	34	42	31	158	29	56	27
162	29	N-NITROSO-BIS(2-HYDROXYPROPYL)AMINE														
			45	100	44	88	42	85	43	73	70	56	88	48	41	38
162	30	N-NITROSO-BIS(2-METHOXYETHYL)AMINE														
			45	100	59	33	42	19	58	17	60	16	57	15	86	13
164	31	N-NITROSO-2,6-DICYANOPIPERIDINE														
			80	100	53	77	92	52	164	52	107	45	134	28	40	25
168	32	N-NITROSO-3,4-DICHLOROPYRROLIDINE														
			42	100	39	46	68	46	41	44	168	44	75	42	67	38
170	33	N-NITROSO-BIS(2-CHLOROETHYL)AMINE														
			42	100	121	68	63	60	90	42	123	24	91	21	35	19
170	34	N-NITROSO-4-TERTBUTYLPIPERIDINE														
			170	100	140	81	57	72	42	58	56	49	55	46	41	35
177	35	N-NITROSONORNICOTINE														
			105	100	118	66	177	60	147	47	78	44	51	33	104	33
179	36	N-NITROSO-1,1-DIMETHYL-3(2-CHLOROETHYL)UREA														
			72	100	44	41	42	23	30	12	56	11	45	11	115	10
180	37	N-NITROSO-METHYL N-PHENYLCARBAMATE														
			93	100	65	89	123	68	94	28	39	17	77	13	30	13

MW	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
182	38	N-NITROSO-3,4-DICHLOROPIPERIDINE														
			42	100	116	42	182	42	82	41	53	35	184	28	89	24
190	39	N-NITROSO-BIS(2-ETHOXYETHYL)AMINE														
			59	100	45	84	72	65	56	36	57	31	42	29	100	29
190	40	N-NITROSO-4-PHENYLPIPERIDINE														
			160	100	42	43	91	43	56	39	131	30	55	17	104	12
191	41	N-NITROSOMETHOMYL														
			59	100	74	62	104	58	58	50	47	46	88	41	42	40
195	42	N-NITROSO-2-BROMOETHYLUREA														
			42	100	30	95	56	75	31	23	116	16	41	11	87	9
198	43	N-NITROSO-BIS-(2-CHLOROPROPYL)AMINE														
			42	100	41	91	70	73	135	60	77	37	104	25	63	22
200	44	1,4-DINITROSO-2,3,5,6-TETRAMETHYLPIPERAZINE														
			97	100	70	98	44	89	41	71	140	71	42	56	56	31
207	45	N-NITROSO-1,1-DIETHYL-3(2-CHLOROETHYL)UREA														
			100	100	72	76	44	33	56	22	30	14	58	12	57	6
214	46	N-NITROSOMETHYLUNDECYLAMINE														
			197	100	43	80	44	71	73	49	74	49	184	36	42	34
219	47	N-NITROSOALDICARB														
			89	100	173	66	41	59	44	34	85	34	30	33	55	31
222	48	N-NITROSOLANDRIN														
			135	100	136	81	121	76	91	33	79	12	39	8	137	7
227	49	N-NITROSO-1-METHYL-3,3-BIS(2-CHLOROETHYL)UREA														
			63	100	168	71	56	68	42	64	170	46	30	40	65	33
238	50	N-NITROSOBAYGON														
			109	100	110	35	81	18	151	14	43	8	152	6	52	5
244	51	N-NITROSOATRAZINE														
			215	100	173	49	200	47	185	44	201	38	70	36	217	35
250	52	N-NITROSOBUXTEN														
			121	100	107	57	163	48	93	35	91	28	164	26	122	24
250	53	N-NITROSOCARBOFURAN														
			163	100	135	58	107	43	164	39	149	23	91	19	117	18
256	54	N-NITROSO-3,4-DIBROMOPYRROLIDINE														
			68	100	41	51	39	41	177	34	179	34	67	29	42	27
270	55	N-NITROSODIOCTYLAMINE														
			49	100	84	67	43	55	57	50	86	47	41	37	155	34
270	56	N-NITROSO-3,4-DIBROMOPIPERIDINE														
			82	100	55	36	191	34	193	33	38	29	53	28	80	21
275	57	N-NITROSO-1,1,3-TRIS(2-CHLOROETHYL)UREA														
			65	100	92	34	63	32	56	20	54	19	42	17	168	12
278	58	N-NITROSO-BIS(2,2-DIETHOXYETHYL)AMINE														
			103	100	75	62	47	58	61	21	89	18	233	10	44	7
312	59	N-NITROSOMETHYLOCTADECYLAMINE														
			295	100	296	24	282	21	44	16	43	14	57	9	73	8
326	60	N-NITROSODIDECYLAMINE														
			309	100	183	64	57	39	43	36	310	22	71	21	85	21
382	61	N-NITROSODIDODECYLAMINE														
			365	100	43	46	57	34	366	29	44	27	58	26	55	20

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	M/E	INT
30	15	N-NITROSO-2-HYDROXYETHYLUREA														
			30	100	42	70	57	38	41	7	117	7	89	7	58	5
30	20	N-NITROSONORBUTYLUREA														
			30	100	41	97	44	82	56	50	59	48	57	42	39	38
30	23	N-NITROSO-N-METHYL-D3-N'-NITROGUANIDINE														
			30	100	44	91	42	44	72	42	46	39	60	34	57	29
30	26	N-NITROSO-BIS(2-CYANOETHYL)AMINE														
			30	100	40	94	54	85	42	76	43	42	81	39	52	15
34	24	N-NITROSO-ETHYL N-ETHYL-D5-CARBAMATE														
			34	100	30	70	58	33	45	27	44	20	61	17	46	16
41	14	N-NITROSODIALLYLAMINE														
			41	100	39	39	42	23	109	18	54	10	68	9	81	8
42	12	N-NITROSOETHYL-2-HYDROXYETHYLAMINE														
			42	100	57	58	56	53	43	50	31	36	58	32	87	23
42	21	N-NITROSO-3-CHLOROPIPERIDINE														
			42	100	55	70	56	39	43	38	30	36	40	36	82	36
42	22	N-NITROSO-4-CHLOROPIPERIDINE														
			42	100	148	70	55	43	82	30	43	25	56	23	150	23
42	32	N-NITROSO-3,4-DICHLOROPYRROLIDINE														
			42	100	39	46	68	46	41	44	168	44	75	42	67	38
42	33	N-NITROSO-BIS(2-CHLOROETHYL)AMINE														
			42	100	121	68	63	60	90	42	123	24	91	21	35	19
42	38	N-NITROSO-3,4-DICHLOROPIPERIDINE														
			42	100	116	42	182	42	82	41	53	35	184	28	89	24
42	42	N-NITROSO-2-BROMOETHYLUREA														
			42	100	30	95	56	75	31	23	116	16	41	11	87	9
42	43	N-NITROSO-BIS-(2-CHLOROPROPYL)AMINE														
			42	100	41	91	70	73	135	60	77	37	104	25	63	22
43	27	N-NITROSO-BIS(2-OXOPROPYL)AMINE														
			43	100	86	78	42	55	85	11	84	10	30	10	58	8
43	16	N-NITROSO-BIS(2-HYDROXYETHYL)AMINE														
			43	100	42	46	74	29	55	27	56	25	87	25	72	24
44	17	N-NITROSO-2-FLUOROETHYLUREA														
			44	100	92	71	59	47	47	35	102	29	93	28	46	26
45	10	N-NITROSOMETHYL-D3-ETHYLAMINE														
			45	100	91	92	46	78	33	24	30	21	43	21	59	20
45	29	N-NITROSO-BIS(2-HYDROXYPROPYL)AMINE														
			45	100	44	88	42	85	43	73	70	56	88	48	41	38
45	30	N-NITROSO-BIS(2-METHOXYETHYL)AMINE														
			45	100	59	33	42	19	58	17	60	16	57	15	86	13
49	55	N-NITROSODIOCTYLAMINE														
			49	100	84	67	43	55	57	50	86	47	41	37	155	34
50	11	N-NITROSODIETHYL-D10-AMINE														
			50	100	112	88	62	77	44	67	70	60	64	52	71	46
55	19	N-NITROSO-3,5-DIMETHYLPIPERIDINE														
			55	100	42	95	41	74	142	66	39	33	83	29	56	26
56	25	N-NITROSO-2-CHLOROETHYL UREA														
			56	100	42	96	41	21	116	17	57	11	40	9	44	7
57	28	N-NITROSODISECBUTYLAMINE														
			57	100	41	56	70	48	84	34	42	31	158	29	56	27
59	39	N-NITROSO-BIS(2-ETHOXYETHYL)AMINE														
			59	100	45	84	72	65	56	36	57	31	42	29	100	29
59	41	N-NITROSOMETHOMYL														
			59	100	74	62	104	58	58	50	47	46	88	41	42	40
61	18	N-NITROSO-ETHYL N-METHYL-D3-CARBAMATE														
			61	100	78	34	46	24	45	22	76	16	60	14	63	14

BASE	PAGE		M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
63	49	N-NITROSO-1-METHYL-3,3-BIS(2-CHLOROETHYL)UREA														
			63	100	168	71	56	68	42	64	170	46	30	40	65	33
65	57	N-NITROSO-1,1,3-TRIS(2-CHLOROETHYL)UREA														
			65	100	92	34	63	32	56	20	54	19	42	17	168	12
68	54	N-NITROSO-3,4-DIBROMOPYRROLIDINE														
			68	100	41	51	39	41	177	34	179	34	67	29	42	27
72	36	N-NITROSO-1,1-DIMETHYL-3(2-CHLOROETHYL)UREA														
			72	100	44	41	42	23	30	12	56	11	45	11	115	10
80	31	N-NITROSO-2,6-DICYANOPIPERIDINE														
			80	100	53	77	92	52	164	52	107	45	134	28	40	25
82	56	N-NITROSO-3,4-DIBROMOPIPERIDINE														
			82	100	55	36	191	34	193	33	38	29	53	28	80	21
89	47	N-NITROSOALDICARB														
			89	100	173	66	41	59	44	34	85	34	30	33	55	31
93	37	N-NITROSO-METHYL N-PHENYLCARBAMATE														
			93	100	65	89	123	68	94	28	39	17	77	13	30	13
97	44	1,4-DINITROSO-2,3,5,6-TETRAMETHYLPIPERAZINE														
			97	100	70	98	44	89	41	71	140	71	42	56	56	31
100	45	N-NITROSO-1,1-DIETHYL-3(2-CHLOROETHYL)UREA														
			100	100	72	76	44	33	56	22	30	14	58	12	57	6
103	58	N-NITROSO-BIS(2,2-DIETHOXYETHYL)AMINE														
			103	100	75	62	47	58	51	21	89	18	233	10	44	7
105	35	N-NITROSONORNICOTINE														
			105	100	118	66	177	60	147	47	78	44	51	33	104	33
109	50	N-NITROSOBAYGON														
			109	100	110	35	81	18	151	14	43	8	152	6	52	5
121	52	N-NITROSOBUXTEN														
			121	100	107	57	163	48	93	35	91	28	164	26	122	24
124	13	N-NITROSO-BIS(CYANOMETHYL)AMINE														
			124	100	40	75	67	33	41	21	39	10	53	7	38	7
135	48	N-NITROSOLANDRIN														
			135	100	136	81	121	76	91	33	79	12	39	8	137	7
160	40	N-NITROSO-4-PHENYLPIPERIDINE														
			160	100	42	43	91	43	56	39	131	30	55	17	104	12
163	53	N-NITROSOCARBOFURAN														
			163	100	135	58	107	43	164	39	149	23	91	19	117	18
170	34	N-NITROSO-4-TERTBUTYLPIPERIDINE														
			170	100	140	81	57	72	42	58	56	49	55	46	41	35
197	46	N-NITROSOMETHYLUNDECYLAMINE														
			197	100	43	80	44	71	73	49	74	49	184	36	42	34
215	51	N-NITROSOATRAZINE														
			215	100	173	49	200	47	185	44	201	38	70	36	217	35
295	59	N-NITROSOMETHYLOCTADECYLAMINE														
			295	100	296	24	282	21	44	16	43	14	57	9	73	8
309	60	N-NITROSODIDECYLAMINE														
			309	100	183	64	57	39	43	36	310	22	71	21	85	21
365	61	N-NITROSODIDODECYLAMINE														
			365	100	43	46	57	34	366	29	44	27	58	26	55	20

3.1 PREPARATION OF COMPOUNDS

Many of the N-nitroso compounds were prepared by reaction of the secondary or tertiary 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*.

Many of the polyfunctional or substituted nitrosamines were prepared by rather specific techniques, depending upon the available starting materials. These procedures have been and will be published in papers describing the results of carcinogenicity testing of each compound.

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.

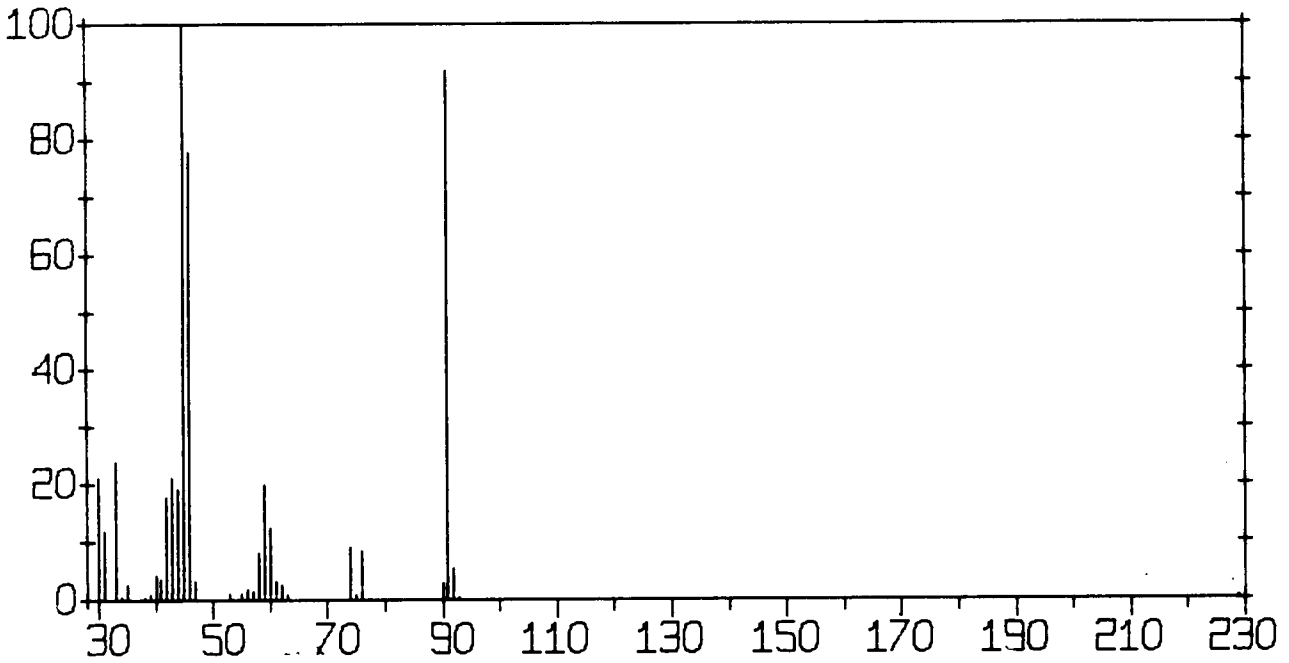
3.2 MASS SPECTROMETRY

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.

4.0 MASS SPECTRA

N-NITROSOMETHYL-D3-ETHYLAMINE
MW = 91 C3.H5.D3.N2.O

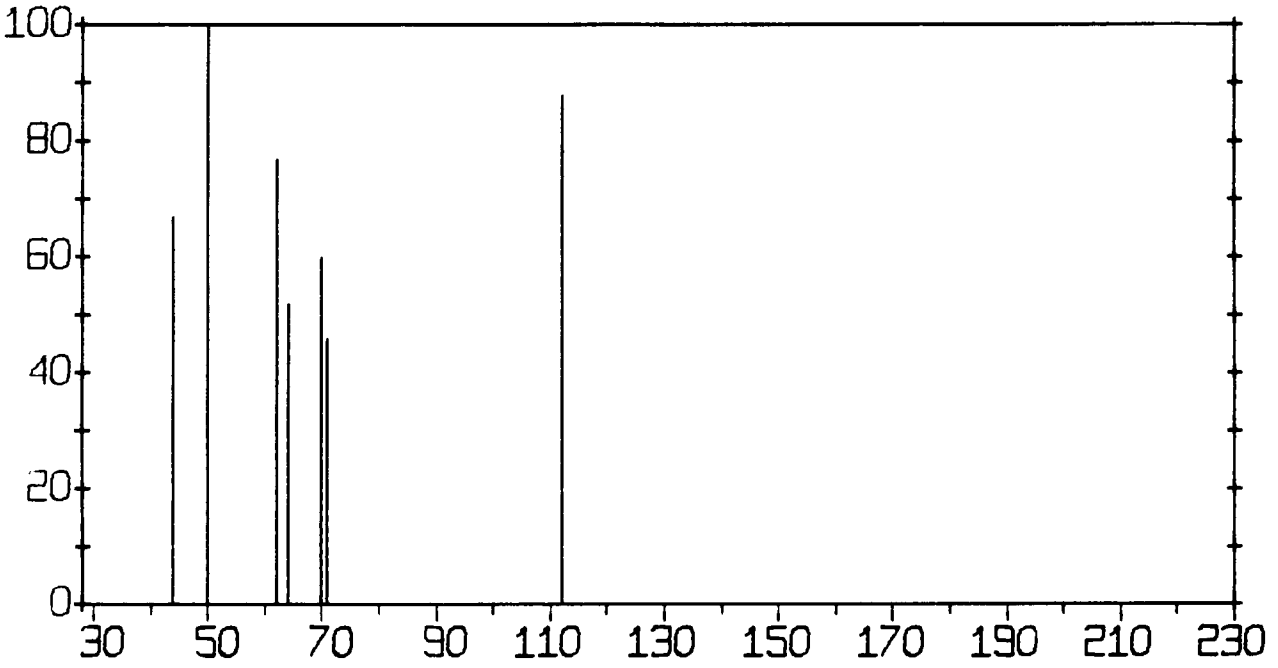
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	21.2	40.0	4.2	47.0	3.3	60.0	12.4	76.0	8.6
31.0	12.0	41.0	3.6	53.0	1.0	61.0	3.2	77.0	0.2
33.0	24.0	42.0	18.0	55.0	1.0	62.0	2.6	90.0	3.0
34.0	0.5	43.0	21.2	56.0	2.0	63.0	0.6	91.0	92.0
35.0	2.6	44.0	19.2	57.0	1.6	74.0	9.2	92.0	5.5
38.0	0.6	45.0	100.0	58.0	8.2	75.0	0.6	93.0	0.6
39.0	0.6	46.0	78.0	59.0	20.0				



N-NITROSODIETHYL-D10-AMINE
MW = 112 C4.D10.N2.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
44.0	67.0	62.0	77.0	70.0	60.0	71.0	46.0	112.0	88.0
50.0	100.0	64.0	52.0						

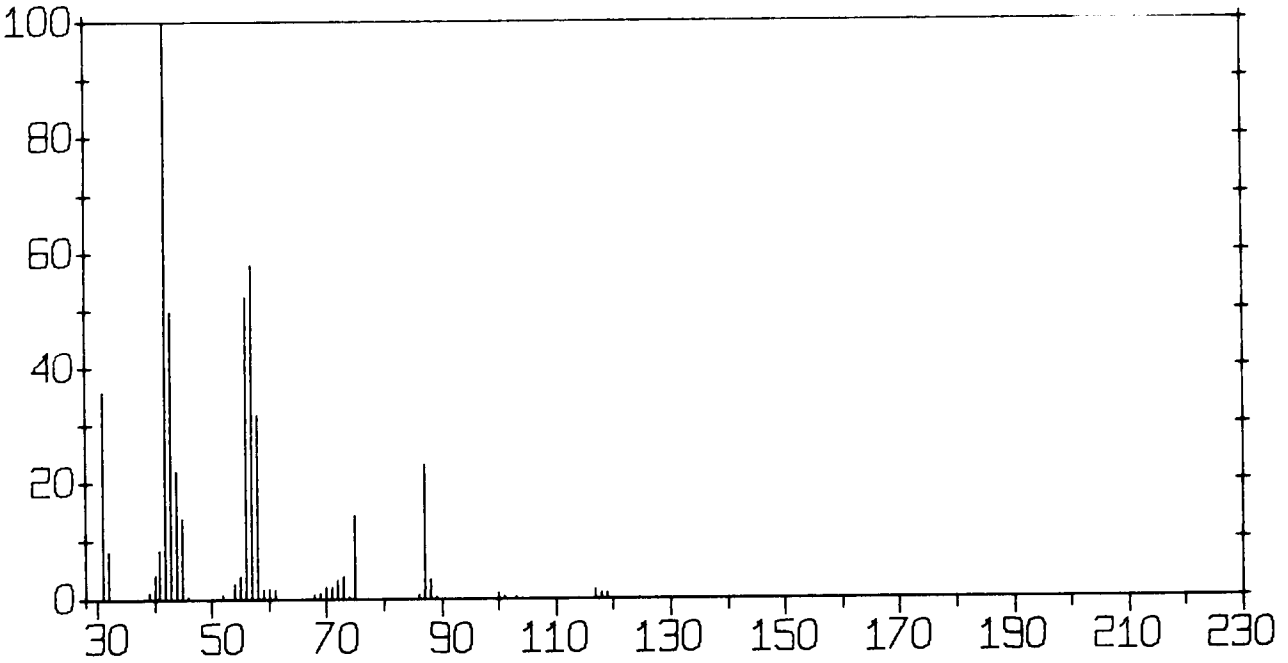
MAJOR PEAKS ONLY



N-NITROSOETHYL-2-HYDROXYETHYLAMINE
MW = 118 C4.H10.N2.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
31.0	36.1	45.0	13.8	59.0	1.6	72.0	3.6	89.0	0.6
32.0	8.3	46.0	0.5	60.0	1.9	73.0	3.8	100.0	1.0
39.0	1.3	52.0	0.7	61.0	1.6	74.0	0.5	101.0	0.4
40.0	4.1	54.0	2.7	68.0	0.6	75.0	14.4	103.0	0.3
41.0	8.6	55.0	3.8	69.0	0.8	86.0	0.7	117.0	1.8
42.0	100.0	56.0	52.7	70.0	2.3	87.0	23.3	118.0	1.1
43.0	50.0	57.0	58.3	71.0	2.2	88.0	3.4	119.0	0.8
44.0	22.2	58.0	31.9						

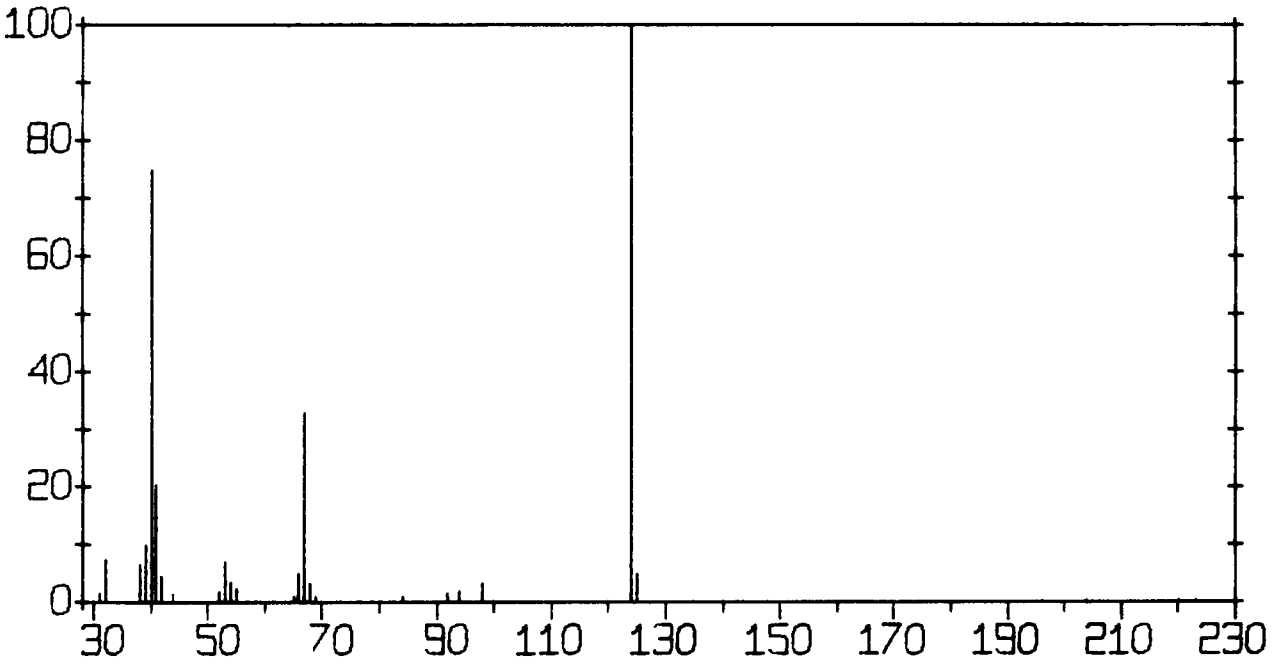
OBSERVED METASTABLES
36.0,



N-NITROSO-BIS(CYANOMETHYL)AMINE
MW = 124 C4.H4.N4.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
31.0	1.5	41.0	20.5	54.0	3.5	68.0	3.2	94.0	2.0
32.0	7.5	42.0	4.5	55.0	2.2	69.0	0.7	98.0	3.2
38.0	6.5	44.0	1.2	65.0	0.7	84.0	0.7	124.0	100.0
39.0	10.0	52.0	1.7	66.0	5.0	92.0	1.4	125.0	5.0
40.0	75.0	53.0	7.0	67.0	33.0				

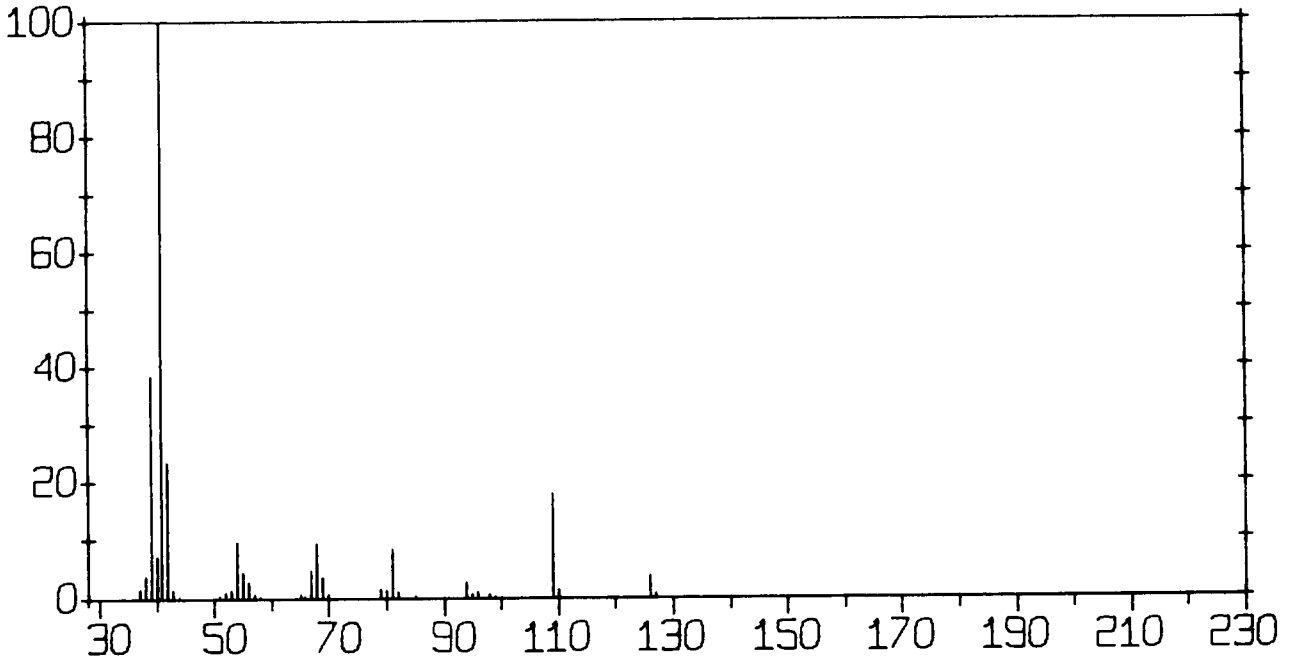
OBSERVED METASTABLES
29.9,



N-NITROSODIALLYLAMINE
MW = 126 C6.H10.N2.O

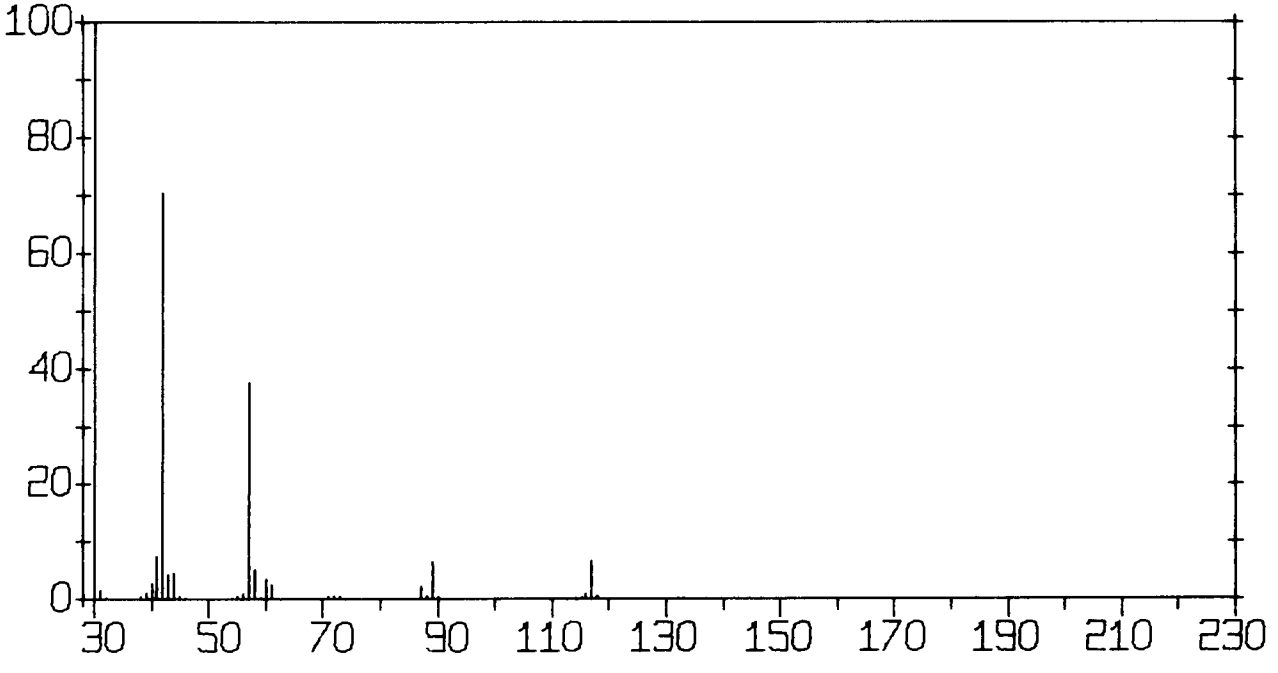
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
37.0	1.6	51.0	0.5	58.0	0.5	79.0	1.6	96.0	1.1
38.0	3.9	52.0	1.0	65.0	0.6	80.0	1.4	98.0	0.6
39.0	38.5	53.0	1.4	66.0	0.4	81.0	8.4	99.0	0.5
40.0	7.2	54.0	9.6	67.0	4.9	82.0	1.2	109.0	18.0
41.0	100.0	55.0	4.5	68.0	9.3	85.0	0.5	110.0	1.3
42.0	23.4	56.0	3.0	69.0	3.8	94.0	2.7	126.0	4.0
43.0	1.5	57.0	0.8	70.0	0.6	95.0	0.7	127.0	0.6
44.0	0.5								

OBSERVED METASTABLES
60.2, 94.3,



N-NITROSO-2-HYDROXYETHYLUREA
MW = 133 C3.H7.N3.O3

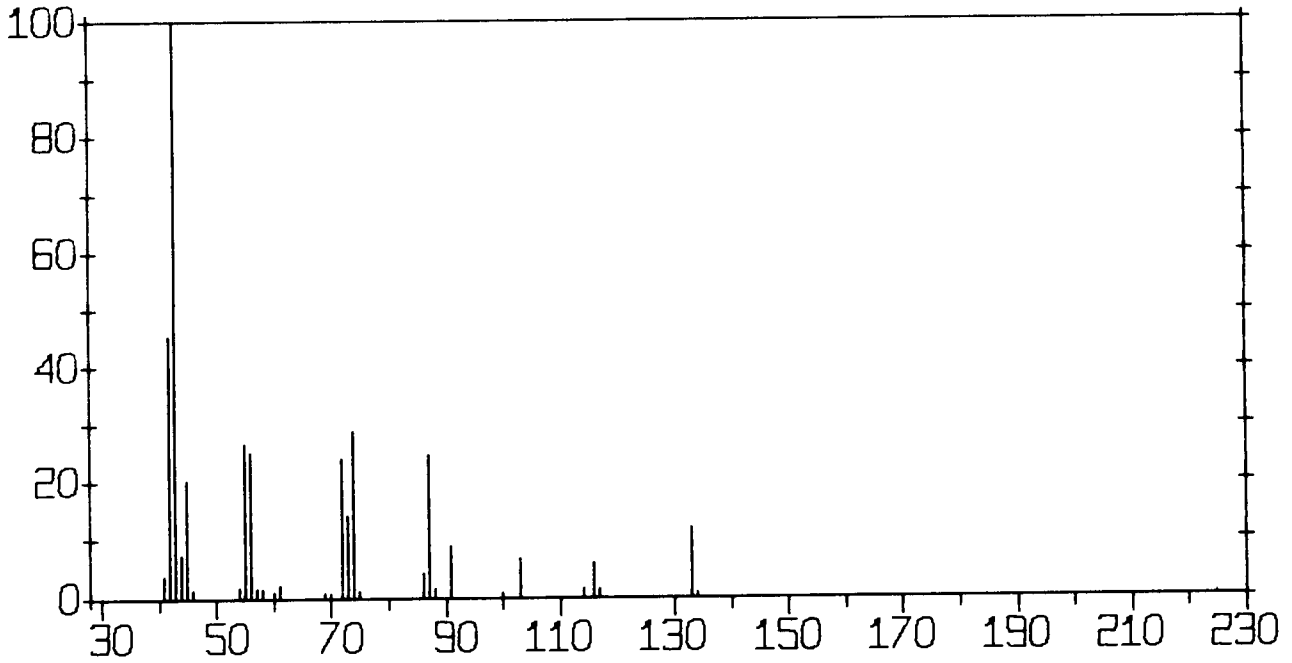
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	42.0	70.4	56.0	0.7	72.0	0.4	115.0	0.3
31.0	1.4	43.0	4.1	57.0	37.7	73.0	0.5	116.0	0.7
32.0	0.2	44.0	4.5	58.0	5.2	87.0	2.2	117.0	6.8
38.0	0.5	45.0	0.4	59.0	0.3	88.0	0.5	118.0	0.4
39.0	0.9	46.0	0.3	60.0	3.5	89.0	6.5	132.0	0.2
40.0	2.7	54.0	0.1	61.0	2.5	90.0	0.5	133.0	0.3
41.0	7.4	55.0	0.4	71.0	0.5	114.0	0.1		



N-NITROSO-BIS(2-HYDROXYETHYL)AMINE
MW = 134 C4.H10.N2.O3

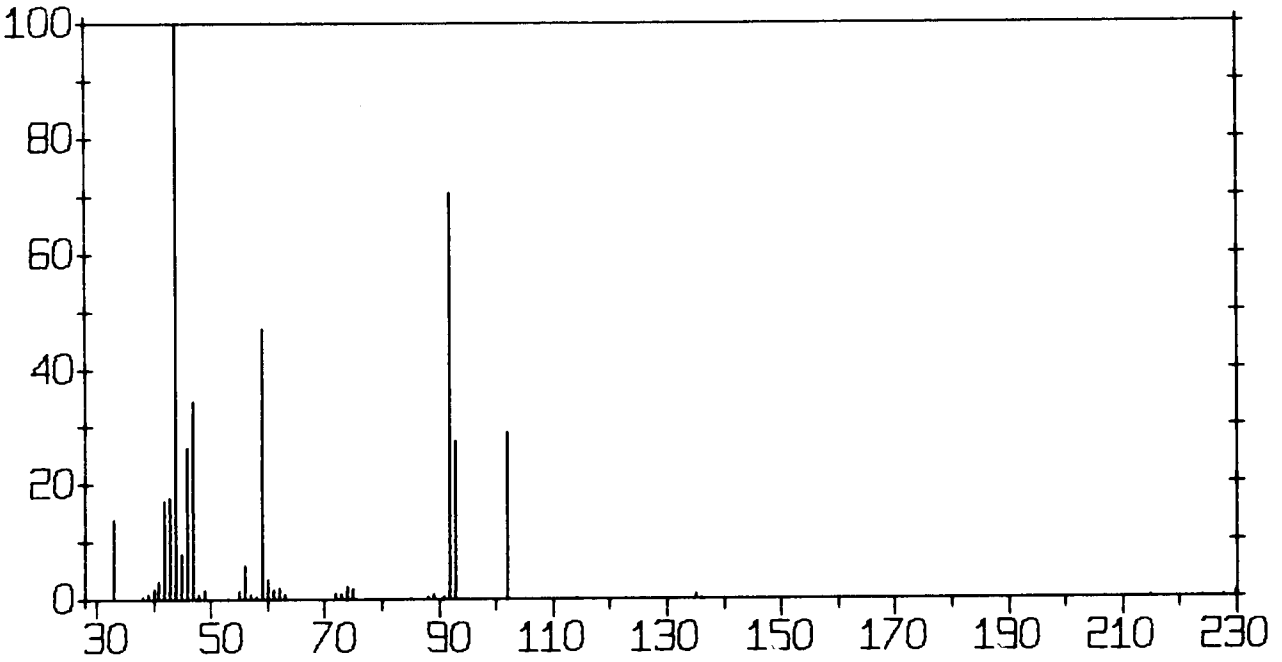
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
41.0	4.1	54.0	2.0	61.0	2.1	75.0	1.1	103.0	6.7
42.0	45.5	55.0	26.8	69.0	0.6	86.0	4.3	114.0	1.8
43.0	100.0	56.0	25.3	70.0	0.6	87.0	24.6	116.0	5.9
44.0	7.4	57.0	1.8	72.0	24.2	88.0	1.8	117.0	1.4
45.0	20.5	58.0	1.7	73.0	14.1	91.0	8.9	133.0	11.9
46.0	1.4	60.0	1.1	74.0	29.1	100.0	0.7	134.0	0.6

OBSERVED METASTABLES
65.3,



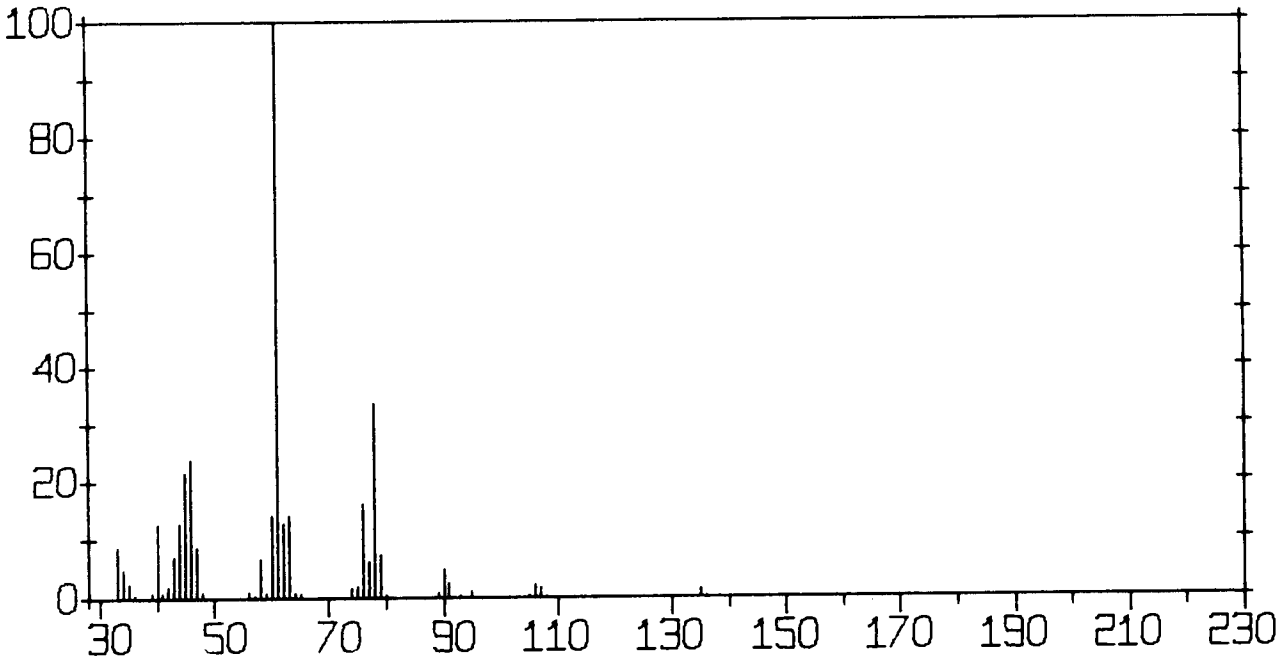
N-NITROSO-2-FLUOROETHYLUREA
MW = 135 C3.H6.N3.O2.F

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
33.0	13.8	45.0	8.0	57.0	0.6	72.0	0.8	91.0	0.3
38.0	0.4	46.0	26.3	58.0	0.5	73.0	0.7	92.0	70.8
39.0	0.6	47.0	34.7	59.0	47.2	74.0	2.2	93.0	27.7
40.0	2.0	48.0	0.8	60.0	3.7	75.0	1.9	102.0	29.1
41.0	3.1	49.0	1.6	61.0	1.8	85.0	0.2	114.0	0.1
42.0	17.2	53.0	0.3	62.0	2.0	88.0	0.3	135.0	0.6
43.0	17.7	55.0	1.5	63.0	0.8	89.0	0.6	136.0	0.3
44.0	100.0	56.0	5.9						



N-NITROSO-ETHYL N-METHYL-D3-CARBAMATE
MW = 135 C4.H5.D3.N2.O3

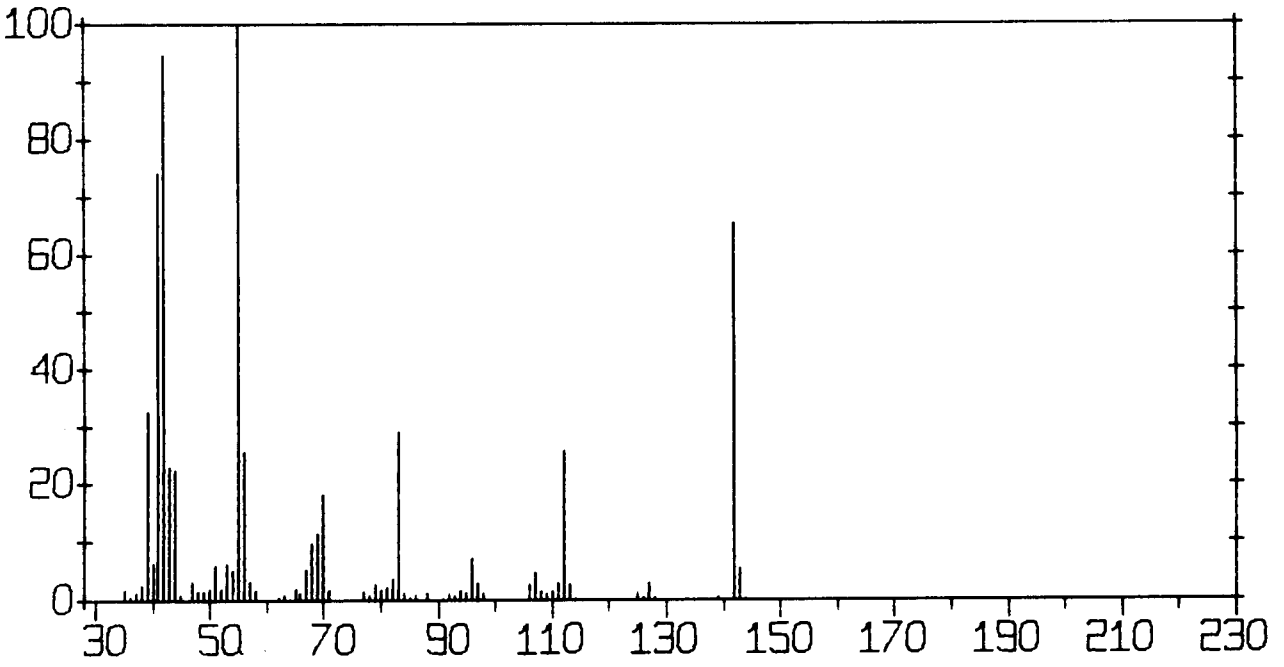
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
33.0	8.6	44.0	13.0	60.0	14.1	76.0	16.3	93.0	0.4
34.0	5.1	45.0	21.7	61.0	100.0	77.0	6.3	95.0	1.1
35.0	2.6	46.0	23.9	62.0	13.0	78.0	33.6	105.0	0.5
36.0	0.5	47.0	8.6	63.0	14.1	79.0	7.5	106.0	2.1
39.0	0.6	48.0	0.9	64.0	0.6	80.0	0.4	107.0	1.6
40.0	13.0	56.0	0.9	65.0	0.8	89.0	0.7	108.0	0.3
41.0	0.8	57.0	0.5	74.0	1.8	90.0	5.0	135.0	1.5
42.0	1.9	58.0	6.7	75.0	1.9	91.0	2.3	136.0	0.2
43.0	7.2	59.0	0.7						



N-NITROSO-3,5-DIMETHYLPIPERIDINE
MW = 142 C7.H14.N2.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
35.0	1.8	50.0	1.9	67.0	5.5	86.0	0.7	110.0	1.4
36.0	0.4	51.0	6.0	68.0	9.6	88.0	1.1	111.0	2.9
37.0	1.2	52.0	2.0	69.0	11.3	91.0	0.3	112.0	25.8
38.0	2.5	53.0	6.2	70.0	18.2	92.0	1.3	113.0	2.7
39.0	32.7	54.0	5.1	71.0	1.7	93.0	0.7	114.0	0.3
40.0	6.2	55.0	100.0	77.0	1.5	94.0	1.7	125.0	1.2
41.0	74.1	56.0	25.8	78.0	0.6	95.0	1.3	126.0	0.5
42.0	94.8	57.0	3.2	79.0	2.7	96.0	7.2	127.0	3.1
43.0	23.1	58.0	1.7	80.0	2.0	97.0	3.1	128.0	0.5
44.0	22.4	62.0	0.4	81.0	2.2	98.0	1.3	139.0	0.3
45.0	0.8	63.0	0.8	82.0	3.7	106.0	2.7	142.0	65.5
47.0	3.2	64.0	0.3	83.0	29.3	107.0	4.8	143.0	5.5
48.0	1.6	65.0	1.8	84.0	1.1	108.0	1.3	144.0	0.3
49.0	1.3	66.0	1.0	85.0	0.4	109.0	0.8		

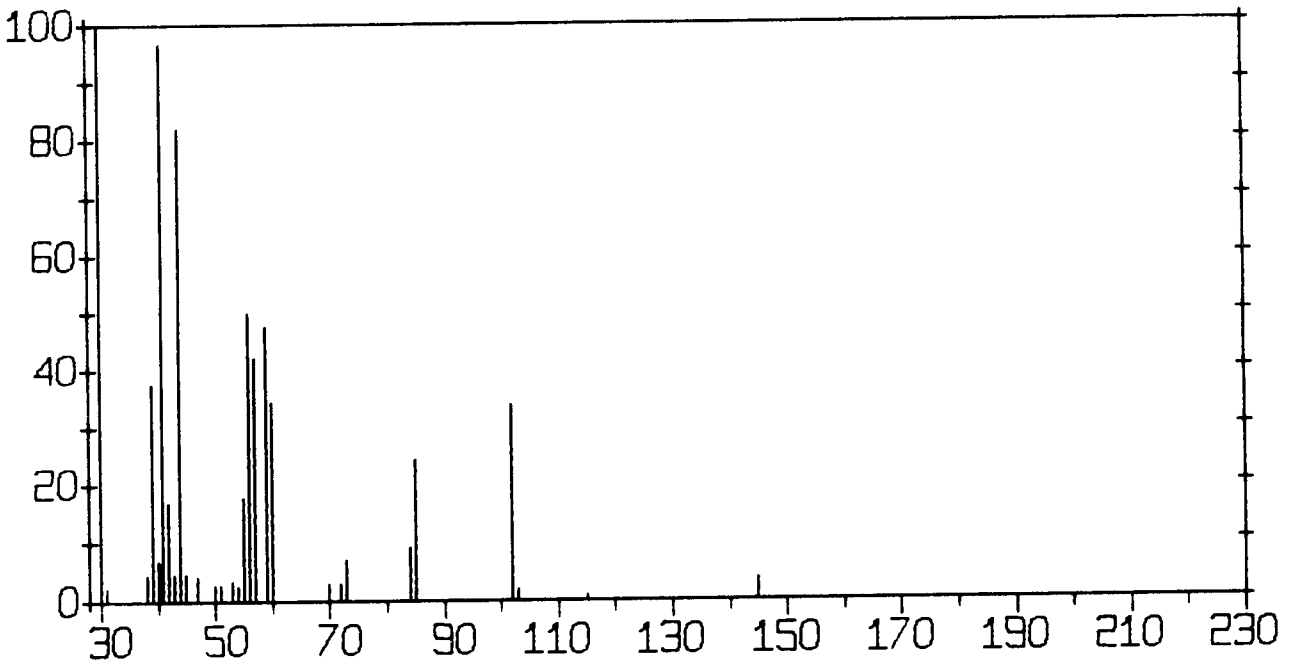
OBSERVED METASTABLES
36.5, 61.5,



N-NITROSONORBUTYLUREA
MW = 145 C5.H11.N3.O2

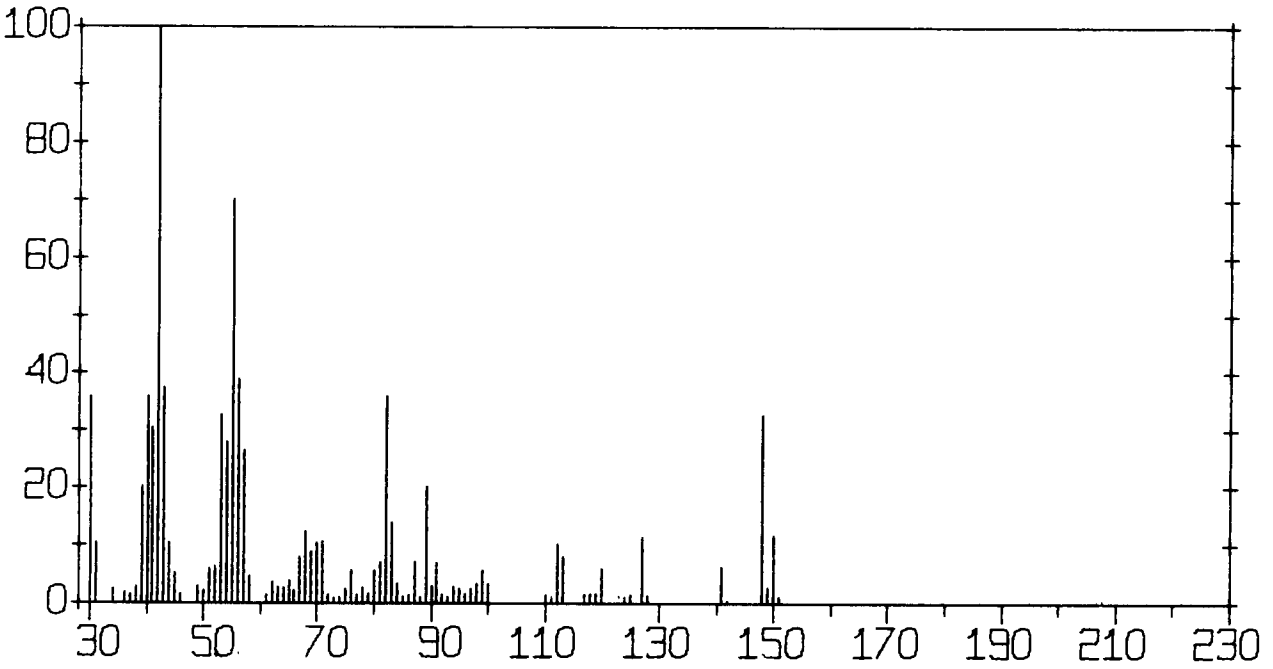
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	42.0	16.8	51.0	2.6	59.0	47.7	85.0	24.4
31.0	2.3	43.0	4.6	53.0	3.4	60.0	34.4	102.0	33.8
38.0	4.4	44.0	82.2	54.0	2.5	70.0	2.8	103.0	1.8
39.0	37.7	45.0	4.6	55.0	17.7	72.0	3.1	115.0	0.6
40.0	6.8	47.0	4.2	56.0	50.0	73.0	7.2	145.0	3.7
41.0	96.6	50.0	2.6	57.0	42.2	84.0	9.2	146.0	0.3

OBSERVED METASTABLES
29.4, 34.3, 40.7, 70.8, 91.0,



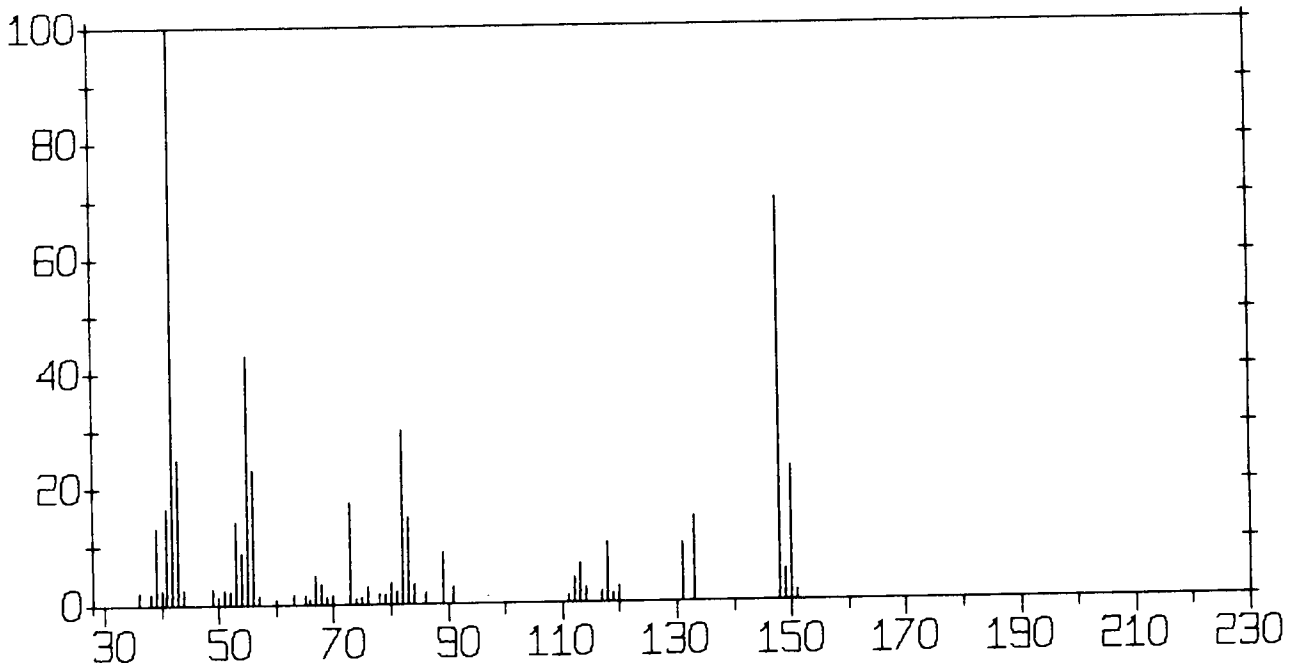
N-NITROSO-3-CHLOROPIPERIDINE
MW = 148 C5.H9.N2.O.CL

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	35.9	52.0	6.2	71.0	10.7	88.0	0.9	113.0	8.1
31.0	10.6	53.0	32.8	72.0	1.5	89.0	20.3	117.0	1.4
34.0	2.5	54.0	28.1	73.0	1.0	90.0	3.1	118.0	1.8
36.0	2.0	55.0	70.3	74.0	1.0	91.0	7.0	119.0	1.7
37.0	1.4	56.0	39.0	75.0	2.5	92.0	1.5	120.0	6.0
38.0	3.1	57.0	26.5	76.0	5.7	93.0	0.9	123.0	1.0
39.0	20.3	58.0	4.8	77.0	1.5	94.0	3.1	124.0	0.9
40.0	35.9	61.0	1.4	78.0	2.6	95.0	2.5	125.0	1.4
41.0	30.4	62.0	3.7	79.0	1.8	96.0	1.8	127.0	11.4
42.0	100.0	63.0	2.6	80.0	5.7	97.0	2.5	128.0	1.2
43.0	37.5	64.0	2.6	81.0	7.3	98.0	3.4	141.0	6.2
44.0	10.4	65.0	3.9	82.0	35.9	99.0	5.7	142.0	0.6
45.0	5.3	66.0	2.3	83.0	14.0	100.0	3.5	148.0	32.8
46.0	1.8	67.0	7.9	84.0	3.4	110.0	1.5	149.0	2.6
49.0	3.1	68.0	12.5	85.0	0.9	111.0	1.2	150.0	11.7
50.0	2.1	69.0	9.0	86.0	1.5	112.0	10.3	151.0	0.9
51.0	5.9	70.0	10.6	87.0	7.3				



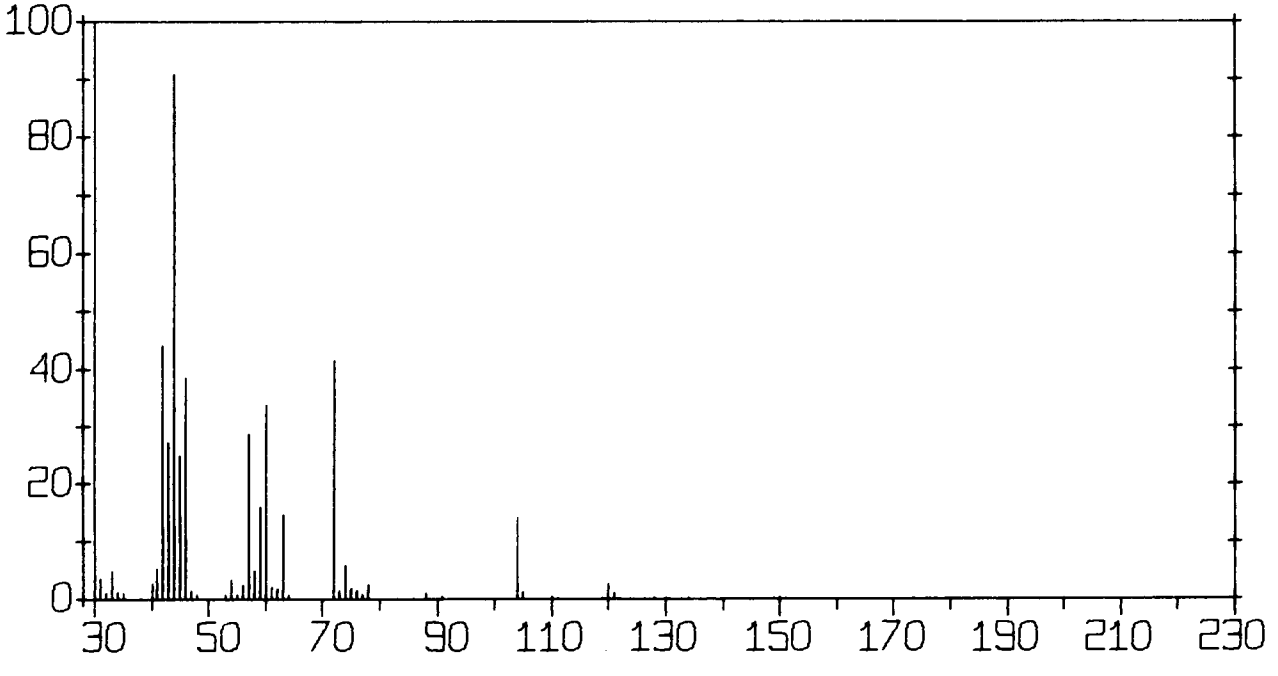
N-NITROSO-4-CHLOROPIPERIDINE
MW = 148 C5.H9.N2.O.CL

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
36.0	2.3	52.0	2.1	68.0	3.5	82.0	30.0	117.0	2.0
38.0	2.0	53.0	14.1	69.0	1.1	83.0	15.0	118.0	10.1
39.0	13.3	54.0	8.6	70.0	1.5	84.0	3.5	119.0	1.5
40.0	2.5	55.0	43.3	73.0	17.5	86.0	2.0	120.0	2.8
41.0	16.6	56.0	23.3	74.0	0.8	89.0	8.6	131.0	10.0
42.0	100.0	57.0	1.5	75.0	1.1	91.0	3.0	133.0	14.6
43.0	25.0	60.0	0.8	76.0	3.0	97.0	1.0	148.0	70.0
44.0	2.5	63.0	1.6	78.0	1.6	111.0	1.1	149.0	5.5
49.0	2.8	65.0	1.5	79.0	1.6	112.0	4.3	150.0	23.3
50.0	1.1	66.0	0.8	80.0	3.8	113.0	6.8	151.0	1.6
51.0	2.5	67.0	5.0	81.0	2.3	114.0	2.5		



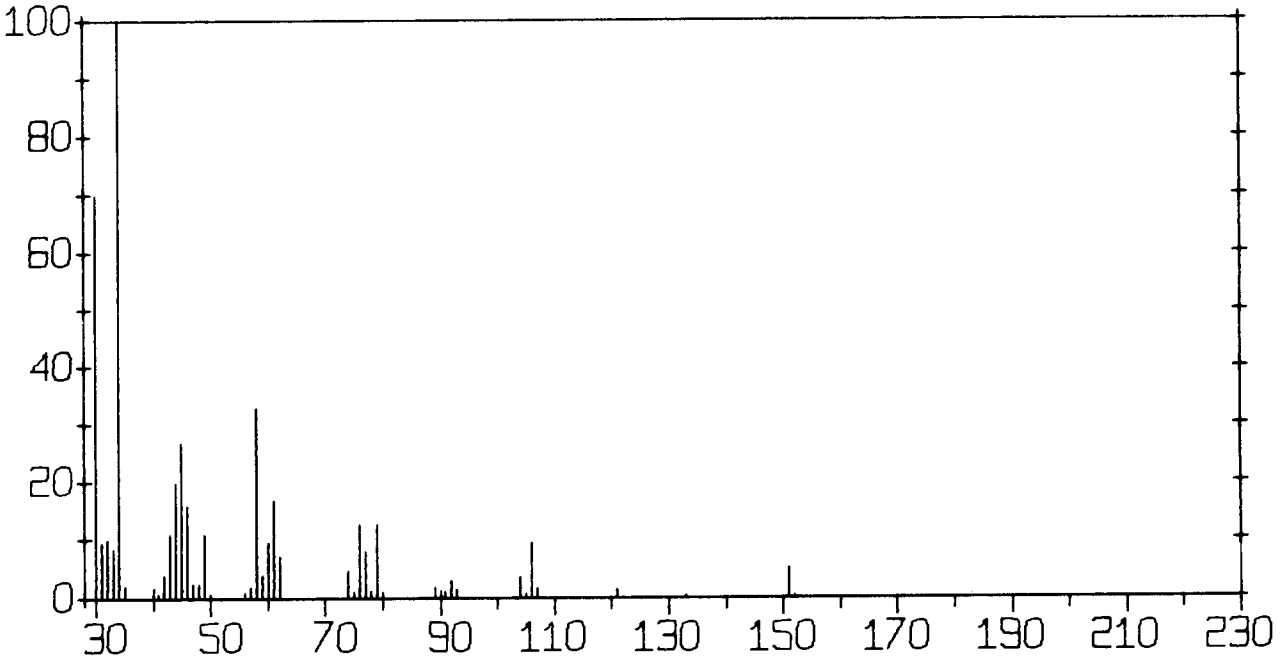
N-NITROSO-N-METHYL-D3-N'-NITROGUANIDINE
MW = 150 C2.H2.D3.N5.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	44.0	90.9	58.0	5.0	75.0	2.0	119.0	0.1
31.0	3.8	45.0	25.0	59.0	15.9	76.0	1.5	120.0	2.8
32.0	0.9	46.0	38.6	60.0	34.0	77.0	0.7	121.0	1.0
33.0	5.0	47.0	1.5	61.0	2.2	78.0	2.5	122.0	0.2
34.0	1.1	48.0	0.7	62.0	1.9	88.0	1.1	128.0	0.1
35.0	0.9	53.0	0.7	63.0	14.7	91.0	0.5	130.0	0.1
40.0	2.8	54.0	3.4	64.0	0.8	104.0	14.3	134.0	0.1
41.0	5.4	55.0	0.8	72.0	41.8	105.0	1.3	149.0	0.1
42.0	44.3	56.0	2.3	73.0	1.5	110.0	0.6	150.0	0.4
43.0	27.2	57.0	28.6	74.0	5.9	111.0	0.1	151.0	0.2



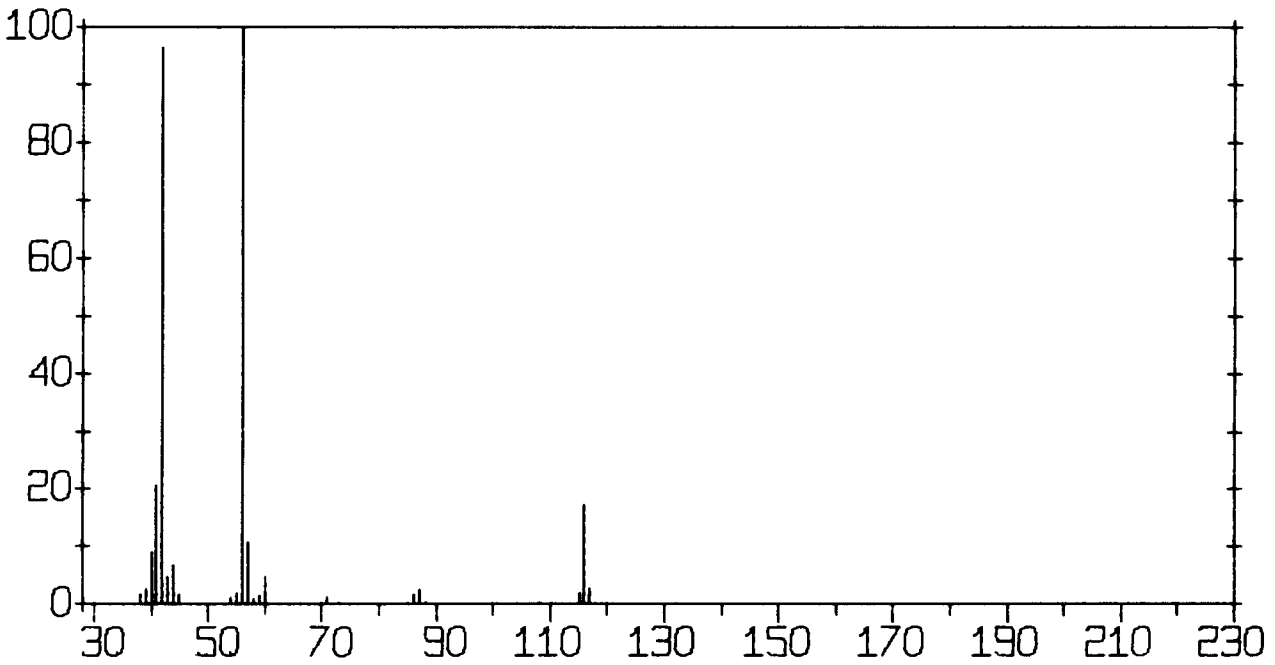
N-NITROSO-ETHYL N-ETHYL-D5-CARBAMATE
MW = 151 C5.H5.D5.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	70.0	43.0	11.0	57.0	2.1	77.0	8.0	104.0	3.8
31.0	9.5	44.0	20.0	58.0	33.0	78.0	1.3	105.0	0.8
32.0	10.0	45.0	27.0	59.0	3.9	79.0	12.8	106.0	9.5
33.0	8.5	46.0	16.0	60.0	9.5	80.0	1.0	107.0	1.8
34.0	100.0	47.0	2.5	61.0	17.0	89.0	2.0	121.0	1.6
35.0	2.2	48.0	2.4	62.0	7.3	90.0	1.4	122.0	0.3
40.0	2.1	49.0	11.0	74.0	4.8	91.0	1.0	133.0	0.6
41.0	0.8	50.0	0.7	75.0	0.9	92.0	3.1	151.0	5.3
42.0	4.1	56.0	1.1	76.0	12.8	93.0	1.6	152.0	0.4



N-NITROSO-2-CHLOROETHYL UREA
MW = 151 C3.H6.N3.O2.CL

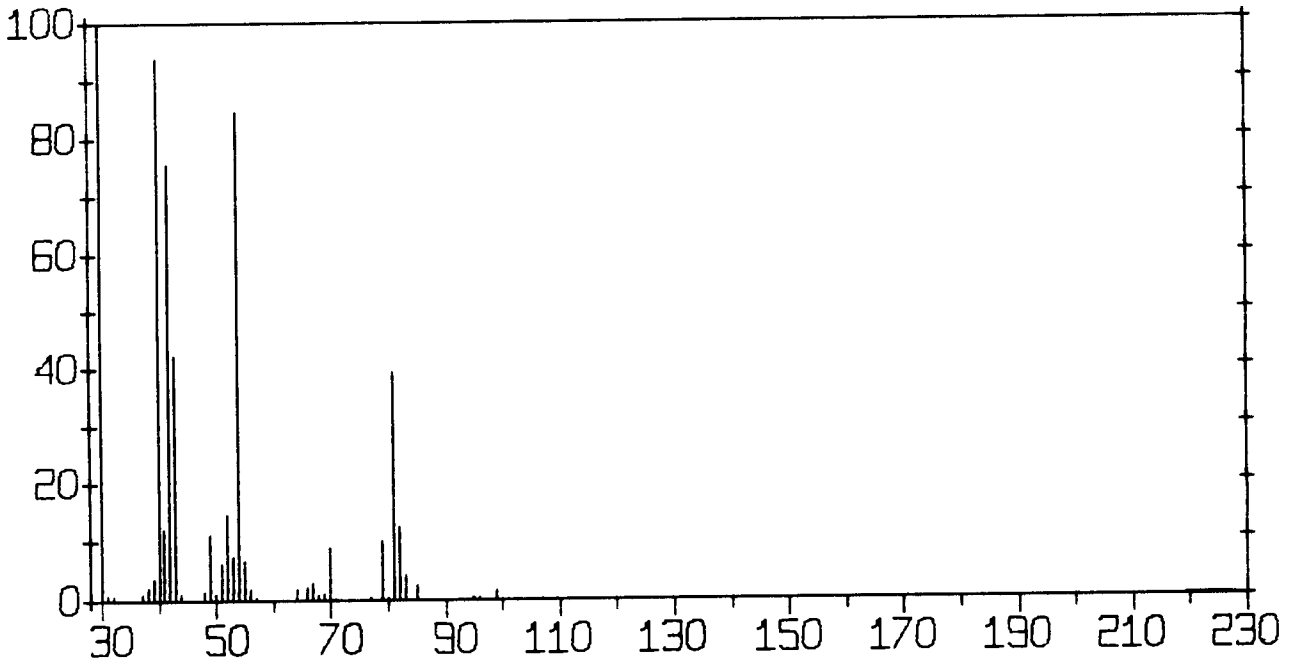
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
38.0	1.7	44.0	6.7	58.0	0.6	73.0	0.2	10.0	0.2
39.0	2.6	45.0	1.6	59.0	1.4	85.0	0.2	108.0	0.3
40.0	8.9	54.0	1.0	60.0	4.6	86.0	1.7	115.0	1.8
41.0	20.7	55.0	2.1	70.0	0.3	87.0	2.5	116.0	17.1
42.0	96.4	56.0	100.0	71.0	1.1	88.0	0.2	117.0	2.8
43.0	4.6	57.0	10.7						



N-NITROSO-BIS(2-CYANOETHYL)AMINE
MW = 152 C6.H8.N4.O

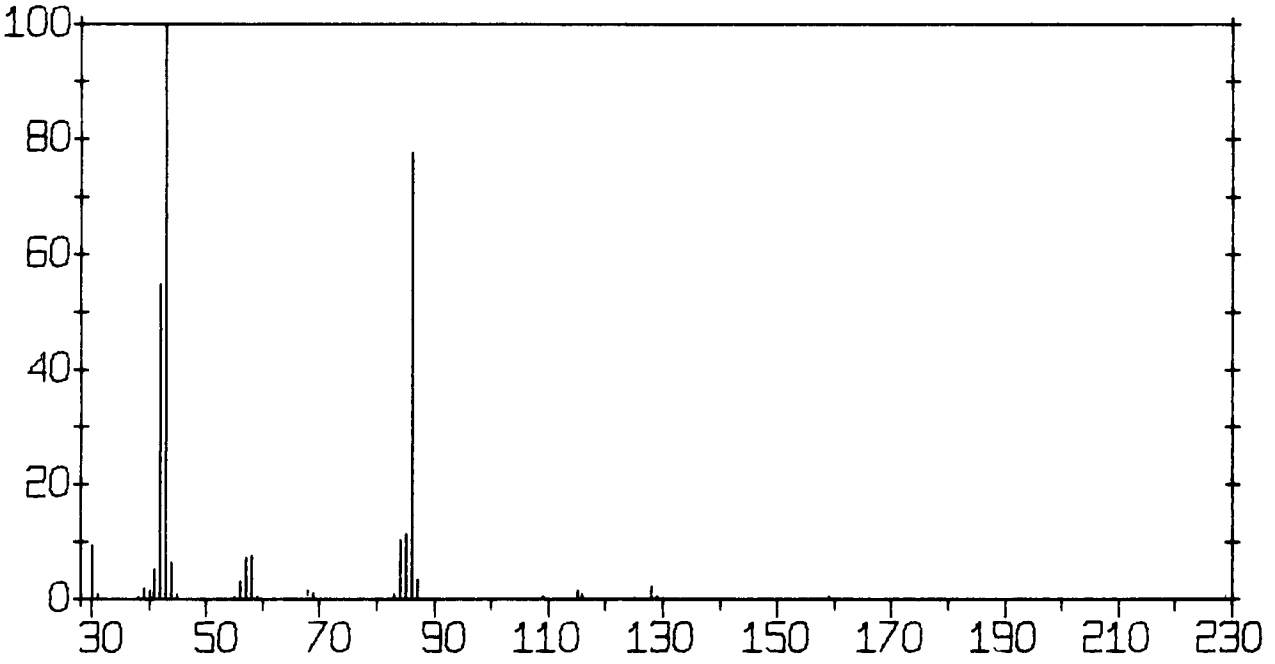
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	100.0	42.0	75.7	52.0	14.8	67.0	3.0	81.0	39.3
31.0	0.7	43.0	42.4	53.0	7.5	68.0	0.7	82.0	12.4
32.0	0.7	44.0	1.0	54.0	84.8	69.0	0.8	83.0	4.2
37.0	0.9	47.0	1.0	55.0	6.6	70.0	8.8	85.0	2.5
38.0	2.2	48.0	1.6	56.0	1.9	71.0	0.3	95.0	0.6
39.0	3.7	49.0	11.2	57.0	0.5	77.0	0.4	96.0	0.4
40.0	93.9	50.0	0.9	64.0	1.9	79.0	10.0	99.0	1.7
41.0	12.1	51.0	6.3	66.0	2.2	80.0	0.4	107.0	0.3

OBSERVED METASTABLES
58.6, 82.5,



N-NITROSO-BIS(2-OXOPROPYL)AMINE
MW = 158 C6.H10.N2.O3

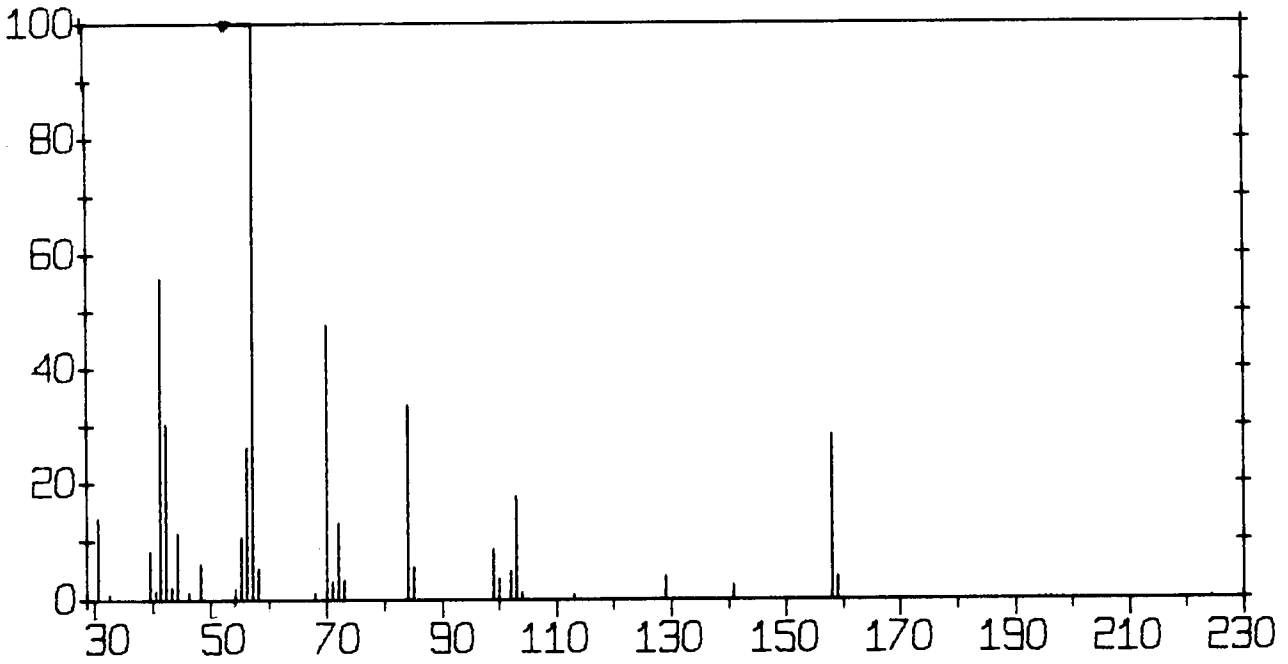
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	9.5	43.0	100.0	59.0	0.3	86.0	77.8	128.0	2.2
31.0	0.6	44.0	6.5	66.0	0.3	87.0	3.5	129.0	0.5
38.0	0.4	45.0	0.6	68.0	1.3	109.0	0.5	130.0	0.0
39.0	1.9	55.0	0.4	69.0	1.0	115.0	1.5	158.0	0.1
40.0	1.5	56.0	3.1	83.0	0.7	116.0	0.8	159.0	0.4
41.0	5.5	57.0	7.5	84.0	10.3	125.0	0.1	160.0	0.0
42.0	54.8	58.0	7.7	85.0	11.3				



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

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	14.0	44.0	11.5	58.0	5.5	84.0	33.7	104.0	1.3
32.0	0.8	46.0	1.3	68.0	1.1	85.0	5.7	113.0	0.8
39.0	8.2	48.0	6.2	70.0	47.7	99.0	8.8	129.0	4.0
40.0	1.5	54.0	2.0	71.0	3.3	100.0	3.7	141.0	2.4
41.0	56.0	55.0	11.1	72.0	13.3	102.0	5.1	158.0	28.6
42.0	30.6	56.0	26.6	73.0	3.5	103.0	17.7	159.0	4.0
43.0	2.2	57.0	100.0						

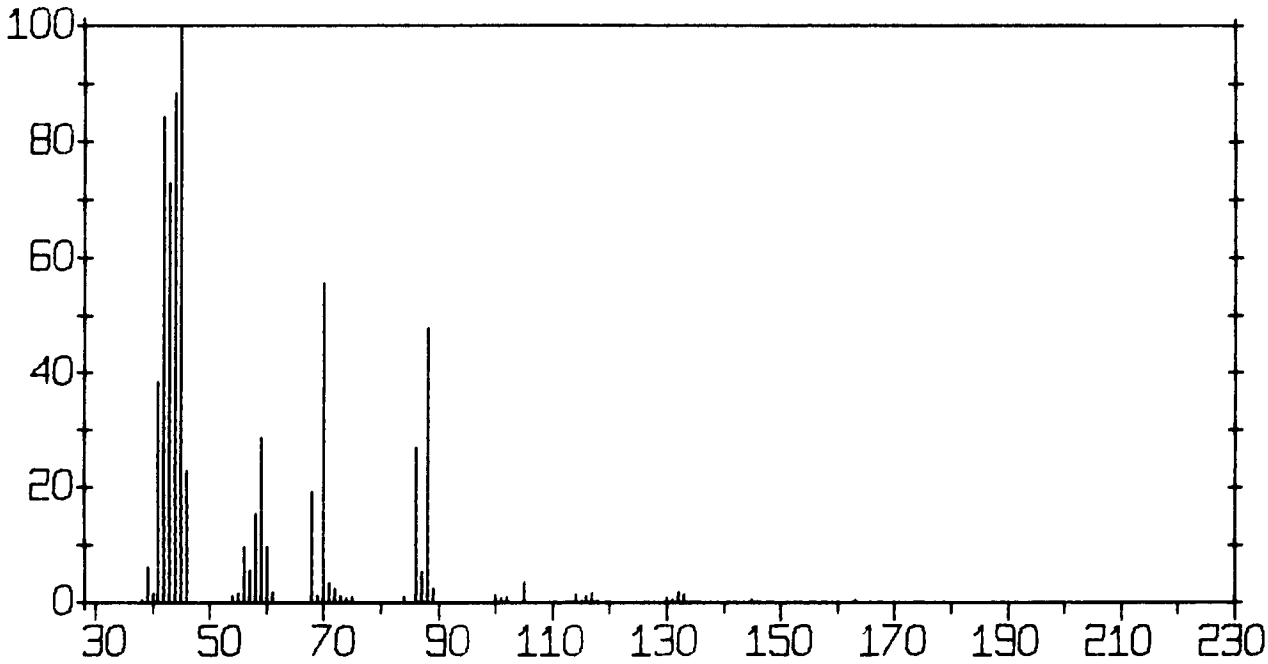
OBSERVED METASTABLES
29.5,



N-NITROSO-BIS(2-HYDROXYPROPYL)AMINE
MW = 162 C6.H14.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
38.0	0.5	55.0	1.8	70.0	55.7	88.0	48.0	117.0	1.7
39.0	6.1	56.0	9.8	71.0	3.4	89.0	2.5	118.0	0.3
40.0	1.8	57.0	5.7	72.0	2.5	100.0	1.3	130.0	0.6
41.0	38.4	58.0	15.3	73.0	1.0	101.0	0.7	131.0	0.5
42.0	84.6	59.0	28.8	74.0	0.6	102.0	1.1	132.0	2.1
43.0	73.0	60.0	9.8	75.0	0.9	105.0	3.8	133.0	1.5
44.0	88.4	61.0	1.9	84.0	0.9	114.0	1.5	145.0	0.3
45.0	100.0	68.0	19.2	86.0	26.9	115.0	0.3	146.0	0.1
46.0	23.0	69.0	1.0	87.0	5.3	116.0	0.9	163.0	0.5
54.0	1.3								

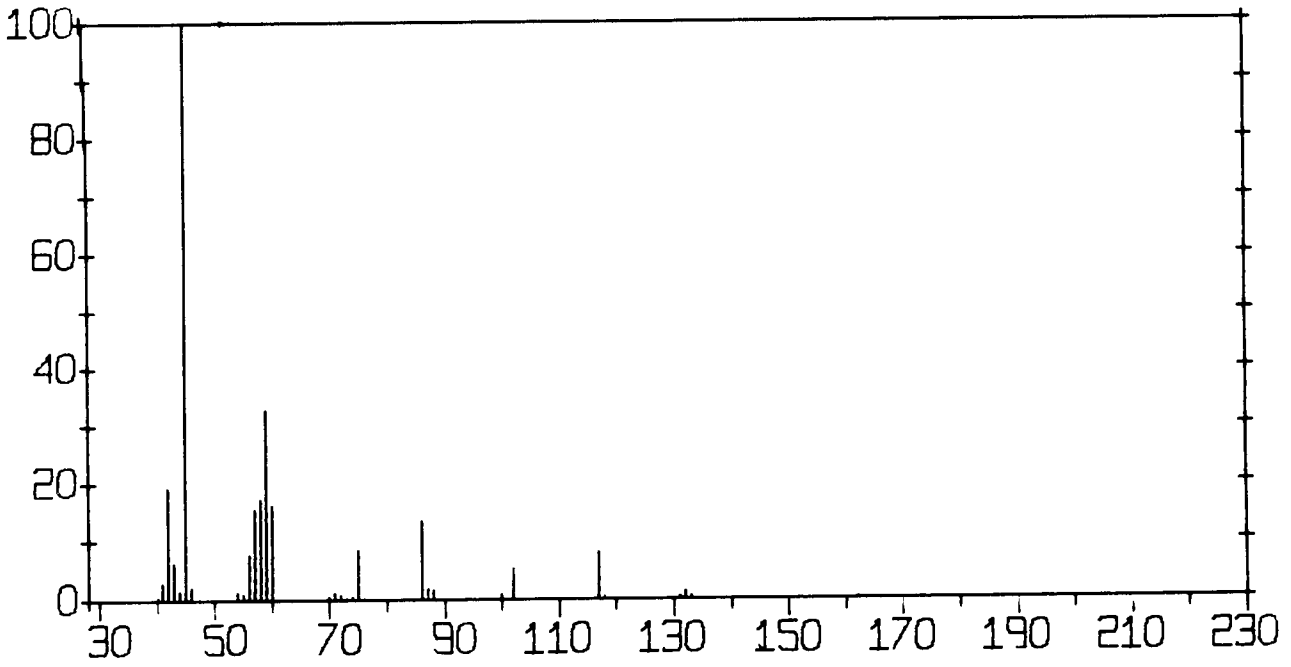
OBSERVED METASTABLES
55.7, 98.5,



N-NITROSO-BIS(2-METHOXYETHYL)AMINE
MW = 162 C6.H14.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
40.0	0.4	54.0	1.2	70.0	0.5	76.0	0.3	117.0	8.0
41.0	2.8	55.0	1.0	71.0	1.0	86.0	13.4	118.0	0.4
42.0	19.2	56.0	7.6	72.0	0.7	87.0	1.9	131.0	0.5
43.0	6.1	57.0	15.3	73.0	0.3	88.0	1.6	132.0	1.2
44.0	1.4	58.0	17.3	74.0	0.3	100.0	0.6	133.0	0.5
45.0	100.0	59.0	32.6	75.0	8.4	102.0	5.3	162.0	0.1
46.0	2.3	60.0	16.1						

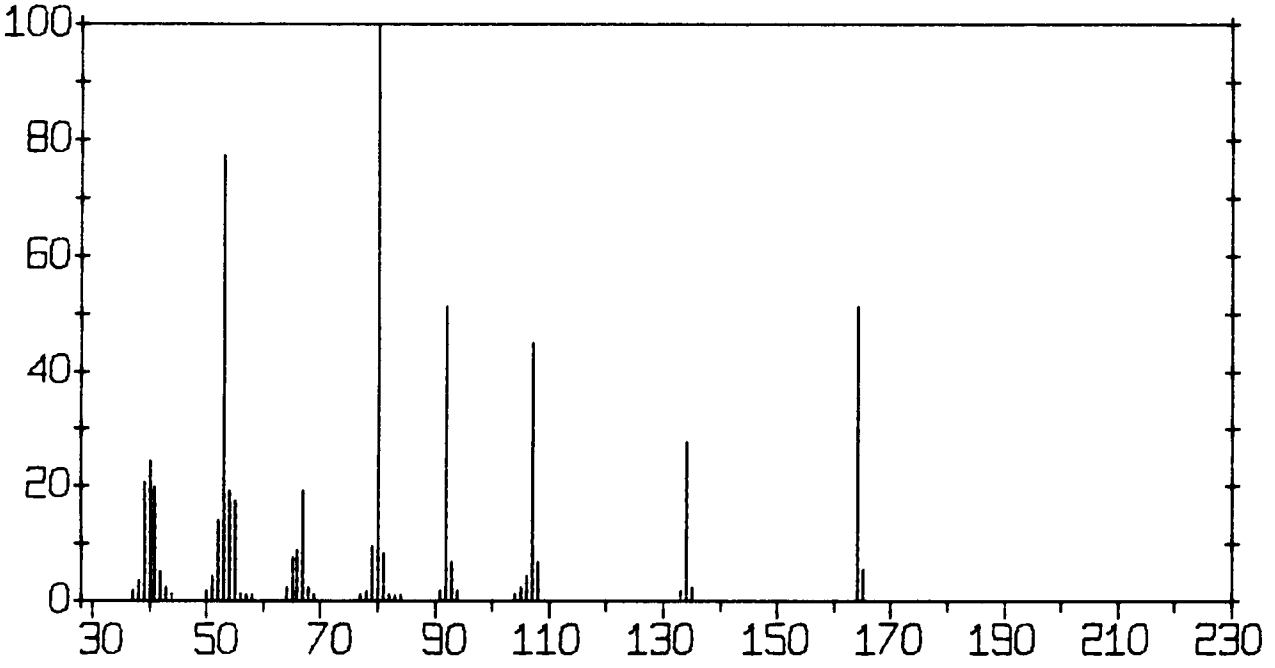
OBSERVED METASTABLES
78.8,



N-NITROSO-2,6-DICYANOPIPERIDINE
MW = 164 C7.H8.N4.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
37.0	1.9	51.0	4.5	65.0	7.7	81.0	8.3	105.0	2.5
38.0	3.8	52.0	14.1	66.0	9.0	82.0	1.2	106.0	4.5
39.0	20.6	53.0	77.4	67.0	19.3	83.0	1.2	107.0	45.1
40.0	24.5	54.0	19.3	68.0	2.5	84.0	1.2	108.0	7.0
41.0	20.0	55.0	17.4	69.0	1.2	91.0	1.9	133.0	1.9
42.0	5.1	56.0	1.2	77.0	1.2	92.0	51.6	134.0	27.7
43.0	2.5	57.0	1.2	78.0	1.9	93.0	7.0	135.0	2.5
44.0	1.2	58.0	1.2	79.0	9.6	94.0	1.9	164.0	51.6
50.0	1.9	64.0	2.5	80.0	100.0	104.0	1.2	165.0	5.8

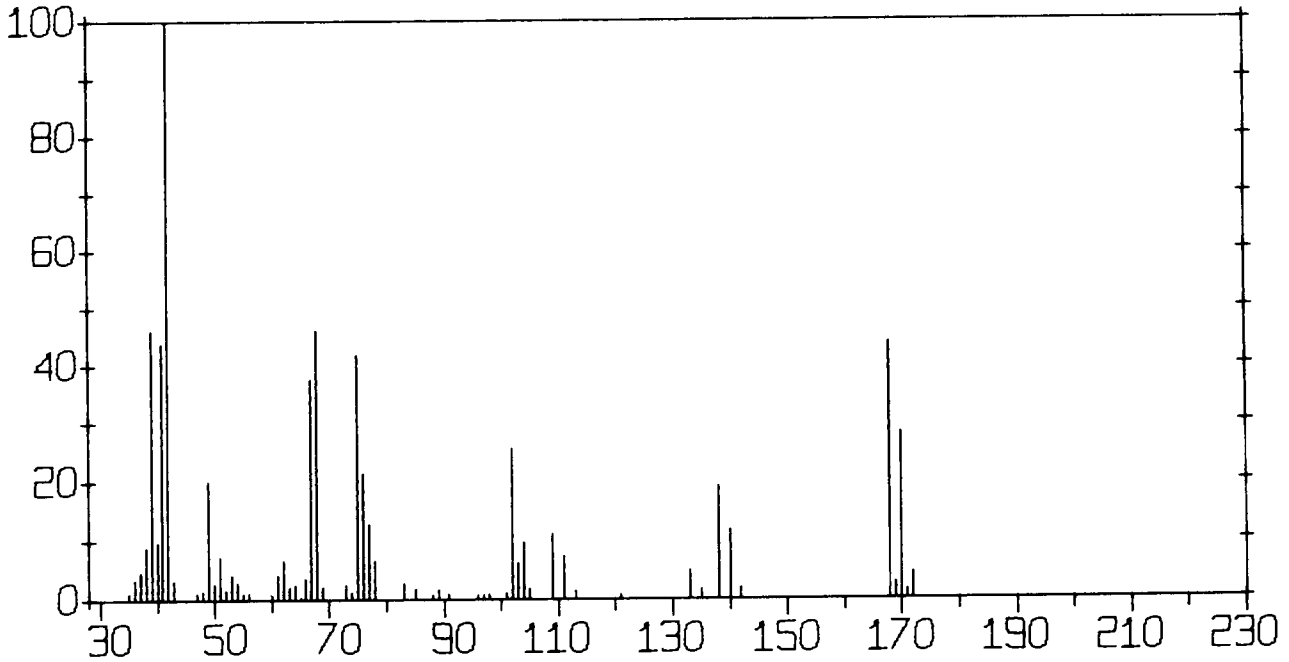
OBSERVED METASTABLES
85.4, 109.5,



N-NITROSO-3,4-DICHLOROPYRROLIDINE
MW = 168 C4.H6.N2.O.CL2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
35.0	1.0	51.0	7.5	67.0	37.8	89.0	1.6	113.0	1.3
36.0	3.5	52.0	1.6	68.0	46.2	91.0	0.6	121.0	0.7
37.0	4.8	53.0	4.2	69.0	2.3	96.0	0.7	133.0	5.0
38.0	9.0	54.0	2.9	73.0	2.5	97.0	0.7	135.0	1.6
39.0	46.2	55.0	1.0	74.0	1.1	98.0	0.7	138.0	19.3
40.0	9.8	56.0	0.8	75.0	42.0	101.0	1.0	140.0	11.7
41.0	44.1	60.0	0.6	76.0	21.4	102.0	25.6	142.0	2.0
42.0	100.0	61.0	4.2	77.0	13.0	103.0	6.3	168.0	44.1
43.0	3.1	62.0	6.7	78.0	6.7	104.0	9.6	169.0	2.7
47.0	0.8	63.0	2.3	83.0	2.7	105.0	2.1	170.0	28.1
48.0	1.3	64.0	2.5	85.0	1.9	109.0	11.3	171.0	1.5
49.0	20.1	65.0	0.5	88.0	0.7	111.0	7.5	172.0	4.4
50.0	2.7	66.0	3.7						

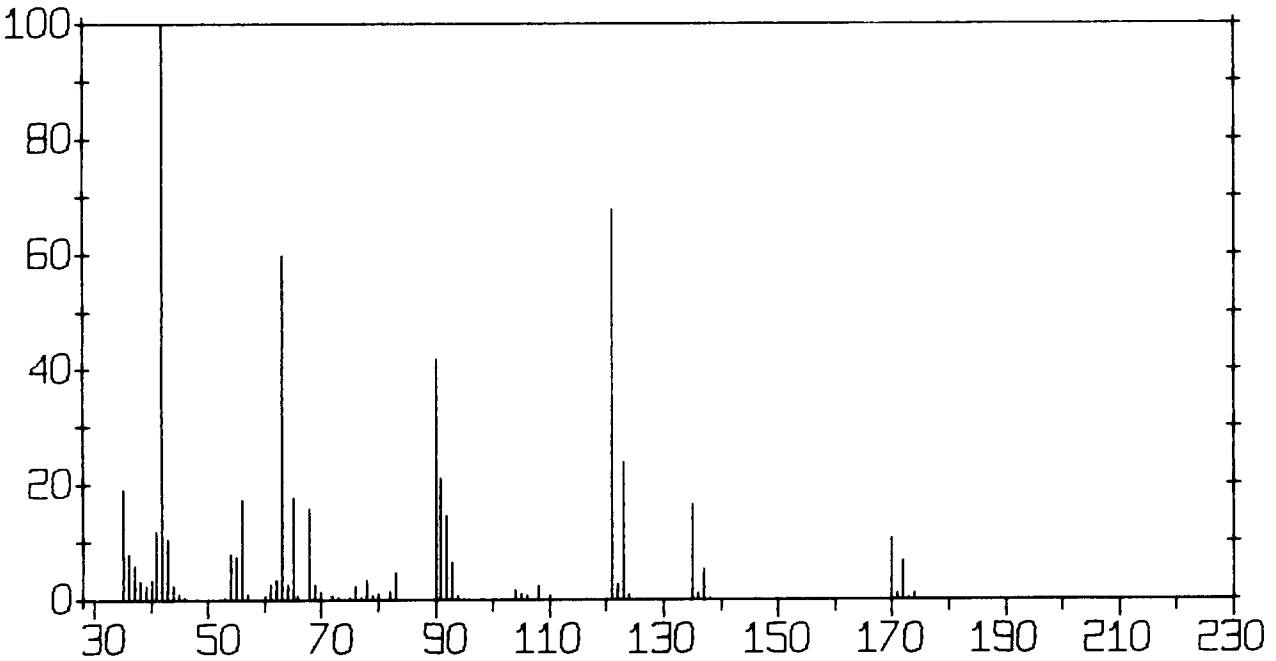
OBSERVED METASTABLES
113.4, 115.3,



N-NITROSO-BIS(2-CHLOROETHYL)AMINE
MW = 170 C4.H8.N2.O.CL2

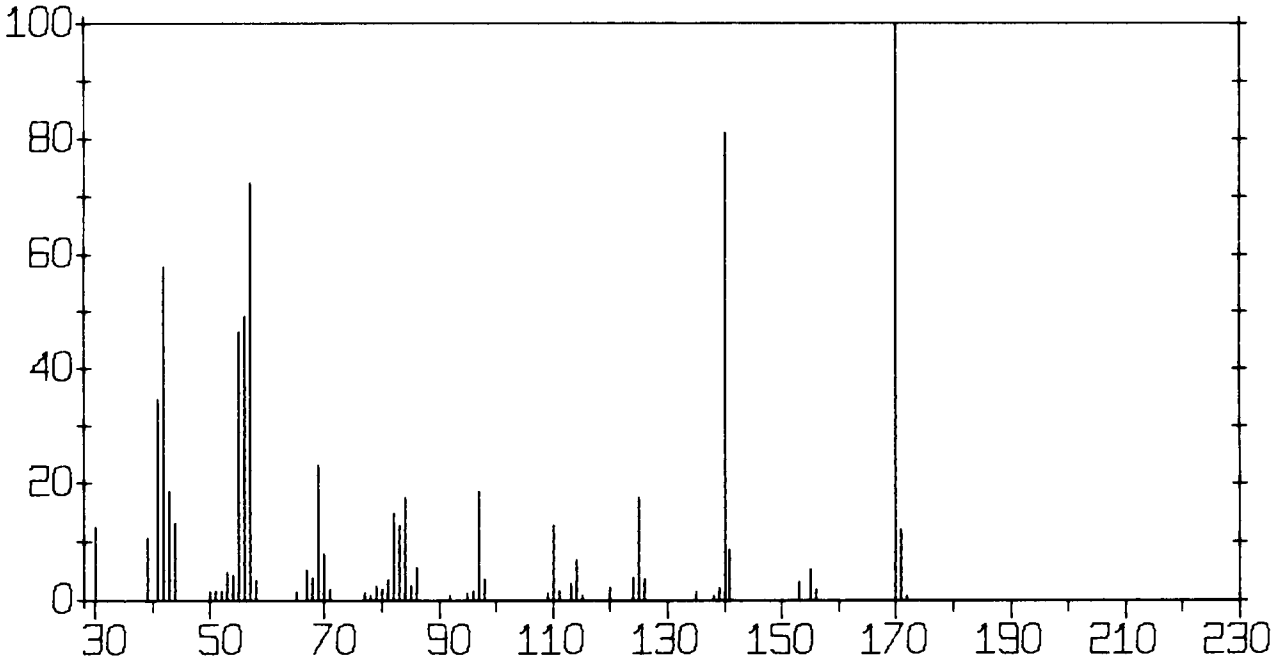
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
35.0	19.2	53.0	0.5	68.0	16.0	83.0	4.8	122.0	2.8
36.0	8.0	54.0	8.0	69.0	2.8	90.0	42.0	123.0	24.0
37.0	6.0	55.0	7.6	70.0	1.4	91.0	21.2	124.0	0.8
38.0	3.2	56.0	17.6	72.0	0.6	92.0	14.8	135.0	16.8
39.0	2.4	57.0	0.8	73.0	0.4	93.0	6.4	136.0	0.9
40.0	3.6	60.0	0.6	75.0	0.5	94.0	0.7	137.0	5.2
41.0	12.0	61.0	2.8	76.0	2.6	104.0	1.6	138.0	0.5
42.0	100.0	62.0	3.6	77.0	0.4	105.0	1.0	170.0	10.8
43.0	10.4	63.0	60.0	78.0	3.6	106.0	0.6	171.0	1.0
44.0	2.4	64.0	2.8	79.0	0.6	108.0	2.5	172.0	6.8
45.0	1.1	65.0	18.0	80.0	0.9	110.0	0.7	173.0	0.4
46.0	0.4	66.0	0.6	82.0	1.6	121.0	68.0	174.0	1.0

OBSERVED METASTABLES
107.2, 66.9,



N-NITROSO-4-TERTBUTYLPIPERIDINE
MW = 170 C9.H18.N2.O

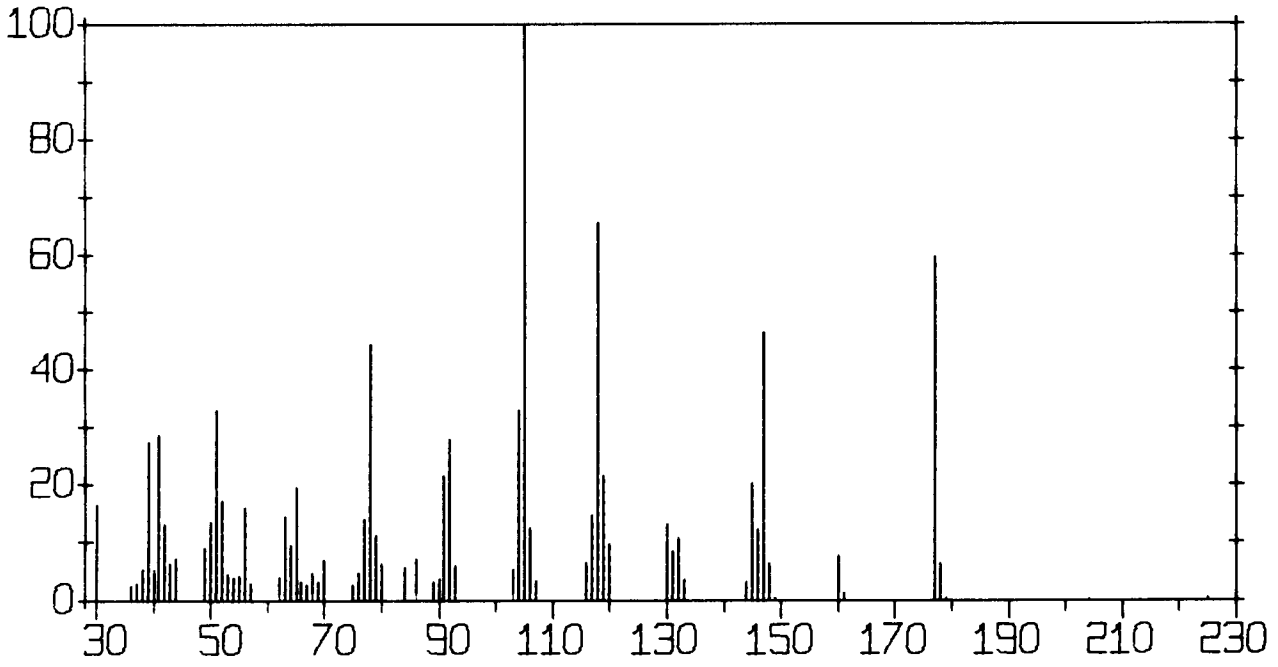
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	12.4	56.0	49.2	80.0	2.0	98.0	3.7	135.0	1.4
39.0	10.7	57.0	72.4	81.0	3.7	109.0	1.1	138.0	0.8
41.0	34.7	58.0	3.7	82.0	15.0	110.0	13.0	139.0	2.3
42.0	57.9	65.0	1.4	83.0	13.0	111.0	1.7	140.0	81.1
43.0	18.8	67.0	5.2	84.0	17.3	113.0	2.8	141.0	8.6
44.0	13.3	68.0	4.0	85.0	2.6	114.0	6.9	153.0	3.1
50.0	1.4	69.0	23.1	86.0	5.7	115.0	0.8	155.0	5.5
51.0	1.7	70.0	8.1	92.0	0.8	120.0	2.3	156.0	2.0
52.0	1.7	71.0	2.0	95.0	1.1	124.0	4.0	170.0	100.0
53.0	4.9	77.0	1.1	96.0	1.7	125.0	17.3	171.0	11.8
54.0	4.3	78.0	0.8	97.0	18.8	126.0	3.7	172.0	0.8
55.0	46.3	79.0	2.6						



N-NITROSONORNICOTINE
MW = 177 C9.H11.N3.O

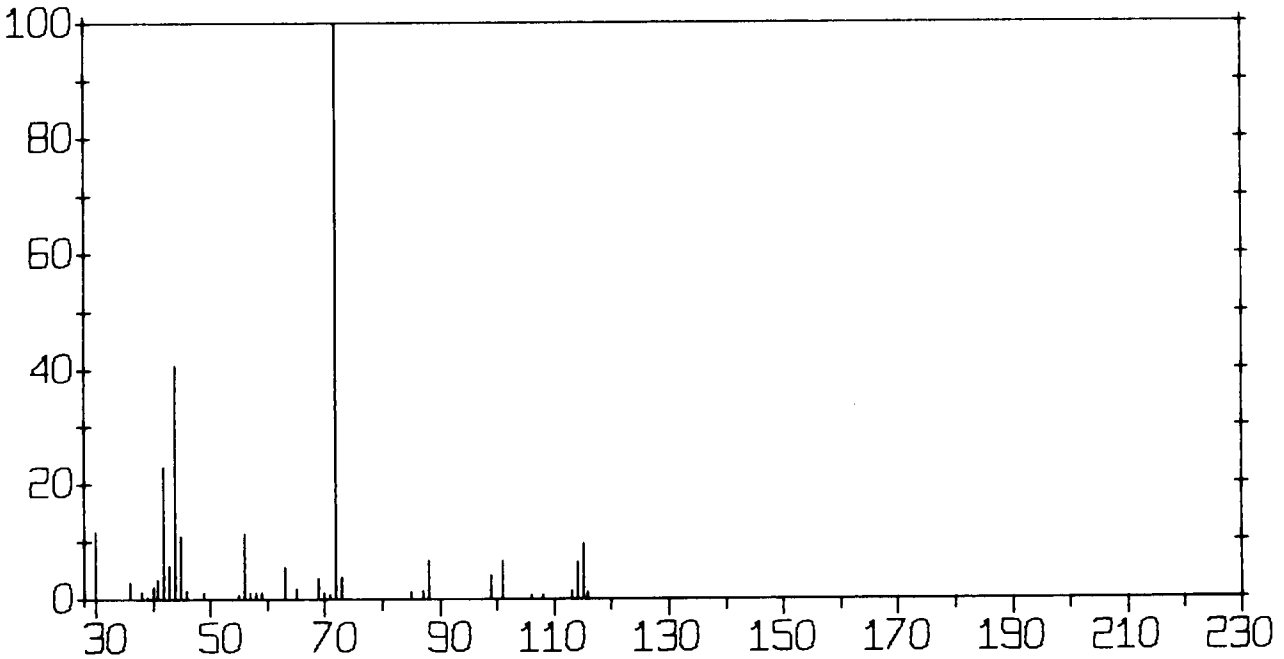
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	16.4	53.0	4.5	70.0	6.9	93.0	6.0	132.0	10.6
36.0	2.4	54.0	3.9	75.0	2.7	103.0	5.5	133.0	3.7
37.0	2.8	55.0	4.3	76.0	4.7	104.0	32.9	144.0	3.3
38.0	5.5	56.0	16.0	77.0	13.9	105.0	100.0	145.0	20.1
39.0	27.5	57.0	2.8	78.0	44.4	106.0	12.5	146.0	12.3
40.0	5.3	62.0	4.1	79.0	11.3	107.0	3.4	147.0	46.5
41.0	28.8	63.0	14.4	80.0	6.1	116.0	6.3	148.0	6.1
42.0	13.1	64.0	9.4	84.0	5.7	117.0	14.8	149.0	0.6
43.0	6.1	65.0	19.5	86.0	7.2	118.0	65.8	160.0	7.8
44.0	7.2	66.0	3.2	89.0	3.2	119.0	21.6	161.0	1.3
49.0	9.0	67.0	2.6	90.0	3.7	120.0	9.6	177.0	59.6
50.0	13.5	68.0	4.7	91.0	21.3	130.0	13.3	178.0	6.2
51.0	32.9	69.0	3.2	92.0	27.9	131.0	8.4	179.0	0.4
52.0	17.2								

OBSERVED METASTABLES
58.0, 75.0, 81.3, 104.1, 122.0, 143.0, 144.7, 144.7, 159.5, 176.5,



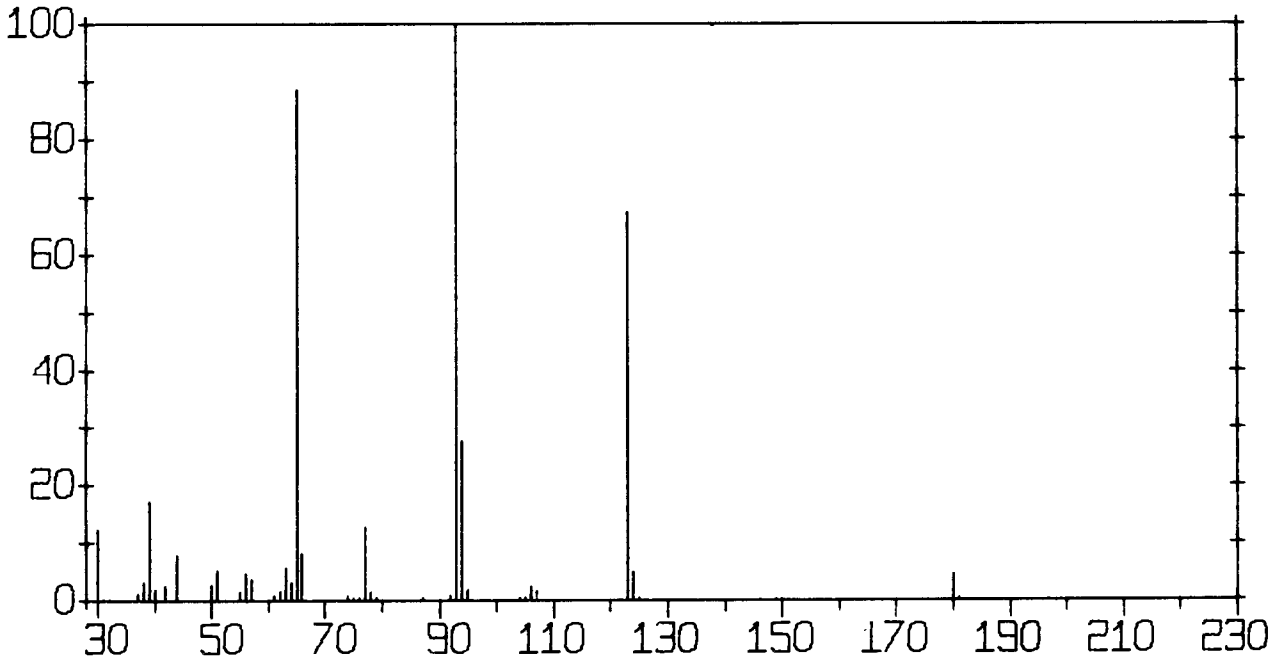
N-NITROSO-1,1-DIMETHYL-3(2-CHLOROETHYL)UREA
MW = 179 C5.H10.N3.O2.CL

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	11.7	43.0	6.0	57.0	1.1	71.0	0.7	101.0	6.7
36.0	3.0	44.0	41.0	58.0	1.1	72.0	100.0	106.0	0.7
38.0	1.1	45.0	11.0	59.0	1.3	73.0	4.1	108.0	0.8
39.0	0.5	46.0	1.5	63.0	5.7	85.0	1.1	113.0	1.4
40.0	2.2	49.0	1.2	65.0	1.8	87.0	1.5	114.0	6.4
41.0	3.4	55.0	0.6	69.0	3.7	88.0	6.7	115.0	9.6
42.0	23.2	56.0	11.4	70.0	0.8	99.0	4.2	116.0	1.1



N-NITROSO-METHYL N-PHENYLCARBAMATE
MW = 180 C8.H8.N2.O3

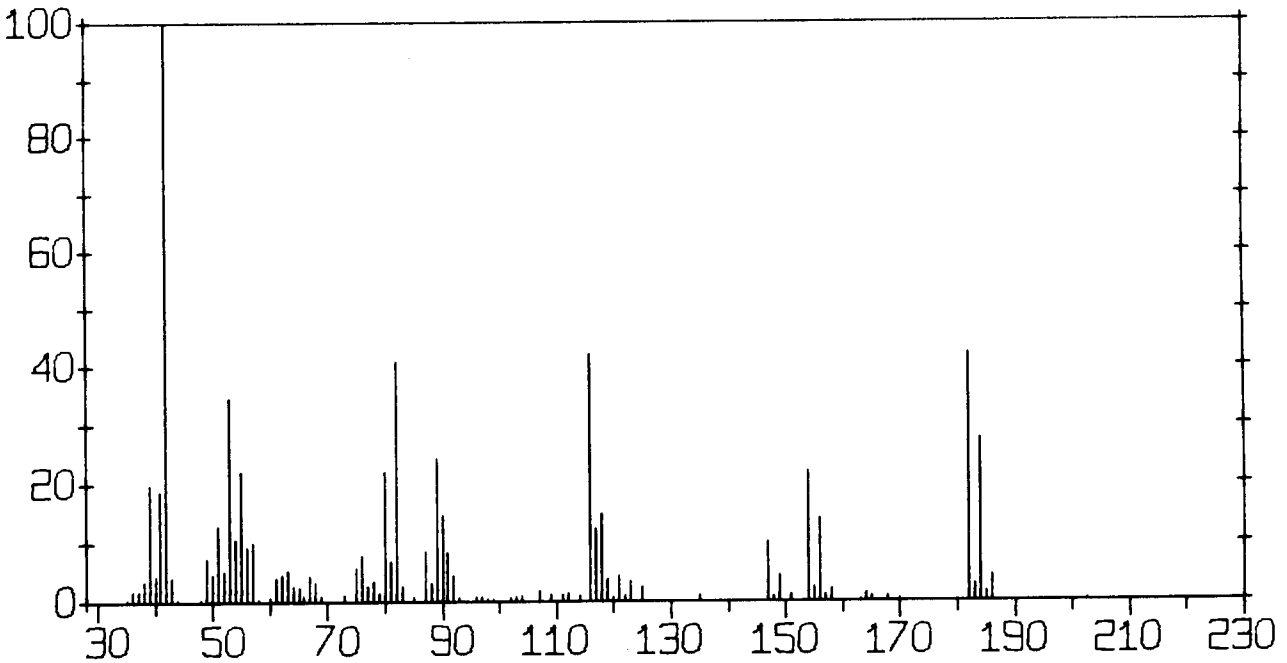
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	12.5	50.0	2.7	65.0	88.7	87.0	0.5	107.0	1.7
31.0	0.3	51.0	5.1	66.0	8.3	92.0	0.6	123.0	67.5
32.0	0.1	55.0	1.5	74.0	0.7	93.0	100.0	124.0	5.0
37.0	0.9	56.0	4.7	75.0	0.3	94.0	27.8	125.0	0.3
38.0	3.3	57.0	3.8	76.0	0.4	95.0	2.1	149.0	0.3
39.0	17.2	61.0	0.6	77.0	12.9	104.0	0.5	150.0	0.2
40.0	1.9	62.0	1.8	78.0	1.4	105.0	0.4	180.0	4.5
42.0	2.5	63.0	5.6	79.0	0.3	106.0	2.5	181.0	0.3
44.0	7.9	64.0	3.3						



N-NITROSO-3,4-DICHLOROPIPERIDINE
MW = 182 C5.H8.N2.O.CL2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
35.0	0.6	56.0	9.5	79.0	1.4	103.0	0.8	148.0	0.7
36.0	1.8	57.0	10.2	80.0	22.2	104.0	0.8	149.0	4.4
37.0	1.8	58.0	0.4	81.0	7.1	107.0	2.0	151.0	1.1
38.0	3.7	60.0	0.7	82.0	41.1	109.0	1.1	154.0	22.2
39.0	20.0	61.0	4.2	83.0	2.6	111.0	1.1	155.0	2.4
40.0	4.4	62.0	4.6	85.0	0.6	112.0	1.3	156.0	14.2
41.0	18.8	63.0	5.5	87.0	8.6	114.0	1.0	157.0	1.1
42.0	100.0	64.0	2.6	88.0	3.3	116.0	42.2	158.0	2.3
43.0	4.2	65.0	2.4	89.0	24.4	117.0	12.4	163.0	0.4
44.0	0.5	66.0	0.9	90.0	14.6	118.0	14.8	164.0	1.3
48.0	0.4	67.0	4.4	91.0	8.4	119.0	4.0	165.0	0.8
49.0	7.5	68.0	3.5	92.0	4.4	120.0	0.6	168.0	0.8
50.0	4.6	69.0	0.9	93.0	0.7	121.0	4.4	170.0	0.4
51.0	12.8	73.0	1.2	96.0	0.6	122.0	1.0	182.0	42.2
52.0	5.3	75.0	6.0	97.0	0.6	123.0	3.7	183.0	2.8
53.0	34.6	76.0	8.0	98.0	0.4	125.0	2.4	184.0	27.7
54.0	10.6	77.0	2.6	99.0	0.5	135.0	1.0	185.0	1.7
55.0	22.2	78.0	3.7	102.0	0.8	147.0	10.2	186.0	4.4

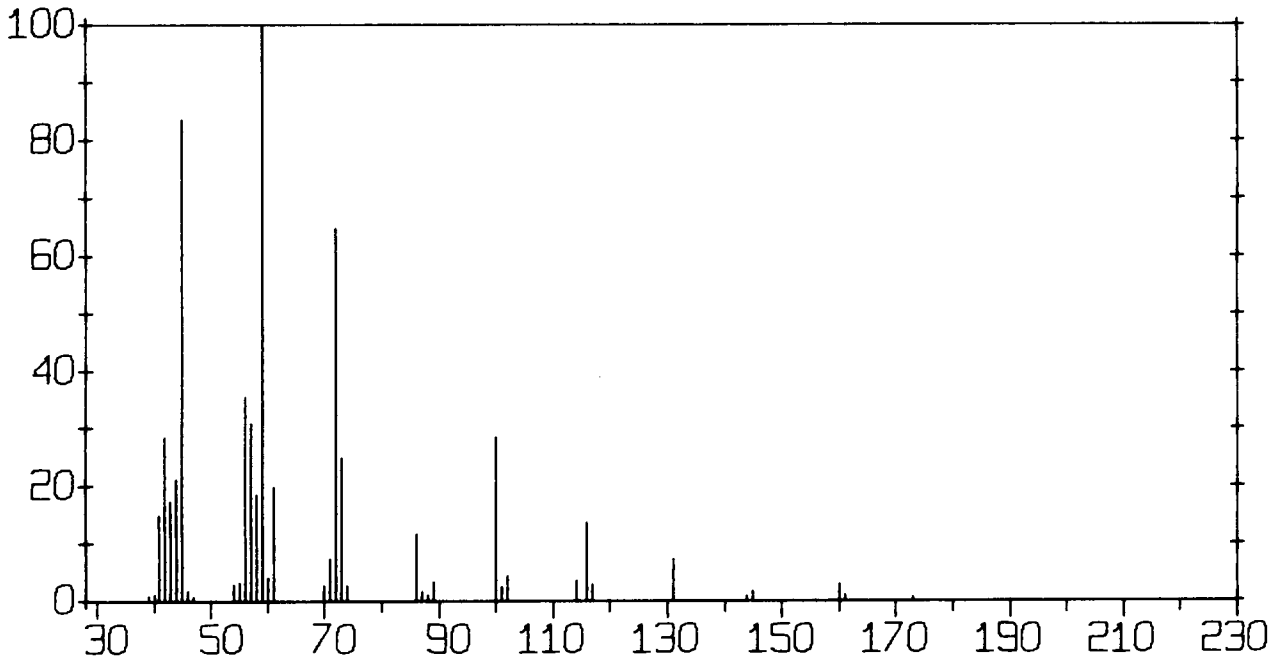
OBSERVED METASTABLES
126.9, 128.9,



N-NITROSO-BIS(2-ETHOXYETHYL)AMINE
MW = 190 C8.H18.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
39.0	0.7	47.0	0.8	61.0	20.0	88.0	0.9	131.0	7.5
40.0	1.0	54.0	3.1	70.0	2.7	89.0	3.5	144.0	0.8
41.0	15.0	55.0	3.3	71.0	7.5	100.0	28.7	145.0	1.7
42.0	28.7	56.0	35.8	72.0	65.0	101.0	2.6	160.0	3.0
43.0	17.5	57.0	31.1	73.0	25.0	102.0	4.6	161.0	0.9
44.0	21.2	58.0	18.7	74.0	2.7	114.0	3.8	173.0	0.7
45.0	83.7	59.0	100.0	86.0	11.8	116.0	13.7	190.0	0.2
46.0	2.0	60.0	4.3	87.0	1.8	117.0	3.0		

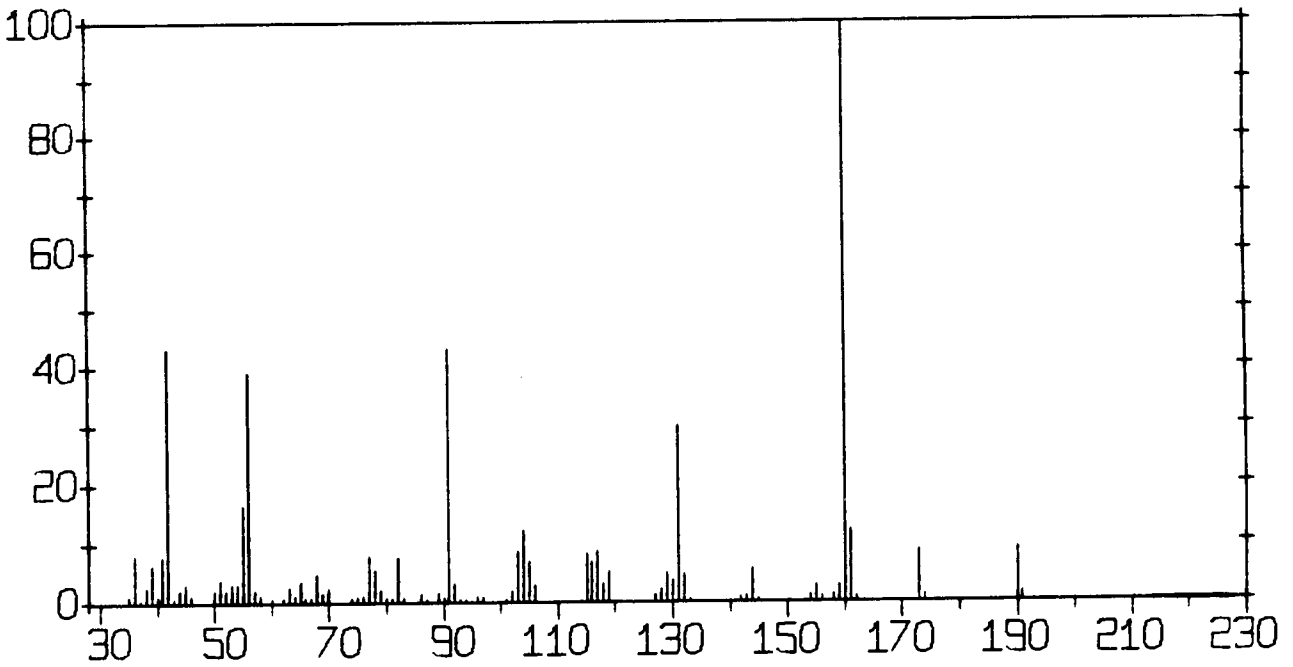
OBSERVED METASTABLES
76.3,



N-NITROSO-4-PHENYLPIPERIDINE
MW = 190 C11.H14.N2.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
35.0	1.0	56.0	39.3	78.0	5.6	102.0	2.0	141.0	0.3
36.0	8.3	57.0	2.3	79.0	2.3	103.0	8.6	142.0	0.7
37.0	0.4	58.0	1.1	80.0	0.8	104.0	12.3	143.0	1.0
38.0	2.8	60.0	0.6	81.0	0.7	105.0	7.0	144.0	5.6
39.0	6.5	62.0	0.6	82.0	7.6	106.0	3.0	145.0	0.4
40.0	0.9	63.0	2.6	83.0	0.7	114.0	0.3	154.0	0.9
41.0	8.0	64.0	0.9	86.0	1.6	115.0	8.3	155.0	2.8
42.0	43.3	65.0	3.8	87.0	0.4	116.0	7.0	156.0	0.6
43.0	0.7	66.0	0.6	89.0	1.7	117.0	8.6	158.0	1.3
44.0	2.2	67.0	0.8	90.0	0.7	118.0	3.1	159.0	2.6
45.0	3.1	68.0	5.0	91.0	43.3	119.0	5.3	160.0	100.0
46.0	1.1	69.0	1.7	92.0	3.3	127.0	1.3	161.0	12.3
50.0	2.1	70.0	2.5	93.0	0.4	128.0	2.3	162.0	0.8
51.0	4.0	73.0	0.3	94.0	0.5	129.0	5.0	173.0	8.6
52.0	2.3	74.0	0.8	95.0	0.3	130.0	3.6	174.0	1.1
53.0	3.1	75.0	0.9	96.0	1.0	131.0	30.0	190.0	9.0
54.0	3.1	76.0	1.3	97.0	0.7	132.0	4.6	191.0	1.4
55.0	16.6	77.0	8.0	101.0	0.4	133.0	0.4		

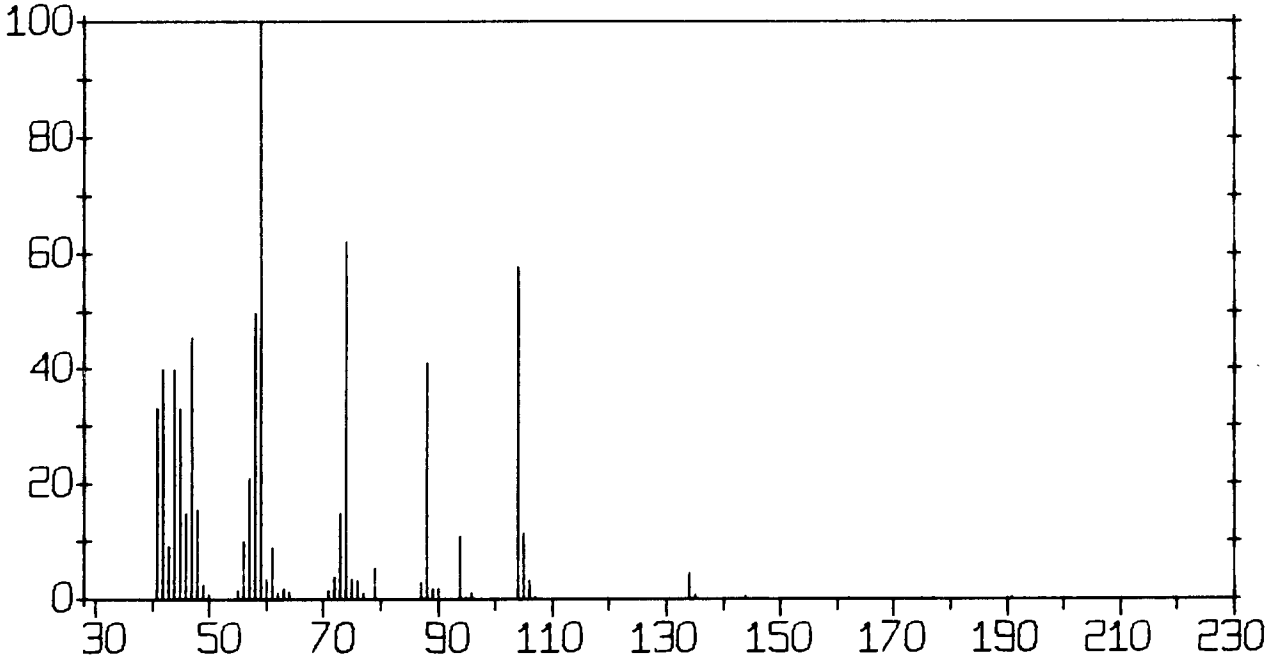
OBSERVED METASTABLES
107.3, 134.7,



N-NITROSOMETHOMYL
MW = 191 C5.H9.N3.O3.S

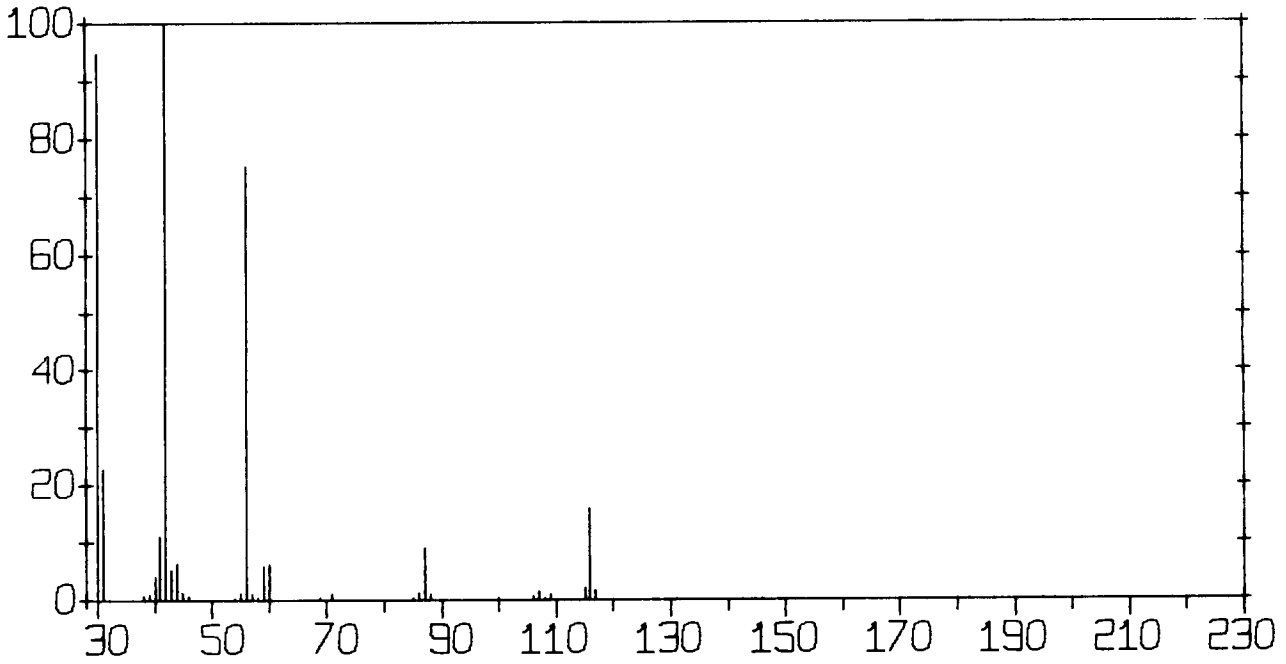
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	33.3	44.0	40.0	59.0	100.0	76.0	3.3	105.0	11.5
31.0	10.8	45.0	33.3	60.0	3.5	77.0	1.0	106.0	3.3
32.0	1.4	46.0	14.8	61.0	9.1	79.0	5.5	107.0	0.6
33.0	0.8	47.0	45.5	62.0	0.9	87.0	3.1	134.0	4.4
35.0	0.7	48.0	15.5	63.0	2.1	88.0	41.1	135.0	0.7
38.0	3.7	49.0	2.4	64.0	1.1	89.0	2.0	144.0	0.4
39.0	6.4	50.0	0.7	71.0	1.5	90.0	2.0	162.0	0.3
40.0	18.8	55.0	1.4	72.0	4.0	94.0	10.8	175.0	0.1
41.0	33.3	56.0	10.0	73.0	15.1	95.0	0.5	177.0	0.1
42.0	40.0	57.0	21.1	74.0	62.2	96.0	1.0	190.0	0.1
43.0	9.3	58.0	50.0	75.0	3.5	104.0	57.7	191.0	0.6

OBSERVED METASTABLES
52.7, 80.7,



N-NITROSO-2-BROMOETHYLUREA
MW = 195 C3.H6.N3.O2.BR

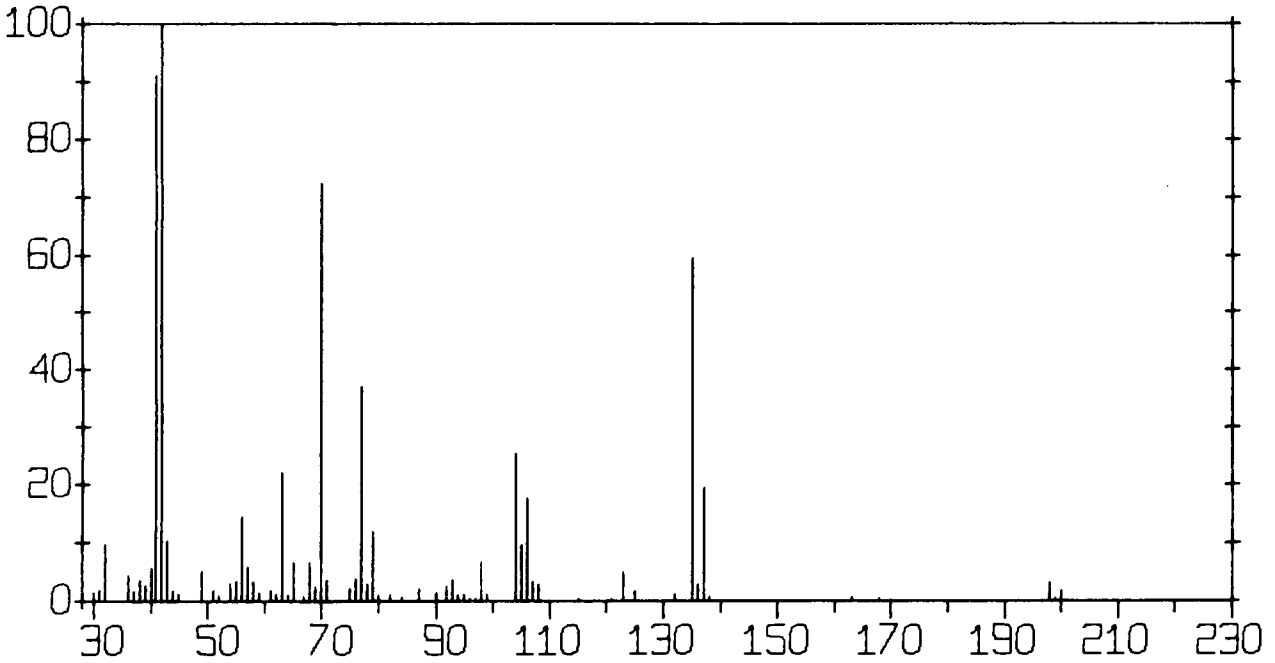
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	95.0	43.0	5.2	58.0	0.5	87.0	9.1	116.0	16.0
31.0	22.9	44.0	6.5	59.0	6.0	88.0	0.9	117.0	1.8
32.0	0.3	45.0	1.1	60.0	6.2	100.0	0.6	131.0	0.2
38.0	0.8	46.0	0.6	69.0	0.4	106.0	0.6	146.0	0.2
39.0	1.0	54.0	0.4	70.0	0.3	107.0	1.3	180.0	0.1
40.0	4.2	55.0	1.2	71.0	1.0	108.0	0.6	182.0	0.1
41.0	11.1	56.0	75.4	85.0	0.4	109.0	1.1	195.0	0.1
42.0	100.0	57.0	0.9	86.0	1.2	115.0	2.2	197.0	0.1



N-NITROSO-BIS-(2-CHLOROPROPYL)AMINE
MW = 198 C6.H12.N2.O.CL2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	1.4	52.0	0.8	70.0	72.5	95.0	1.1	132.0	1.3
31.0	2.0	54.0	3.1	71.0	3.7	96.0	0.5	135.0	59.8
32.0	9.8	55.0	3.4	75.0	2.2	97.0	0.5	136.0	2.9
36.0	4.5	56.0	14.5	76.0	4.1	98.0	7.0	137.0	19.6
37.0	1.8	57.0	6.0	77.0	37.2	99.0	1.1	138.0	0.8
38.0	3.7	58.0	3.5	78.0	2.9	104.0	25.4	163.0	0.8
39.0	2.7	59.0	1.5	79.0	11.9	105.0	9.8	165.0	0.2
40.0	5.6	61.0	1.9	80.0	0.9	106.0	17.6	168.0	0.4
41.0	91.1	62.0	1.2	82.0	1.2	107.0	3.5	170.0	0.2
42.0	100.0	63.0	22.3	84.0	0.7	108.0	2.9	198.0	3.3
43.0	10.3	64.0	1.0	87.0	2.1	115.0	0.5	199.0	0.4
44.0	1.9	65.0	6.8	90.0	1.4	121.0	0.5	200.0	2.0
45.0	1.1	67.0	0.7	92.0	2.7	123.0	5.2	201.0	0.3
49.0	5.2	68.0	6.6	93.0	3.7	125.0	1.7	202.0	0.3
51.0	1.8	69.0	2.5	94.0	1.0				

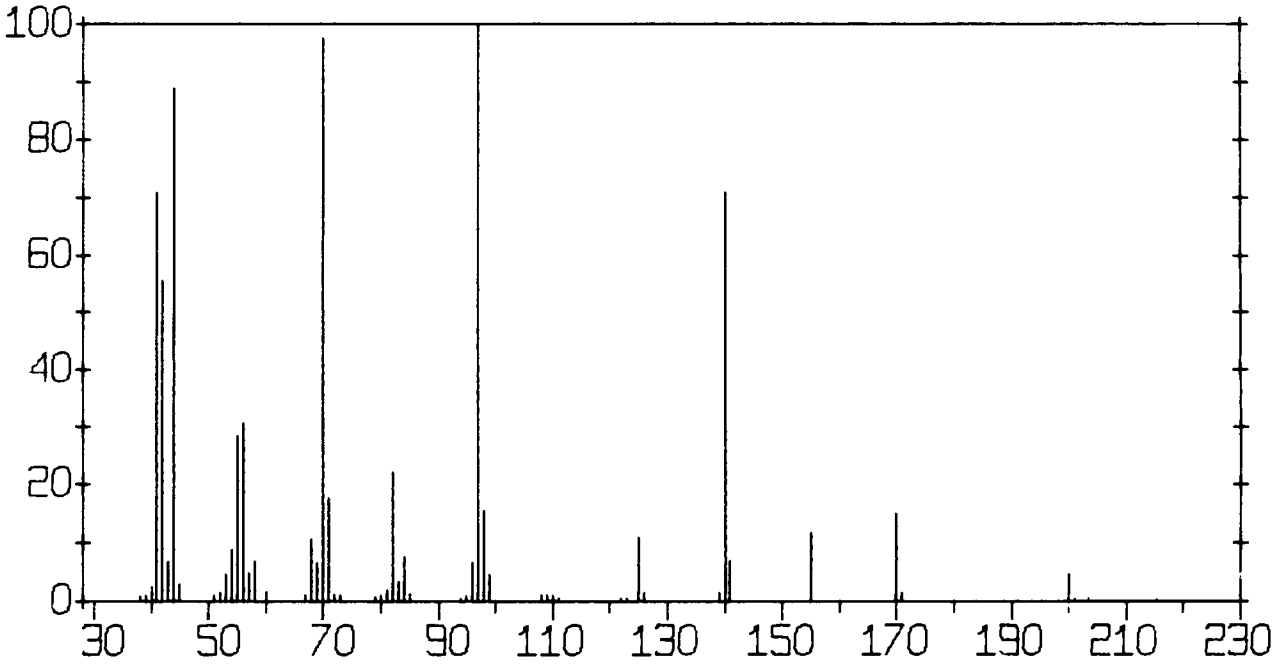
OBSERVED METASTABLES
80.1, 82.0,



1,4-DINITROSO-2,3,5,6-TETRAMETHYLPIPERAZINE
MW = 200 C8.H16.N4.O2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
38.0	0.6	54.0	9.1	72.0	1.1	96.0	6.6	125.0	10.8
39.0	1.1	55.0	28.4	73.0	1.0	97.0	100.0	126.0	1.5
40.0	2.4	56.0	30.6	79.0	0.8	98.0	15.5	139.0	1.4
41.0	71.1	57.0	4.8	80.0	1.0	99.0	4.7	140.0	71.1
42.0	55.5	58.0	6.8	81.0	1.8	108.0	1.3	141.0	6.8
43.0	7.1	60.0	1.7	82.0	22.2	109.0	0.8	155.0	11.7
44.0	88.8	67.0	1.1	83.0	3.5	110.0	1.0	170.0	14.8
45.0	3.1	68.0	10.6	84.0	7.7	111.0	0.5	171.0	1.5
51.0	1.0	69.0	6.6	85.0	1.2	122.0	0.6	200.0	4.6
52.0	1.4	70.0	97.7	94.0	0.6	123.0	0.5	201.0	0.6
53.0	4.6	71.0	17.7	95.0	0.6				

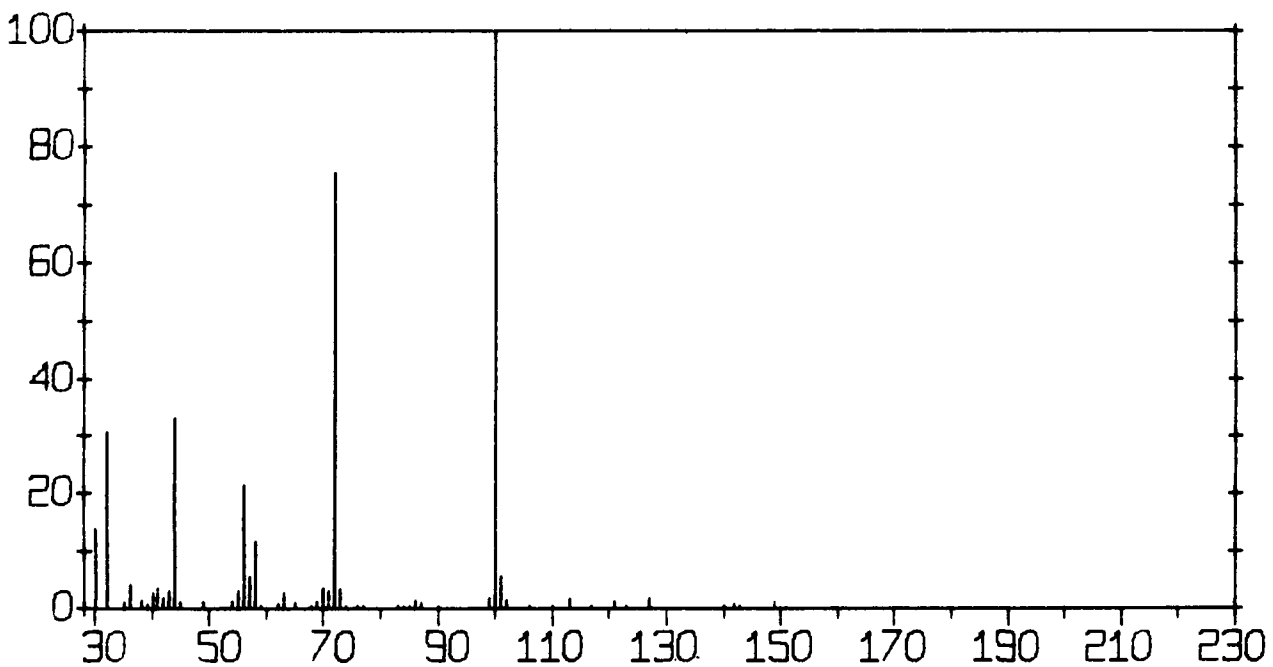
OBSERVED METASTABLES
67.1, 69.2, 81.8, 115.2, 144.5,



N-NITROSO-1,1-DIETHYL-3(2-CHLOROETHYL)UREA
MW = 207 C7.H14.N3.O2.CL

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	14.0	45.0	1.0	68.0	0.4	85.0	0.5	117.0	0.5
32.0	30.6	49.0	1.2	69.0	1.1	86.0	1.4	121.0	1.2
35.0	0.8	54.0	1.2	70.0	3.8	87.0	0.9	123.0	0.3
36.0	4.3	55.0	3.2	71.0	3.2	90.0	0.5	127.0	1.9
38.0	1.5	56.0	21.6	72.0	75.6	99.0	1.9	140.0	0.4
39.0	0.7	57.0	5.7	73.0	3.6	100.0	100.0	141.0	0.2
40.0	2.7	58.0	11.7	74.0	0.5	101.0	5.7	142.0	0.8
41.0	3.7	59.0	0.5	76.0	0.4	102.0	1.6	143.0	0.3
42.0	1.9	62.0	0.7	77.0	0.5	106.0	0.4	149.0	0.8
43.0	3.1	63.0	3.0	83.0	0.5	110.0	0.4	150.0	0.1
44.0	33.3	65.0	1.0	84.0	0.5	113.0	1.7	151.0	0.3

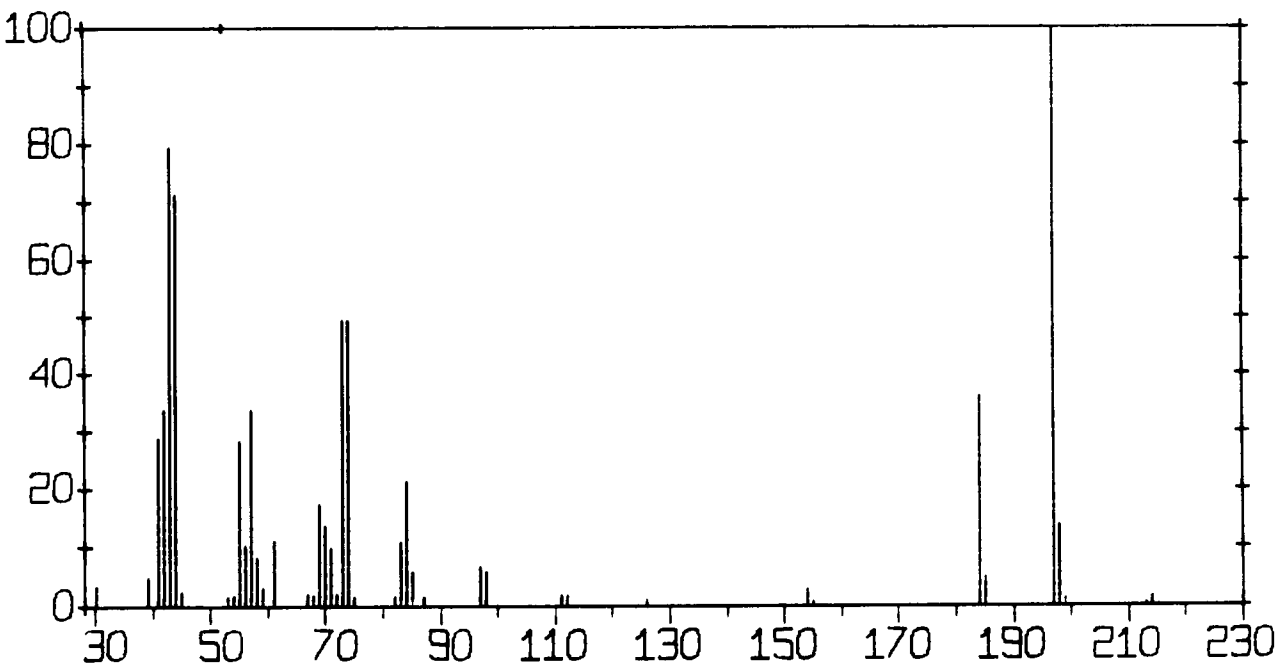
OBSERVED METASTABLES
51.8,



N-NITROSOMETHYLUNDECYLAMINE
MW = 214 C12.H26.N2.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	3.4	55.0	28.5	70.0	13.7	85.0	6.0	184.0	36.2
39.0	4.9	56.0	10.2	71.0	10.0	87.0	1.7	185.0	4.9
41.0	29.1	57.0	34.0	72.0	2.1	97.0	6.7	197.0	100.0
42.0	34.0	58.0	8.2	73.0	49.4	98.0	5.9	198.0	13.7
43.0	79.6	59.0	3.1	74.0	49.4	111.0	1.9	199.0	1.2
44.0	71.4	61.0	11.2	75.0	1.7	112.0	2.0	213.0	0.5
45.0	2.5	67.0	2.1	82.0	1.6	126.0	1.3	214.0	1.6
53.0	1.7	68.0	2.0	83.0	10.9	154.0	2.9	215.0	0.2
54.0	2.0	69.0	17.5	84.0	21.4	155.0	0.7		

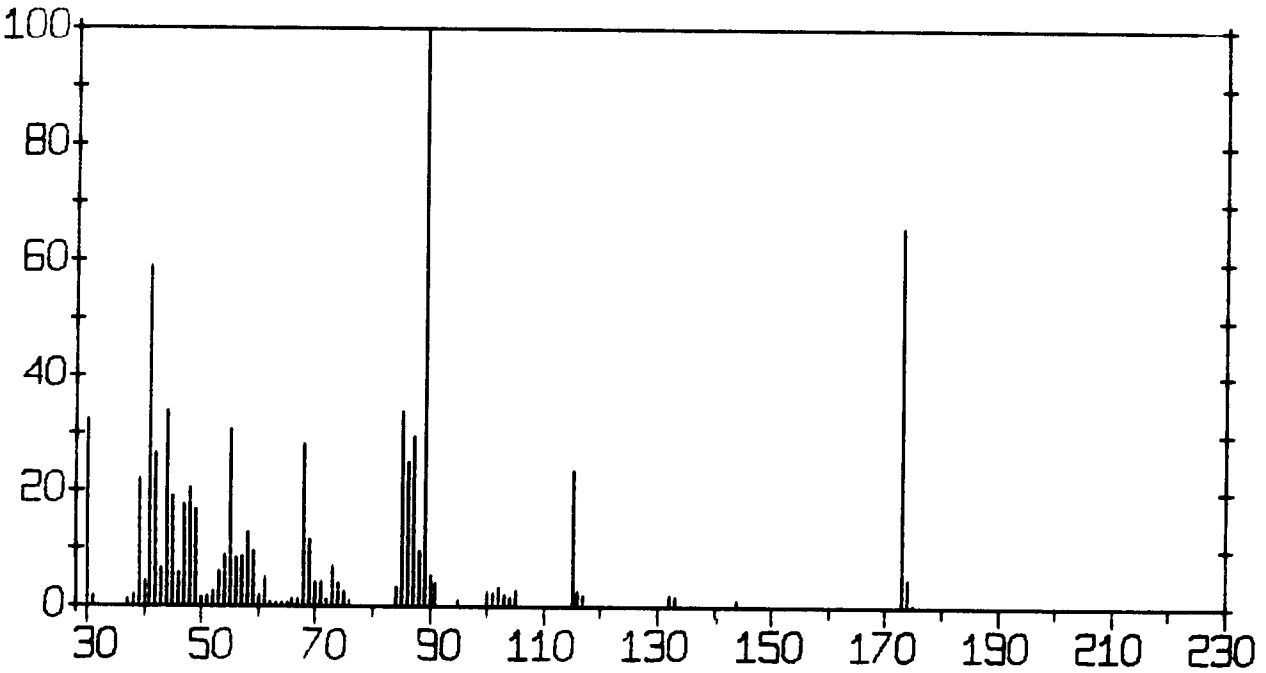
OBSERVED METASTABLES
181.5, 120.5,



N-NITROSOALDICARB
MW = 219 C7.H13.N3.O3.S

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	32.5	49.0	17.0	63.0	0.6	84.0	3.5	104.0	1.7
31.0	2.0	50.0	1.6	64.0	0.7	85.0	34.0	105.0	3.1
37.0	1.1	51.0	2.0	65.0	0.6	86.0	25.1	115.0	23.7
38.0	2.2	52.0	2.8	66.0	1.4	87.0	29.6	116.0	2.8
39.0	22.2	53.0	6.2	67.0	1.4	88.0	9.6	117.0	2.3
40.0	4.5	54.0	9.0	68.0	28.1	89.0	100.0	132.0	2.2
41.0	59.2	55.0	31.1	69.0	11.8	90.0	5.4	133.0	1.9
42.0	26.6	56.0	8.5	70.0	4.1	91.0	4.2	144.0	1.2
43.0	6.6	57.0	8.7	71.0	4.5	95.0	1.0	173.0	65.9
44.0	34.0	58.0	13.0	72.0	1.2	100.0	2.8	174.0	5.0
45.0	19.2	59.0	9.7	73.0	7.2	101.0	2.5	175.0	0.5
46.0	5.9	60.0	2.2	74.0	4.1	102.0	3.5	219.0	0.3
47.0	17.7	61.0	5.1	75.0	2.6	103.0	2.2	220.0	0.0
48.0	20.7	62.0	0.8	76.0	1.1				

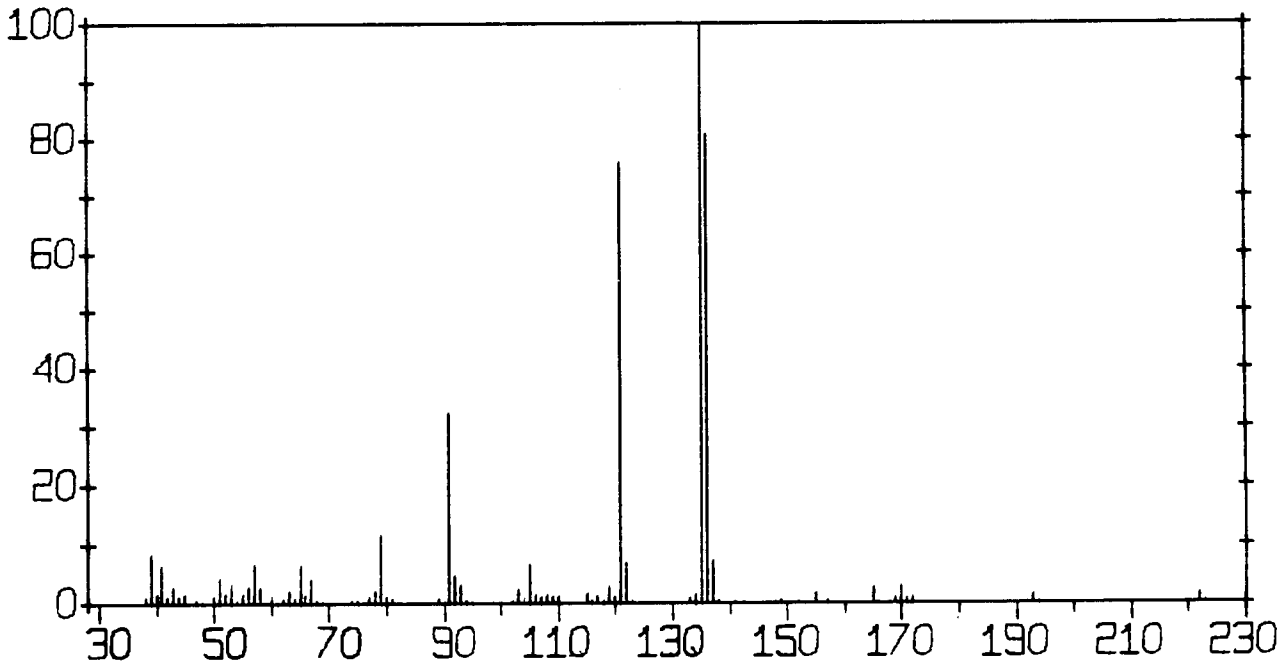
OBSERVED METASTABLES
136.7,



N-NITROSOLANDRIN
MW = 222 C11.H14.N2.O3

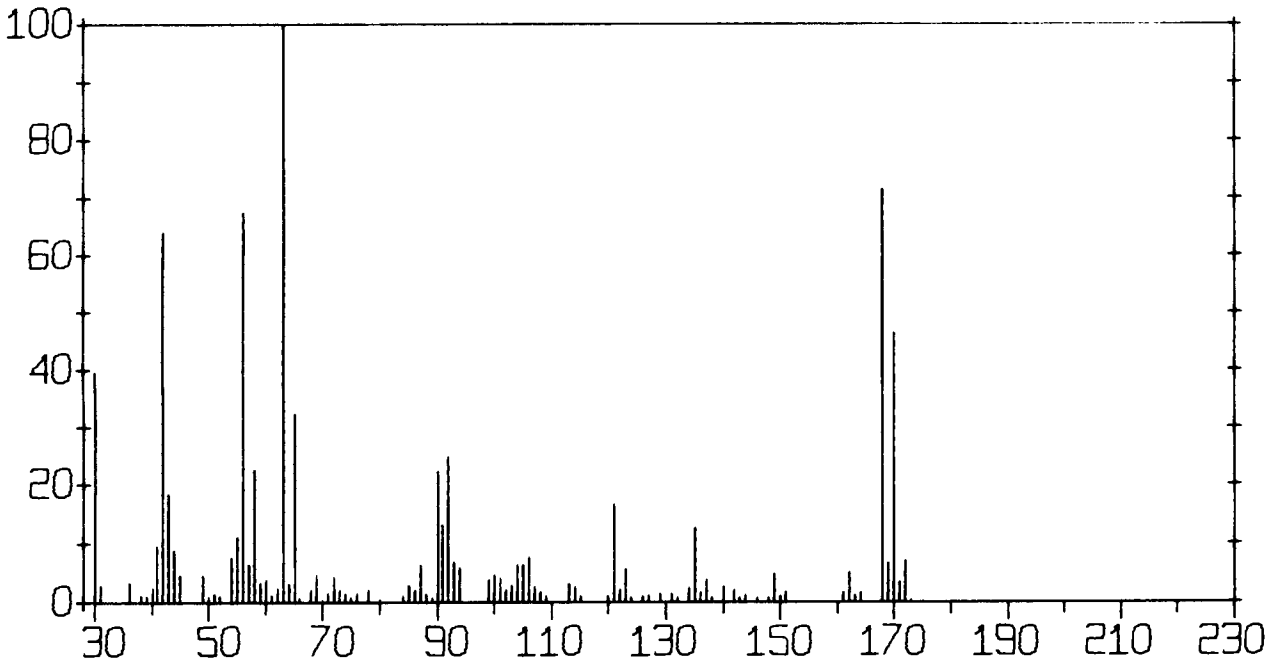
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
38.0	0.9	58.0	2.6	80.0	0.9	110.0	1.2	148.0	0.3
39.0	8.4	59.0	0.3	81.0	0.6	115.0	1.8	149.0	0.3
40.0	1.6	60.0	1.2	87.0	0.2	116.0	0.4	151.0	0.3
41.0	6.4	61.0	0.2	89.0	0.7	117.0	1.3	152.0	0.2
42.0	0.9	62.0	0.6	90.0	0.3	118.0	0.5	155.0	1.7
43.0	2.9	63.0	2.1	91.0	32.5	119.0	3.0	157.0	0.5
44.0	1.1	64.0	0.7	92.0	4.7	120.0	0.9	165.0	2.8
45.0	1.8	65.0	6.7	93.0	3.2	121.0	75.9	166.0	0.3
47.0	0.3	66.0	1.5	94.0	0.5	122.0	6.9	169.0	1.1
48.0	0.2	67.0	4.2	95.0	0.3	123.0	0.4	170.0	2.9
50.0	1.3	68.0	0.4	102.0	0.4	133.0	0.6	171.0	0.6
51.0	4.3	69.0	0.2	103.0	2.5	134.0	1.4	172.0	0.9
52.0	1.8	74.0	0.4	104.0	0.8	135.0	100.0	192.0	0.1
53.0	3.4	75.0	0.4	105.0	6.7	136.0	81.0	193.0	1.5
54.0	0.4	76.0	0.3	106.0	1.5	137.0	7.2	194.0	0.2
55.0	1.7	77.0	0.9	107.0	0.9	138.0	0.4	222.0	1.8
56.0	2.9	78.0	2.1	108.0	1.5	141.0	0.2	223.0	0.2
57.0	6.7	79.0	11.7	109.0	1.3	147.0	0.1		

OBSERVED METASTABLES
46.5, 84.8, 95.4, 101.4, 107.7, 113.0,



N-NITROSO-1-METHYL-3,3-BIS(2-CHLOROETHYL)UREA
MW = 227 C6.H11.N3.O2.CL2

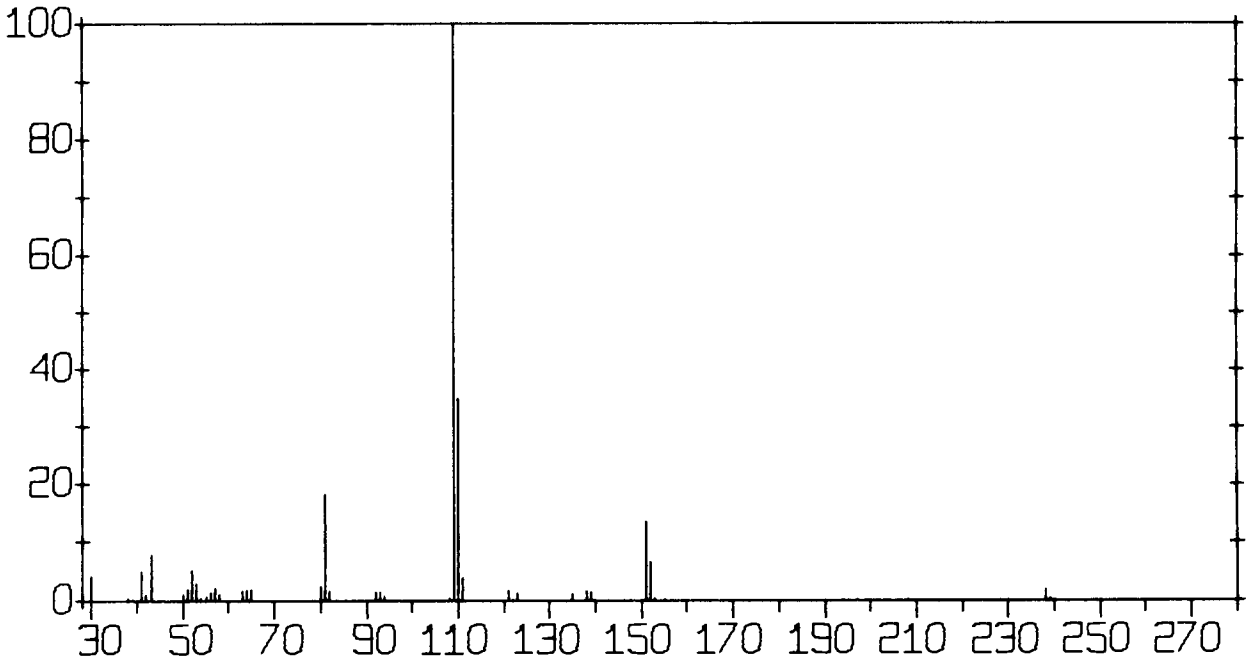
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	39.8	59.0	3.3	85.0	3.0	109.0	0.8	140.0	2.6
31.0	3.0	60.0	3.9	86.0	2.1	113.0	3.3	142.0	2.3
36.0	3.5	61.0	1.3	87.0	6.4	114.0	2.8	143.0	0.7
38.0	1.1	62.0	2.5	88.0	1.4	115.0	0.9	144.0	1.2
39.0	1.1	63.0	100.0	89.0	0.8	120.0	0.9	146.0	0.7
40.0	2.5	64.0	3.2	90.0	22.5	121.0	16.7	148.0	0.8
41.0	9.8	65.0	32.5	91.0	13.2	122.0	2.3	149.0	5.0
42.0	64.2	66.0	0.7	92.0	25.0	123.0	5.7	150.0	1.0
43.0	18.5	68.0	2.2	93.0	6.9	124.0	0.7	151.0	1.9
44.0	8.9	69.0	4.8	94.0	5.8	126.0	1.0	161.0	1.8
45.0	4.6	70.0	0.5	99.0	3.9	127.0	1.1	162.0	5.1
49.0	4.6	71.0	1.7	100.0	4.8	129.0	1.5	163.0	1.3
50.0	0.9	72.0	4.4	101.0	4.2	131.0	1.4	164.0	1.7
51.0	1.5	73.0	2.3	102.0	2.3	132.0	0.6	168.0	71.4
52.0	0.9	74.0	1.5	103.0	3.0	134.0	2.5	169.0	6.7
54.0	7.6	75.0	0.7	104.0	6.4	135.0	12.8	170.0	46.4
55.0	11.2	76.0	1.7	105.0	6.4	136.0	1.8	171.0	3.5
56.0	67.8	78.0	2.1	106.0	7.8	137.0	4.1	172.0	7.1
57.0	6.6	80.0	0.5	107.0	2.8	138.0	0.8	173.0	0.6
58.0	22.8	84.0	1.1	108.0	2.0				



N-NITROSOBAYGON
MW = 238 C11.H14.N2.O4

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	4.3	53.0	2.8	80.0	2.5	111.0	4.1	153.0	0.5
38.0	0.6	54.0	0.5	81.0	18.1	121.0	1.8	155.0	0.3
39.0	0.2	55.0	0.6	82.0	1.6	122.0	0.3	194.0	0.0
41.0	4.9	56.0	1.4	92.0	1.4	123.0	1.1	197.0	0.1
42.0	1.0	57.0	2.1	93.0	1.4	135.0	0.9	208.0	0.1
43.0	7.8	58.0	1.0	94.0	0.6	138.0	1.6	238.0	2.0
50.0	0.9	63.0	1.6	108.0	0.4	139.0	1.5	239.0	0.4
51.0	1.9	64.0	2.0	109.0	100.0	151.0	13.6	240.0	0.0
52.0	5.1	65.0	1.9	110.0	35.0	152.0	6.3		

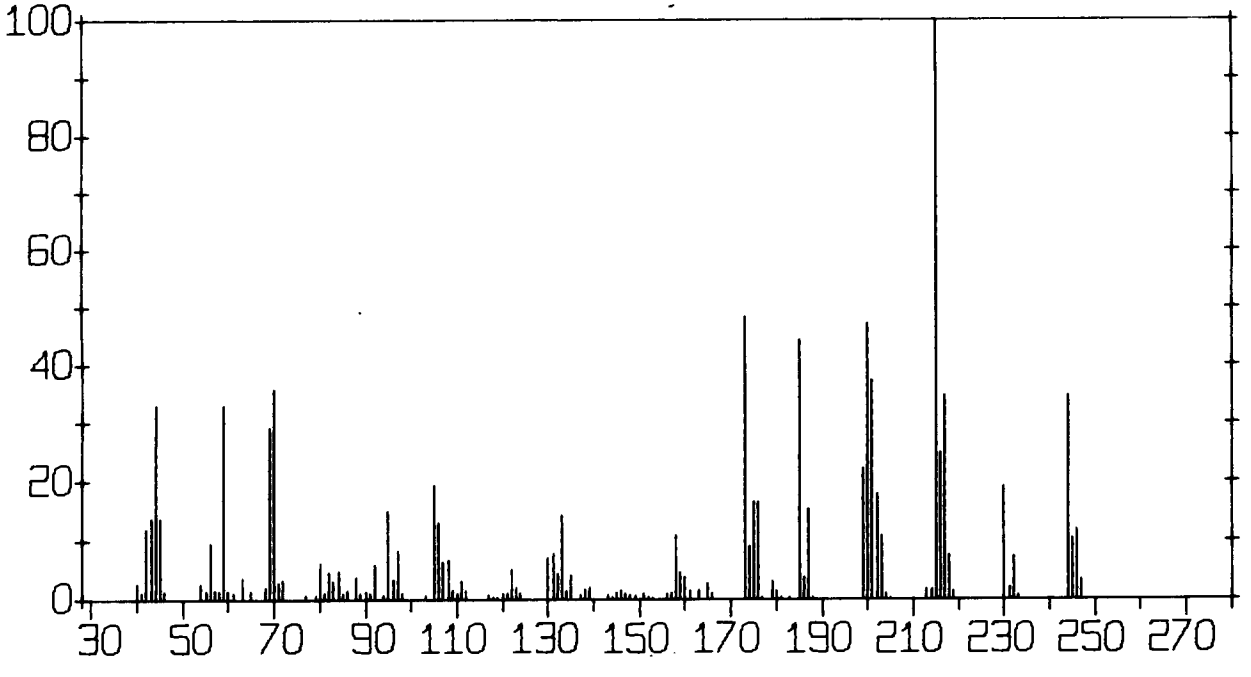
OBSERVED METASTABLES
59.6, 60.3, 78.7, 79.6, 95.8, 96.3,



N-NITROSOATRAZINE
MW = 244 C8.H13.N6.O.CL

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
40.0	2.7	81.0	1.2	117.0	0.7	152.0	0.5	199.0	22.2
41.0	1.2	82.0	4.7	118.0	0.6	153.0	0.5	200.0	47.2
42.0	12.2	83.0	3.3	119.0	0.5	156.0	0.9	201.0	37.5
43.0	13.8	84.0	5.0	120.0	1.0	157.0	1.3	202.0	18.0
44.0	33.3	85.0	0.9	121.0	1.2	158.0	11.1	203.0	11.1
45.0	13.8	86.0	1.8	122.0	5.2	159.0	4.7	204.0	1.1
46.0	1.5	88.0	3.8	123.0	2.3	160.0	3.8	205.0	0.5
54.0	2.7	89.0	1.1	124.0	1.0	161.0	1.6	210.0	0.3
55.0	1.4	90.0	1.5	130.0	7.2	163.0	1.6	213.0	1.9
56.0	9.7	91.0	1.0	131.0	8.0	165.0	2.7	214.0	1.9
57.0	1.7	92.0	6.1	132.0	4.4	166.0	1.2	215.0	100.0
58.0	1.5	94.0	0.6	133.0	14.4	173.0	48.6	216.0	25.0
59.0	33.3	95.0	15.2	134.0	1.5	174.0	9.1	217.0	34.7
60.0	1.4	96.0	3.6	135.0	4.1	175.0	16.6	218.0	7.7
61.0	1.2	97.0	8.6	137.0	0.7	176.0	16.6	219.0	1.5
63.0	3.8	98.0	1.3	138.0	1.9	177.0	0.5	230.0	19.1
65.0	1.3	103.0	0.7	139.0	2.2	179.0	3.3	231.0	2.2
68.0	2.3	105.0	19.4	143.0	0.7	180.0	1.5	232.0	7.5
69.0	29.1	106.0	13.3	144.0	0.5	181.0	0.3	233.0	0.7
70.0	36.1	107.0	6.3	145.0	1.3	183.0	0.5	244.0	34.7
71.0	3.0	108.0	6.6	146.0	1.8	185.0	44.4	245.0	10.5
72.0	3.4	109.0	1.6	147.0	1.0	186.0	3.8	246.0	11.9
77.0	0.7	110.0	1.1	148.0	0.6	187.0	15.5	247.0	3.6
79.0	0.8	111.0	3.3	149.0	0.6	188.0	0.5	248.0	0.3
80.0	6.3	112.0	1.6	151.0	0.9				

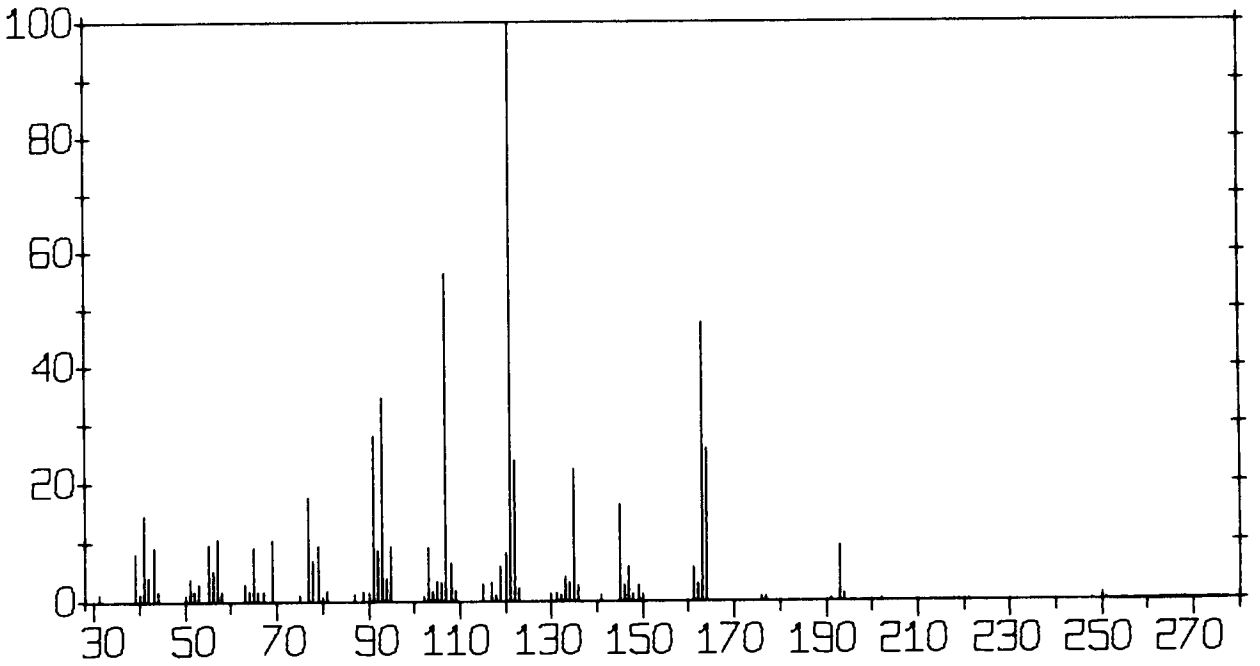
OBSERVED METASTABLES
139.1, 141.0,



N-NITROSOBUXTEN
MW = 250 C13.H18.N2.O3

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
31.0	1.1	65.0	9.1	95.0	9.5	123.0	2.1	162.0	2.9
39.0	8.2	66.0	1.6	102.0	0.8	130.0	1.1	163.0	47.8
40.0	1.2	67.0	1.6	103.0	9.1	131.0	1.5	164.0	26.0
41.0	14.7	69.0	10.4	104.0	1.7	132.0	0.9	176.0	0.6
42.0	4.1	75.0	1.0	105.0	3.4	133.0	4.3	177.0	0.7
43.0	9.1	77.0	17.8	106.0	3.2	134.0	3.3	191.0	0.5
44.0	1.6	78.0	6.9	107.0	56.5	135.0	22.6	193.0	9.5
50.0	1.0	79.0	9.5	108.0	6.5	136.0	2.7	194.0	1.2
51.0	3.9	80.0	0.8	109.0	1.9	141.0	0.9	202.0	0.4
52.0	1.7	81.0	1.9	115.0	2.9	145.0	16.5	218.0	0.2
53.0	2.9	87.0	1.3	117.0	3.2	146.0	2.7	219.0	0.1
55.0	9.7	89.0	1.8	118.0	1.0	147.0	6.0	220.0	0.1
56.0	5.2	90.0	1.4	119.0	6.0	148.0	1.3	221.0	0.2
57.0	10.6	91.0	28.2	120.0	8.2	149.0	2.6	248.0	0.0
58.0	1.7	92.0	8.6	121.0	100.0	150.0	1.2	250.0	1.0
63.0	3.0	93.0	34.7	122.0	23.9	161.0	5.6	251.0	0.2
64.0	1.6	94.0	3.9						

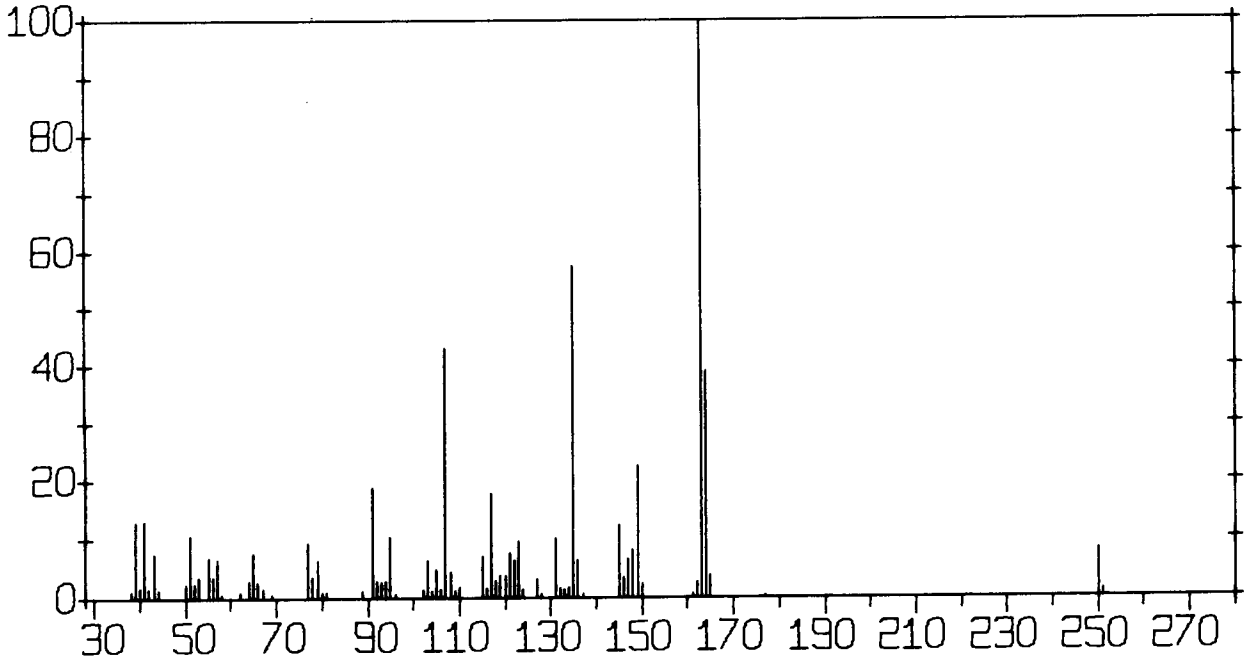
OBSERVED METASTABLES
71.5, 84.8, 111.8, 129.0, 137.7,



N-NITROSOCARBOFURAN
MW = 250 C12.H14.N2.O4

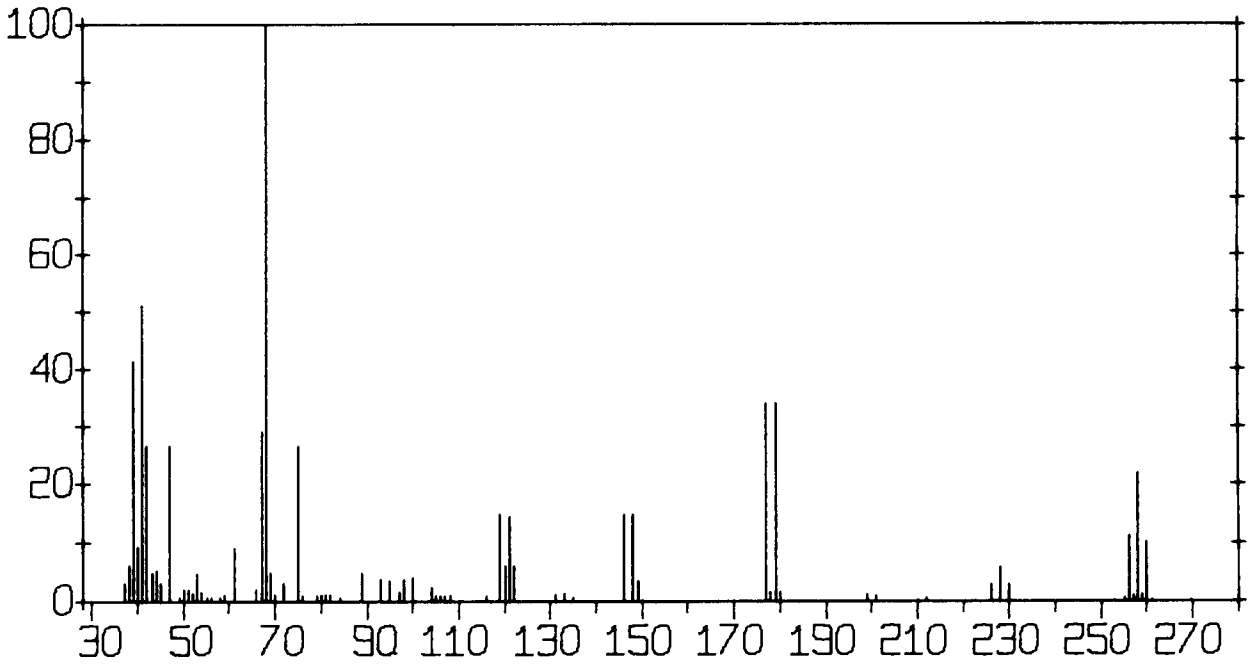
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
38.0	1.3	65.0	7.6	103.0	6.5	123.0	9.6	150.0	2.4
39.0	12.9	66.0	2.7	104.0	1.3	124.0	1.4	161.0	0.8
40.0	2.0	67.0	1.7	105.0	4.9	127.0	3.2	162.0	2.6
41.0	13.1	69.0	0.6	106.0	1.5	128.0	0.7	163.0	100.0
42.0	1.6	77.0	9.4	107.0	43.2	131.0	10.3	164.0	39.1
43.0	7.8	78.0	3.7	108.0	4.5	132.0	1.7	165.0	3.9
44.0	1.5	79.0	6.5	109.0	1.1	133.0	1.5	176.0	0.2
50.0	2.4	80.0	1.0	110.0	1.9	134.0	2.0	177.0	0.4
51.0	10.7	81.0	1.0	115.0	7.2	135.0	57.7	178.0	0.2
52.0	2.4	89.0	1.1	116.0	1.8	136.0	6.3	190.0	0.3
53.0	3.7	91.0	18.9	117.0	17.9	137.0	0.7	191.0	0.1
55.0	7.0	92.0	3.0	118.0	3.0	145.0	12.5	221.0	0.1
56.0	3.7	93.0	2.7	119.0	4.1	146.0	3.5	222.0	0.1
57.0	6.8	94.0	2.8	120.0	3.9	147.0	6.8	250.0	8.2
58.0	0.6	95.0	10.5	121.0	7.8	148.0	8.2	251.0	1.2
62.0	0.8	96.0	0.7	122.0	6.3	149.0	22.6	252.0	0.1
64.0	2.8	102.0	1.4						

OBSERVED METASTABLES
84.8, 111.1, 111.8, 113.5,



N-NITROSO-3,4-DIBROMOPYRROLIDINE
MW = 256 C4.H6.N2.O.BR2

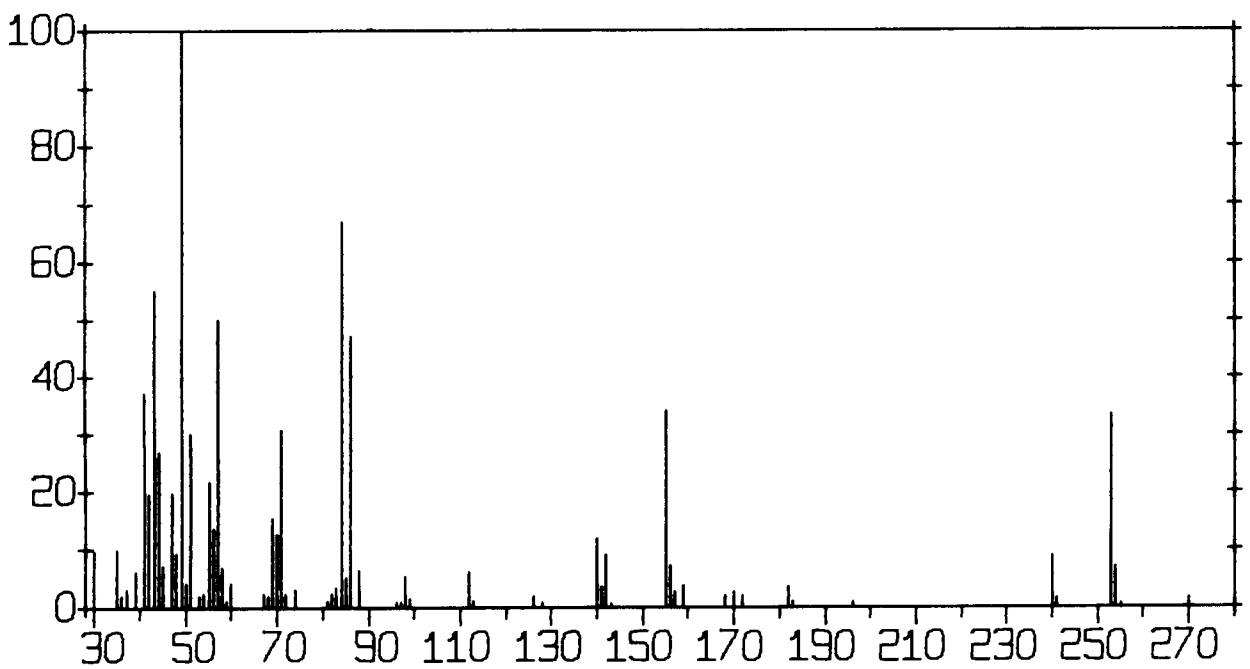
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
37.0	3.1	55.0	0.8	81.0	1.2	119.0	14.8	199.0	1.2
38.0	6.3	56.0	0.7	82.0	1.3	120.0	6.3	201.0	1.0
39.0	41.4	58.0	0.7	84.0	0.8	121.0	14.6	210.0	0.4
40.0	9.5	59.0	1.2	89.0	4.8	122.0	6.3	212.0	0.6
41.0	51.2	61.0	9.2	93.0	3.9	131.0	1.2	226.0	2.9
42.0	26.8	66.0	2.1	95.0	3.6	133.0	1.4	228.0	6.0
43.0	5.1	67.0	29.2	97.0	1.7	135.0	0.6	230.0	2.9
44.0	5.6	68.0	100.0	98.0	3.9	146.0	15.1	253.0	0.3
45.0	3.1	69.0	4.8	100.0	4.1	148.0	15.1	255.0	0.7
47.0	26.8	70.0	1.2	104.0	2.4	149.0	3.6	256.0	11.2
49.0	0.6	72.0	3.1	105.0	0.9	150.0	0.5	257.0	0.9
50.0	2.1	75.0	26.8	106.0	1.0	177.0	34.1	258.0	21.9
51.0	2.1	76.0	0.9	107.0	0.9	178.0	1.8	259.0	1.3
52.0	1.4	79.0	1.0	108.0	0.9	179.0	34.1	260.0	10.2
53.0	5.1	80.0	1.2	116.0	0.9	180.0	1.8	261.0	0.6
54.0	1.7								



N-NITROSODIOCTYLAMINE
MW = 270 C16.H34.N2.O

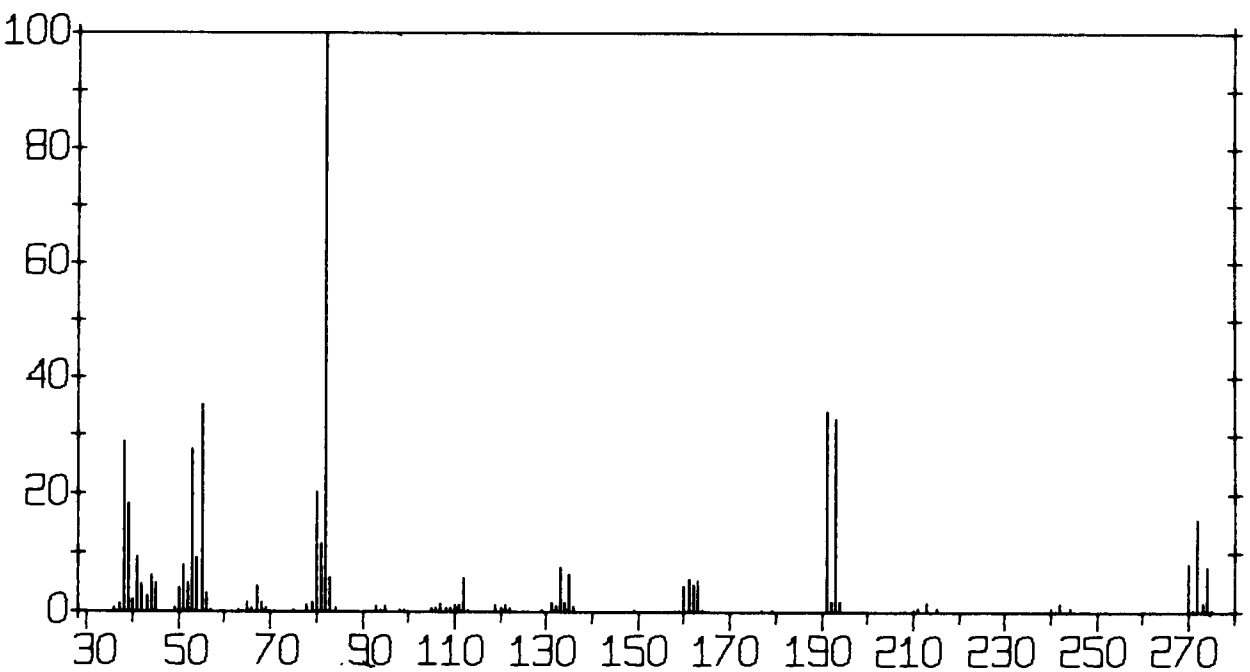
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	9.6	51.0	30.3	72.0	2.4	112.0	6.3	170.0	2.7
35.0	10.0	53.0	2.1	74.0	3.1	113.0	1.2	172.0	2.1
36.0	2.3	54.0	2.4	81.0	1.2	126.0	2.1	182.0	3.7
37.0	3.2	55.0	22.0	82.0	2.4	128.0	0.8	183.0	1.1
39.0	6.2	56.0	13.7	83.0	3.6	140.0	12.0	196.0	0.9
41.0	37.2	57.0	50.3	84.0	67.2	141.0	3.7	240.0	9.0
42.0	19.6	58.0	6.8	85.0	5.1	142.0	9.3	241.0	1.7
43.0	55.1	59.0	1.3	86.0	47.2	143.0	0.8	253.0	33.4
44.0	26.8	60.0	4.3	88.0	6.4	155.0	34.1	254.0	6.8
45.0	7.2	67.0	2.5	96.0	1.0	156.0	7.2	255.0	0.8
47.0	20.0	68.0	2.3	97.0	0.9	157.0	2.7	269.0	0.3
48.0	9.5	69.0	15.5	98.0	5.5	159.0	4.0	270.0	1.6
49.0	100.0	70.0	12.7	99.0	1.7	168.0	2.3	271.0	0.3
50.0	4.1	71.0	31.0						

OBSERVED METASTABLES
236.9,



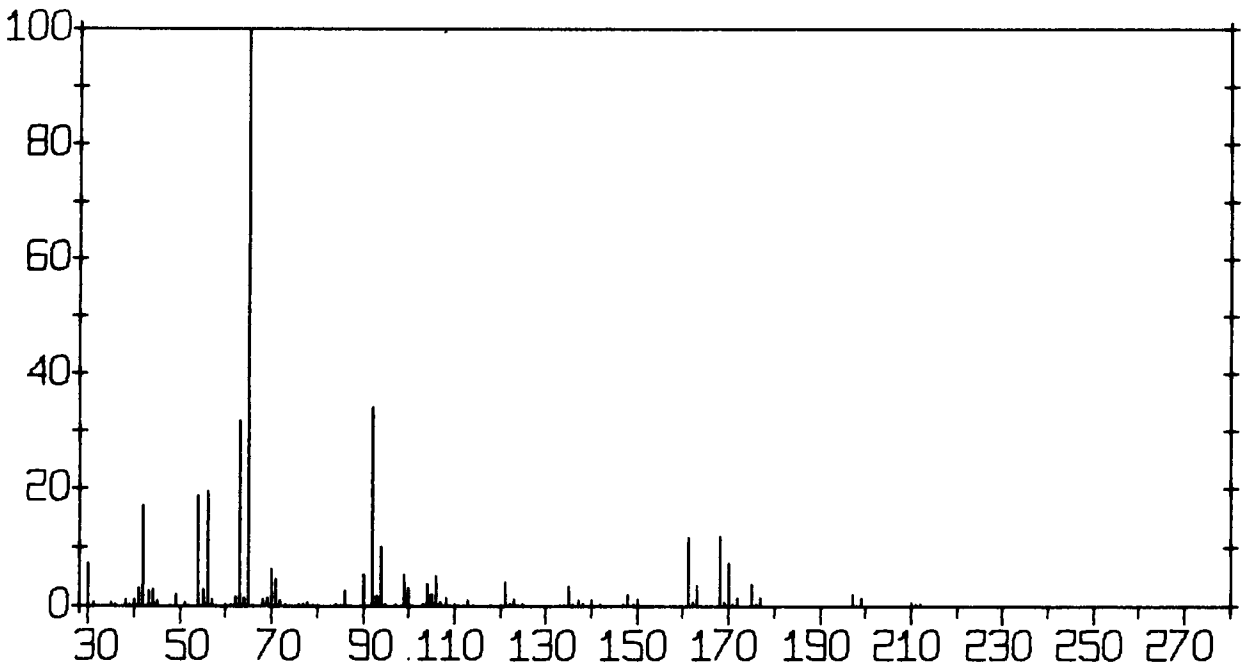
N-NITROSO-3,4-DIBROMOPIPERIDINE
MW = 270 C5.H8.N2.O.BR2

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
36.0	0.6	63.0	0.4	95.0	0.9	133.0	7.6	194.0	1.9
37.0	1.3	64.0	0.3	98.0	0.5	134.0	1.8	199.0	0.2
38.0	28.9	65.0	1.7	99.0	0.6	135.0	6.5	208.0	0.3
39.0	18.4	66.0	0.7	105.0	0.8	136.0	1.0	210.0	0.3
40.0	2.3	67.0	4.4	106.0	0.7	149.0	0.3	211.0	0.8
41.0	9.4	68.0	1.7	107.0	1.5	151.0	0.2	213.0	1.7
42.0	4.7	69.0	0.8	108.0	0.8	158.0	0.2	215.0	0.7
43.0	2.6	70.0	0.3	109.0	0.8	159.0	0.3	240.0	0.7
44.0	6.3	71.0	0.3	110.0	1.3	160.0	4.4	241.0	0.3
45.0	5.0	75.0	0.5	111.0	1.1	161.0	5.7	242.0	1.5
49.0	0.7	78.0	1.3	112.0	6.0	162.0	4.7	243.0	0.2
50.0	4.2	79.0	1.7	113.0	0.5	163.0	5.5	244.0	0.6
51.0	7.8	80.0	20.5	119.0	1.1	164.0	0.5	270.0	8.1
52.0	5.0	81.0	11.8	120.0	0.7	177.0	0.3	271.0	0.6
53.0	27.6	82.0	100.0	121.0	1.1	179.0	0.3	272.0	15.7
54.0	9.2	83.0	6.0	122.0	0.7	191.0	34.2	273.0	1.4
55.0	35.5	84.0	0.7	129.0	0.3	192.0	2.1	274.0	7.6
56.0	3.1	93.0	1.0	131.0	1.7	193.0	32.8	275.0	0.5
57.0	0.5	94.0	0.4	132.0	0.9				



N-NITROSO-1,1,3-TRIS(2-CHLOROETHYL)UREA
MW = 275 C7.H12.N3.O2.CL3

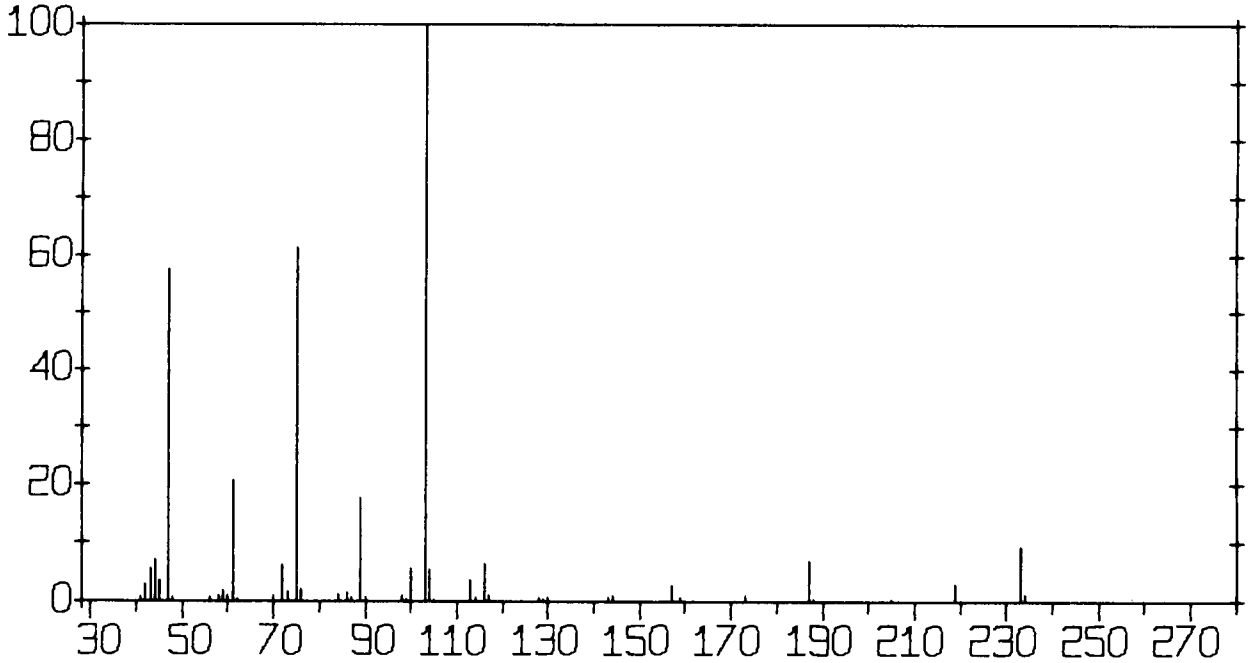
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
30.0	7.6	61.0	0.6	90.0	5.4	118.0	0.3	163.0	3.8
31.0	0.7	62.0	1.8	91.0	0.2	120.0	0.2	164.0	0.3
35.0	0.7	63.0	31.9	92.0	34.2	121.0	4.2	168.0	11.9
36.0	0.4	64.0	1.4	93.0	2.0	122.0	0.6	169.0	0.6
38.0	1.1	65.0	100.0	94.0	10.2	123.0	1.3	170.0	7.6
39.0	0.4	66.0	0.2	95.0	0.4	124.0	0.2	171.0	0.4
40.0	1.2	68.0	1.1	97.0	0.4	125.0	0.3	172.0	1.4
41.0	3.3	69.0	1.6	99.0	5.6	133.0	0.2	175.0	4.0
42.0	17.1	70.0	6.3	100.0	3.1	134.0	0.3	176.0	0.3
43.0	2.8	71.0	4.6	101.0	0.2	135.0	3.5	177.0	1.3
44.0	3.0	72.0	0.9	103.0	0.5	136.0	0.4	197.0	2.3
45.0	0.9	73.0	0.5	104.0	4.0	137.0	1.0	198.0	0.2
48.0	0.2	74.0	0.2	105.0	2.1	138.0	0.4	199.0	1.4
49.0	2.2	76.0	0.6	106.0	5.3	140.0	0.9	201.0	0.2
51.0	0.7	77.0	0.4	107.0	0.8	142.0	0.6	209.0	0.2
52.0	0.2	78.0	0.8	108.0	1.3	147.0	0.6	210.0	0.8
54.0	19.0	79.0	0.1	109.0	0.2	148.0	2.3	211.0	0.4
55.0	3.0	80.0	0.2	110.0	0.3	149.0	0.6	212.0	0.5
56.0	19.7	84.0	0.3	111.0	0.2	150.0	1.1	213.0	0.2
57.0	1.2	85.0	0.3	112.0	0.2	151.0	0.1	214.0	0.1
58.0	0.3	86.0	2.7	113.0	1.0	161.0	11.8	217.0	0.0
60.0	0.5	87.0	0.3	114.0	0.2	162.0	0.8	219.0	0.0



N-NITROSO-BIS(2,2-DIETHOXYETHYL)AMINE
MW = 278 C12,H26,N2,O5

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
41.0	0.7	60.0	1.0	87.0	0.6	114.0	0.6	173.0	0.9
42.0	3.0	61.0	20.7	89.0	17.6	116.0	6.5	187.0	6.9
43.0	5.7	62.0	0.4	90.0	0.7	117.0	1.0	188.0	0.4
44.0	7.3	70.0	1.1	98.0	1.0	128.0	0.6	203.0	0.3
45.0	3.8	72.0	6.1	99.0	0.5	129.0	0.5	205.0	0.3
47.0	57.6	73.0	1.7	100.0	5.7	130.0	0.6	219.0	3.0
48.0	0.6	75.0	61.5	103.0	100.0	143.0	0.7	220.0	0.3
56.0	0.7	76.0	2.1	104.0	5.3	144.0	1.0	233.0	9.6
58.0	0.9	84.0	1.1	105.0	0.5	157.0	2.6	234.0	1.1
59.0	2.1	86.0	1.5	113.0	3.8	159.0	0.8		

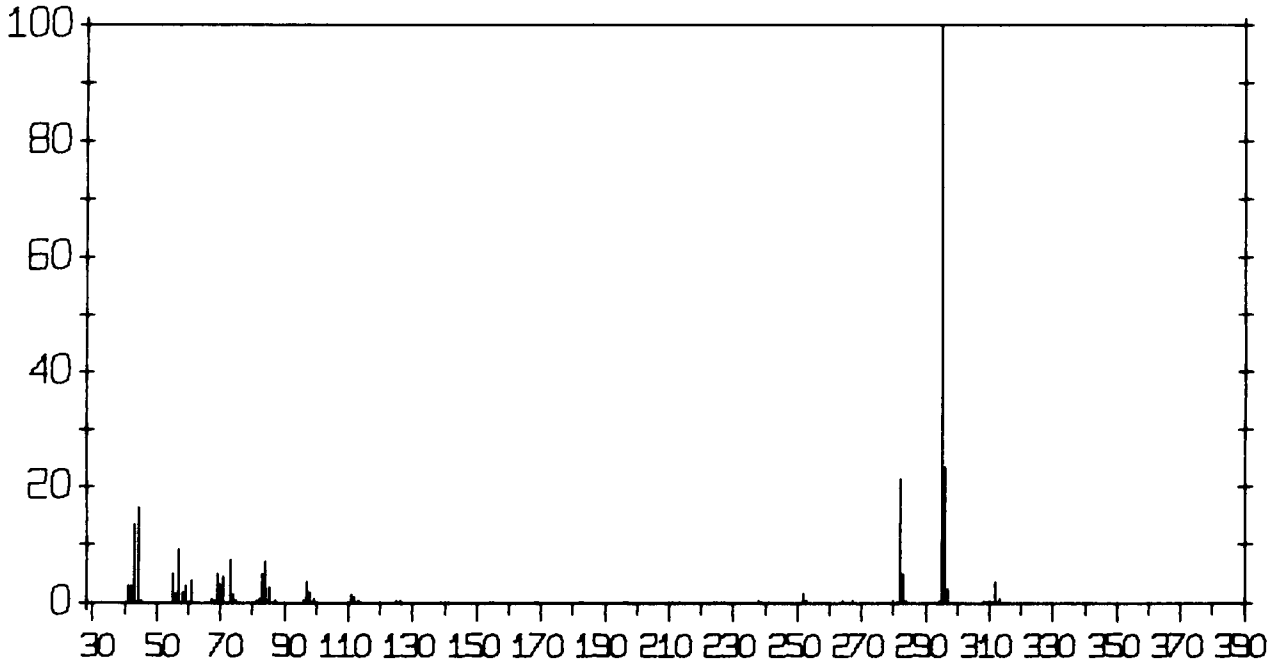
OBSERVED METASTABLES
54.6, 150.1,



N-NITROSOMETHYLOCTADECYLAMINE
MW = 312 C19.H40.N2.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
41.0	2.9	73.0	7.5	113.0	0.4	211.0	0.1	282.0	21.4
42.0	3.0	74.0	1.5	125.0	0.5	213.0	0.1	283.0	5.0
43.0	13.5	75.0	0.5	126.0	0.5	224.0	0.1	284.0	0.5
44.0	16.4	81.0	0.5	139.0	0.2	225.0	0.2	293.0	0.2
45.0	0.5	82.0	0.7	140.0	0.3	226.0	0.1	294.0	0.4
55.0	5.0	83.0	5.0	141.0	0.2	227.0	0.1	295.0	100.0
56.0	1.6	84.0	7.1	154.0	0.2	238.0	0.4	296.0	23.5
57.0	9.2	85.0	2.7	155.0	0.2	239.0	0.2	297.0	2.5
58.0	2.0	87.0	0.5	168.0	0.2	241.0	0.1	298.0	0.1
59.0	3.0	96.0	0.5	169.0	0.2	252.0	1.6	308.0	0.4
61.0	3.9	97.0	3.7	182.0	0.2	253.0	0.5	309.0	0.2
67.0	0.6	98.0	2.0	183.0	0.2	264.0	0.4	310.0	0.5
68.0	0.5	99.0	0.7	196.0	0.1	267.0	0.4	311.0	0.2
69.0	5.0	111.0	1.5	197.0	0.1	280.0	0.5	312.0	3.7
70.0	3.3	112.0	0.9	210.0	0.1	281.0	0.3	313.0	0.8
71.0	4.4								

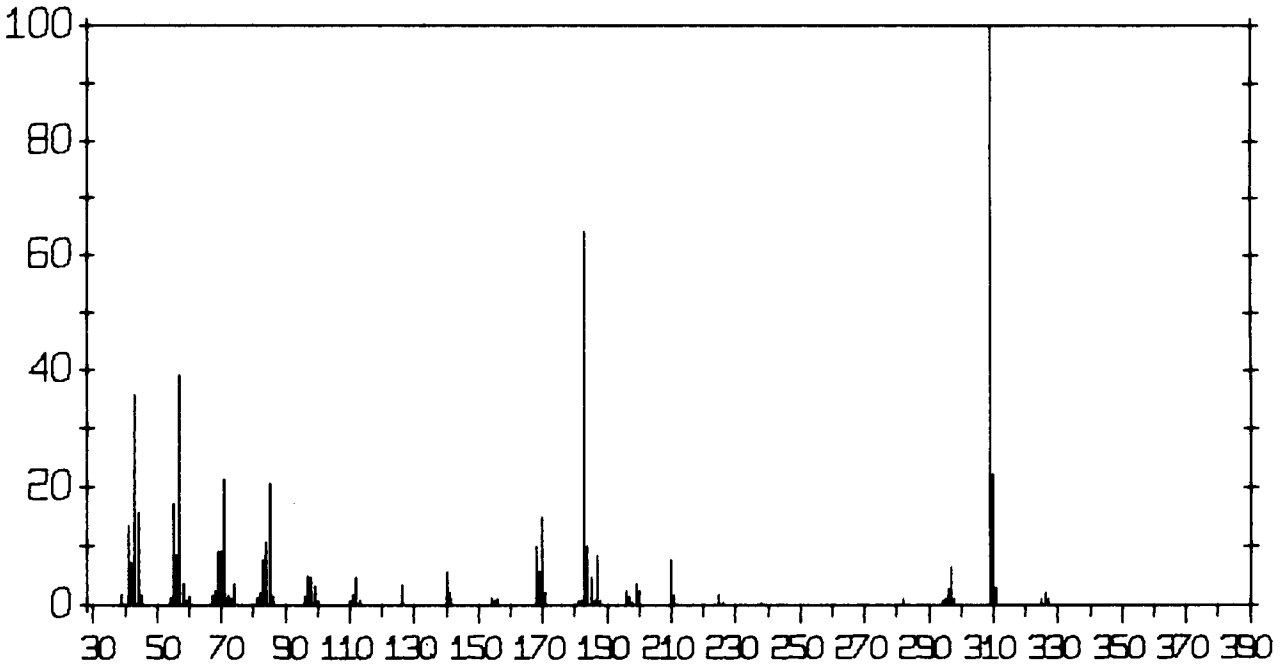
OBSERVED METASTABLES
215.3,



N-NITROSODIDECYLAMINE
MW = 326 C20.H42.N2.O

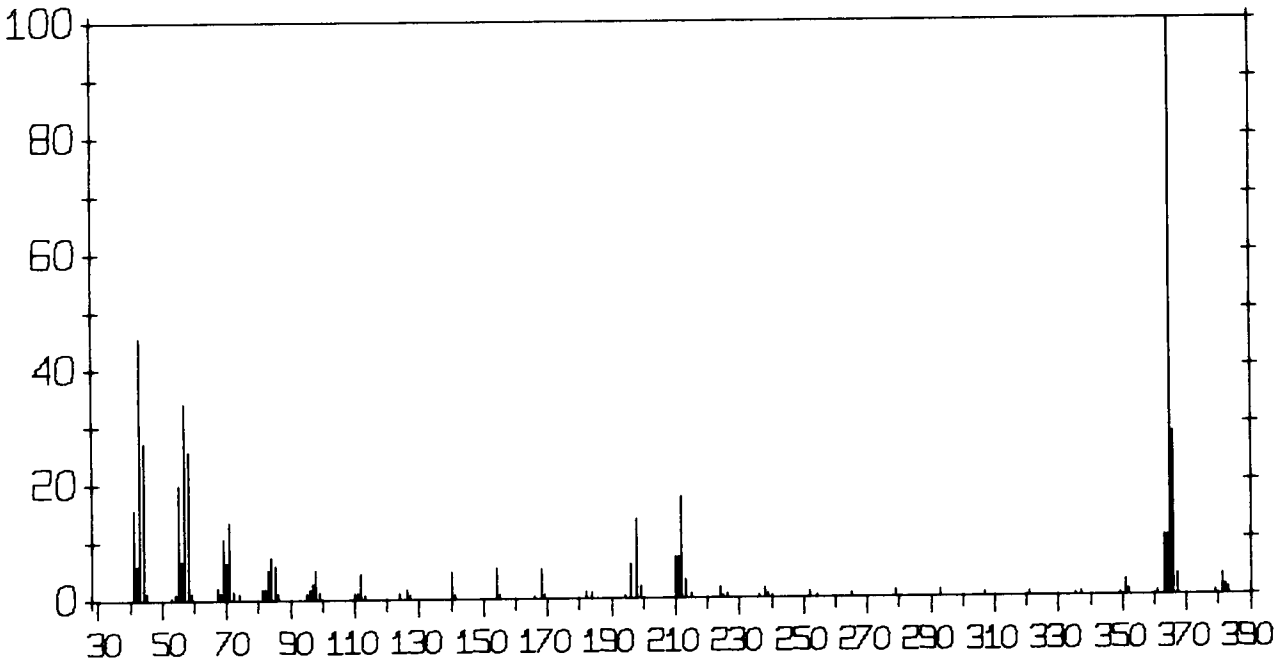
M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
39.0	2.0	70.0	9.2	100.0	0.7	181.0	0.6	225.0	2.0
41.0	13.5	71.0	21.4	110.0	0.7	182.0	0.7	226.0	0.5
42.0	7.1	72.0	1.6	111.0	1.7	183.0	64.2	238.0	0.5
43.0	35.7	73.0	0.9	112.0	4.6	184.0	10.0	282.0	1.0
44.0	15.7	74.0	3.6	113.0	0.8	185.0	4.6	294.0	0.8
45.0	1.8	81.0	1.3	126.0	3.4	186.0	0.7	295.0	1.0
54.0	1.3	82.0	2.3	140.0	5.7	187.0	8.5	296.0	2.7
55.0	17.1	83.0	7.8	141.0	2.1	188.0	0.7	297.0	6.4
56.0	8.5	84.0	10.7	154.0	1.2	196.0	2.5	298.0	0.9
57.0	39.2	85.0	20.7	155.0	0.6	197.0	1.4	309.0	100.0
58.0	3.8	86.0	1.5	156.0	1.0	198.0	0.5	310.0	22.1
59.0	0.8	96.0	1.4	168.0	10.0	199.0	3.7	311.0	2.9
60.0	1.5	97.0	5.0	169.0	5.7	200.0	2.5	325.0	1.0
67.0	1.7	98.0	4.6	170.0	15.0	210.0	7.8	326.0	2.2
68.0	2.5	99.0	3.1	171.0	2.1	211.0	1.6	327.0	0.9
69.0	9.2								

OBSERVED METASTABLES
167.4, 292.9,



N-NITROSODIDODECYLAMINE
MW = 382 C24.H50.N2.O

M/E	INT	M/E	INT	M/E	INT	M/E	INT	M/E	INT
41.0	15.7	72.0	1.6	124.0	1.0	211.0	7.1	321.0	0.6
42.0	6.0	74.0	0.9	126.0	1.7	212.0	17.7	335.0	0.4
43.0	45.7	81.0	2.0	127.0	0.7	213.0	3.1	337.0	0.6
44.0	27.1	82.0	2.0	140.0	4.8	215.0	0.6	349.0	0.4
45.0	1.1	83.0	5.1	141.0	0.7	224.0	2.0	351.0	2.8
53.0	0.6	84.0	7.4	154.0	5.4	225.0	0.4	352.0	1.0
54.0	1.0	85.0	6.0	155.0	0.7	226.0	0.6	361.0	0.6
55.0	20.0	86.0	0.9	166.0	0.4	236.0	0.4	363.0	10.5
56.0	6.8	95.0	1.0	168.0	5.1	238.0	1.8	364.0	10.5
57.0	34.2	96.0	1.6	169.0	0.8	239.0	0.8	365.0	100.0
58.0	25.7	97.0	2.7	182.0	1.3	240.0	0.4	366.0	28.5
59.0	1.3	98.0	5.1	184.0	0.9	252.0	0.8	367.0	3.7
67.0	2.1	99.0	1.1	194.0	0.4	254.0	0.4	379.0	0.6
68.0	1.3	110.0	1.0	196.0	6.0	265.0	0.7	381.0	0.7
69.0	10.8	111.0	0.9	198.0	14.0	279.0	1.1	382.0	1.6
70.0	6.5	112.0	4.5	199.0	2.2	293.0	1.3	383.0	1.2
71.0	13.4	113.0	0.7	210.0	7.1	307.0	0.8		



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