

INFRARED PRISM COLLECTION

**1980
CUMULATIVE
NUMERICAL
INDEX**

No.1 - 59000



**STANDARD
SPECTRA**

Sadtler Research Laboratories

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Researchers, Editors & Publishers

Printed in the United States of America

ISBN 0 8456 0048 6

INTRODUCTION

The 1980 Cumulative Numerical Index for Infrared Prism Standard Spectra contains the 59,000 pure compounds for which Sadtler Research Laboratories has issued prism infrared reference spectra through January 1980.

This index also includes the spectrum numbers of the same compounds as published in the companion Sadtler publications of 48,000 infrared grating spectra, 48,000 ultraviolet spectra, 32,000 60 MHz nuclear magnetic resonance spectra and 7,000 carbon-13 NMR spectra.

In addition to Sadtler spectra, the column of this index titled NMR includes the reference number of spectra published by Varian Associates and JEOL (Japan Electron Optics Laboratory Co., Ltd.). The Varian numbers are preceded by the letter V and the JEOL numbers either by the symbol * representing 100 MHz spectra, the letter F for ^{19}F spectra and the letter J for 60 MHz spectra.

The inclusion of the reference spectrum numbers for a variety of instrumental techniques provides the user with the ability to rapidly locate all available spectral data for compound identification or characterization.

This index may also be used in conjunction with the corresponding Sadtler Standard Prism Spec-Finder[®] publication to identify the reference spectrum numbers located by that comparison technique or other computerized data search and comparison methods such as the IRIS[®] system. Space limitations prevent inclusion of cross-references to the collections of Raman spectra, 100 MHz nuclear magnetic resonance spectra, fluorescence spectra and infrared vapor phase spectra, therefore each of these publications contains its own individual set of indexes.

During the past years those published infrared prism spectra which are not available in the infrared grating format have been re-issued and renumbered in the Sadtler Standard Grating Spectra publication to provide maximum obtainable data to the user of that collection. The entries for these spectra, numbered from 38001P to 48487P, are included in the column titled GRATING and denoted by the P suffix.

The naming of the chemical compounds in the Sadtler reference spectra collections closely follows the Chemical Abstracts (CA) system of nomenclature, whereby the parent name is assigned on the basis of a predefined order of functionality and the arrangement of substitutions to the parent compound in alphabetical order. Recently CA has revised its nomenclature system but the new alterations are not incorporated in the Sadtler indexes at this time. In addition to the systematized names, many cross-references to frequently used trivial names are also included in this index.

Whenever there is more than one spectrum available in any collection for a given compound, the alternative spectrum numbers are listed below the initial entry in this index. Similarly the infrared spectra of some compounds were run in various media when this additional information was pertinent. The media are designated at the end of the name in the index entry by the following abbreviations:

- B - Between Salts (neat)
- C - Cell
- F - Film
- G - Gas
- K - KBr
- M - Mineral Oil Mull
- S - Solution

Since the Sadtler indexing system is totally computerized, certain limitations are imposed in nomenclature symbolism. Deviations which appear in the printed index are as follows:

- / (slash) - Read as parenthesis, bracket, or brace
- ▢ (lozenge) - Read as indication of superscripting
(See last of the examples on the next page)
- PR - Read as "prime". Therefore 2PR is read as 2'.
- * (asterisk) - Also read as "prime"

Lack of provision for Greek letters, super or subscripts (except as noted above) or lower case letters causes the following changes from normal notation:

- A - Read as a or α
- B - Read as b or β
- G - Read as g or γ
- D - Read as d or δ
- O - Read as o, ortho or oxygen
- M - Read as m or meta
- N - Read as normal or nitrogen
- P - Read as p, para or phosphorus
- S - Read as s (symmetrical) or sulfur
- D & L - Still retain their original significance when used in conjunction with carbohydrates.

Some examples illustrating the variations to be encountered are shown on the opposite page.

Chemical Abstracts System

s-Triazine, 4-amino-6-(p-bromoanilino)-1,2-dihydro-2,2-dimethyl-,

Benz[a] anthracene-7,12-dione

Chryseno[6,5-d] oxazole

Spiro[cyclopropane-1,9'-fluorene],2-acetyl-,

Tricyclo[3,3,1,1^{3,7}] decane

Sadtler Index

S-TRIAZINE, 4-AMINO-6-/P-BROMOANILINO/-1,2-DIHYDRO-2,2-DIMETHYL-,

BENZ/A/ANTHRACENE-7,12-DIONE

CHRYSENO/6,5-D/OXAZOLE

SPIRO/CYCLOPROPANE-1,9PR-FLUORENE/,2-ACETYL-,

or

SPIRO/CYCLOPROPANE-1,9*FLUORENE/,2-ACETYL-,

TRICYCLO/3,3,1,1^{3,7}/DECANE

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NAME	PRISM	GRATING	UV	NMR	C-13
PROPANE, 2-NITRO-,	1	1	1	V 41	1601
PROPANE, 2-NITRO-,	1	1	1	13155	1601
BUTYL ALCOHOL, TERT-,	2	2		V 423	1602
BUTYL ALCOHOL, TERT-,	2	2		10198	1602
2-PROPANOL, 2-METHYL-,	2	2		V 423	1602
2-PROPANOL, 2-METHYL-,	2	2		10198	1602
BENZOYL CHLORIDE	3	5402	2	3147	1
ACETIC ACID, ETHYL ESTER	4	3		10291	401
ACETIC ACID, ETHYL ESTER	4	3		V 79	401
ETHYL ACETATE	4	3		10291	401
ETHYL ACETATE	4	3		V 79	401
PHOSPHONIC DICHLORIDE, PHENYL-,	5	33801	21873	8044	4801
ANILINE, N,N-DIMETHYL-,	6	4	3	1	2
ETHANE, NITRO-,	7	5	4	2	402
TOLUENE, A-CHLORO-,	8	6	5	3	3
BENZYL CHLORIDE	8	6	5	3	3
2-PICOLINE	9	7	6	566	403
2-PICOLINE	9	7	6	J 192	403
BROMOFORM	10	8		6375	1603
METHANE, TRIBROMO-,	10	8		6375	1603
O-XYLENE	11	9	7	10199	4
O-XYLENE	11	9	7	V 201	4
BENZENE, NITRO-,	12	10	8	4	1401
PALMITIN, 2-OLEO-1,3-DI-,	13	41001P			
DODECANOIC ACID	14	11		10325	5
LAURIC ACID	14	11		10325	5
PYRIDINE	15	12	9	10200	1201
PYRIDINE	15	12	9	V 96	1201
ISOBUTYL ALCOHOL	16	13		7219	801
PALMITIN, 2-STEARO-1,3-DI-,	17	41002P			
2-NAPHTHOL	18	8001	2551	3230	4601
XANTHYLIUM TETRACHLOROFERRATE/III/,	19	41003P			
4-/9-ETHYLCARBAZOL-3-YL/METHYLENE/-					
1,2,3,4-TETRAHYDRO-,					
PHOSPHORIC ACID, TRI-M-TOLYL ESTER	20	8002	10	301	1604
M-TOLYL PHOSPHATE	20	8002	10	301	1604
CHOLINE CHLORIDE, CARBAMATE	21	21001		8045	
CARBACHOL	21	21001		8045	
O-TOLYL PHOSPHATE	22	15001		7011	1605
PHTHALIC ACID, BIS/2-METHOXYETHYL/	23	14	11	1120	6
ESTER					
ADIPIC ACID, BIS/2-ETHYLHEXYL/	24	8003		2913	1606
ESTER					
FORMIC ACID	25	15		6653	2801
PHTHALIC ACID, BIS/2-BUTOXYETHYL/	26	16	12	1399	1607
ESTER					
ETHANE, 1,1-BIS/P-CHLOROPHENYL/-	27	15014			4401
2,2,2-TRICHLORO-,					
DDT	27	15014			4401
PHTHALIC ACID, BIS/2-ETHYLHEXYL/	28	18401	22080	9392	5201
ESTER					
ACETIC ACID, BENZYLIDENE-,	29	18402	3452	10168	7
ACETIC ACID, BENZYLIDENE-,	29	18402	3452	V 230	7
ACRYLIC ACID, 3-PHENYL-,	29	18402	3452	10168	7
ACRYLIC ACID, 3-PHENYL-,	29	18402	3452	V 230	7
CINNAMIC ACID	29	18402	3452	10168	7
CINNAMIC ACID	29	18402	3452	V 230	7
FORMIC ACID, STYRYL-,	29	18402	3452	10168	7
FORMIC ACID, STYRYL-,	29	18402	3452	V 230	7
1-NAPHTHOL	30	8004	2045	5	4602
4-PICOLINE	31	17	13	889	8
4-PICOLINE	31	17	13	J 194	8
3-PICOLINE	32	18	14	890	9
3-PICOLINE	32	18	14	* 136	9
P-CRESOL	33	8005	15	9491	1608
BENZENE, CHLORO-,	34	19	16	714	1402
ETHANE, 1,2-DICHLORO-,	35	20		7304	1609
ACETIC ACID, TRICHLORO-,	36	29681		6	10
PHTHALIC ACID, DICYCLOHEXYL ESTER	37	3837	225	1199	124
PHOSPHONOTHIOIC ACID, PHENYL-,	38	41004P	17		
O,O-DIPHENYL ESTER					
ISOBENZOFURAN, 1,3-DIHYDRO-1,3-	39	21002	18	10133	
DIOXO-,					
1,3-ISOBENZOFURANDIONE	39	21002	18	10133	
PHTHALIC ANHYDRIDE	39	21002	18	10133	
P-DIOXANE	40	21		1193	11
P-DIOXIN, TETRAHYDRO-,	40	21		1193	11
CYCLOHEXANOL	41	10960		7	1610
CYCLOHEXANONE, 4-METHYL-,	42	24506	19	8	404
PROPANE, 1-NITRO-,	43	22	20	10192	
PROPANE, 1-NITRO-,	43	22	20	V 42	
2-PENTANONE, 4-METHYL-,	44	23	21	10201	405
2-PENTANONE, 4-METHYL-,	44	23	21	V 139	405
P-TOLUENETHIOL	45	8006	11403	V 168	4603
P-TOLUENETHIOL	45	8006	11403	17031	4603

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NAME	PRISM	GRATING	UV	NMR	C-13
2-NAPHTHYLAMINE	46	33001	22	25001	
PHOSPHONIC ACID, PHENYL-, DIALLYL ESTER	47	41005P	23		
HEXADECANOIC ACID	48	8007		14716	4604
PALMITIC ACID	48	8007		14716	4604
SULFAMERAZINE	49	41006P	24	8370	4605
SULFANILAMIDE, N<1-/-4-METHYL-2- PYRIMIDINYL/-,	49	41006P	24	8370	4605
OCTADECANOIC ACID	50	21003		9661	4606
STEARIC ACID	50	21003		9661	4606
ACETYSALICYLIC ACID	51	32501	25	18001	4607
ASPIRIN	51	32501	25	18001	4607
SALICYLIC ACID, ACETATE	51	32501	25	18001	4607
1-PENTANOL	52	205		10132	802
PENTYL ALCOHOL	52	205		10132	802
PHENYL SULFONE	53	24	26	17333	4001
QUINOLINE, 1-BENZOYL-6-METHYL- 1,2,3,4-TETRAHYDRO-,	54	41007P			
PYRIMIDINE, 4,6-DICHLORO-,	55	8008	27	7335	4402
ACETIC ACID, DIFLUORO-, METHYL ESTER	56	41008P	28	11478	
ETHANE, IODO-,	57	28501		10202	12
ETHANE, IODO-,	57	28501		V 13	12
ETHYL IODIDE	57	28501		10202	12
ETHYL IODIDE	57	28501		V 13	12
ACETIC ACID, 2-ETHYLBUTYL ESTER	58	15002		7305	803
METHANE, IODO-,	59	28502		7872	13
METHYL IODIDE	59	28502		7872	13
NONANOIC ACID	60	24507		9	14
PELARGONIC ACID	60	24507		9	14
METHANE, NITRO-,	61	25	29	9146	4002
STYRENE, POLYMER	62	41009P			
PENTANE, 1-CHLORO-,	63	28503		8238	
1-PROPANOL	64	10961		10	4003
1-PROPANOL	64	10961		V 43	4003
PROPYL ALCOHOL	64	10961		10	4003
PROPYL ALCOHOL	64	10961		V 43	4003
ACETOACETIC ACID, METHYL ESTER	65	15003		10319	1611
2-PENTANOL, 4-METHYL-,	66	10933		4279	15
BUTYRIC ACID, 2-ETHYL-,	67	15004		6654	16
DIPHENYLAMINE	68	8009	30	11	17
ACETAMIDE	69	15005		4280	406
ACETIC ANHYDRIDE	70	29126		9879	18
FORMALDEHYDE, BIS/2-CHLOROETHYL/ ACETAL	71	36001		1194	19
METHANE, BIS/2-CHLOROETHOXY/-,	71	36001		1194	19
ETHER, BIS/2-CHLOROETHYL/,	72	10993		4299	20
CHLOREX	72	10993		4299	20
ETHANOL, 2-CHLORO-,	73	29682		10320	21
ETHANOL, 2-CHLORO-,	73	29682		V 12	21
FURAN, TETRAHYDRO-,	74	24001		14667	22
FURAN, TETRAHYDRO-,	74	24001		* 132	22
FURAN, TETRAHYDRO-,	74	24001		V 77	22
1-BUTANOL	75	10934		7200	23
BUTYL ALCOHOL	75	10934		7200	23
ACETIC ACID	76	29891		16864	24
ACETIC ACID	76	29891		V 8	24
ETHANE, 1,2-BIS/2-CHLOROETHOXY/-,	77	15006		7306	25
ETHYL PYROPHOSPHATE	78	15007		7627	
PYROPHOSPHORIC ACID, TETRAETHYL ESTER	78	15007		7627	
BENZENE, 1-CHLORO-2-ETHYL-,	79	26	32	1111	1612
ISOCTANE /SO-CALLED/	80	433		3432	1613
PENTANE, 2,2,4-TRIMETHYL-,	80	433		3432	1613
BENZENE, M-DINITRO-,	81	27	33	10134	4004
BARBITURIC ACID, 5-SEC-BUTYL-5- ETHYL-, SODIUM DERIVATIVE	82	28			4608
BUTABARBITAL, SODIUM DERIVATIVE	82	28			4608
HOMATROPINE, METHOBROMIDE	83	21004	34	10238	
HOMATROPINIUM BROMIDE, 8-METHYL-,	83	21004	34	10238	
TROPINE, MANDELATE, METHOBROMIDE	83	21004	34	10238	
BENZENE, 1,3-DIFLUORO-4-NITRO-,	84	8010		8239	
PHENOL, P-ETHOXY-,	85	24508	35	12	26
STEARIN, TRI-,	86	8011		17251	4609
STEARIN, TRI-,	86	8011		V 368	4609
PALMITIN, TRI-,	87	719		10290	
PALMITIN, 1-MONO-,	88	15257		7198	4802
STEARIN, 1,3-DI-,	89	8012		2400	
GUAIACOL	90	8013	36	3149	805
PHENOL, O-METHOXY-,	90	8013	36	3149	805
TOLUENE, O-CHLORO-,	91	29	37	13	1614
3,4-PYRIDINEDIMETHANOL, 5-HYDROXY-6- METHYL-, HYDROCHLORIDE	92	30	38	17264	5001
PYRIDOXINE, HYDROCHLORIDE	92	30	38	17264	5001

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NAME	PRISM	GRATING	UV	NMR	C-13
PYRIDOXOL, HYDROCHLORIDE	92	30	38	17264	5001
VITAMIN B6, HYDROCHLORIDE	92	30	38	17264	5001
AMMONIA	93	33002			
ACETONE, PEROXIDE TRIMER	94	15258		7288	4610
HEXOXONANE, 1,2,4,5,7,8-, 3,3,6,6,- 9,9-HEXAMETHYL	94	15258		7288	4610
ETHER, HEXYL,	95	41010P		7307	27
HEXYL ETHER	95	41010P		7307	27
ETHYLENE GLYCOL, DIFORMATE	96	41011P		12894	
FORMIC ACID, ETHYLENE ESTER	96	41011P		12894	
ETHANOL, 2-//2-AMINOETHYL/AMINO/-,	97	15009		7308	1615
CYCLOHEXYL PEROXIDE	98	41012P			
4-HEPTANONE, 2,6-DIMETHYL-,	99	31	39	10135	806
4-HEPTANONE, 2,6-DIMETHYL-,	99	31	39	10897	806
MORPHOLINE	100	10962		10193	28
MORPHOLINE	100	10962		V 83	28
OXAZINE, 2H-1,4-, TETRAHYDRO-,	100	10962		10193	28
OXAZINE, 2H-1,4-, TETRAHYDRO-,	100	10962		V 83	28
ACETOACETIC ACID, ETHYL ESTER	101	32	40	10321	1616
ETHER, ISOPROPYL,	102	28976		7258	29
ISOPROPYL ETHER	102	28976		7258	29
1-BUTANOL, 2-ETHYL-,	103	10963		14	30
BUTYL PHOSPHITE	104	33		6655	
ETHYL PHOSPHITE	105	34		19891	4611
BUTYL ETHER	106	15010		6656	1617
ETHER, BUTYL,	106	15010		6656	1617
PROPIONIC ANHYDRIDE	107	15011		6657	407
ACETIC ACID, 2-ETHYLHEXYL ESTER	108	15012		7309	31
MESITYL OXIDE	109	18001	41	13213	
3-PENTEN-2-ONE, 4-METHYL-,	109	18001	41	13213	
ETHYL PHOSPHITE	110	34		29632	2802
2-HEPTANOL	111	15013		7310	32
FURFURYL ALCOHOL, TETRAHYDRO-,	112	10964		1554	33
2-FURALDEHYDE	113	35	42	10203	1618
2-FURALDEHYDE	113	35	42	V 95	1618
FURFURAL	113	35	42	10203	1618
FURFURAL	113	35	42	V 95	1618
FURFUROLE	113	35	42	10203	1618
FURFUROLE	113	35	42	V 95	1618
S-TETROXANE, 3,3,6,6-TETRAMETHYL-,	114	41013P			
PROPIONIC ACID, 8-HYDROXY-, LACTONE	115	36002		10204	
PROPIONIC ACID, 8-HYDROXY-, LACTONE	115	36002		V 409	
FLAVANONE, 3,3*,4*,7-TETRAHYDROXY-,	116	8014			
FUSTIN	116	8014			
FLAVANONE, 3,3*,4*,5*,7-PENTA- HYDROXY-,	117	8015		8240	
ROBINETIN, DIHYDRO-,	117	8015		8240	
URACIL, 6-METHYL-5-NITRO-,	118	8016			
CYCLOHEXANE, /TRIFLUOROMETHYL/- UNDECAFLURO-,	119	33003			
ETHER, BIS/2-CHLORO-1-METHYLETHYL/, 2,5-HEXANEDIONE	120	10994			
ACETONE, ACETONYL-,	121	15015	43	2709	34
2-CYCLOHEXEN-1-ONE, 3,5,5-TRIMETHYL-,	121	15015	43	2709	34
ISOPHORONE	122	36	44	7311	4612
ETHANOL, 2-AMINO-,	122	36	44	7311	4612
2-FURANMETHANOL	123	33004		9143	4613
2-FURANMETHANOL	124	10765	45	17032	1619
FURFURYL ALCOHOL	124	10765	45	V 102	1619
FURFURYL ALCOHOL	124	10765	45	17032	1619
BUTYRIC ACID	125	37		V 102	1619
2-FURANCARBOXYLIC ACID	126	38	46	7312	1801
2-FUROIC ACID	126	38	46	10235	4614
PYROMUCIC ACID	126	38	46	10235	4614
ETHANE, 2,2-BIS/P-CHLOROPHENYL/- 1,1,1-TRICHLORO-,	127	15014	47	15	4401
THIOPHENE, 2-ISOPROPENYL- 3,4,5-TRICHLORO-,	128	41014P			
EPICHLOROHYDRIN	129	10935		16	1802
PROPANE, 1-CHLORO-2,3-EPOXY-,	129	10935		16	1802
PENICILLIN, BENZYL-, S,S-DIOXIDE, METHYL ESTER	130	15251	48	6908	
PENICILLIN G, S,S-DIOXIDE, METHYL ESTER	130	15251	48	6908	
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2- CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-PHENYLACETAMIDO/-, 4,4-DIOXIDE, METHYL ESTER	130	15251	48	6908	
BUTYRIC ACID, 2-AMINO-4-/METHYL- THIO/-,	131	39		13494	4615
METHIONINE	131	39		13494	4615
4-OXAZOLECARBOXYLIC ACID, 2-BENZYL-, ETHYL ESTER	132	41015P			
ACETURIC ACID	133	40		6658	4616

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NAME	PRISM	GRATING	UV	NMR	C-13
GLYCINE, N-ACETYL-,	133	40		6658	4616
PHENETHYLAMINE, DL-A-METHYL-,	134	41016P	49		
ETHANOL, 2,2PR-/PHENYLIMINO/DI-, F	135	10843	1670	9777	807
ETHANOL, 2,2PR-/PHENYLIMINO/DI-, F	135	10843	1670	8133	807
2-PROPANOL, 1,1PR,1PRPR-NITRILOTRI-,	136	33802		10322	
SALICYLIC ACID, 5-SULFO-,	137	29551	50	16001	4617
BUTYL PHOSPHATE	138	29683		6338	1803
O-TOLUIC ACID	139	41	51	17	4618
M-TOLUIC ACID	140	42	52	18	4619
MERCURY, ACETOXYPHENYL-,	141	21005	53	10205	4803
MERCURY, /ACETATO/PHENYL-,	141	21005	53	10205	4803
MERCURY, ACETOXYPHENYL-,	141	21005	53	10205	4803
AZELAIC ACID	142	15259		6060	4620
NONANEDIOIC ACID	142	15259		6060	4620
ETHANOL, 2-/DIETHYLAMINO/-,	143	33330		7047	35
2-PENTANOL, 4-METHYL-, ACETATE	144	43		521	36
FLUOREN-2-AMINE	145	233	54	18667	
2-FLUORENAMINE	145	233	54	18667	
BENZENE, P-DICHLORO-,	146	44	55	715	37
BENZOIC ACID, P-CHLORO-,	147	45	56	10266	4621
ISOCYANIC ACID, 4-METHYL-M-PHENYL- ENE ESTER	148	29893	15732	17271	2001
ACETIC ACID, /P-/ISOPENTYLOXY/- PHENYL/-,	149	41017P		13156	
ETHANOL, 2-BUTOXY-, PHOSPHATE	150	41018P			
ACETAMIDE, N-METHYL-2-PHENYL-,	151	46	58	6359	4622
FLAVONE, 3-/6-B-L-RHAMNOPYRANO- SIDO-D-GLUCOPYRANOSYL/OXY/-3PR,4PR,5,7- TETRAHYDROXY-, DIHYDRATE	152	21006	59		
QUERCETIN, 3-RUTINOSIDE, DIHYDRATE	152	21006	59		
RUTIN	152	21006	59		
BENZENE, P-DIHYDROXY-,	153	47	60	10350	38
P-BENZENEDIOL	153	47	60	10350	38
HYDROQUINOL	153	47	60	10350	38
HYDROQUINONE	153	47	60	10350	38
QUINOL	153	47	60	10350	38
ACETAMIDE, N-/DIBENZO-P-DIOXIN-2- YL/-,	154	41019P			
ANILINE, N-/2-NAPHTHYL/-,	155	48	61	10206	4804
2-NAPHTHYLAMINE, N-PHENYL-,	155	48	61	10206	4804
FORMAMIDE, N,N-DIMETHYL-,	156	29552		9537	408
FORMAMIDE, N,N-DIMETHYL-,	156	29552		9287	408
FORMAMIDE, N,N-DIMETHYL-,	156	29552		V 39	408
BENZYL ALCOHOL	157	985	62	9374	1804
BENZYL ALCOHOL	157	985	62	V 161	1804
METHANOL, PHENYL-,	157	985	62	9374	1804
METHANOL, PHENYL-,	157	985	62	V 161	1804
A-TOLUENOL	157	985	62	9374	1804
A-TOLUENOL	157	985	62	V 161	1804
CHLORAL	158	41020P		10362	4005
CHLORAL, HYDRATE	158	41020P		10362	4005
1,1-ETHANEDIOL, 2,2,2-TRICHLORO-,	158	41020P		10362	4005
1-DECANOL	159	10965		10207	2803
1-DECANOL	159	10965		V 282	2803
ACETANILIDE	160	49	63	5235	4201
1-OCTANOL	161	15016		6392	1805
FORMIC ACID, DITHIOBIS/THIO-, O,O- DIISOPROPYL ESTER	162	15260		6551	4623
3-PENTANONE, 2,4-DIMETHYL-,	163	14537		8242	1806
ACETIC ACID, ISOBUTYL ESTER	164	50		8590	39
ACETIC ACID, PHENYL-, METHYL ESTER	165	4764	64	19	40
CYCLOHEXANONE	166	51	65	10208	409
CINNAMIC ACID, METHYL ESTER	167	52	66	20	4624
3,5-PYRIDINEDICARBOXYLIC ACID	168	53	15733	6659	4625
GLYCERIN	169	10001		4979	41
GLYCEROL	169	10001		4979	41
PROPANETRIOL, 1,2,3-,	169	10001		4979	41
1-OCTADECANOL	170	54		6360	4626
CYCLOPENTANONE	171	55	67	1195	42
THIOPHENE	172	29684	68	10285	1202
THIOFURAN	172	29684	68	10285	1202
THENOYL CHLORIDE	173	36003			
2-THIOPHENECARBONYL CHLORIDE	173	36003			
2-THIOPHENECARBOXALDEHYDE	174	56	69	10165	43
2-THIOPHENECARBOXALDEHYDE	174	56	69	V 94	43
TOLUENE, 2,4-DINITRO-,	175	8017	2550	3229	4627
DNT	175	8017	2550	3229	4627
THIOPHENE-2-CARBOXYLIC ACID	176	963	70	523	4805
2-THIOPHENECARBOXYLIC ACID	176	963	70	523	4805
THIOPHENE, 2-NITRO-,	177	57	71	31622	
ETHANE, PENTACHLORO-,	178	33331		21132	44
ANILINE, N-/1-NAPHTHYL/-,	179	58	72	21	4628
1-NAPHTHYLAMINE, N-PHENYL-,	179	58	72	21	4628
CYCLOHEXANE	180	59		1196	1403
CYCLOHEXANE	180	59		* 150	1403

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NAME	PRISM	GRATING	UV	NMR	C-13
ADIPIC ACID, DIISOBUTYL ESTER	181	36501		23001	1404
ETHANE, 1,1,2,2-TETRACHLORO-	182	60		10209	45
ETHANE, 1,1,2,2-TETRACHLORO-	182	60		J 119	45
TOLUENE, M-NITRO-	183	61	73	22	2002
CINNAMYL ALCOHOL	184	8018	74	23	46
2-PROPEN-1-OL, 3-PHENYL-	184	8018	74	23	46
ETHYLENE, TRICHLORO-	185	62		9266	410
CINCHONINIC ACID, 6-METHYL-2-PHENYL-, ETHYL ESTER	186	15261	75	6276	4629
NEOCINCHOPHEN	186	15261	75	6276	4629
NOVATOPHAN	186	15261	75	6276	4629
8-QUINOLINOL	187	63	76	24	4630
ETHYL ALCOHOL	188	64		16002	808
ETHYL ALCOHOL	188	64		V 14	808
ETHANOL	188	64		16002	808
ETHANOL	188	64		V 14	808
SPIRITS	188	64		16002	808
SPIRITS	188	64		V 14	808
ISOPROPYL ALCOHOL	189	65		14604	47
ISOPROPYL ALCOHOL	189	65		V 44	47
2-PROPANOL	189	65		14604	47
2-PROPANOL	189	65		V 44	47
PROPIONITRILE	190	33332		1877	1807
CYCLOHEXANE, CHLORO-	191	8019		25	48
BENZENE, ETHOXY-	192	4826	77	26	4202
BENZENE, ETHOXY-	192	4826	77	J 102	4202
PHENETOLE	192	4826	77	26	4202
PHENETOLE	192	4826	77	J 102	4202
PROPANE, 1-CHLORO-	193	66		6660	
CYCLOHEXANE, METHYL-	194	68		27	49
CYCLOHEXANE, METHYL-	194	67		* 151	49
STYRENE, A-METHYL-	195	8020	78	9908	50
STYRENE, A-METHYL-	195	8020	78	V 232	50
BENZENE, TETRAHYDRO-	196	29892		3409	1808
CYCLOHEXENE	196	29892		3409	1808
M-XYLENE, A,A,A, APR, APR, APR-HEXAFLUORO-	197	8021	9754	1476	809
FORMAMIDE, N-/2-HYDROXYETHYL/-	198	33803		21801	4631
CYCLOHEXANEVALERIC ACID	199	15017		6376	1809
CARBAMIC ACID, DIMETHYLDITHIO-, SODIUM SALT	200	41021P		21802	4632
BENZENEPHOSPHINIC ACID	201	69	2285	6012	3601
PHOSPHINIC ACID, PHENYL-	201	69	2285	6012	3601
UREA, 1,3-DI-O-TOLYL-2-THIO-	202	14368	16326	17230	4806
UREA, 1,3-DI-O-TOLYL-2-THIO-	202	14368	16326	4399	4806
UREA, 1,3-DI-O-TOLYL-2-THIO-	202	15018	16326	17230	4806
COUMALIC ACID	203	15019	79	6491	4633
GLUTAMIC ACID, 4-/HYDROXY-METHYLENE/-, D-LACTONE	203	15019	79	6491	4633
2H-PYRAN-5-CARBOXYLIC ACID, 2-OXO-	203	15019	79	6491	4633
METHANE, BROMOCHLORO-	204	28977		6661	51
ANILINE, M-NITRO-	205	70	80	13454	5801
PENICILLIN, BENZYL-	206	41022P		81	
PENICILLIN G	206	41022P		81	
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6-/2-PHENYLACETAMIDO/-	206	41022P		81	
ISOBORNEOL, ACETATE	207	71		524	2003
2-AZEPINONE, HEXAHYDRO-	208	15262		6492	1620
E-CAPROLACTAM	208	15262		6492	1620
HEXAMETHYLENIMINE, 2-OXO-	208	15262		6492	1620
MYRISTOYL CHLORIDE	209	29685		17033	52
FURAN, 2-METHYL-	210	28978	82	6662	411
SYLVAN	210	28978	82	6662	411
PENTYLAMINE, 1-METHYL-	211	33005		28	53
P-TOLUIDINE, 3-NITRO-	212	33333	4691	23002	810
CYCLOHEXANEBUTYRIC ACID	213	24509		10097	
CYCLOHEXANEACETIC ACID	214	15020		6377	811
HYDROCINNAMALDEHYDE, P-ISOPROPYL-A-METHYL-	215	41023P		31623	
ANILINE, N,N-DIETHYL-	216	72	83	716	412
ETHER, BUTYL VINYL	217	33334		6510	1810
CARBONIC ACID, 2-BUTOXYETHYL ESTER, DIESTER WITH DIETHYLENE GLYCOL	218	41024P			
DIETHYLENE GLYCOL, BIS/2-BUTOXY-ETHYL CARBONATE/	218	41024P			
1-PROPENE, 1,1-DICHLORO-3,3-DI-FLUORO-	219	41025P			
ETHER, ISOPROPYL VINYL	220	41026P			
ETHER, 2-CHLOROETHYL VINYL	221	73		10136	54
1-HEXADECANOL	222	15263		24001	4203
CARBONIC ACID, BUTYL ESTER, DIESTER WITH DIETHYLENE GLYCOL	223	28504		13205	
DIETHYLENE GLYCOL, BIS/BUTYL CARBONATE/	223	28504		13205	

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NAME	PRISM	GRATING	UV	NMR	C-13
CARBONIC ACID, PHENYL ESTER, DIESTER WITH DIETHYLENE GLYCOL	224	41027P	84		
DIETHYLENE GLYCOL, BIS/PHENYL CARBONATE/	224	41027P	84		
TOLUENE, O-CHLORO-A,A,A-TRIFLUORO-,	225	74	85	10137	2401
TOLUENE, P-CHLORO-A,A,A-TRIFLUORO-,	226	75	86	1177	2004
TRIETHYLAMINE	227	76		29	55
ETHER, ETHYL VINYL,	228	10936		7313	56
ETHER, ETHYL VINYL,	228	10936		* 110	56
XANTHYLIUM TETRACHLOROFERRATE/III/ 4-//2,5-DIMETHYL-1-OCTYL-3-PYRRL/- METHYLENE/-1,2,3,4-TETRAHYDRO-,	229	41028P			
TOLUENE, M-CHLORO-A,A,A-TRIFLUORO-,	230	15021	87	18328	4807
ETHER, 2-METHOXYETHYL VINYL,	231	25086		7314	57
TOLUENE, A,A,A-TRIFLUORO-,	232	28979	88	6569	1811
BENZOTRIFLUORIDE	232	28979	88	6569	1811
ACETONE	233	77	89	9288	413
2-PROPANONE	233	77	89	9288	413
1-NAPHTHOIC ACID, 2-HYDROXY-,	234	78	90	13433	4634
AS-TRIAZINE, 5,6-DIMETHYL-3-PHENYL-,	235	41029P	91		
TOLUENE, M-NITRO-A,A,A-TRIFLUORO-,	236	8022	92	6904	
ETHYLENE, TETRACHLORO-,	237	79			1812
TOLUENE, 4-CHLORO-3-NITRO-A,A,A- TRIFLUORO-,	238	80	93	466	2804
2,4-PENTANEDIOL, 2-METHYL-,	239	15022		7315	1813
4,5-OCTANEDIOL	240	15023		10323	
BENZENE, VINYL-,	241	81	94	6408	4006
CINNAMENE	241	81	94	6408	4006
PHENETHYLENE	241	81	94	6408	4006
STYRENE	241	81	94	6408	4006
STYROL	241	81	94	6408	4006
BENZENE, ISOPROPYL-,	242	8023	95	10183	58
BENZENE, ISOPROPYL-,	242	8023	95	V 240	58
CUMENE	242	8023	95	10183	58
CUMENE	242	8023	95	V 240	58
PROPANE, 2-CHLORO-,	243	36502		6866	59
BICYCLO/2.2.1/HEPTAN-2-ONE, 1,7,7- TRIMETHYL-,	244	15264	96	30	4635
2-CAMPHANONE	244	15264	96	30	4635
CAMPHOR	244	15264	96	30	4635
ALANINE, 3-/3,4-DIHYDROXYPHENYL/-, D-/PLUS/-,	245	8024	15808	14668	
BENZENE, ETHYL-,	246	82	97	10210	1621
BENZENE, ETHYL-,	246	82	97	V 505	1621
BENZENE, SEC-BUTYL-,	247	83	98	31	60
BENZENE, SEC-BUTYL-,	247	83	98	* 155	60
ETHANOL, 2-PHENOXY-,	248	84	99	10211	61
ETHANOL, 2-PHENOXY-,	248	84	99	V 506	61
ETHANOL, 2-/P-SEC-BUTYLPHENOXY/-, CYCLOHEXANEPROPIONIC ACID	249	15024	100	6663	1814
BENZOIC ACID, O-CHLORO-,	250	15025		6378	1815
P-ACETOPHENETIDIDE	251	85	101	10212	4808
P-ACETOPHENETIDIDE	252	4849	102	10213	4636
PHENACETIN	252	4849	102	V 267	4636
PHENACETIN	252	4849	102	10213	4636
PHENOL, 2,4-DINITRO-,	253	86	3234	13483	4637
ETHANOL, 2-METHOXY-,	254	87		32	62
RHODANIC ACID	255	88	2964	10214	4638
RHODANINE	255	88	2964	10214	4638
4-THIAZOLIDINONE, 2-THIOXO-, CYCLOHEXANEHEXANOIC ACID	255	88	2964	10214	4638
M-CRESOL, 6-TERT-BUTYL-,	256	24510		10184	4639
TOLUENE, 2,4-DINITRO-,	257	89	103	525	2005
DNT	258	8017	2550	3229	4627
ETHANOL, 2-/P-TERT-BUTYLPHENOXY/-, BENZOIC ACID, 2,4-DIHYDROXY-, TRIHYDRATE	258	8017	2550	3229	4627
B-RESORCYLIC ACID, TRIHYDRATE	259	15026	104	6664	1816
BUTYRONITRILE	260	90	105	9527	5002
M-CRESOL, 4,6-DI-TERT-BUTYL-,	261	29686		33	63
M-CRESOL, 4,6-DI-TERT-BUTYL-,	262	4896	379	10197	
BUTYRIC ACID, 2-PHENYL-, ETHYL ESTER	262	4896	106	10197	
MALONIC ACID, ETHYLPHENYL-, DIETHYL ESTER	263	15027	107	6641	
1,3-BUTANEDIOL	264	8025	1728	302	1817
1,3-BUTANEDIOL	265	91		10176	1818
CHLOROTONE	265	91		V 86	1818
2-PROPANOL, 2-METHYL-1,1,1-TRI- CHLORO-,	266	10937		9396	4640
1,2-PROPANEDIOL	266	10937		9396	4640
1,2-PROPANEDIOL	267	92		9449	2805
1,2-PROPANEDIOL	267	92		9450	2805
1,2-PROPANEDIOL	267	92		V 45	2805
A-PROPYLENE GLYCOL	267	92		9449	2805
A-PROPYLENE GLYCOL	267	92		9450	2805
A-PROPYLENE GLYCOL	267	92		V 45	2805

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NAME	PRISM	GRATING	UV	NMR	C-13
BENZENE, O-DIHYDROXY-,	268	29687	108	17034	64
BENZENE, O-DIHYDROXY-,	268	29687	108	V 124	64
PYROCATECHOL	268	29687	108	17034	64
PYROCATECHOL	268	29687	108	V 124	64
ACETONITRILE	269	33006		9154	65
ETHANOL, 2-FLUORO-,	270	24511		8243	
HEPTANE	271	93		679	414
HEPTANE	271	93		* 144	414
PROPIOPHENONE	272	94	109	34	66
CARBAZOLE, 9-VINYL-,	273	15265			
CYCLOPENTENE, 3-/1-NAPHTHYL/-,	274	41030P			
NAPHTHALENE, 1-/2-CYCLOPENTEN-1- YL/-,	274	41030P			
ALLYL CHLORIDE	275	28001		7833	415
PROPENE, 3-CHLORO-,	275	28001		7833	415
CYCLOHEXANONE, OXIME	276	95		6160	4007
DIPHENETHYLAMINE	277	15028	110	6917	67
INDOLE, 3,3*-METHYLENEDI-,	278	8026	111		
PHENOL, PENTACHLORO-,	279	96	112		
PHENETHYLAMINE	280	8027	113	35	68
ADIPIC ACID	281	24002		4406	4641
2-NAPHTHALENEACETIC ACID, DECAHYDRO- 1-HYDROXY-7-OXO-A,4A,8-TRIMETHYL-, G-LACTONE	282	41031P			
A-SANTONIN, A-TETRAHYDRO-,	282	41031P			
P-CRESOL, 2,6-DI-TERT-BUTYL-,	283	18002	9777	526	4642
ALLYL ALCOHOL	284	97		9730	1819
ALLYL ALCOHOL	284	97		V 34	1819
2-PROPEN-1-OL	284	97		9730	1819
2-PROPEN-1-OL	284	97		V 34	1819
3-PENTANOL, 2,3,4-TRIMETHYL-, ETHER, OCTADECYL VINYL,	285	8028		8244	
O-CRESOL, 4,6-DINITRO-,	286	41032P		10370	5401
DN 2	287	98	2907	3236	1622
DNC	287	98	2907	3236	1622
DNOC	287	98	2907	3236	1622
ANILINE, N-BENZYL-N-ETHYL-,	288	24512	114	1178	1820
BENZYLAMINE, N-ETHYL-N-PHENYL-,	288	24512	114	1178	1820
2-PROPANOL, 2-METHYL-1,1,1-TRI- CHLORO-, HEMIHYDRATE	289	99		6273	4643
CARBAZOLE, 9-VINYL-, POLYMER	290	15029			
2-PYRROLIDINONE, 1-VINYL-, POLYMER	291	15030			
ETHER, METHYL VINYL, POLYMER	292	41033P			
BENZOIC ACID, 8-QUINOLINYL ESTER	293	15031	28586	10390	4644
8-QUINOLINOL, BENZOATE	293	15031	28586	10390	4644
PHENOL, 2,6-DIMETHYL-,	294	100	21874	36	69
2,6-XYLENOL	294	100	21874	36	69
MESITOL	295	8029	115	8657	6401
PHENOL, 2,4,6-TRIMETHYL-,	295	8029	115	8657	6401
HEMIMELLITENOL	296	36751	116	6013	4645
PHENOL, 3,4,5-TRIMETHYL-,	296	36751	116	6013	4645
2-BUTANONE	297	101		10292	70
2-BUTANONE	297	101		V 76	70
KETONE, METHYL ETHYL,	297	101		10292	70
KETONE, METHYL ETHYL,	297	101		V 76	70
2-PENTENE, 2,4,4-TRIMETHYL-,	298	33007		7336	1821
1-BUTENE, 3,4-EPOXY-,	299	33008		19474	4008
OXIRANE, VINYL-,	299	33008		19474	4008
MALIC ACID, CMPD WITH 2-BENZYL- 2-THIOPSEUDOUREA	300	41034P			
PSEUDOUREA, 2-BENZYL-2-THIO-, MALATE	300	41034P			
BENZENESULFONAMIDE, P-AMINO-,	301	102	117	9685	4009
SULFANILAMIDE	301	102	117	9685	4009
DESEPTYL	301	102	117	9685	4009
PRONTOSIL ALBUM	301	102	117	9685	4009
PRONTYLIN	301	102	117	9685	4009
PROPANAL /LIQUID/	302	24003		14669	
PROPIONALDEHYDE /LIQUID/	302	24003		14669	
PROPIONIC ACID, ETHYL ESTER	303	103		6665	
PENTANOIC ACID	304	10844		5995	416
VALERIC ACID	304	10844		5995	416
ACETONITRILE, /5-ACETYL-2-ETHOXY- PHENYL/-,	305	41035P	118		
HEPTANAL	306	29688		9267	2806
PROPANOIC ACID	307	104		5996	417
PROPIONIC ACID	307	104		5996	417
CAPROIC ACID	308	24004		37	418
HEXANOIC ACID	308	24004		37	418
PROPIONIC ACID, PROPYL ESTER	309	105		38	
TRIMETHYLENE TRISULFIDE	310	29894		25002	
TRITHIACYCLOHEXANE, 1,3,5-,	310	29894		25002	
S-TRITHIANE	310	29894		25002	
TRITHIOFORMALDEHYDE	310	29894		25002	

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NAME	PRISM	GRATING	UV	NMR	C-13
SULFANILAMIDE, N<1-/2-THIAZOLYL/-,	311	106	119	6666	4809
SULFATHIAZOLE	311	106	119	6666	4809
SULFANILAMIDE, N<1-/PYRAZINYL/-,	312	48477P			
SULFAPYRAZINE	312	48477P			
M-TOLUENETHIOL	313	29689	21875	9799	2006
XANTHIC ACID, ETHYL-, ETHYL ESTER	314	29690		17035	
SULFIDE, METHYL PHENYL,	315	33944	120	19831	71
SULFIDE, METHYL PHENYL,	315	33944	120	V 490	71
ACETIC ACID, MERCAPTO-,	316	21703		10969	
GLYCOLIC ACID, 2-THIO-,	316	21703		10969	
BENZENETHIOL	317	24513	2919	8245	72
PHENYL DISULFIDE	318	107	2094	286	73
ETHYL SULFIDE	319	29127		10215	74
PHENYL SULFIDE	320	108	121	39	75
PHENOTHIAZINE	321	109	122	9237	4403
PHENOTHIAZINE	321	109	122	8246	4403
10H-PHENOTHIAZINE	321	109	122	9237	4403
10H-PHENOTHIAZINE	321	109	122	8246	4403
THIODIPHENYLAMINE	321	109	122	9237	4403
THIODIPHENYLAMINE	321	109	122	8246	4403
1,2-BENZISOSULFONAZOLE, 3-OXO-,	322	110	15734	6667	4010
1,2-BENZISOTHIAZOLIN-3-ONE, 1,1-DIOXIDE	322	110	15734	6667	4010
1,2-BENZISOTHIAZOL-3-OL, 1,1-DIOXIDE	322	110	15734	6667	4010
SACCHARIN	322	110	15734	6667	4010
ALANINE, 3,3PR-DITHIODI-,	323	111			
CYSTEINE, L-/MINUS/-,	323	111			
THIAMINE, HYDROCHLORIDE	324	18003	123	13482	4404
THIAZOLIUM CHLORIDE, 3-//4-AMINO-2- METHYL-5-PYRIMIDINYL/METHYL/-5-/2- HYDROXYETHYL/-4-METHYL-, HYDROCHLORIDE	324	18003	123	13482	4404
VITAMIN B1, HYDROCHLORIDE	324	18003	123	13482	4404
ANEURINE	324	18003	123	13482	4404
ETHYL DISULFIDE	325	36752	124	17036	419
CYSTEINE, L-/PLUS/-, HYDROCHLORIDE	326	41036P			
BENZOIC ACID, O-MERCAPTO-,	327	15032	125	6668	
1-PROPANETHIOL LIQUID	328	29553		16981	
2-PROPANETHIOL	329	29554		16933	
2-PROPANETHIOL	329	29554		V 396	
1-PROPANETHIOL, 2-METHYL-,	330	41037P		3410	
2-NAPHTHALENETHIOL	331	21007	126	17037	4405
BENZOYL PEROXIDE	332	36004	127	7604	
BUTANAL	333	29691		17038	
BUTANAL	333	29691		V 78	
BUTYRALDEHYDE	333	29691		17038	
BUTYRALDEHYDE	333	29691		V 78	
LAUROYL PEROXIDE	334	9994		3845	4646
DODECANOYL PEROXIDE	334	9994		3845	4646
PHTHALIC ACID, BIS/2-ETHYLBUTYL/ ESTER	335	41038P	128		
BUTYRIC ACID, PROPYL ESTER	336	29692		12108	
BUTYRIC ACID, METHYL ESTER	337	29693		6669	812
BUTYRIC ACID, BUTYL ESTER	338	112		6463	76
PROPIONIC ACID, PENTYL ESTER	339	113		40	77
2-HEPTANONE	340	10966		41	420
BUTYRIC ACID, ETHYL ESTER	341	114		42	78
HEXANAL	342	15033			
ANILINE, N,N-DIMETHYL-P-//A,A,A- TRIFLUORO-M-TOLYL/AZO/-,	343	41039P	129	10418	
ANILINE, N,N-DIMETHYL-P-//P- FLUOROPHENYL/AZO/-,	344	15034	130	7532	
ANILINE, N,N-DIMETHYL-P-//O- FLUOROPHENYL/AZO/-,	345	15035	131	7533	
ANILINE, N,N-DIMETHYL-P-/O-	346	15266	132	7534	4406
ANILINE, N,N-DIMETHYL-P-/O-	346	44688P	132	7534	4406
ANILINE, N,N-DIMETHYL-P-/PHENYL- AZO/-,	347	21685	133	10351	4407
ANILINE, N-METHYL-P-/PHENYL-AZO/-,	348	15267	134	18329	4408
ANILINE, N-METHYL-P-/PHENYL-AZO/-,	348	15267	134	4313	4408
ANILINE, N,N-DIMETHYL-P-/P- TOLYL-AZO/-,	349	15036	135	7535	
AZO BENZENE	350	115	136	43	79
BENZENE AZOBENZENE	350	115	136	43	79
XANTHINE, 2,6-DITHIO-7-METHYL-,	351	8030			
ANILINE, N-METHYL-P-/M-TOLYL-AZO/-,	352	15268	137	10742	
XANTHINE, 2,6-DITHIO-,	353	8031			
M-TOLUIDINE, N,N-DIMETHYL-P- /PHENYL-AZO/-,	354	15269	138	7536	4409
MALONIC ACID, CHMPD WITH 2-BENZYL- 2-THIOPSEUDUREA	355	41040P			
PSEUDUREA, 2-BENZYL-2-THIO-, HYDROGEN MALONATE	355	41040P			
2-PENTANONE, 4-HYDROXY-4-METHYL-,	356	116	139	303	2807
ANILINE, N,N-DIMETHYL-P-//M- FLUOROPHENYL/AZO/-,	357	15037	140	7537	4410

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NAME	PRISM	GRATING	UV	NMR	C-13
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-2-THIENYL/ACETAMIDO/-, PENICILLIN, /2-THENYL/-,	397	41053P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 6-2-/P-ALLYLOXY-PHENYL/ACETAMIDO/-3,3-DIMETHYL-7-OXO- PENICILLIN, /P-/ALLYLOXY/BENZYL/-,	397 398	41053P 41054P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-6-2- /ISOPROPYLTHIO/ACETAMIDO-7-OXO- PENICILLIN, //ISOPROPYLTHIO/- METHYL/-,	398 399 399	41054P 41055P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-//2-PHENOXYETHYL/THIO/ACETAMIDO/-, PENICILLIN, //2-PHENOXYETHYL/- THIO/METHYL/-,	400 400	41056P 41056P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-/3-THIENYLTHIO/ACETAMIDO/-, PENICILLIN, //3-THIENYLTHIO/- METHYL/-,	401 401	41057P 41057P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 6-2-/CYCLOPENTYLACET- AMIDO/-3,3-DIMETHYL-7-OXO- PENICILLIN, /CYCLOPENTYLMETHYL/-,	402 402	41058P 41058P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-6-2-/P- METHOXYPHENOXY/ACETAMIDO-7-OXO- PENICILLIN, //P-METHOXYPHENOXY/- METHYL/-,	403 403	41059P 41059P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 6-2-/BUTYLTHIO/ACET- AMIDO/-3,3-DIMETHYL-7-OXO- PENICILLIN, //BUTYLTHIO/METHYL/-,	404 404	41060P 41060P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 6-2-/P-CHLOROPHENYL/ ACETAMIDO-3,3-DIMETHYL-7-OXO- PENICILLIN, /P-CHLOROBENZYL/-,	405 405	41061P 41061P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 6-2-/P-BROMOPHENYL/ ACETAMIDO/-3,3-DIMETHYL-7-OXO- PENICILLIN, /P-BROMOBENZYL/-,	406 406	41062P 41062P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-6-2-/P- IODOPHENYL/ACETAMIDO-7-OXO- PENICILLIN, /P-IODOBENZYL/-,	407 407	41063P 41063P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-PHENOXYACETAMIDO/-, PENICILLIN, /PHENOXYMETHYL/-, ALANINE, N-FORMYL-3-PHENYL-, DL-,	408 409 410	41064P 8034 41065P		8247	
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-6-2-/P- FLUOROPHENYL/ACETAMIDO-7-OXO- PENICILLIN, /P-FLUOROBENZYL/-, BENZOIC ACID, O-//ETHYLMERCURI/- THIO/-, SODIUM SALT MERCURY, //O-CARBOXYPHENYL/THIO/- ETHYL-, SODIUM SALT MERTHIOLATE THIMEROSAL	410 411 411 411 411 411 411 412	41065P 15042 15042 15042 15042 15042 15042 41066P		7612 7612 7612 7612	
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-//3-PHENYLPROPYL/THIO/ACETAMIDO/-, PENICILLIN, //3-PHENYLPROPYL/- THIO/METHYL/-,	412 412	41066P 41066P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-//A,A,A-TRIFLUORO-N-TOLYL/THIO/ACET- AMIDO/-, PENICILLIN, //A,A,A-TRIFLUORO-M- TOLYL/THIO/METHYL/-,	413 413	41067P 41067P			
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2-CARBOXYLIC ACID, 3,3-DIMETHYL-7-OXO-6- /2-/PHENETHYLTHIO/ACETAMIDO/-, PENICILLIN, //PHENETHYLTHIO/- METHYL/-, BENZENESULFONYL CHLORIDE BENZENESULFINIC ACID, SODIUM SALT ACETIC ACID, THIO- ACETIC ACID, THIO- PHENYL SULFOXIDE PHENYL SULFOXIDE	414 414 415 416 417 417 418 418	41068P 41068P 118 15043 33335 33335 15271 15271	154 18349 5090 5090	3150 6670 18330 V 7 6014 12288	90 4204

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NAME	PRISM	GRATING	UV	NMR	C-13
BENZENE, METHYL-,	419	119	155	10216	91
BENZENE, METHYL-,	419	119	155	V 157	91
TOLUENE	419	119	155	10216	91
TOLUENE	419	119	155	V 157	91
ETHANOL, 2-/4-CHLORO-2-NITRO- PHENOXY/-,	420	41069P	156		
BENZANILIDE, THIO-,	421	29694	24499	21803	4416
BUTYL SULFONE	422	33009		17039	92
SULFAMETHAZINE	423	15044		6671	4417
SULFANILAMIDE, N<1-/4,6-DIMETHYL- 2-PYRIMIDINYL/-,	423	15044		6671	4417
METHANEDIOL, HYDROGEN SULFOXYLATE, SODIUM SALT, DIHYDRATE	424	21009		10166	4647
SODIUM FORMALDEHYDESULFOXYLATE, DIHYDRATE	424	21009		10166	4647
SULFOXYLIC ACID, /HYDROXYMETHYL/ ESTER, SODIUM SALT, DIHYDRATE	424	21009		10166	4647
PEROXIDE, BIS/3-CARBOXYPROPIONYL/, DIPHENYLAMINE, 4-ISOPROPOXY-,	425	41070P			
BENZOIC ACID, THIO-, S-BENZYL ESTER	426	15045	157		
TRYPTOPHAN, N-BENZOYL-, L-,	427	28507	158	13154	
ANILINE, 2,5-DIMETHOXY-,	428	41071P	159		
ANILINE, 2,5-DIMETHOXY-,	429	21010	2087	11258	1203
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2- CARBOXYLIC ACID, 6-/2-/3-CHLORO-2- BUTENYL/THIO/ACETAMIDO/-3,3-DIMETHYL-7- OXO-, POTASSIUM SALT	429	21010	2087	V 508	1203
4-THIA-1-AZABICYCLO/3.2.0/HEPTANE-2- CARBOXYLIC ACID, 6-/2-/3-CHLORO-2- BUTENYL/THIO/ACETAMIDO/-3,3-DIMETHYL-7- OXO-, POTASSIUM SALT	430	41072P			
PENICILLIN, ///3-CHLORO-2-BUTENYL/- THIO/METHYL/-, POTASSIUM SALT	430	41072P			
ACETONITRILE, 3,4-DIMETHOXYPHENYL-, HOMOVERATRONITRILE	431	24514	160	10267	4418
ALANINE, 3-/3-INDOLYL/-,	431	24514	160	10267	4418
3-INDOLEPROPIONIC ACID, A-AMINO-, TRYPTOPHAN, DL-,	432	8612	3453	27501	
HEXYLAMINE	432	8612	3453	27501	
NIACIN	433	28227		46	1825
NICOTINIC ACID	434	120	161	14671	
3-PYRIDINECARBOXYLIC ACID	434	120	161	14671	
HEXANOIC ACID, 2,6-DIAMINO-, HYDROCHLORIDE	435	8036		13207	4419
LYSINE, HYDROCHLORIDE, DL-,	435	8036		13207	4419
ALANINE, PHENYL-, DL-,	436	121	20765	17174	4420
ALANINE, PHENYL-, DL-,	436	29842	20765	17174	4420
HYDROCINNAMIC ACID, A-AMINO-,	436	121	20765	17174	4420
HYDROCINNAMIC ACID, A-AMINO-,	436	29842	20765	17174	4420
TRIAZOLE, 1H-1,2,4-, 3-/2-HYDROXY- ETHYLAMINO/-,	437	41073P			
CYCLOPENTANE, BROMO-,	438	15046		6225	93
PIPERAZINE, 2,6-DIMETHYL-,	439	15047		7688	4648
M-TOLUIC ACID, 2-/2,4,6-TRIMETHYL- BENZOYL/-, METHYL ESTER	440	41074P			
BASIC FUCHSINE	441	8037	21876		
FUCHSINE	441	8037	21876		
2,4-XYLIDINE, A<4-/P-AMINOPHENYL/- A<4-/4-IMINO-2,5-CYCLOHEXADIEN-1-YL- IDENE/-,	441	8037	21876		
QUINOLINE, 3-BENZYL-6-METHOXY-,	442	32001			
BENZOPHENONE, 2,2PR,4,6-TETRA- METHYL-,	443	32002			
O-TOLUIC ACID, 6-/2,4,6-TRIMETHYL- BENZOYL/-, METHYL ESTER	444	41075P			
4-NONANONE, 2,6,8-TRIMETHYL-,	445	15048		7316	423
ANILINE, 2,5-DIETHOXY-,	446	122	2088	660	4421
CARBAMIDE	447	123		16982	6801
UREA	447	123		16982	6801
FUMARIC ACID, DISODIUM SALT	448	8038		1544	4422
SODIUM FUMARATE	448	8038		1544	4422
ETHANOL, 2-/3-AMINOPROPYL/AMINO/-,	449	124		19607	
ETHER, 2,3-EPOXYPROPYL PHENYL,	450	15049	9785	25003	94
PROPANE, 1,2-EPOXY-3-PHENOXY-,	450	15049	9785	25003	94
GLUTAMIC ACID, SODIUM SALT	451	15050		6178	4423
GLUTARIC ACID, 2-AMINO-, SODIUM SALT	451	15050		6178	4423
SODIUM GLUTAMATE	451	15050		6178	4423
GUANIDINE, NITRATE	452	15051		13305	
BUTYRIC ACID, 2-AMINO-3-METHYL-,	453	21011		10363	4424
VALINE, DL-,	453	21011		10363	4424
HYDRACRYLIC ACID, 2-AMINO-,	454	21012		13157	4425
SERINE, DL-,	454	21012		13157	4425
TRYPTOPHAN, N-ACETYL-, DL-,	455	592	15735	13597	
UREA, AMIDINO-, SULFATE, DIHYDRATE	456	15252			
2-FUROIC ACID, HYDRAZIDE	457	8039		355	6402
BENZENESULFONIC ACID, 3,5-DIAMINO-, SODIUM SALT	458	41076P			