SADTLER COMMERCIAL INFRARED GRATING SPECTRA—STEROIDS 1983

Vol. 4: S7511K—S11000K

With Numerical, Alphabetical
Molecular Formula and Classes
Index to IR Grating
Vols. 1—4

SADTLER RESEARCH LABORATORIES
Division of Bio-Rad Laboratories, Inc.

STEROID SPECTRA

Volume 4

S751K - S1000K

Creative Chemists Since 1874

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The publication of the physical data of the Sadtler Standard Spectra and the Sadtler Commercial Spectra is intended to be descriptive. The samples of the materials represented have come generally from other sources than our own laboratories and frequently without the donors' knowledge of their part in this publication.

On the other hand every effort is made by Sadtler Research Laboratories, a division of Bio-Rad Laboratories, Inc. to assure the reliability of the published spectra. When improved data is available or errors are called to our attention, we revise and reissue the proper replacement spectra.

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SADTLER STEROID INFRARED GRATING SPECTRA

This group of 250 infrared grating spectra, numbered S 751 K to S 1000 K inclusive, is an addition to the ***Sadtler Steroid Spectra***.

In compiling this particular catalog, a Digilab model FTS-14 or FTS-15 interferometer-based spectrometer was employed, scanning the region from 4000 to 450 cm^{-1}. The spectra are presented in a linear frequency (wavenumber) vs. transmittance format. All data were measured at an optical retardation of 0.25 which corresponds to 4 cm^{-1} nominal spectral resolution.

Standard techniques have been developed in our laboratories to insure that the spectra published are of the best possible quality and reproducible for comparison and identification purposes. The preferred sample preparation methods are capillary cells for liquids, cast films from a suitable solvent for samples with melting points below 72° C, and KBr wafers for solids with melting points above 72° C.

When the KBr method cannot be used for solids due to a reaction between KBr and the compound, the split mull sample preparation technique is used. The sample is mulled in mineral oil, spread between AgCl plates and the entire spectrum is measured. The sample is then mulled in a perfluorinated hydrocarbon, spread between AgCl plates and the spectrum is measured again. Finally, the two spectra are merged where the perfluorinated hydrocarbon data are used from 4000 cm^{-1} to 1330 cm^{-1} and the mineral oil data are used from 1330 cm^{-1} to 450 cm^{-1}. This method provides a complete spectrum of the compound without interference from the mineral oil or the perfluorinated hydrocarbon mulling compounds. Each spectrum printed is clearly labelled with the sample preparation technique used.

There are four different KBr wafer sample preparation techniques used at Sadtler: KBr 0, KBr 1, KBr 2 and KBr 3. Each of these techniques uses the same general procedure for preparing the sample in the KBr matrix, but each technique incorporates certain modifications, where required, to obtain different levels of quantitative information. The general procedure is that for technique KBr 1 and this procedure is given below in detail. The remaining techniques present only modifications in the KBr]1 technique to obtain the specified quantitative information.

KBr 0

KBr 0 is not a quantitative technique. This technique is used when heating of the sample causes its decomposition. In this case, a KBr wafer containing a small amount of H_2O is placed in the reference beam to compensate for the free water absorbed during mixing. The KBr 1 procedure is followed except that the sample is neither dried or weighed.

This procedure is used for samples with melting points $> 120^{o}$ C and when > 10 mg of sample are available for analysis.

Equipment required:

Stainless Steel Capsules with ¼ inch ball bearing (i.e. Part numbers 3114 and 6117, Crescent Dental Company, Lyons, Illinois)

Mechanical Vibrator (i.e. Model 3A Wig-L-Bug, Crescent Dental Company)

13 mm Die and Press

Temperature Controlled Vacuum Oven

Dry Box

Analytical Balance (± 0.001 mg accuracy)

Analytical Balance (± 0.1 mg accuracy)

1.) Place ∿ 10 mg of the sample in a stainless steel capsule and grind with a mechanical vibrator for 1 minute. It is important that grinding time be kept constant, since absorbance depends on particle size. The sample is ground in a dry box and purged with dry air to eliminate excessive moisture absorption by the sample.

2.) Dry the ground sample in a vacuum oven with a dish of P_2O_5 at 72^{o} C and 252 mm Hg for 2 hours.

3.) Weigh out 0.300 - 0.800 mg of the sample to the nearest 0.001 mg and add it to a new capsule.

4.) Place the capsule on a balance, tare, and add ∿ 400 mg KBr. Be sure that the sample is at the bottom of the capsule with the KBr on top of the sample. Then, weigh to the nearest 0.1 mg.

5.) Grind the sample without the ball bearing for 20 seconds, then grind again with the ball bearing in the capsule for an additional 20 seconds. Perform the grinding in a dry box purged with dry air to eliminate excessive moisture absorption.

6.) Place the sample in the die, then apply 252 mm Hg vacuum for 30 seconds; press the pellet using 8 tons of pressure for 30 seconds. Triple press the pellet by alternately applying and releasing the 8 tons of pressure (slowly), being sure to keep the vacuum applied during the entire cycle to produce clear pellets.

7.) Dry the pellet overnight in a vacuum oven (72^{o} C at 252 mm Hg with a dish of P_2O_5) to remove free H_2O in the KBr.

8.) Remove the pellet from the oven and, if it is cloudy, re-press it for 30 seconds using 8 tons of pressure.

9.) Weigh the pellet to the nearest milligram.

10.) Measure the spectrum. If the spectrum contains a H_2O band at 3500 cm^{-1} greater than 10% transmission in intensity, then the pellet should be dried for another 8 - 12 hours. The amount of sample lost in the process is proportional to the amount of KBr lost; therefore, the weight of the sample is given by:

$$\text{Weight of sample in the pellet} = \frac{\text{wt. of pellet}}{\text{original wt. of KBr}} \times \text{original wt. of sample}$$

11.) The weight of sample used to measure an unknown spectrum can be approximated by comparing the unknown spectrum with the quantitative information found on the corresponding reference spectrum. This first approximation can be calculated by either of two methods. The first method is based on having access to the fully digitized reference spectrum for computation of areas under the curve. The second method uses peak height measurements and yields less accuracy than the first method.

a. Determination of the weight of an unknown using a fully digitized unknown spectrum and a fully digitized reference spectrum.

1. Convert the spectrum to absorbance, if it is not already an absorbance spectrum.

2. Calculate the area under the curve over the frequency region of interest for the unknown.

3. Calculate the area under the curve over the same frequency region using Sadtler's digitized reference spectrum.

4. Calculate the weight of the unknown using the following equation:

$$\text{weight of the unknown} = \frac{\text{wt. of sample for Sadtler's reference spectrum} \times \text{total absorbance for the unknown}}{\text{total absorbance for the Sadtler's reference spectrum}}$$

b. Determination of the weight of an unknown using peak height measurements from Sadtler's hard copy reference spectra in percent transmission.

1. Using the unknown spectrum, draw a line tangential to the baseline extremities of the peak of interest.

2. Determine the maximum transmittance at the center of the peak along the drawn baseline.

3. Measure the minimum transmittance at the apex of the peak.

4. Determine the absorbance of the unknown by subtracting the minimum from the maximum % transmission,

$$\%T_{max} - \%T_{min} = \%T,$$

then, subtract the percent transmission from 100% T to determine the peak percent transmission for the sample,

$$100\%T - \%T = \text{Peak } \%T_{UNK}$$

Determine the absorbance for the unknown according to the equation,

$$ABS_{UNK} = -\log(\text{Peak } \%T_{UNK}).$$

5. Determine the reference sample absorbance by using Sadtler's hard copy reference spectrum and repeat steps 1 through 4 for the reference compound.

6. Determine the scaling factor used on Sadtler's hard copy spectrum to compensate for the reference spectrum being scale expanded,

$$\text{Scaling Factor} = \frac{92}{T\ \text{min} - T\ \text{max.}}$$

7. To obtain the corrected transmittance of the peak of interest in Sadtler's hard copy spectrum, divide the $\%\ T_{SADT}$ by the scaling factor found in step 6,

$$\text{Corrected } \%\ T_{SADT} = \frac{\%\ T_{SADT}}{\text{Scaling Factor.}}$$

Subtract this value from 100%,

$$100\% - \text{True } \%\ T_{SADT} = \text{Peak } \%\ T_{SADT},$$

and convert to absorbance using the equation,

$$ABS_{SADT} = -\log \text{Peak } \%\ T_{SADT}.$$

8. Obtain the weight of the unknown according to,

$$Wt_{UNK} = \frac{Wt_{SADT}}{ABS_{SADT}} \times ABS_{UNK}$$

KBr 2

This technique is used for samples with melting points between 72° C and 120° C, and when > 10 mg of sample are available for analysis. The procedure is the same as that for KBr 1 except step 2 below should be substituted for step 2 in the KBr 1 technique.

2. Dry the powdered sample in a vacuum at 252 mm Hg with a dish of P_2O_5 for 2 hours. ***Do not apply heat.***

KBr 3

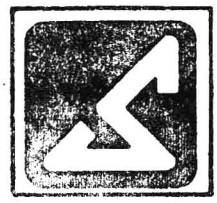
This technique is used when there is < 10 mg of sample available for analysis and the melting point is > 120° C. The procedure is the same as that for KBr 1 except skip step 1 and substitute step 5 on the next page for step 5 in the KBr 1 technique.

5.) Grind the sample without the ball bearing for 20 seconds, then with the ball bearing for an additional 60 seconds. Perform all grinding in a dry box purged with dry air to eliminate excessive moisture absorption.

All compounds are of at least 98% purity and each spectrum is labelled with the following information.

1. Name, according to the Chemical Abstracts system of nomenclature
2. Structural Formula
3. Molecular Formula
4. Molecular Weight
5. Physical Data (when available)
6. Source of Sample
7. Method of Sample Preparation

Four indexes are provided with this collection. They are the Numerical, the Alphabetical, the Molecular Formula and the Chemical Class. The index is a composite and it lists this new group as well as the previous published volumes.



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INDEXES TO STEROIDS

Volumes 1 - 4

Creative Chemists Since 1874

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NUMERICAL INDEX

NUMERICAL INDEX

This index contains 1000 Steroid compounds listed in numerical sequence.

The method of naming the chemical compounds in the Sadtler reference spectra collections closely follows the Chemical Abstracts (CA) nomenclature system which was in operation prior to the publication of the CA Ninth Collective Index. Briefly, this system assigns the parent name on the basis of a predefined priority of functionality (the Sadtler Chemical Classes Index is comparable to this priority table) and then the substituents to the parent name are listed after it in alphabetical sequence. The simple example shown below will illustrate this point. In addition to the systematized names, many cross-references to frequently used trivial names are also included in this index.

Example I

The compound $HO-CH_2-CH_2-CH_2-C\equiv N$

could be named as
(a) HYDRACRYLONITRILE
(b) PROPIONITRILE, 3-HYDROXY-,
(c) 1-PROPANOL, 3-CYANO-,

The index includes (a) which is a commonly-accepted name and (b) which is the systematic name but not (c) since the nitrile functionality always takes precedence over the hydroxy group in the priority table.

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
<	(lozenge)	–	Read as indication of superscripting
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.

STEROIDS

NUMERICAL INFRARED INDEX

	MFG CODE	GRATING	PRISM	NMR	UV	FICHE
5A-ANDROSTANE-17B-CARBOXYLIC ACID		S 1P	S 1			S 1
5A-ANDROSTANE-17A-CARBOXYLIC ACID, METHYL ESTER		S 2P	S 2			S 2
5A-PREGNAN-3B-OL		S 3P	S 3			S 3
5A-PREGNAN-3B-OL, ACETATE		S 4P	S 4			S 4
5A-PREGNANE, 3B-METHOXY-		S 5P	S 5			S 5
5A-ANDROSTANE-17B-CARBOXYLIC ACID, 3B-HYDROXY-		S 6P	S 6			S 6
5A-ANDROSTANE-17B-CARBOXYLIC ACID, 3B-HYDROXY-, METHYL ESTER		S 7P	S 7			S 7
5A-ANDROSTANE-17B-CARBOXYLIC ACID, 3B-HYDROXY-, ACETATE		S 8P	S 8			S 8
5A-ANDROSTANE-17B-CARBOXYLIC ACID, 3B-HYDROXY-, METHYL ESTER, ACETATE		S 9P	S 9			S 9
5B-ANDROSTANE-17B-CARBOXYLIC ACID, 3B-HYDROXY-, METHYL ESTER, ACETATE		S 10P	S 10			S 10
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B-HYDROXY-, METHYL ESTER, ACETATE		S 11P	S 11			S 11
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-, METHYL ESTER, 3-ACETATE		S 12P	S 12			S 12
ANDROSTANE-17A-CARBOXYLIC ACID, 5B,14B-, METHYL ESTER, ACETATE		S 13P	S 13			S 13
5B-ANDROSTANE-17B-CARBOXYLIC ACID, 3B-HYDROXY-19-OXO-, METHYL ESTER, ACETATE		S 14P	S 14			S 14
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B-HYDROXY-19-OXO-, METHYL ESTER, ACETATE		S 15P	S 15			S 15
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-, METHYL ESTER		S 16P	S 16			S 16
5B-ANDROST-14-ENE-17B-CARBOXYLIC ACID, 3B-HYDROXY-11-OXO-, METHYL ESTER, ACETATE		S 17P	S 17			S 17
ANDROST-8-ENE-17A-CARBOXYLIC ACID, 5B,14B-, 3A-HYDROXY-11-OXO-, METHYL ESTER, ACETATE		S 18P	S 18			S 18
5A-CHOLESTAN-3-ONE, 1A,2A-EPOXY-		S 19P	S 19			S 19
ANDROST-5-ENE-17B-CARBOXYLIC ACID, 3B-HYDROXY-, METHYL ESTER, ACETATE		S 20P	S 20			S 20
5A-ANDROSTANE-17B-CARBOXYLIC ACID, 3-OXO-, METHYL ESTER		S 21P	S 21			S 21
ANDROST-4-ENE-17B-CARBOXYLIC ACID, 3-OXO-, METHYL ESTER		S 22P	S 22			S 22
5A-ANDROST-1-ENE-17B-CARBOXYLIC ACID, 3-OXO-, METHYL ESTER		S 23P	S 23			S 23
ANDROSTA-1,4-DIENE-17B-CARBOXYLIC ACID, 3-OXO-, METHYL ESTER		S 24P	S 24			S 24
5A-ANDROSTANE-17B-CARBOXYLIC ACID, 1A,2A-EPOXY-3-OXO-, METHYL ESTER		S 25P	S 25			S 25
5A-ANDROSTANE-17B-CARBOXYLIC ACID, 2A-BROMO-3-OXO-, METHYL ESTER		S 26P	S 26			S 26
5A-CHOLESTAN-3-ONE		S 27P	S 27			S 27
5A-CHOLEST-1-EN-3-ONE		S 28P	S 28			S 28
CHOLESTA-1,4-DIEN-3-ONE		S 29P	S 29			S 29
5B-ANDROST-1-ENE-17B-CARBOXYLIC ACID, 3-OXO-, METHYL ESTER		S 30P	S 30			S 30
ESTRA-2,5/10/-DIENE-16A,17B-DIOL, 3-METHOXY-		S 31P	S 31			S 31
5B-ANDROSTANE-17B-CARBOXYLIC ACID, 3-OXO-, METHYL ESTER		S 32P	S 32			S 32
5B-CHOLESTAN-3-ONE		S 33P	S 33			S 33
COPROSTAN-3-ONE		S 33P	S 33			S 33
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 14-HYDROXY-3-OXO-, METHYL ESTER		S 34P	S 34			S 34
5A-ANDROSTANE-17B-CARBOXYLIC ACID, METHYL ESTER		S 35P	S 35			S 35
5B-ANDROSTANE-17B-CARBOXYLIC ACID, METHYL ESTER		S 36P	S 36			S 36
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 14-HYDROXY-, METHYL ESTER		S 37P	S 37			S 37
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 14-HYDROXY-		S 38P	S 38			S 38
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 14-HYDROXY-, G-LACTONE		S 39P	S 39			S 39
5B-ANDROST-14-ENE-17B-CARBOXYLIC ACID, 3B-HYDROXY-, METHYL ESTER, ACETATE		S 40P	S 40			S 40
5B-ANDROST-8/14/-ENE-17B-CARBOXYLIC ACID, 3B-HYDROXY-, METHYL ESTER, ACETATE		S 41P	S 41			S 41

	MFG CODE	GRATING	PRISM	NMR	UV	FICHE
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-, METHYL ESTER		S 42P	S 42			S 42
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-,		S 43P	S 43			S 43
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-, G-LACTONE, ACETATE		S 44P	S 44			S 44
5B-ANDROSTANE-17B-CARBOXYLIC ACID, 14A,15A-EPOXY-3B-HYDROXY-, METHYL ESTER, ACETATE		S 45P	S 45			S 45
5B-ANDROSTANE-17B-CARBOXYLIC ACID, 8,14-EPOXY-3B-HYDROXY-, METHYL ESTER, ACETATE		S 46P	S 46			S 46
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-15-OXO-, METHYL ESTER, 3-ACETATE		S 47P	S 47			S 47
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-15-OXO-,		S 48P	S 48			S 48
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-15-OXO-, METHYL ESTER		S 49P	S 49			S 49
ANDROSTANE-17B-CARBOXYLIC ACID, 5B,14B-, 3B,14-DIHYDROXY-15-OXO-, G-LACTONE, ACETATE		S 50P	S 50			S 50
ANDROSTANE-3B,14-DIOL, 5B,14B-, 17B-/HYDROXYMETHYL/-, 3,17-DIACETATE		S 51P	S 51			S 51
21-NOR-5B,14B-PREGNANE-3B,14,20-TRIOL, 3,20-DIACETATE		S 51P	S 51			S 51
5B-ANDROST-14-ENE-17B-METHANOL, 3B-HYDROXY-, DIACETATE		S 52P	S 52			S 52
21-NOR-5B-PREGN-14-ENE-3B,20-DIOL, DIACETATE		S 52P	S 52			S 52
5B-ANDROSTANE-17B-METHANOL, 14A,15A-EPOXY-3B-HYDROXY-, DIACETATE		S 53P	S 53			S 53
21-NOR-5B-PREGNANE-3B,20-DIOL, 14A,15A-EPOXY-, DIACETATE		S 53P	S 53			S 53
5B-CHOLANIC ACID		S 54P	S 54			S 54
5B-CHOLAN-24-OIC ACID		S 54P	S 54			S 54
ANDROST-5-EN-17-ONE, 3B-HYDROXY-, ACETATE		S 55P	S 55			S 55
5A-ANDROSTAN-17-ONE, 3B-HYDROXY-,		S 56P	S 56			S 56
EPIANDROSTERONE		S 56P	S 56			S 56
ANDROST-5-EN-17-ONE, 3B-HYDROXY-,		S 57P	S 57			S 57
ANDROST-4-ENE-3,17-DIONE		S 58P	S 58			S 58
5A-ANDROSTAN-17-ONE, 3A-HYDROXY-,		S 59P	S 59			S 59
ANDROSTERONE		S 59P	S 59			S 59
ANDROSTA-1,4-DIEN-3-ONE, 17B-HYDROXY-,		S 60P	S 60			S 60
ANDROST-5-ENE-3B,17B-DIOL, DI-ACETATE		S 61P	S 61			S 61
ANDROST-5-ENE-3B,17B-DIOL		S 62P	S 62			S 62
ANDROST-5-ENE-3B,17B-DIOL, 17-METHYL-		S 63P	S 63			S 63
ESTRA-1,3,5/10/-TRIEN-17-ONE, 3-HYDROXY-, BENZOATE		S 64P	S 64			S 64
ESTRONE, BENZOATE		S 64P	S 64			S 64
PREGN-4-EN-3,20-DIONE, 21-HYDROXY-		S 65P	S 65			S 65
5A-CHOLESTAN-3-OL		S 66P	S 66			S 66
PREGNA-5,17(20)-DIEN-20-ONE, 21-HYDROXY-, ACETATE		S 67P	S 67			S 67
CHOLESTAN-3B-OL		S 68P	S 68			S 68
17A-PREGN-4-EN-20-YN-3-ONE, 17-HYDROXY-,		S 69P	S 69			S 69
TESTOSTERONE, 17-ETHYNYL-,		S 69P	S 69			S 69
ESTRADIOL, 3-BENZOATE		S 70P	S 70			S 70
ESTRA-1,3,5/10/-TRIENE-3,17B-DIOL, 3-BENZOATE		S 70P	S 70			S 70
PREGNANE-3A,20B-DIOL		S 71P	S 71			S 71
ANDROST-4-EN-3-ONE, 17B-HYDROXY-, PROPIONATE		S 72P	S 72			S 72
TESTOSTERONE, PROPIONATE		S 72P	S 72			S 72
5A-ANDROSTAN-17-ONE, 3A-HYDROXY-, BENZOATE		S 73P	S 73			S 73
PREGN-5-EN-20-ONE, 3B-HYDROXY-,		S 74P	S 74			S 74
PREGN-4-ENE-3,20-DIONE, 21-HYDROXY-,		S 75P	S 75			S 75
ANDROST-4-EN-3-ONE, 17B-HYDROXY-,		S 76P	S 76			S 76
TESTOSTERONE		S 76P	S 76			S 76
ANDROST-4-EN-3-ONE, 17B-HYDROXY-, ACETATE		S 77P	S 77			S 77
TESTOSTERONE, ACETATE		S 77P	S 77			S 77

	MFG CODE	GRATING	PRISM	NMR	UV	FICHE
ANDROST-4-EN-3-ONE, 17B-HYDROXY-17-METHYL-,		S 78P	S 78			S 78
ESTRADIOL		S 79P	S 79			S 79
ESTRA-1,3,5/10/-TRIENE-3,17B-DIOL		S 79P	S 79			S 79
METAGENIN, TRIACETATE		S 80P	S 80			S 80
SPIROSTAN-2B,3B,11-TRIOL, 5B,25D-, TRIACETATE		S 80P	S 80			S 80
CHOLESTAN-7-ONE, 6-BROMO-3B-HYDROXY-, ACETATE		S 81P	S 81			S 81
METAGENIN		S 82P	S 82			S 82
SPIROSTAN-2B,3B,11-TRIOL, 5B,25D-,		S 82P	S 82			S 82
5A-CHOLESTAN-7-ONE, 6,6-DIBROMO-3B-HYDROXY-, BENZOATE		S 83P	S 83			S 83
SMILAGENIN, ACETATE		S 84P	S 84			S 84
SPIROSTAN-3B-OL, 5B,25D-, ACETATE		S 84P	S 84			S 84
GITOGENIN		S 85P	S 85			S 85
SPIROSTAN-2A,3B-DIOL, 5A,25D-,		S 85P	S 85			S 85
GITOGENIN, DIACETATE		S 86P	S 86			S 86
SPIROSTAN-2A,3B-DIOL, 5A,25D-, DI-ACETATE		S 86P	S 86			S 86
SPIROSTAN-2B,3A-DIOL, 5B,25D-,		S 87P	S 87			S 87
YAMOGENIN		S 87P	S 87			S 87
SPIROSTAN-2B,3A-DIOL, 5B,25D-, DI-ACETATE		S 88P	S 88			S 88
YAMOGENIN, DIACETATE		S 88P	S 88			S 88
B-ALANINE, N-CHOLOYL-,		S 89P	S 89			S 89
B-ALANINE, N-/3A,7A,12A-TRIHYDROXY-CHOLANOYL/-,		S 89P	S 89			S 89
HECOGENIN		S 90P	S 90			S 90
SPIROSTAN-12-ONE, 5A,25D-, 3B-HYDROXY-,		S 90P	S 90			S 90
SMILAGENIN		S 91P	S 91			S 91
SPIROSTAN-3B-OL, 5B,25D-,		S 91P	S 91			S 91
DIOSGENIN		S 92P	S 92			S 92
25D-SPIROST-5-EN-3B-OL		S 92P	S 92			S 92
DIOSGENIN, ACETATE		S 93P	S 93			S 93
25D-SPIROST-5-EN-3B-OL, ACETATE		S 93P	S 93			S 93
DIGITOGENIN		S 94P	S 94			S 94
SPIROSTAN-2A,3B,15B-TRIOL, 5A,25D-,		S 94P	S 94			S 94
SARSASAPOGENIN		S 95P	S 95			S 95
SPIROSTAN-3B-OL, 5B,25L-,		S 95P	S 95			S 95
SPIROSTAN-1B,2B,3A-TRIOL, 5B,25D-,		S 96P	S 96			S 96
TOKOROGENIN		S 96P	S 96			S 96
GLYCINE, N-/3,7,12-TRIOXOCHOLAN-OYL/-, SODIUM SALT		S 97P	S 97			S 97
GLYCOCHOLANIC ACID, 3,7,12-TRIOXO-, SODIUM SALT		S 97P	S 97			S 97
GLYCODEHYDROCHOLIC ACID, SODIUM SALT		S 97P	S 97			S 97
CHOLESTAN-7-ONE, 6,6-DIBROMO-3B-HYDROXY-, ACETATE		S 98P	S 98			S 98
SARSASAPOGENIN, ACETATE		S 99P	S 99			S 99
SPIROSTAN-3B-OL, 5B,25L-, ACETATE		S 99P	S 99			S 99
KOGAGENIN		S 100P	S 100			S 100
SPIROSTAN-1B,2B,3A,5-TETROL, 5B,25D-,		S 100P	S 100			S 100
HECOGENIN, ACETATE		S 101P	S 101			S 101
SPIROSTAN-12-ONE, 5A,25D-, 3B-HYDROXY-, ACETATE		S 101P	S 101			S 101
GLYCINE, N-/3,7,12-TRIOXOCHOLAN-OYL/-,		S 102P	S 102			S 102
GLYCODEHYDROCHOLIC ACID		S 102P	S 102			S 102
KOGAGENIN, ACETATE		S 103P	S 103			S 103
SPIROSTAN-1B,2B,3A,5-TETROL, 5B,25D-, ACETATE		S 103P	S 103			S 103
SPIROSTAN-1B,2B,3A-TRIOL, 5B,25D-,		S 104P	S 104			S 104
TOKOROGENIN, ACETATE		S 104P	S 104			S 104
CHOLEST-5-ENE-16,22-DIONE, 3B,27-DIHYDROXY-, DIACETATE		S 105P	S 105			S 105
CRYPTOGENIN, DIACETATE		S 105P	S 105			S 105
KRYPTOGENIN, DIACETATE		S 105P	S 105			S 105
ERGOSTA-5,7,22-TRIEN-3B-OL		S 106P	S 106			S 106
ERGOSTEROL		S 106P	S 106			S 106
STIGMASTA-5,22-DIEN-3B-OL		S 107P	S 107			S 107
STIGMASTEROL		S 107P	S 107			S 107
CHOLEST-4-EN-3-ONE		S 108P	S 108			S 108
PEROXYACETIC ACID, 20,20-DIESTER WITH 3A,20,20-TRIHYDROXY-5B-PREGNAN-11-ONE, 3-ACETATE		S 109P	S 109			S 109
5B-PREGNAN-11-ONE, 20,20-DIHYDRO-PEROXY-3A-HYDROXY-, TRIACETATE		S 109P	S 109			S 109
5B-ANDROSTAN-11-ONE, 17,17-DIHYDRO-PEROXY-3A-HYDROXY-, 3-ACETATE		S 110P	S 110			S 110

	MFG CODE	GRATING	PRISM	NMR	UV	FICHE
HYDROPEROXIDE, /3A-HYDROXY-11-OXO-5B-ANDROSTAN-17-YLIDENE/DI-, 3-ACETATE		S 110P	S 110			S 110
5B-ANDROSTAN-11-ONE, 17B,17PRB-/3,6-DIMETHYL-S-TETROXANE-3,6-DIYL/BIS/3A-HYDROXY-, DIACETATE		S 111P	S 111			S 111
HYDROPEROXIDE, /3A-HYDROXY-11-OXO-5B-PREGNAN-20-YLIDENE/DI-, 3-ACETATE		S 112P	S 112			S 112
5B-PREGNAN-11-ONE, 20,20-DIHYDKO-PEROXY-3A-HYDROXY-, 3-ACETATE		S 112P	S 112			S 112
HYDROPEROXIDE, /21-HYDROXY-20-OXO-PREGN-4-EN-3-YLIDENE/DI-, 21-ACETATE		S 113P	S 113			S 113
PREGN-4-EN-20-ONE, 3,3-DIHYDRO-PEROXY-21-HYDROXY-, 21-ACETATE		S 113P	S 113			S 113
HYDROPEROXIDE, /20-OXOPREGN-4-EN-3-YLIDENE/DI-,		S 114P	S 114			S 114
PREGN-4-EN-20-ONE, 3,3-DIHYDRO-PEROXY-,		S 114P	S 114			S 114
PREDNISOLONE, 21-ACETATE		S 115P	S 115			S 115
PREGNA-1,4-DIENE-3,20-DIONE, 11B,17,21-TRIHYDROXY-, 21-ACETATE		S 115P	S 115			S 115
PREDNISOLONE		S 116P	S 116			S 116
PREGNA-1,4-DIENE-3,20-DIONE, 11B,17,21-TRIHYDROXY-,		S 116P	S 116			S 116
PREGN-5-EN-20-ONE, 3B,21-DI-HYDROXY-, 21-ACETATE		S 117P	S 117			S 117
1H-BENZ/E/INDENE-6-PROPIONIC ACID, 2,3.3A,4,5,5A,6,9,9A,9B-DECAHYDRO-3,7-DIHYDROXY-3A,6-DIMETHYL-, D-LACTONE, BENZOATE		S 118P	S 118			S 118
4-OXAANDROST-5-EN-3-ONE, 17B-HYDROXY-, BENZOATE		S 118P	S 118			S 118
1H-BENZ/E/INDENE-6-PROPIONIC ACID, 3,7-DIHYDROXY-3A,6-DIMETHYLDODECA-HYDRO-, D-LACTONE, ISOMER		S 119P	S 119			S 119
4-OXA-5A-ANDROSTAN-3-ONE, 17B-HYDROXY-,		S 119P	S 119			S 119
1H-BENZ/E/INDENE-6-PROPIONIC ACID, 3,7-DIHYDROXY-3A,6-DIMETHYLDODECA-HYDRO-, D-LACTONE, ISOMER		S 120P	S 120			S 120
4-OXA-5B-ANDROSTAN-3-ONE, 17B-HYDROXY-,		S 120P	S 120			S 120
1H-BENZ/E/INDENE-6-PROPIONIC ACID, 3,7-DIHYDROXY-3A,6-DIMETHYLDODECA-HYDRO-, D-LACTONE, BENZOATE, ISOMER		S 121P	S 121			S 121
4-OXA-5B-ANDROSTAN-3-ONE, 17B-HYDROXY-, BENZOATE		S 121P	S 121			S 121
1H-BENZ/E/INDENE-6-PROPIONIC ACID, 3,7-DIHYDROXY-3A,6-DIMETHYLDODECA-HYDRO-, D-LACTONE, BENZOATE, ISOMER		S 122P	S 122			S 122
4-OXA-5A-ANDROSTAN-3-ONE, 17B-HYDROXY-, BENZOATE		S 122P	S 122			S 122
1H-BENZ/E/INDENE-6-PROPIONIC ACID, 3A,6-DIMETHYL-3-HYDROXYDODECAHYDRO-7-OXO-, BENZOATE		S 123P	S 123			S 123
3,5-SECO-A-NORANDROSTAN-3-OIC ACID, 17B-HYDROXY-5-OXO-, BENZOATE		S 123P	S 123			S 123
1H-BENZ/E/INDENE-6-PROPIONIC ACID, 7-ALLYLOXY-3,7-DIHYDROXYDODECAHYDRO-, D-LACTONE, BENZOATE		S 124P	S 124			S 124
4-OXAANDROSTAN-3-ONE, 5-ALLYLOXY-17B-HYDROXY-, BENZOATE		S 124P	S 124			S 124
ANDROST-5-EN-17-ONE, 3B-HYDROXY-, POTASSIUM SULFATE		S 125P	S 125			S 125
ANDROST-5-EN-17-ONE, 3B-HYDROXY-, P-TOLUENESULFONATE		S 126P	S 126			S 126
3,5-CYCLOANDROSTAN-17-ONE, 6B-HYDROXY-,		S 127P	S 127			S 127
3,5-CYCLOCHOLEST-6-ENE		S 128P	S 128			S 128
3-CHOLESTEROL		S 129P	S 129			S 129
3,5-CYCLOCHOLESTAN-6B-OL		S 129P	S 129			S 129
ANDROST-5-EN-17-ONE, 3B-HYDROXY-, HYDROGEN SULFATE, PYRIDINE SALT		S 130P	S 130			S 130
ANDROST-5-EN-3-ONE, 4,4-DIMETHYL-17B-HYDROXY-,		S 131P	S 131			S 131
ANDROSTAN-3-ONE, 17B-HYDROXY-2A-METHYL-, PROPIONATE		S 132P	S 132			S 132
DIHYDROTESTOSTERONE, 2A-METHYL-, PROPIONATE		S 132P	S 132			S 132
ANDROSTAN-3-ONE, 17B-HYDROXY-6B-METHYL-,		S 133P	S 133			S 133
DIHYDROTESTOSTERONE, 6B-METHYL-,		S 133P	S 133			S 133
ANDROST-4-EN-3-ONE, 17B-HYDROXY-7A-METHYL-, PROPIONATE, HYDRATE		S 134P	S 134			S 134
CHOLANIC ACID, 3,3-ETHYLENEDIOXY-		S 135P	S 135			S 135

	MFG CODE	GRATING	PRISM	NMR	UV	FICHE
CHOL-6-ENIC ACID, 3,3-ETHYLENE-DIOXY-12-OXO-, METHYL ESTER		S 136P	S 136			S 136
CHOLANIC ACID, 3,3-ETHYLENEDIOXY-, METHYL ESTER		S 137P	S 137			S 137
CHOLANIC ACID, 3,3-ETHYLENEDIOXY-7A-HYDROXY-12-OXO-, METHYL ESTER, ACETATE		S 138P	S 138			S 138
CHOLANIC ACID, 7,12-DIOXO-3,3-ETHYLENEDIOXY-, METHYL ESTER		S 139P	S 139			S 139
CHOLANIC ACID, 3,3-ETHYLENEDIOXY-7A-HYDROXY-12-OXO-,		S 140P	S 140			S 140
CHOLANIC ACID, 3,3-ETHYLENEDIOXY-12-OXO-,		S 141P	S 141			S 141
CHOLANIC ACID, 7,12-DIOXO-3,3-ETHYLENEDIOXY-,		S 142P	S 142			S 142
1,4-CHRYSENEDIONE, 8-METHOXY-2,3,4A,-4B,5,6,12,12A-OCTAHYDRO-, ISOMER		S 143P	S 143			S 143
D-HOMO-18-NORESTRA-1,3,5/10/,9/11/-TETRAENE-15,17A-DIONE, 3-METHOXY-,		S 143P	S 143			S 143
1,4-CHRYSENEDIONE, 8-METHOXY-2,3,4A,-4B,5,6,12,12A-OCTAHYDRO-, ISOMER		S 144P	S 144			S 144
D-HOMO-18-NOR-14B-ESTRA-1,3,5/10/,-9/11/-TETRAENE-15,17A-DIONE, 3-METHOXY-,		S 144P	S 144			S 144
1,4-CHRYSENEDIONE, 8-METHOXY-2,3,4A,-4B,5,6,12,12A-OCTAHYDRO-, ISOMER		S 145P	S 145			S 145
D-HOMO-18-NOR-13A,14B-ESTRA-1,3,5/10/,9/11/-TETRAENE-15,17A-DIONE, 3-METHOXY-,		S 145P	S 145			S 145
CHOLANIC ACID, 3B-HYDROXY-12-OXO-, ACETATE		S 146P	S 146			S 146
CORTICOSTERONE, DEOXY-, ACETATE		S 147P	S 147			S 147
PREGN-4-ENE-3,20-DIONE, 21-HYDROXY-, ACETATE		S 147P	S 147			S 147
5B-CHOLANIC ACID, 3A,6A-DIHYDROXY-,		S 148P	S 148			S 148
HYODEOXYCHOLIC ACID		S 148P	S 148			S 148
ANDROST-5-ENE-3B,17A-DIOL		S 149P	S 149			S 149
CHRYSENONE, 1/2H/-, 3,4,4A,11,12,-12A-HEXAHYDRO-, ISOMER		S 150P	S 150			S 150
D-HOMO-18-NOR-13A,14B-ESTRA-1,3,5/10/,6,8-PENTAEN-17A-ONE		S 150P				150
CHRYSENEDIONE, 1,11-, 2,3,4,4A,-12,12A-HEXAHYDRO-, ISOMER		S 151P				151
D-HOMO-18-NOR-13A,14B-ESTRA-1,3,5/10/,6,8-PENTAENE-11,17A-DIONE		S 151P				151
CHRYSENONE, 1/2H/-, 3,4,4A,11,12,-12A-HEXAHYDRO-8-METHOXY-, ISOMER		S 152P	S 152			S 152
D-HOMO-18-NOR-13A,14B-ESTRA-1,3,5/10/,6,8-PENTAEN-17A-ONE, 3-METHOXY-,		S 152P	S 152			S 152
CHRYSENEDIONE, 1,11-, 2,3,4,4A,-12,12A-HEXAHYDRO-8-METHOXY-, ISOMER		S 153P	S 153			S 153
D-HOMO-18-NOR-13A,14B-ESTRA-1,3,5/10/,6,8-PENTAENE-11,17A-DIONE, 3-METHOXY-,		S 153P	S 153			S 153
CARD-20/22/-ENOLIDE, 5B,14B-, 3B,14-DIHYDROXY-, 3-DIGITOXOSIDE		S 154P	S 154			S 154
CARD-20/22/-ENOLIDE, 5B,14B-, 3B,14-DIHYDROXY-, 3-DIGITOXOSIDE		S 154P	S 154			S 154
DIGITOXIGENIN, 3-DIGITOXOSIDE		S 154P	S 154			S 154
CORTICOSTERONE, 17A-HYDROXY-, 21-SUCCINATE, SODIUM SALT		S 155P	S 155			S 155
CORTISOL, 21-/HYDROGEN SUCCINATE/, SODIUM SALT		S 155P	S 155			S 155
PREGN-4-ENE-3,20-DIONE, 11B,17-DIHYDROXY-, 21-/HYDROGEN SUCCINATE/, SODIUM SALT		S 155P	S 155			S 155
PREGN-4-EN-18-OIC ACID, 3,20-DIOXO-,		S 156P	S 156			S 156
PREGN-4-EN-3-ONE, 18,20-EPOXY-20-HYDROXY-,		S 157P	S 157			S 157
ALDACTONE		S 158P	S 158			S 158
17A-PREGN-4-ENE-21-CARBOXYLIC ACID, 17-HYDROXY-7A-MERCAPTO-3-OXO-, G-LACTONE, ACETATE		S 158P	S 158			S 158
PREGN-4-EN-3-ONE, 20,21-DIHYDROXY-18,20-EPOXY-,		S 159P	S 159			S 159
5A-CHOLESTAN-6-ONE, 3B,5-DIHYDROXY-, 3-ACETATE		S 160P	S 160			S 160
5A-CHOLESTANE-3B,5,6B-TRIOL, 3,6-DIACETATE		S 161P	S 161			161
5A-CHOLESTANE-3B,4B-DIOL DIACETATE		S 162P	S 162			162
CHOLEST-5-ENE-3B,4B-DIOL, DIACETATE		S 163P	S 163			S 163

	MFG CODE	GRATING	PRISM	NMR	UV	FICHE
CHOLEST-5-ENE-33,4B-DIOL, 4-ACETATE		S 164P	S 164			S 164
CHOLEST-5-ENE-3B,4B-DIOL, 3-ACETATE		S 165P	S 165			S 165
PREGNEMOLONE, ACETATE		S 166P	S 166			S 166
PREGN-5-EN-20-ONE, 3B-HYDROXY-, ACETATE		S 166P	S 166			S 166
CORTISONE, 21-ACETATE		S 167P	S 167			S 167
PREGN-4-ENE-3,11,20-TRIONE, 17,21-DIHYDROXY-, 21-ACETATE		S 167P	S 167			S 167
CORTISOL, 21-ACETATE		S 168P	S 168			S 168
HYDROCORTISONE, 21-ACETATE		S 168P	S 168			S 168
PREGN-4-ENE-3,20-DIONE, 11B,17,21-TRIHYDROXY-, 21-ACETATE		S 168P	S 168			S 168
14B-LANOSTANE-3B,7A-DIOL		S 169P	S 169			S 169
14B-CHOLANIC ACID, 3B-HYDROXY-4,4,14-TRIMETHYL-, METHYL ESTER		S 170P	S 170			S 170
TRINOR-14B-LANOSTAN-24-OIC ACID, 25,26,27-, 3B-HYDROXY-, METHYL ESTER		S 170P	S 170			S 170
14B-LANOST-5-ENE-7,11-DIONE, 3B-HYDROXY-, ACETATE		S 171P	S 171			S 171
14B-LANOST-8-ENE-7,11-DIONE, 3B-HYDROXY-, ACETATE		S 172P	S 172			S 172
14B-LANOST-8-ENE-3,7-DIONE		S 173P	S 173			S 173
14B-LANOSTAN-7-ONE, 3B,11B-DIHYDROXY-, DIACETATE		S 174P	S 174			S 174
14B-LANOSTAN-3-ONE, 7A,11B-DIHYDROXY-, DIACETATE		S 175P	S 175			S 175
14B-LANOST-9/11/-ENE-3B,7B-DIOL, DIACETATE		S 176P	S 176			S 176
14B-LANOST-8-ENE-3,7,11-TRIONE		S 177P	S 177			S 177
14B-LANOSTAN-11-ONE, 3B,7A-DIHYDROXY-;		S 178P	S 178			S 178
18-NORANDROST-13-EN-3-ONE, 17,17-DIMETHYL-,		S 179P	S 179			S 179
CHOLESTAN-3A-OL, 3-METHYL-,		S 180P	S 180			S 180
14B-LANOSTAN-11-ONE, 3B,7A-DIHYDROXY-, 3-ACETATE		S 181P	S 181			S 181
14B-LANOST-5-ENE-3,7,11-TRIONE		S 182P	S 182			S 182
14B-LANOST-8-EN-3B-OL		S 183P	S 183			S 183
14B-LANOST-5-ENE-7,11-DIONE, 3B-HYDROXY-, BENZOATE		S 184P	S 184			S 184
14B-LANOSTANE-3,7-DIONE, 11B-HYDROXY-, ACETATE		S 185P	S 185			S 185
14B-LANOSTANE-3B,7B-DIOL, DIBENZOATE		S 186P	S 186			S 186
14B-LANOST-8-ENE, 3B-HYDROXY-, ACETATE		S 187P	S 187			S 187
14B-CHOLANIC ACID, 3B-HYDROXY-4,4,14-TRIMETHYL-, METHYL ESTER, ACETATE		S 188P	S 188			S 188
TRINOR-14B-LANOSTAN-24-OIC ACID, 25,26,27-, 3B-HYDROXY-, METHYL ESTER, ACETATE		S 188P	S 188			S 188
CHOLEST-5-ENE, 3B-METHYL-,		S 189P	S 189			S 189
CHOLESTANE, 3B-METHYL-,		S 190P	S 190			S 190
14B-LANOSTANE-3B,17B-DIOL, DIACETATE		S 191P	S 191			S 191
CHOLEST-2-ENE, 3-METHYL-,		S 192P	S 192			S 192
14B-LANOSTA-7,9/11/-DIEN-3B-OL, ACETATE		S 193P	S 193			S 193
14B-CHOLANIC ACID, 7,11-DIOXO-3B-HYDROXY-4,4,14-TRIMETHYL-,		S 194P	S 194			S 194
TRINOR-14B-LANOSTAN-24-OIC ACID, 25,26,27-, 7,11-DIOXO-3B-HYDROXY-,		S 194P	S 194			S 194
ALLOPREGNAN-20-ONE, 3B-HYDROXY-4,4,14B-TRIMETHYL-,		S 195P	S 195			S 195
PREGNAN-20-ONE, 5A,14B-, 3B-HYDROXY-4,4,14-TRIMETHYL-,		S 195P	S 195			S 195
14B-LANOSTAN-11-ONE, 3B,7B-DIHYDROXY-, DIACETATE		S 196P	S 196			S 196
14B-CHOL-8-ENIC ACID, 7,11-DIOXO-3B-HYDROXY-4,4,14-TRIMETHYL-, ACETATE		S 197P	S 197			S 197
TRINOR-14B-LANOST-8-EN-24-OIC ACID, 25,26,27-, 7,11-DIOXO-3B-HYDROXY-, ACETATE		S 197P	S 197			S 197
LANOST-8-EN-7,11-DIONE, 3B-HYDROXY-,		S 198P	S 198			S 198
14B-CHOLANIC ACID, 7,11-DIOXO-3B-HYDROXY-4,4,14-TRIMETHYL-, METHYL ESTER, ACETATE		S 199P	S 199			S 199
TRINORLANOSTAN-24-OIC ACID, 25,26,-27-, 7,11-DIOXO-3B-HYDROXY-, METHYL ESTER, ACETATE		S 199P	S 199			S 199
LANOSTAN-3-ONE		S 200P	S 200			S 200
LANOSTANE-3B,7B,11B-TRIOL, TRI-ACETATE		S 201P	S 201			S 201
LANOSTANE-3B,7A-DIOL, DIACETATE		S 202P	S 202			S 202
LANOSTANE-3B,7B,11B-TRIOL, 11-ACETATE		S 203P	S 203			S 203