



IS NIR Spectra

Starter (1043 spectra)

The NIR sublibrary "IS NIR Spectra Starter (1043 spectra)" includes selection of common organic and inorganic chemicals, common pharmaceutical related substances and common polymers. It has been designed for beginners on the field of NIR spectroscopy.

The near infrared spectral library „IS NIR Spectra“ is a unique collection of NIR (near infrared) digital spectra. The spectra have been collected in range 4200-10000 cm⁻¹ (=2.4 – 1 micrometers).

„IS NIR Spectra“ is the biggest and newest NIR library available on the market. This spectral library has been designed for users who use their NIR spectrometer not only for quantitative and chemometric analysis, but also want to identify unknown samples or just want to use the library as reference spectra database.

IS means "Integrating Sphere" and at the same time "Identify Sample".

Technical parameters:

The „IS NIR Spectra“ were collected using the FT-NIR Spectrometer equipped with Integrating Sphere Accessory.

Resolution: standard 4cm⁻¹

Customized resolution: upon special request the spectra can be delivered in customized resolution to reach better correspondence with spectra collected by customer NIR instrument

Spectral range in wavenumbers units: 4200-10000 cm⁻¹

Spectral range in wavelength units: 2.4 – 1 micrometers

Only one spectrum/compound covering the mentioned spectral range

Typical text information about the sample includes (when available):

Compound name including synonyms

CAS number

Chemical formula

Molecular weight

Additional information about the sample like manufacturer and comments.

Download a free NIR library of 30 NIR spectra to check the compatibility of you instrument with the „IS NIR Spectra“.

Samples were selected and NIR spectra collected 2010-2012.

IS NIR Spectra – Starter

1043 NIR spectra

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This library is available as digital searchable library compatible with your spectroscopic software. Visit the „Download“ section of our webpage to select the correct library format. The spectra are available in wavenumbers (cm-1) units or wavelength (micrometer) units. Also the library can be delivered with SEARCH software or in *.pdf format (if you do not have a spectroscopic software).

The near infrared spectral library „IS NIR Spectra“ can be purchased as a complete collection of over 6049 spectra or as following application specific sublibraries.

Ordering Code	Library Name	Number of Spectra
ISNNCM-X	IS NIR Complete Collection	6049
IS NIR Sublibraries*:		
ISNNST-X	IS NIR Starter	1043
ISNNPH-X	IS NIR Pharma, Drugs	1340
ISNNPO-X	IS NIR Polymers, Additives	1740
ISNNHA-X	IS NIR Hazardous, Toxic	1718
ISNNDY-X	IS NIR Dyes, Pigments	1005

* all sublibraries spectra are included in the complete collection ISNNCM-X and have the same technical parameters

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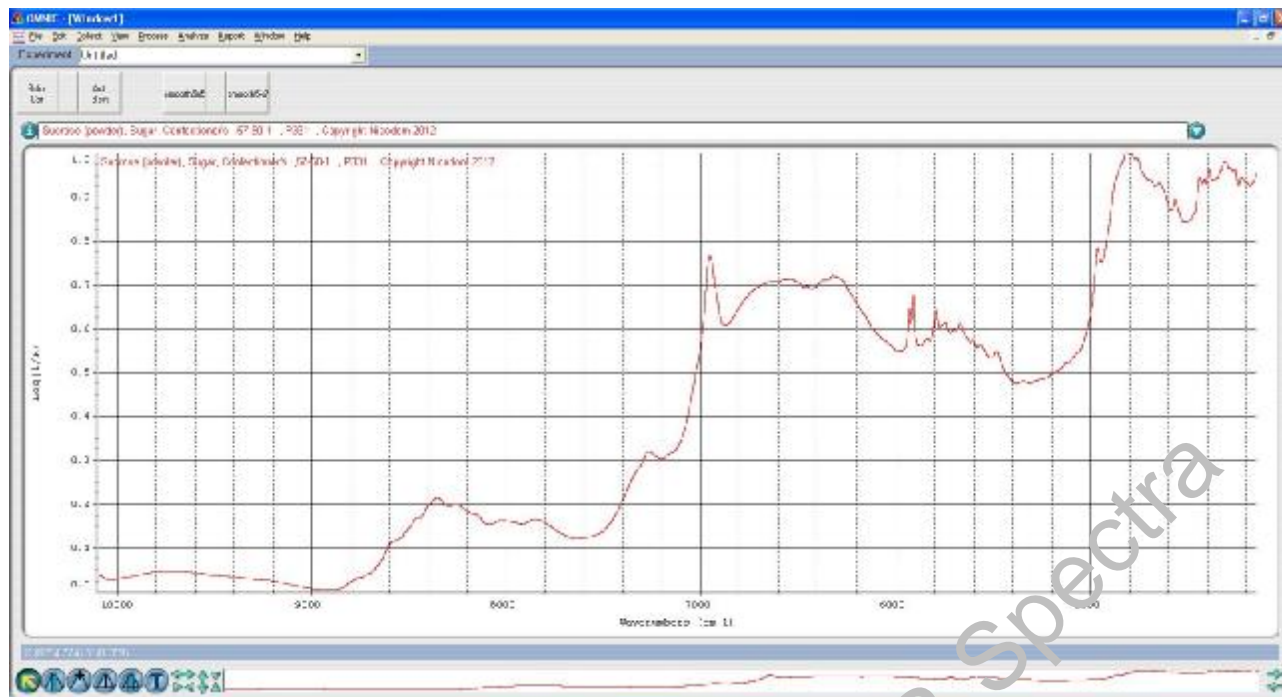
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Example Spectra

Pictures: NIR spectrum of Sucrose (powder), C₁₂H₂₂O₁₁, CAS: 57-50-1, in cm⁻¹ units (range 4200-10000 cm⁻¹), the second spectrum in micrometers (2.4 – 1 micrometers), both resolution 4cm⁻¹, Copyright Nicodom 2012



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List of Spectra /Compound Names

Starch Tapioca
Citric Acid
Sucrose (powder), Sugar, Confectioner's
Talc
L-Ascorbic acid, Vitamin C
Polystyrene high impact #1
Urea
D-Glucose Monohydrate
Polyvinylchloride
Zein
Poly(methyl methacrylate)
Phenoxy resin
Poly(ethylene oxide)
Titanium Dioxide
Ethanol
Toluene
Benzoic acid
Bicarbonate of soda
Acetylsalicylic acid
Benzene
L-Alanine
L-Arginine
L-Histidine
L-Proline
L-Serine
Naphthalene
Glycine
L(+)-Tartaric acid
Teflon
Poly(vinyl alcohol)
Cellulose Microcrystalline (Vivapur 105)
Cellophane
Cellulose Acetate
Poly(diallylphthalate)
Nylon 11
Phenol-formaldehyde resin
Paragum 501 (Polyacrylate)
Poly(acrylamide) #1
Poly(acrylic acid) m.w.4000000
Poly(ethylene dimethacrylate)

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Poly(methacrylic acid) #2
Polyacrylate
Nylon 610
Ultramid C-35
Buna CB HX 529 SIC, Polymer PB type
Poly(butadiene) (55% cis & trans, 45% vinyl)
Poly(butadiene), phenyl terminated
Polyisoprene cis #1
Poly(cyclohexylene terephthalate)
Poly(diethylene hexachlor endomethylene tetrahydrophthalate)
Poly(diethylene phthalate)
Poly(diethylene tetrahydrophthalate)
Poly(dipropylene endomethylene tetrahydrophthalate)
Poly(dipropylene hexachlor endomethylene tetrahydrophthalate)
Poly(dipropylene isophthalate)
Poly(ethylene endomethylene tetrahydrophthalate)
Poly(ethylene hexachlor endomethylene tetrahydrophthalate)
Poly(ethylene isophthalate)
Poly(ethylene maleate)
Poly(hexandiol 1,6 maleinadipate)
Poly(isopropylene endomethylene tetrahydrophthalate)
Poly(neopentylene adipate)
Poly(neopentylene fumarate)
Poly(neopentylene hexachlor endomethylene tetrahydrophthalate)
Poly(neopentylene isophthalate)
Poly(neopentylene phthalate)
Poly(neopentylene succinate)
Poly(neopentylene terephthalate)
Poly(propylene maleate)
Poly(propylene succinate)
Poly(trimethylpentylen adipate)
Poly(trimethylpentylen endomethylene tetrahydrophthalate)
Poly(trimethylpentylen maleate)
Poly(trimethylpentylen sebacate)
Polyester, adipic Acid
Polyethylene plasticized #2
Acacia gum
Carrageenan
Gum arabic
Paraform
Paraldehyde
PEG 7 Glyceryl Cocoate
Poly(diallylphthalate) #1
Poly(N-vinyl carbazole), Luvican

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Poly(vinyl acetate) #2
Poly(vinyl isobutyl ether)
Polyether polyol
HIPS/HDPE alloy #2
HIPS/PP/PA6 alloy
Polypropylene with rubber content
Polypropylene, isotactic #1
Polypropylene+Vistalon 719, 1:1
Polystyrene, dicarboxy terminated
Polyurethane #1
Poly(propylene glycol) 500
Bisphenol-A-polycarbonate, 20% glass reinforced
Epon 828
Epoxy Resin
Epoxy resin, Bisphenol A + epichlorohydrin
Melamine-urea-formaldehyde resin #1
Melamine-urea-formaldehyde resin #2
Phenol resin #1
Phenolic Resin
Dimeticone
Poly(methylphenylsiloxane) fluid
Silicone rubber #1
Acrylic Copolymer with Styrene
Lotryl 35MA08
Ploxamer 105 (PEG-PPG copolymer)
Poly(acrylonitrile:butadiene)
Poly(acrylonitrile:divinylbenzene)
Poly(alpha-methylstyrene-block-butadiene)
Poly(ethylene:tetrafluoroethylene)
Poly(styrene:ethylacrylate)
Poly(styrene:n-butyl methacrylate)
Poly[(2,3-epoxypropyl methacrylate):styrene:(ethylene dimethacrylate)]
Poly[(acrylic acid):(2-ethylhexyl acrylate):styrene]
Poly[(acrylic acid):(butyl acrylate):2-(hydroxyethyl methacrylate):styrene]
Poly[(acrylic acid):(butyl acrylate):styrene]
Poly[(acrylic acid):(ethyl acrylate):(2-hydroxyethyl methacrylate):styrene]
Poly[(divinyl benzene):styrene]
Poly[styrene-co-acrylonitrile-co-(divinyl benzene)]
Polypropylene-graft-maleic anhydride
Ultramid 6A, Poly[caprolactam:(hexamethylene adipamide)]
Vinylpyrrolidone-Vinylacetate Copolymer
Cycloc G 101, Copolymer ABS type
Poly(methyl methacrylate):(butyl methacrylate)
Poly[(2,3-epoxypropyl methacrylate):(ethylene dimethacrylate)]

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Poly[(acrylic acid):(2-hydroxyethyl methacrylate)]
Poly[(acrylic acid):(butyl acrylate):(ethyl acrylate):(2-ethylhexyl acrylate):(methacryl amide)]
Poly[(acrylic acid):(butyl acrylate):(methacryl amide):(methyl methacrylate)]
Poly[(acrylic acid):(butyl acrylate):(methyl methacrylate)]
Poly[(acrylic acid):(butyl acrylate):]
Poly[(acrylic acid):(ethyl acrylate):(methacryl amide):(methyl methacrylate)]
Poly[(acrylic acid):(ethyl acrylate)]
Poly[(acrylic acid):acrylonitrile]
Poly[(ethyl acrylate):(methacrylic acid)]
Poly[acrylonitrile:(butyl acrylate):(methacryl amide)]
Poly(butadiene::styrene)
Poly(styrene::butadiene) ABA block (28% styrene), Kraton D 1101
Poly(styrene::butadiene) graft
Poly(styrene::isoprene) ABA block (14% styrene)
Dutral TER 9046, Copolymer EPDM type
Poly(ethylene:propylene:diene) (50% ethylene, 4% diene)
Poly(ethylene:propylene:diene) (50% ethylene, 8% diene)
Escorene ultra UL 00723, Copolymer EVA type
Evatane 1005 VN 4, Copolymer EVA type
Levapren 8338, Copolymer EVA type
Miravithen D23EA, Copolymer EVA type
Poly(ethylene:propylene), Daplen KSR 4525
Poly(ethylene:propylene), Keltan 740
Poly(propylene:ethylene), Novolen 2900NC
Kibisan 127, Copolymer SAN type
Poly(styrene:acrylonitrile) (70% styrene)
Poly(vinylidene fluoride) #1
Xanthan gum
Acetylated distarch adipate
Agar powder
Starch, Maize Starch Pregelatinised
Macrogol 1500, Poly(ethylene glycol) 1500
Poly(4,4-dipropoxy-2,2-diphenyl propane fumarate)
Poly(dianol 22 tetrahydrophthalate)
Poly(dianol 33 adipate)
Poly(dianol 33 endomethylene tetrahydrophthalate)
Poly(dianol 33 fumarate)
Poly(dianol 33 isophthalate)
Poly(dianol 33 maleate)
Poly(dianol 33 tetrahydrophthalate)
Antioxidant 2246
Chimasorb 944
Cyasorb UV 3346

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Hostanox 03
Hostavin N30 (HALS)
Irgafos 168
Irganox 1010 + Irganox 168
Irganox 1076
Irganox 1330
Tris(2,4-di-tert-butylphenyl) phosphite
Irganox 3114
Leucopur EGM
Millad 3988
Tinuvin 622
Uvinul 4050 H
Candelilla wax
Carnauba wax
Carnauba wax yellow
Ceresin
Cetaceum, Cetyl Palmitate 15
Chlorinated paraffin
Ethoxylated Lanoline 4000
Lanolin Anhydrous
Wax, Yellow Bees Wax
Tween 21, POE (4) sorbitan monolaurate
Tween 60, POE (20) Sorbitan Monopalmitate
2-Benzothiazolethiol
Aliquat 336
Aluminium acetate basic
Aluminium Hydroxide
Ethylene/Vinylacetate copolymer with Aluminium Oxide pigment
Aluminium Stearate
Aluminosilicate
Ammonium Bromide
Bis (2-hydroxyethyl) tallow amine
Brij 35, Polyoxyethylene (35) Lauryl Ether
Calcium Oxide
Dibutylphthalate
Diethylenetriamine
Di-isononyl Phthalate
Disodium EDTA
Edetate Dipotassium Magnesium
Erucamide
Ethyl palmitate
Glycerides of fatty acids C12-C22
Glycerides of natural fatty acids
Glycerol Stearate

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Glyceryl Stearate
Gum Tragacanth
Hexadecanoic Acid, Palmitic acid
Iron (III) Hydroxide
Iron (III) Oxide monohydrate, yellow
Kaolin, Aluminum silicate dihydrate
Loxamid E, Stearoamides mixture
Magnesium acetate tetrahydrate
Magnesium Chloride
Magnesium Chloride Hexahydrate
Magnesium Stearate
Manganese stearate
Mono and Diglycerides of fatty acids
Nacrelon S-30 (pearlescent pigment)
Octadecanoic Acid, Stearic Acid
Oxide Aluminium
Quartz
Silipor 600
Sodium Metasilicate
Sodium Silicate
Sorbitan tristearate
Succinimide
Triton, X-100
Tween 65, POE (20) sorbitan tristearate
2,6-Di-tert-butyl-p-cresol
Color masterbatch Poly[ethylene-co-(vinyl acetate)] + 45% benzimidazolone
Color masterbatch Poly[ethylene-co-(vinyl acetate)] + 45% yellow pigment #2
Color masterbatch Polyethylene + 30% red pigment #3
Color masterbatch Polyethylene + 30% yellow pigment #2
Color masterbatch Polyethylene + 30% yellow pigment #4
Color masterbatch Polyethylene + 45% yellow pigment
Color masterbatch Polyethylene + 60% brown pigment
Color masterbatch Polyethylene + 60% Fe-oxide
Color masterbatch Polyethylene + 60% yellow pigment #3
Color masterbatch Polyethylene + 75% white pigment
Color masterbatch Polypropylene + 70% white pigment
Color masterbatch Polypropylene + brown pigment
Color masterbatch Polypropylene + white pigment
Color masterbatch Polypropylene + yellow pigment #1
Color masterbatch Polystyrene + 30%, Sb, Ni, Ti-oxide
Color masterbatch Polystyrene + 50% brown pigment
Color masterbatch Polystyrene + 50% white pigment
Color masterbatch Poly(styrene-co-acrylonitrile) + 50% white pigment
(E)-Anethole

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1,2-Dicyanobenzene
1-Docosanol
1-Heptadecanol
1-Heptene
1-Methyl-4-piperidone
1-Octadecanol
2-(Dibutylamino) ethanol
2-Methoxybenzaldehyde
2-Methoxynaphthalene
4-Aminosalicylic acid sodium salt
4-Methyl-2-pentanone
4-Vinylcyclohexene dioxide
5,5-Dimethyl-1,3-cyclohexanedione
6-Aminohexanoic acid
Acetanilide
Aluminium Chlorohydrate
Ammonium Acetate
Azelaic acid
Bentonite
Benzotriazole
Beta-cyclodextrine
Butylated hydroxyanisole, BHA
Calcium chloride dihydrate
Calcium Hydroxide
Calcium Lactate
Carbonate Sodium Decahydrate
Carbonate Zinc Basic
Chloral hydrate
Chlorodiphenylphosphine
Cinnamic Acid
Citric Acid Monohydrate
Cocoamidopropyl Hydroxysultaine
Cyclododecanone
D-(+)-Malic acid
Dextrin
D-Galactonic acid g-lactone
Di(ethylene glycol) distearate
Diethyl t-butylmalonate
Diphosphate Tetrasodium
Dodecanoic acid
Ethyl caprylate
Ethyl maltol
Ethylene glycol diformate
Gallotannin

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Inositol
Iodoform
Iron Citrate
Isopropyl Glycidyl Ether
Isostearyl isostearate
Itaconic acid
L-Lactic acid
L-Lactic acid, Sodium salt
L-Malic acid
Magnesium Carbonate Basic Hydrate
Metabisulfite Potassium
Myristic acid
Stearate Calcium
Oil of Peppermint, Menthol
Orthoboric Acid
Ostion (HPLC sorbent)
Pentasodium triphosphate
Pentyl propionate
Persulfate Ammonium
Persulfate Sodium
Phenyl Salicylate
Phosphate Ammonium Dibasic
Phosphate Ammonium Monobasic
Phosphate Calcium Dibasic
Phosphate Calcium Monobasic
Phosphate Potassium Monobasic
Phosphate Potassium Tribasic n-hydrate
Phthalide
Potassium chloride
Potassium Nitrate
Ethanecarboxylic acid
Salicylic acid
Sodium Cetylsulfate
Sodium Tetraborate Decahydrate
Stannous Chloride
Sulfate Aluminium
Sulfate Ammonium
Sulfate Ferrous
Sulfate Magnesium
Sulfate Sodium Monobasic
Thiosulfate Sodium
Glycol Bis(Hydroxyethyl) Ether
Zinc salicylate
1,3-Butanediol

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1,5-Cyclooctadiene
1,5-Pentanediol
1-Dodecene
1-Hexadecene
1-Nonanol
1-Propanol
1-Tetradecene
2,3-Butanediol
2-Benzyloxyethanol
2-Butanone
2-Methyl-1-propanol
2-Methyl-2-hexanol
2-Methyl-2-pentanol
2-Octanol
3-Amino-1-propanol
Acetic anhydride
Acrylonitrile
Anethole
Benzaldehyde
Benzyl alcohol
Butyl ether
Butyl formate
Butyraldehyde
Chloroform
Cycloheptanol
Cyclohexanol
Cyclohexanone
Diethyl ethylmalonate
Diethyl malonate
Diethyl methylmalonate
Diethyl oxalate
Diethyl phthalate
Diethyl propylmalonate
Diethyl succinate
Diethylene Glycol Dibutyl Ether
Diethylene glycol dimethyl ether
Dimethyl succinate
2-Dimethylaminoethanol
Dioctylphthalate
2-Oxohexamethyleneimine
Ethyl acetate
Ethyl caproate
Ethyl crotonate
Ethyl dodecanoate

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Ethyl formate
Ethyl Lactate
Ethyl salicylate
Ethylene Diglycol Monoethyl Ether
Ethylene glycol
Ethylene glycol dimethacrylate
Ethylene glycol dimethyl ether
Ethylene glycol monobutyl ether
Ethylene glycol monoethyl ether
Formic acid
g-Butyrolactone
g-Caprolactone
Hexanoic acid
Isoamyl acetate
3-Methyl-1-butanol
Methyl alcohol
Methyl formate
Methyl Palmitate
Methylsalicylate
N,N-Dimethylformamide
N-Methylacetamide
o-Cresol
Oleic acid
Propionaldehyde
Propylene carbonate
Propylene Glycol
t-Butyl Acetate
t-Butyl alcohol
Tributyl phosphate
Tributylin
Trichloroethylene
Triethanolamine
Triethyl citrate
Trioctylamine
Water
Xylenes Mixed
Mineral Oil, light and heavy
1,10-Decanediol= Decamethylene glycol
1,7-Heptanediol= Heptamethylene glycol
1,9-Nonanediol
Allyl alcohol
Cetyl alcohol
Dodecanedioic acid
Ethylenediamine

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Fumaric acid
Glutaric acid
g-Valerolactone
Maleic anhydride
Malonic Acid
Octylamine
Phthalimide
Sebacic Acid
Sodium benzoate
Suberic acid
Succinic acid
Succinic anhydride
trans-1,2-Cyclohexanediol
Hexamethylenetetramine
4,4'-thiobis(2-tert-butyl-5-methylphenol)
Ammonium carbonate
Cyasorb UV 9
Distearyl thiodipropionate
Linoleic Acid
Monoethanolamine
Sodium lauryl sulfate
Phenol
Ethyl Cellulose
Polyvidone Insoluble, Polyvinylpyrrolidone
Caramel
Starch Modified
Starch, Potato Starch Acetyl Oxidized
1,4-Phenylenediamine
Calcium Chloride Powder
Aluminiumsilicate Calcium Sodium
Iron (III) Oxide, Hematite
1,12-Diaminododecane
1,2,4-Triacetoxybenzene
1,2-Bis(diphenylphosphino)ethane
1,5-Dimethylnaphthalene
12-Hydroxydodecanoic acid
1-Adamantanecarboxylic acid
1-Bromohexadecane
1-Bromotetradecane
1-Iodobutane
1-Methylnaphthalene
1-Phenyl-1,2-ethanediol
1-Phenyl-2-thiourea
Isooctane

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2,2'-Azobis(isobutyronitrile)
2,4-Dihydroxybenzaldehyde
2-Ethoxynaphthalene
2-Methylnaphthalene
2-Naphthol
3-Nitrophenol
4-Aminobenzoic acid; PABA
4-Bromoaniline
4-Chlorobutyronitrile
9,10-Dicyanoanthracene
Acetoacetanilide
Allyl sulfide
Ammonium iodide
Anthracene
Benzamide
Benzil
Benzimidazole
Benzyl bromide
Benzyltrimethylammonium chloride
Cetyldimethylamine
Chloroacetamide
Cupric acetate .H2O
Diethyl dithiophosphate, ammonium salt
Di-t-butyl dicarbonate
DL-Camphor
DL-Menthol
Hexamethylbenzene
Hydroquinone
Imidazole
Indole
Lead(II) nitrate
L-Menthol
Methanesulfonic acid
N,N-Dimethyl-p-toluidine
N,N'-Methylenebisacrylamide
n-Dotriacontane
Nicotinic acid = Niacin
o-Tolidine
Phenylurea
Potassium Ferricyanide
Potassium Ferrocyanide
1,3-Benzenediol
Silver Nitrate
Sulfamic acid

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Tetrabutylammonium cyanide
Tetrabutylammonium perchlorate
Tetracosane
Tetraoctylammonium bromide
Thioacetic acid
trans-Cinnamic acid
Tribenzylamine
Triethyl phosphonoacetate
1,10-Dibromodecane
1,2-Dibromoethane
1,2-Dibromopropane
1,2-Dichlorobenzene
1,2-Dichloroethane
1,4-Butanediol diglycidyl ether
1,4-Dibromobutane
1,4-Pentanediol
1-Bromo-3-chloropropane
1-Bromobutane
1-Bromododecane
1-Bromoheptane
1-Bromohexane
1-Chlorohexane
1-Decanol
1-Decene
1-Heptanol
1-Iodohexane
1-Octanol
2-(Ethylamino)ethanol
2,2,2-Trifluoroethanol
2,2'-Dichloroethyl ether
2,2'-Thiodiethanol
2,3-Dimethyl-2-butanol
2-Amino-2-methyl-1-propanol
2-Bromohexanoic acid
2-Bromopentane
2-Chloroethanol
2-Ethoxyethyl acetate
2-Mercaptoethanol
2-Methyl-1-butanol
2-Methyl-2-butanol
2-Nitropropane
3-Acetylpyridine
3-Chloro-1,2-propanediol
4-Isopropyltoluene, p-Cymene

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Acetonitrile
Amyl Acetate
Benzonitrile
Benzyl acetate
Benzyl chloride
Benzylamine
Butyl acetate
n-Butyl vinyl ether
Cyclododecene
Cyclohexane
Cyclohexene
Cyclohexylamine
Cyclohexylmercaptan
Cyclooctanone
Cyclopentane
Cyclopentanol
Cyclopentanone
Decane
Diacetone Alcohol
Dibutyl sulfide
Dichloromethane
Dicyclopentadiene
Diethylamine
Diethylene glycol
Diisobutylketone
Diisopropyl ether
Diisopropylamine
Dodecane
Epichlorhydrin
Ethyl benzoate
Ethyl bromoacetate
Ethyl butyrate
Ethyl chloroacetate
Ethyl cinnamate
Ethylene glycol monomethyl ether
Heptadecane
Heptane
Isoamyl ether
Isobutyronitrile
Methyl benzoate
Methyl dichloroacetate
m-Toluidine
N,N,N',N'-Tetramethylethylenediamine
N,N-Diethylethanolamine

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N,N-Dimethylacetamide
Nitrobenzene
Nitrocyclohexane
Nitroethane
Nitromethane
N-Methylcyclohexylamine
Nonylphenol
o-Toluidine
Phenyl Ether
Phenyl Isocyanate
Piperidine
t-Butylamine
2-Butyne-1,4-Diol
2-Vinylnaphthalene
Acrylamide
Chloromaleic anhydride
Dicyandiamide = Cyanoguanidine
Ethyl Carbamate
Isocyanic acid
Methylamine Hydrochloride
mono-Methyl terephthalate
Oleoyl chloride
Terephthalic acid
Tetrahydrofurfuryl alcohol
L-Lysine Monohydrochloride
L-Asparagine
L-Asparagine *H2O
L-Aspartic acid
L-Cysteine
L-Cysteine HCl
L-Cystine
L-Histidine Hydrochloride Monohydrate
L-Hydroxyproline
L-Isoleucine
L-Leucine
L-Lysine acetate
L-Methionine
L-Ornithine
L-(+)-Ornithine monohydrochloride
L-Threonine
L-Tryptophan
L-Valine
D-Alanine
D-Arginine

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D-Arginine hydrochloride
D-Aspartic acid
DL-Alanine
DL-Asparagine monohydrate
DL-Cystathionine
D-Leucine
DL-Methionine
DL-Phenylalanine
DL-Tryptophan
D-Tryptophan
D-Valine
Histamine
3,4-Dihydroxy-L-Phenylalanine
L-Lysine Monohydrochloride
L-Phenylalanine
L-Tyrosine
Maleic Hydrazide
Guaifenesin
Acetaminophen
Atropine sulfate
Isosorbide 5-Mononitrate
Acetylcysteine
Nonanoic acid vanillylamide
Procaine
Sodium Dichlorisocyanurate
Sodium Salicylate
Sulfanilic acid
Thymol = 3-p-Cymenol
L-Glutamic acid
Bismuth Subnitrate
Sucrose octaacetate
Sulfanilamide
Phosphate Calcium Dibasic, Monetite
4-Ethyl hydroxybenzoate
4-Methyl hydroxybenzoate = Methylparaben
Sorbic Acid
Benzethonium chloride
D-Isoascorbic Acid
3,7-Dimethyl-1,6-octadien-3-yl acetate
4-Allyl-2-methoxyphenol
Sulfate Calcium Dihydrate
Iminodiacetic acid
Sulfate Sodium Anhydrous
Meglumine

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2-Propanol
3-Ethoxy-4-hydroxybenzaldehyde = Ethylvanillin
Maltol
Sulfate Manganese
Dehydroacetic acid
D-Glucose, 2,3,4,5,6-pentaacetate
Phosphate Sodium Tribasic Dodecahydrate
Sulfate Aluminium Potassium Dodecahydrate
Sulfate Magnesium Heptahydrate
2-Phenylphenol
Sulfate Copper Pentahydrate
Lactic Acid
2-Bromo-2-nitro-1,3-propanediol
Sulfate Potassium
Lactitol
Acesulfame K
a-D-Lactose Monohydrate
(+)-S-Carboxymethyl-L-cysteine
1,3-Dicyclohexylurea
2-Aminoisobutyric Acid
3,4-Dihydroxycinnamic acid= Caffeic acid
5-Hydroxy-DL-lysine hydrochloride
Hexadecyl Trimethyl Ammonium Bromide
Chloramine B hydrate
D-(+)-Glucosamine .HCl
D-Glucose 6-phosphate, disodium salt
DL-2-Aminoadipic acid
DL-Homocystine
Flavianic acid hydrate
Galactaric acid
Guanidine Hydrochloride
Heptadecanoic acid
Heptaldehyde
L-(+)-Glutamic acid .HCl
L-Djenkolic Acid
L-Glutamine
Limonene
Methyl-3-aminocrotonate
p-Anisidine
Succinamide
N-t-BOC-L-proline
N-t-BOC-L-valine
Calcium D-pantothenate, Vitamin B5
Dexpanthenol

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1-Dodecanol
Cinnamyl alcohol
1-Valeric acid
1-Undecanol
b-Pinene
Isobutylbenzene
4-Methylmorpholine
3-Dimethylaminopropylamine
Thioanisole
Phenyl isothiocyanate
Methyl cyanoacetate
p-Benzoquinone
2-Pentanone
3-Mercaptopropionic acid
3-Chloroaniline
1,3-Diaminopropane
Acetylacetone
N-Decyl aldehyde
3-(N-Morpholino)propanesulfonic acid; MOPS
2-Acetylfuran
Tetramethylene sulfone
Cyclopentyl bromide
Ethyl 5-bromovalerate
Ethyl benzoylformate
3-(Dimethylamino)propionitrile
Phenylchloroformate
1-Ethyl-2-pyrrolidinone
meso-2,3-Dimercaptosuccinic acid
2,5-Dimethoxy-2,5-dihydrofuran (cis+trans)
2-Fluoroaniline
Crotonaldehyde
N-Formylmorpholine
Epinephrine
3-Methoxypropylamine
N-Acetylglycine
Cystamine dihydrochloride
3,3'-Diaminodipropylamine
3-Methyl-2-butanone
1,1,1-Trichloro-2-methyl-2-propanol
2-Bromoanisole
Promethazine hydrochloride
Iodobenzene
2-Chloropropionic acid
1-Ethyl-2-nitrobenzene

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3-Diethylamino-1-propanol
1-Nitrobutane
3-Chloro-1-propanol
1,1,3,3-Tetramethylurea
1,3-Dioxolane
Barbituric acid
Thioglycolic Acid
trans-1,2-Dibromocyclohexane
Trichloroacetic acid
Pinacol
2-Methyl-1,3-butadiene
Chloroacetone
Isobutanoic acid
Pinene
2-Bromobutyric acid
Salicylaldehyde
Guaiacol
Veratrole
Decahydronaphthalene
N,N-Diethylaniline
2-Chloroaniline
o-Chlorophenol
1,3-Dichloro-2-propanol
Gelatine
p-Nitrophenol
p-Dimethylaminobenzaldehyde
p-Nitrobenzyl bromide
p-Dinitrobenzene
Diaminodiphenylmethane
endo-3-Bromo-d-camphor
3,9-Dibromocamphor
beta-Nitrostyrene
2-(N-Cyclohexylamino)ethanesulfonic acid; CHES
2-Phenoxyethyl isobutyrate
Phenylacetic acid
4'-Methylacetanilide
4'-Aminooxanilic acid
3-Acetyl umbelliferone
Diethyl-3-oxoglutarate
p-Dichlorobenzene
4-Chloroaniline
Betaine
6-Methoxy-1-tetralone
Phloroglucinol, 1,3,5-Benzenetriol

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1-Allyl-2-thiourea
2-Methoxyethylamine
Undecylenic acid
5,6,7,8-Tetrahydro-2-naphthol
Guanidine
3-(Cyclohexylamino)propane-1-sulfonic acid; CAPS
Caryophyllene oxide
1,3-Dichloro-1,4-naphthoquinone
Tris(hydroxymethyl)aminomethane hydrochloride
4-Acetamidophenyl salicylate
Tribromophenol
o-Toluic acid
Anthranilic acid = 2-Aminobenzoic acid
2,4-Dinitrophenylhydrazine
(R)-(+)-N,N-dimethyl-1-(1-naphthyl)ethylamine
3,4-Dimethoxybenzaldehyde
Isosafrole
2-Imidazolidone
2,4-Dinitrotoluene
3-Aminobenzenesulfonic acid
3-Nitrobenzoic acid
N-Acetyl-1,4-phenylenediamine
3-(Chloromethyl) heptane
4-Hydroxybenzaldehyde
Choline
Tris(hydroxymethyl)nitromethane
3-Nitrobenzenesulfonic acid sodium salt
N-Chlorosuccinimide
1,4,5,8-Naphthalenetetracarboxylic acid
1,5-Diaminoanthraquinone
2,4,6-Trinitrobenzoic acid
Naphthionic Acid Sodium Salt
Anthraquinone-2-sulfonic acid, sodium salt, monohydrate
2-Naphthylamine-4,8-disulfonic acid
2,2',4,4',6,6'-Hexanitrodiphenylamine
2-Nitroso-1-naphthol
Naphthoresorcinol
(1,2-Cyclohexylenedinitrilo) tetraacetic acid
2,4-Diaminophenol .2HCl
N-Lauroylsarcosine sodium salt
Salicin
N,N-Dimethyl-4-nitrosoaniline
Nitrilotriacetic acid
3,4-Dihydroxybenzaldehyde = Protocatechualdehyde

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Cyanoacetohydrazide
Rhodanine
1,3,5-Tri-t-butylbenzene
2-Iodohippuric acid
Hexadecyltributylphosphonium bromide
3,7,11,15-Tetramethyl-2-hexadecen-1-ol
Diethyldithiocarbamic acid diethylammonium salt
2-Aminofluorene
2- Aminoethanethiol hydrochloride
Trimethylsulfoxonium iodide
Dimethyl 1,3-acetonedicarboxylate
2,4-Dichloro-1-naphthol
Sodium diethyldithiocarbamate trihydrate
Lead(II) cyanamide hydrate
10-Camphorsulfonyl chloride
L-Canavanine sulfate
Terpin hydrate
2,6-Diisopropylaniline
1,2,3-Tris-(2-cyanoethoxy)propane
L-Alanine-15N
1,4-Diazobicyclo(2.2.2)octane
Xylyl bromide
2-Aminobenzophenone
DL-2-Aminobutyric acid
p-Cyanobiphenyl
Bis-(4-fluoro-3-nitrophenyl)sulfone
Chloromethyl thiocyanate
2,7-Dimethoxynaphthalene
o-Fluoroiodobenzene
Ethyl 2,3-dibromopropionate
1-Iodododecane
Amitriptylinoxide
4-Trifluoromethylmercaptophenol
Ethyl oxalyl chloride
Ninhydrin
Indoline
1,3-Cyclohexanedione
Dimethylamine Hydrochloride
Guanidine Nitrate
Ammonium Pyrrolidine Dithiocarbamate
2,4-Dinitrophenol
Sodium Sulfanilate
1,2-Naphthoquinone-4-sulfonic acid, sodium salt
1-Nitroso-2-naphthol-3,6-disulfonic acid, disodium salt

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2-(Methylthio)ethanol
2-Iodoanisole
N,N'-Diphenylbenzidine
Naphthalene-2-sulfonic acid; sodium salt
Aleuritic acid
4,6-Dinitro-o-cresol
2,6-Dibromoquinone-4-chloroimide
Benzyl sulfide
1,3-Dicyclohexylcarbodiimide
2-Methoxy-1-naphthaldehyde
Aniline sulfate
H Acid
Hydroxylamine hydrochloride
Picronic acid
2-Nitrobenzaldehyde
4-Methylamino-phenol-sulfate
Ethylamine hydrochloride
Glycine methyl ester hydrochloride
DL-Glyceraldehyde
Mordant Violet 39
2-Methyl-6-nitroaniline = 6-Nitro-o-toluidine
6-Acetamidohexanoic acid
2,6-Dinitrophenol
o-Anisic acid
Betaine hydrochloride
1-Acetyl-2-thiourea
3-Methoxybenzaldehyde
DL-2-Bromopropionic acid
4-Cumylphenol
Dimethyl-L-tartrate
Ethyl 2-chloroacetoacetate
1,3,5-Trihydroxybenzene dihydrate
3,5-Dinitrosalicylic acid
2,3,4-Trihydroxybenzoic acid
4-Nitrophthalic acid
2,4-Dimethoxybenzaldehyde
Benzoylhydrazine
Benzoylacetonitrile = beta-Oxohydrocinnamionitrile
2-Iodotoluene
1,2-Diiodobenzene
2,5-Diaminotoluene sulfate
Ethyl-3-nitrobenzoate
4-Iodobenzoic acid
5-Bromo-m-xylene

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4-Nitrobenzoic acid
9-Fluorenone-4-carboxylic acid
Ethylurea
Dibenzoyl-L-tartaric acid Monohydrate
2-Chlorooctane
D-Glucuronic acid
2-Naphthaldehyde
TAPSO, 2-Hydroxy-N-(tris(hydroxymethyl)methyl)-3-aminopropanesulfonic acid
D(+)-Galacturonic acid monohydrate
5-Chloro-1,3-dimethoxybenzene
4'-Hydroxypropiophenone
N,N-Diisopropylethylamine
N-(2-Hydroxyethyl)piperazine-N'-2-ethanesulfonic acid; HEPES
4-Hydroxycinnamic acid
3,3-Diaminobenzidine tetrahydrochloride
Isobutyl-2-ethyl hexanoate
Neopentyl alcohol
Acetone cyanohydrin
1,1,1-Tris(hydroxymethyl)ethane
(-)-Quinic acid
Glycolic acid
Thiosemicarbazide
Dithiooxamid
Trimethylpyruvic acid
1,8-Naphthalic anhydride
Xanthene 9-carboxylic Acid
4-(Trifluoromethoxy)phenol
4-Nitrophenyl acetate
4-Aminoantipyrene
1-Indanone
2-Hydroxy-1,4-naphthoquinone
Phenanthrene
2-Methyl-2-thiopseudourea sulfate
2-Amino-5-naphthol-7-sulfonic acid
Benzenesulfinic acid, sodium salt
Pyrogallol = 1,2,3-Trihydroxybenzene
2,4,6-Trichlorophenol
o-Iodobenzoic acid
2-Nitrophenol
4-Chloro-2-isopropyl-5-methylphenol
Resacetophenone
4-Amino-5-hydroxy-2,7-naphthalenedisulfonic acid
N-Phenylanthranilic acid
1-Phenyl-3-pyrazolidone

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2,3-Dihydroxynaphthalene
4,4'-Diamino-diphenyl
4-Acetylbiphenyl
p-Terphenyl = 1,4-Diphenylbenzene
N,N-Diethyl-1,4-phenylenediamine
2-Azacyclononanone
Benzanilide
Benzyl nicotinate
3,4-Dimethylaniline
2,4-Diaminotoluene
2,5-Dichloroaniline
1,2,4,5-Tetramethylbenzene
2,4,5-Trichlorophenol
2-Chloro-1,1-dimethoxyethane
Phenyltrimethylammonium iodide
4-t-Butylcatechol
2-Chloroaniline-5-sulfonic acid
4-t-Butylphenol
4-Nitrobenzenesulfonyl chloride
m-Toluic acid
3,5-Dinitrobenzoic acid
Aminoguanidine sulfate
p-Aminoacetophenone
p-Toluic acid
4-Hydroxybenzoic acid
Copper(II) glycinate
Diacetone-L-sorbose
p-Azobenzene sulfonic acid
Salicylaldehyde semicarbazone
Ammonium thiocyanate
Sodium borohydride
Hydrazine sulfate
Ammonium fluoride
Sodium cyanoborohydride
Hydroxylamine sulfate
Potassium hexafluorophosphate

List of Spectra /CAS Numbers

100-02-7
100-10-7
100-11-8
100-21-0

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100-25-4
10034-93-2
10034-99-8
10035-04-8
100-37-8
100-39-0
10039-54-0
10043-01-3
10043-52-4
100-44-7
100-46-9
100-47-0
100-51-6
100-52-7
100-60-7
100-68-5
100-97-0
10098-89-2
10099-74-8
10101-41-4
10101-89-0
101-77-9
101-84-8
102-01-2
102-71-6
102-81-8
10293-06-8
10293-10-4
102-96-5
103-36-6
103-47-9
103-60-6
103-71-9
103-72-0
103-82-2
103-84-4
103-85-5
103-89-9
103-90-2
103-92-4
10441-27-7
10442-39-4
104-46-1
104-54-1

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104-94-9
105-34-0
105-36-2
105-39-5
10544-63-5
105-50-0
105-53-3
105-54-4
105-60-2
106-32-1
106-33-2
106-40-1
106-46-7
106-47-8
106-50-3
106-51-4
106-65-0
1068-22-0
106-87-6
106-89-8
106-93-4
107-06-2
107-07-3
107-13-1
107-15-3
107-18-6
107-21-1
107-31-3
107-43-7
107-81-3
1078-19-9
107-87-9
107-88-0
107-96-0
1079-66-9
108-01-0
108-10-1
108-18-9
108-20-3
108-24-7
108-29-2
108-30-5
108-31-6
108-32-7

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108-42-9
108-44-1
108-46-3
108-73-6
108-83-8
108-88-3
108-91-8
108-93-0
108-94-1
108-95-2
109-02-4
109-30-8
109-52-4
109-55-7
109-57-9
109-65-9
109-70-6
109-76-2
109-85-3
109-86-4
109-89-7
109-94-4
110-13-4
110-14-5
110-15-6
110-17-8
110-18-9
110-26-9
110-44-1
110-52-1
110-65-6
110-71-4
110-73-6
110-80-5
110-82-7
110-83-8
110-89-4
11092-32-3
110-94-1
11099-07-3
11113-50-1
111-15-9
111-20-6
111-25-1

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111-29-5
111-34-2
11138-66-2
111-40-0
111-44-4
111-46-6
111-48-8
1116-76-3
111-70-6
111-71-7
111-76-2
111-78-4
111-86-4
111-87-5
111-90-0
111-96-6
1120-01-0
1120-36-1
1122-60-7
112-27-6
112-30-1
112-31-2
112-38-9
112-39-0
112-40-3
112-41-4
112-42-5
112-47-0
112-53-8
1125-78-6
112-69-6
112-71-0
112-73-2
112-77-6
112-80-1
112-82-3
112-84-5
112-92-5
113-00-8
1132-61-2
1135-40-6
1139-30-6
115-95-7
116-54-1

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117-80-6
117-81-7
1185-53-1
118-55-8
118-57-0
118-61-6
118-71-8
118-79-6
118-90-1
118-92-3
1192-62-7
119-26-6
119-36-8
119392-95-9
119-47-1
119-53-9
119-93-7
120-12-7
120-14-9
12027-06-4
120-47-8
120-58-1
120-72-9
120-92-3
120-93-4
121-14-2
12124-97-9
12125-01-8
121-32-4
121-47-1
121-54-0
121-57-3
1217-45-4
121-92-6
122-80-5
123-04-6
123-08-0
123-25-1
123-31-9
123-33-1
123-38-6
123-41-1
123-42-2
123-51-3

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123-56-8
123-63-7
123-66-0
123-72-8
123-86-4
123-92-2
123-94-4
123-96-6
123-99-9
124172-53-8
124-18-5
124-68-5
126-11-4
126-14-7
126-33-0
126-73-8
126-81-8
127-19-5
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