Mass Spectra of N-Nitroso Compounds

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OAK RIDGE NATIONAL LABORATORY

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ANALYTICAL CHEMISTRY AND BIOLOGY DIVISIONS

MASS SPECTRA OF N-NITROSO COMPOUNDS

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SEPTEMBER 1976

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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	101 348 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-DIMETHYLPYPERIDINE	142		75 350 E	19
4-TERTBUTYLPYPERIDINE	170	M 51-54	97 350 E	34
4-PHENYLPYPERIDINE	190	M 66-68	103 351 E	40
NORNICOTINE	177		64 346 W	35
3-CHLOROPYPERIDINE	148		93 350 E	21
4-CHLOROPYPERIDINE	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-DICHLOROPYPERIDINE	182	M 81-82	88 345 W	38
3,4-DIBROMOPYPERIDINE	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	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	79
		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	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-NITROSUATRAZINE							
		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	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-FTHYL-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 40	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	M/E INT
63	49	N-NITROSO-1-METHYL-3,3-BIS(2-CHLOROETHYL)UREA							
		63	100	168	71	56	68	42	64
65	57	N-NITROSO-1,1,3-TRIS(2-CHLOROETHYL)UREA							
		65	100	92	34	63	32	56	20
68	54	N-NITROSO-3,4-DIBROMOPYRROLIDINE							
		68	100	41	51	39	41	177	34
72	36	N-NITROSO-1,1-DIMETHYL-3(2-CHLOROETHYL)UREA							
		72	100	44	41	42	23	30	12
80	31	N-NITROSO-2,6-DICYANOPIPERIDINE							
		80	100	53	77	92	52	164	52
82	56	N-NITROSO-3,4-DIBROMOPIPERIDINE							
		82	100	55	36	191	34	193	33
89	47	N-NITROSOALDICARB							
		89	100	173	66	41	59	44	34
93	37	N-NITROSO-METHYL N-PHENYL CARBAMATE							
		93	100	65	89	123	68	94	28
97	44	1,4-DINITROSO-2,3,5,6-TETRAMETHYLPIPERAZINE							
		97	100	70	98	44	89	41	71
100	45	N-NITROSO-1,1-DIETHYL-3(2-CHLOROETHYL)UREA							
		100	100	72	76	44	33	56	22
103	58	N-NITROSO-BIS(2,2-DIETHOXYETHYL)AMINE							
		103	100	75	62	47	58	31	21
105	35	N-NITROSONORNICOTINE							
		105	100	118	66	177	60	147	47
109	50	N-NITROSOBAYGON							
		109	100	110	35	81	18	151	14
121	52	N-NITROSOBUXTEN							
		121	100	107	57	163	48	93	35
124	13	N-NITROSO-BIS(CYANOMETHYL)AMINE							
		124	100	40	75	67	33	41	21
135	48	N-NITROSOLANDRIN							
		135	100	136	81	121	76	91	33
160	40	N-NITROSO-4-PHENYLPIPERIDINE							
		160	100	42	43	91	43	56	39
163	53	N-NITROSOCARBOFURAN							
		163	100	135	58	107	43	164	39
170	34	N-NITROSO-4-TERTBUTYLPIPERIDINE							
		170	100	140	81	57	72	42	58
197	46	N-NITROSOMETHYLUNDECYLAMINE							
		197	100	43	80	44	71	73	49
215	51	N-NITROSOATRAZINE							
		215	100	173	49	200	47	185	44
295	59	N-NITROSOMETHYLOCTADECYLAMINE							
		295	100	296	24	282	21	44	16
309	60	N-NITROSODIDECYLAMINE							
		309	100	183	64	57	39	43	36
365	61	N-NITROSODIDODECYLAMINE							
		365	100	43	46	57	34	366	29

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 sub-zero 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 C₃H₅D₃N₂O

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 C₄D₁₀N₂O

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						

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N-NITROSOETHYL-2-HYDROXYETHYLAMINE
MW = 118 C₄H₁₀N₂O₂

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 C₄H₄N₄O

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 C₆H₁₀N₂O

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 C₃H₇N₃O₃

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	0.2
41.0	7.4	55.0	0.4	71.0	0.5	114.0	0.1

N-NITROSO-BIS(2-HYDROXYETHYL)AMINE
MW = 134 C₄H₁₀N₂O₃

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 C₃H₆N₃O₂F

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 C₄H₅D₃N₂O₃

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-DIMETHYLPYPERIDINE
 MW = 142 C₇H₁₄N₂O

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
49.0	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 C₅H₁₁N₃O₂

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 C₅H₉N₂O.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 C₅H₅D₅N₂O₃

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	9.5	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	5.2
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 C₆H₈N₄O

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 C₆H₁₀N₂O₃

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 C₈H₁₈N₂O

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 C₆H₁₄N₂O₃

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 C₆H₁₄N₂O₃

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 C₇H₈N₄O

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

95.4, 109.5,

N-NITROSO-3,4-DICHLOROPYRROLIDINE
 MW = 168 C₄H₆N₂O.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	0.9	63.0	2.3	93.0	2.7	105.0	2.1	170.0	28.1
48.0	1.3	64.0	2.9	85.0	1.9	109.0	11.3	171.0	1.9
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 C₄H₈N₂O.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-TERTBUTYLPYPERIDINE
MW = 170 C₉H₁₈N₂O

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 C₉H₁₁N₃O

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 C₅H₁₀N₃O₂Cl

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	2.7	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 C₈H₈N₂O₃

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 C₅H₈N₂O.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-PHENYLPYPERIDINE
MW = 190 C11H14N2O

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	2.3	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 C₅H₉N₃O₃S

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	5.0	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 C₆H₁₂N₂O.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	59.0	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	1.0	69.0	2.5	94.0	1.0				

OBSERVED METASTABLES
 80.1, 82.0,

1,4-DINITROSO-2,3,5,6-TETRAMETHYLPIPERAZINE
MW = 200 C₈H₁₆N₄O₂

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 C₁₂H₂₆N₂O

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

191.5, 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	2.9	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	0.9	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 C₈H₁₃N₆O₂CL

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	175.0	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-NITROSOBUTYRNE
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-NITROSCARBOFURAN
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 C₄H₆N₂O₂Br₂

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 C₁₆H₃₄N₂O

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 C₅H₈N₂O.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 C₁₂H₂₆N₂O₅

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 C₁₉H₄₀N₂O

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 C₂₀H₄₂N₂O

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 C₂₄H₅₀N₂O

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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