



nmr
suite | V11

Available NOW!

Spectral Reference Libraries
400 MHz - 800 MHz

July 2024



The Chenomx Compound Signature Library was acquired using the **Sample Preparation** and **NMR Data Acquisition** standard operating procedures summarized below. Use our method for your samples to match the conditions of our library and improve the accuracy of your results.

1.0 Sample Preparation

Sample Filtration through a 3KDa filter tube.

Chenomx is uniquely designed to identify and quantify small molecules in liquid samples. Filtration is recommended for samples containing large molecules. For a step-by-step guide for *filtering your sample*, visit www.chenomx.com/support to read SOPs C-001 and C-002.

Mix/vortex Sample with an Internal Standard

Chenomx Internal Standard (IS2) contains a DSS Chemical Shape Indicator. For a step-by-step guide to *Internal Standard (IS2)* and *Sample Preparation*, visit chenomx.com/chenomxsupport to read SOP S-001.

2.0 NMR Data Acquisition

NMR Spectral Acquisition

Chenomx uses a 1D-1H NMR pulse sequence. Remember to Export an Uncompressed FID file. Automatically processed FIDs can include automatic phasing and baseline correction, which are not best practice for metabolomics research. Use the following parameters for best results:

Pulse sequence:	noesypr1d (Bruker), or an adaptation of metnoesy (Varian). Varian users can download the pulse sequence C code from chenomx.com/chenomxsupport under the Sample Preparation section of the FAQ.
Solvent:	90% H ₂ O, 10% D ₂ O
Temperature:	25°C
Acquisition time:	4 s
NOE Mixing time:	0.1 s
Initial delay:	0.01 s
Pre-saturation delay:	0.99 s
Steady state scans:	4
Spectral width:	12 ppm

ALANINE, ASPARTATE AND GLUTAMATE METABOLISM

1,3-Diaminopropane
2-Aminobutyrate
2-Oxocaproate
4-Aminobutyrate
Alanine
Asparagine
Aspartate
Glutamate
N-Acetylaspartate
N-Acetylglutamate
N-Acetylglutamine
Pyroglutamate

ALCOHOLS AND POLYOLS

1,3-Dihydroxyacetone
2-Phosphoglycerate
4-Hydroxybutyrate
4-Pyridoxate
5-Hydroxylysine
6-Hydroxynicotinate
Acetoin
Arabinitol
Ascorbate
Chlorogenate
Choline
D-Threitol
Epicatechin
Erythritol
Ethanol
Ethanolamine
Ethylene glycol
Galactarate
Galactitol
Galactonate
Glucarate
Glucitol
Gluconate
Glycerate
Glycerol
Glycolate
Hydroxyacetone
Isopropanol
Kynurenate
Mannitol
Methanol
N-Acetylserotonin
Pantothenate
Propylene glycol
Pyridoxine
Riboflavin
Serotonin
Threonate
Xanthurenate
Xylitol
myo-Inositol
sn-Glycero-3-phosphocholine

AMIDES

1-Methylnicotinamide
Acetamide
Acetaminophen
Allantoin
Biotin
Citruiline
Glycylproline
Homocitrulline
Melatonin
N-Acetylglucosamine
N-Acetylglutamine
N-Acetylserotonin
N-Carbamoyl- β -alanine
N-Methylhydantoin

N6-Acetyllysine
NAD⁺
NADH
NADP⁺
NADPH
Niacinamide
Nicotinamide N-oxide
Riboflavin
UDP-N-Acetylglucosamine
Urea

AMIDO ACIDS

2-Furolyglycine
4-Aminohippurate
Anserine
Asparagine
Carnosine
Glutamine
Glutathione
Glycylproline
Hippurate
N-Acetylaspartate
N-Acetylcysteine
N-Acetylglutamate
N-Acetylglutamine
N-Acetyllysine
N-Acetylornithine
N-Acetyltyrosine
N-Carbamoylaspartate
N-Isovalerylglycine
N-Phenylacetyllysine
N-Phenylacetylphenylalanine
Nicotinurate
N α -Acetyllysine
O-Acetylcarnitine
Pantothenate
Pyroglutamate
Salicylurate
Tiglyglycine

AMINES

1,3-Diaminopropane
1-Methylnicotinamide
3-Hydroxykynurenine
4-Aminohippurate
4-Guanidinobutanoate
4-Pyridoxate
5-Aminolevulinatate
5-Aminopentanoate
5-Hydroxylysine
6-Hydroxynicotinate
Anserine
Anthranilate
Arginine
Cadaverine
Carnitine
Carnosine
Creatine
Creatine phosphate
Creatinine
Dimethylamine
Ethanolamine
Guanidinosuccinate
Guanidoacetate
Histamine
Kynurenate
Kynurenine
Lysine
Methylamine
N,N-Dimethylformamide
N-Acetylornithine
N-Nitrosodimethylamine
NAD⁺
NADH
NADP⁺
Niacinamide
Nicotinate

Nicotinic acid adenine dinucleotide
Nicotinurate
N α -Acetyllysine
O-Acetylcholine
O-Phosphocholine
O-Phosphoethanolamine
Omithine
Putrescine
Pyridoxine
Riboflavin
Serotonin
Taurine
Trigonelline
Trymethylamine
Tyramine
sn-Glycero-3-phosphocholine

AMINO ACIDS

2-Amino adipate
2-Aminobutyrate
2-Furolyglycine
3,5-Dibromotyrosine
3-Aminoisobutyrate
3-Chlorotyrosine
3-Hydroxykynurenine
4-Aminobutyrate
4-Carboxyglutamate
5-Aminopentanoate
5-Hydroxylysine
5-Hydroxytryptophan
Alanine
Alloisoleucine
Arginine
Asparagine
Aspartate
Betaine
Citrulline
Creatine
Creatine phosphate
Cystathionine
Cysteine
Cystine
Glutamate
Glutamine
Glutathione
Glycine
Histidine
Homocitrulline
Homocysteine
Homocystine
Homoserine
Isoleucine
Kynurenine
Leucine
Lysine
Methionine
N,N-Dimethylglycine
N6-Acetyllysine
O-Phosphoserine
Ornithine
Phenylalanine
Piperolate
Proline
S-Adenosylhomosteine
S-Sulfocysteine
Saccharopine
Sarcosine
Serine
Threonine
Tryptophan
Tyrosine
Valine
trans-4-Hydroxy-L-proline
 β -Alanine
 γ -Glutamylphenylalanine
 π -Methylhistidine
 τ -Methylhistidine

ARGININE AND PROLINE METABOLISM

4-Guanidinobutanoate
Agmatine
Creatine
Creatine phosphate
Creatinine
Glycylproline
Guanidinosuccinate
N-Acetylmithine
N-Methylhydantoin
Proline
trans-4-Hydroxy-L-proline

AROMATICS

1-Methylnicotinamide
2-Furoate
2-Phenylpropionate
3-Indoxylsulfate
3-Phenyllactate
3-Phenylpropionate
4-Aminohippurate
4-Pyridoxate
5-Hydroxyindole-3-acetate
5-Hydroxytryptophan
6-Hydroxynicotinate
Acetylalicylate
Anserine
Anthranilate
Benzoate
Carnosine
Cinnamate
Hippurate
Histamine
Histidine
Ibuprofen
Imidazole
Indole-3-acetate
Indole-3-lactate
Kynurenate
Kynurenine
Mandelate
Melatonin
N-Acetylserotonin
N-Phenylacetyllysine
N-Phenylacetylphenylalanine
NAD⁺
NADP⁺
Niacinamide
Nicotinamide N-oxide
Nicotinate
Nicotinic acid adenine dinucleotide
Nicotinurate
Phenylacetate
Phenylalanine
Phthalate
Pyridoxine
Quinolate
Riboflavin
Serotonin
Trigonelline
Tropate
Tryptophan
Urocanate
Xanthurenate
 γ -Glutamylphenylalanine
 π -Methylhistidine
 τ -Methylhistidine

BILE ACID BIOSYNTHESIS

Cholate
Glycocholate
Isocaproate
Taurine

BILE ACIDS

Cholate
Glycocholate

CARBOHYDRATE METABOLISM

2-Phosphoglycerate
Arabinitol
Arabinose
Ascorbate
Cellobiose
Ethanol
Fructose
Fucose
Galactarate
Galactitol
Galactonate
Galactose
Glucarate
Glucitol
Gluconate
Glucose
Glucose-1-phosphate
Glucose-6-phosphate
Glucuronate
Lactose
Maltose
Mannitol
Mannose
N-Acetylglucosamine
Ribose
Sucrose
Threonate
Trehalose
UDP-N-Acetylglucosamine
UDP-galactose
UDP-glucose
UDP-glucuronate
Xylitol
Xylose
myo-Inositol

CARBOXYLIC ACIDS

2,3,4-Trihydroxybenzoate
2,6-Dihydroxybenzoate
2-Amino adipate
2-Ethylacrylate
2-Furoate
2-Hydroxyglutarate
2-Hydroxyphenylacetate
2-Methylglutarate
2-Methylglutarate
2-Oxoglutarate
2-Phenylpropionate
2-Phosphoglycerate
3,4-Dihydroxybenzeneacetate
3-Hydromuconate
3-Hydroxy-3-methylglutarate
3-Hydroxyphenylacetate
3-Methyladipate
3-Methylglutarate
3-Phenylpropionate
4-Carboxyglutamate
4-Guanidinobutanoate
4-Hydroxybenzoate
4-Hydroxyphenylacetate
4-Pyridoxate
5-Hydroxyindole-3-acetate
5-Methoxysalicylate
6-Hydroxynicotinate
Acetylsalicylate
Adipate
Anthranilate
Aspartate
Azelate
Benzoate

Biotin
Cinnamate
Citrate
Citric acid
Desaminotyrosine
Ethylmalonate
Ethylmalonate
Ferulate
Formate
Fumarate
Galactarate
Gentisate
Glucarate
Gluconate
Glutamate
Glutarate
Glutaric acid monomethyl ester
Guanidinosuccinate
Guanidoacetate
Homogentisate
Homovanillate
Ibuprofen
Indole-3-acetate
Isobutyrate
Isocaproate
Isocitrate
Kynurenine
Malate
Maleate
Malonate
Methylmalonate
Methylsuccinate
N-Acetylsuccinate
N-Acetylglutamate
N-Acetylglutamine
N-Carbamoyl-β-alanine
N-Carbamoylaspartate
N-Carbamoylaspartate
Nicotinate
Nicotinic acid adenine dinucleotide
Phenylacetate
Phenylglyoxylate
Phthalate
Pimelate
Protocatechuic acid
Quinolinic acid
Saccharopine
Salicylate
Sebacate
Suberate
Succinate
Syringate
Tartate
Trigonelline
Urocanate
Vanillate
Xanthurenate
cis, cis-Muconate
cis-Aconitate
trans-Aconitate

CYSTEINE AND METHIONINE METABOLISM

Cystathionine
Cysteine
Cystine
Homocysteine
Homocystine
Methionine
N-Acetylcysteine
S-Adenosylhomocysteine
S-Sulfocysteine

D-XYLOSE METABOLISM

D-Threitol

DRUG COMPONENTS

2,3,4-Trihydroxybenzoate
2,6-Dihydroxybenzoate
3,5-Dibromotyrosine
5-Methoxysalicylate
Acetaminophen
Acetylsalicylate
Azelaic acid
Ibuprofen
Imidazole
Lactulose
Levulinic acid
N-Phenylacetylphenylalanine
Oxypurine
Salicylic acid
Salicylic acid
Thymol
Valproic acid

ENVIRONMENTAL POLLUTANTS

1,6-Anhydro-β-D-glucose
2-Furoic acid
2-Hydroxyisobutyrate
2-Hydroxyvaleric acid
2-Phenylpropionic acid
Acetamide
Butanone
Isoeugenol
Mandelic acid
N,N-Dimethylformamide
N-Nitrosodimethylamine
Phthalate

FATTY ACIDS

2-Octenoic acid
Acetic acid
Butyric acid
Caproic acid
Caprylic acid
Isovaleric acid
Propionic acid
Valeric acid
Valproic acid

FOOD COMPONENTS

1,3-Dimethyluracil
1,7-Dimethylxanthine
2-Furoylglycine
3-Methylxanthine
Acetoin
Adipic acid
Caffeine
Chlorogenic acid
Dimethyl sulfone
Epicatechin
Erythritol
Ferulate
Gallate
Glutaric acid monomethyl ester
Isobutyrate
Pyrocatechol
Syringic acid
Theophylline
Trigonelline
Vanillate

GLYCINE, SERINE AND THREONINE METABOLISM

2-Oxobutyrate
5-Aminolevulinic acid
Betaine
Glycine
Guanidoacetate
Homoserine
Hydroxyacetone
N,N-Dimethylglycine
N-Acetylglycine
N-Isovalerylglycine
O-Phosphoserine
Sarcosine
Serine
Threonine

HISTIDINE METABOLISM

Anserine
Carnosine
Histamine
Histidine
Urocanic acid
β-Alanine
π-Methylhistidine
τ-Methylhistidine

HYDROXY ACIDS

2-Hydroxy-3-methylvaleric acid
2-Hydroxybutyrate
2-Hydroxyglutaric acid
2-Hydroxyisobutyrate
2-Hydroxyisocaproic acid
2-Hydroxyisovaleric acid
2-Hydroxyvaleric acid
3,4-Dihydroxymandelic acid
3-Hydroxy-3-methylglutaric acid
3-Hydroxybutyrate
3-Hydroxyisobutyrate
3-Hydroxyisovaleric acid
3-Hydroxymandelic acid
3-Phenylactic acid
4-Hydroxy-3-methoxymandelic acid
4-Hydroxybutyrate
4-Hydroxyphenyllactate
Carnitine
Chlorogenic acid
Citric acid
Galactonic acid
Gallate
Glyceric acid
Glycolic acid
Homoserine
Indole-3-lactate
Isocitric acid
Lactic acid
Malic acid
Mandelic acid
Serine
Tartaric acid
Threonine
Threonic acid
Tropic acid
trans-4-Hydroxy-L-proline

INTERNAL STANDARDS

DSS (Chemical Shape Indicator)
DSS-d6 (Chemical Shape Indicator)
Fumaric acid
Maleic acid

KETO ACIDS

2-Oxobutyrate
2-Oxocaproic acid
2-Oxoglutaric acid
2-Oxoisocaproic acid
2-Oxovaleric acid
3-Hydroxykynurenine
2-Methyl-2-oxovaleric acid
5-Aminolevulinic acid
Acetoacetic acid
Kynurenine
Levulinic acid
Pyruvic acid
Succinylacetic acid

KETONE BODY METABOLISM

3-Hydroxy-3-methylglutaric acid
3-Hydroxybutyrate
Acetoacetic acid
Acetone

KETONES

Acetoacetic acid
Acetoin
Acetone
Butanone
Creatinine
Hydroxyacetone
Phenylglyoxylate
Succinylacetic acid

LIPID METABOLISM

1,3-Dihydroxyacetone
2-Hydroxybutyrate
2-Hydroxyglutaric acid
2-Methylglutaric acid
2-Octenoic acid
3-Hydroxymuconic acid
3-Methyladipic acid
4-Aminohippuric acid
4-Hydroxybutyrate
Butyrate
Caproic acid
Caprylic acid
Carnitine
Choline
Ethanolamine
Ethylmalonate
Glutaric acid
Glyceric acid
Glycerol
Isopropanol
Maleic acid
Malonic acid
Methylsuccinate
O-Acetylcarnitine
O-Acetylcholine
O-Phosphocholine
O-Phosphoethanolamine
Propionic acid
Propylene glycol
Sebacic acid
Suberic acid
Valeric acid
sn-Glycero-3-phosphocholine

LYSINE METABOLISM

2-Amino adipic acid
5-Aminopentanoic acid
5-Hydroxylysine
Homocitrulline

Lysine
N6-Acetyllysine
Nα-Acetyllysine
Pimelic acid
Pipelic acid
Saccharopine

METHANE METABOLISM

Dimethylamine
Methanol
Methylamine
Trimethylamine
Trimethylamine N-oxide

MONOSACCHARIDES AND DISACCHARIDES

1,6-Anhydro-β-D-glucose
Arabinose
Cellobiose
Fructose
Fucose
Galactose
Glucose
Glucose-1-phosphate
Glucose-6-phosphate
Glucuronic acid
Lactose
Lactulose
Maltose
Mannose
N-Acetylglucosamine
NAD⁺
NADH
NADP⁺
NADPH
Nicotinic acid adenine dinucleotide
Ribose
Sucrose
Trehalose
UDP-N-Acetylglucosamine
UDP-galactose
UDP-glucose
UDP-glucuronic acid
Xylose

N-OXIDES

Nicotinamide N-oxide
Trimethylamine N-oxide

NUCLEOTIDES AND NUCLEOSIDES

2'-Deoxyadenosine
2'-Deoxyguanosine
2'-Deoxyinosine
2'-Deoxyuridine
ADP
AMP
ATP
Adenosine
Cytidine
GTP
Guanosine
IMP
Inosine
NAD⁺
NADH
NADP⁺
NADPH
Nicotinic acid adenine dinucleotide
S-Adenosylhomocysteine

Thymidine
UDP-N-Acetylglucosamine
UDP-galactose
UDP-glucose
UDP-glucuronate
Uridine
Xanthosine
dCTP
dTTP

ORGANOHALIDES

3,5-Dibromotyrosine
3-Chlorotyrosine

PHENOLS

2,3,4-Trihydroxybenzoate
2,6-Dihydroxybenzoate
2-Hydroxyphenylacetate
3,4-Dihydroxybenzeneacetate
3,4-Dihydroxymandelate
3,5-Dibromotyrosine
3-Chlorotyrosine
3-Hydroxykynurenine
3-Hydroxymandelate
3-Hydroxyphenylacetate
4-Hydroxy-3-methoxymandelate
4-Hydroxybenzoate
4-Hydroxyphenylacetate
4-Hydroxyphenyllactate
5-Hydroxyindole-3-acetate
5-Hydroxytryptophan
5-Methoxysalicylate
Acetaminophen
Catechol
Chlorogenate
Desaminotyrosine
Epicatechin
Ferulate
Gallate
Gentisate
Homogentisate
Homovanillate
Isoeugenol
N-Acetyltyrosine
Phenol
Protocatechuete
Pyrocatechol
Salicylate
Salicylurate
Syringate
Thymol
Tyramine
Tyrosine
Vanillate
o-Cresol
p-Cresol

PHENYLALANINE AND TYROSINE METABOLISM

2-Hydroxyphenylacetate
3,4-Dihydroxybenzeneacetate
3,4-Dihydroxymandelate
3-Chlorotyrosine
3-Hydroxymandelate
3-Hydroxyphenylacetate
3-Phenyllactate
3-Phenylpropionate
4-Hydroxy-3-methoxymandelate
4-Hydroxybenzoate
4-Hydroxyphenylacetate
4-Hydroxyphenyllactate
Benzoate
Catechol
Cinnamate
Desaminotyrosine

Gentisate
Hippurate
Homogentisate
Homovanillate
N-Acetyltyrosine
N-Phenylacetyltyrosine
Phenol
Phenylacetate
Phenylalanine
Phenylglyoxylate
Protocatechuete
Succinylacetone
Tropate
Tyramine
Tyrosine
cis,cis-Muconate
o-Cresol
p-Cresol
γ-Glutamylphenylalanine

PHOSPHATES

2-Phosphoglycerate
Creatine phosphate
Glucose-1-phosphate
Glucose-6-phosphate
O-Phosphocholine
O-Phosphoethanolamine
O-Phosphoserine
sn-Glycero-3-phosphocholine

PURINE AND PYRIMIDINE METABOLISM

2'-Deoxyadenosine
2'-Deoxyguanosine
2'-Deoxyinosine
2'-Deoxyuridine
3-Aminoisobutyrate
5,6-Dihydrothymine
5,6-Dihydrouracil
ADP
AMP
ATP
Adenine
Adenosine
Allantoin
Cytidine
Cytosine
GTP
Guanosine
Hypoxanthine
IMP
Inosine
Methylmalonate
N-Carbamoyl-β-alanine
Pyrimidine
Thymidine
Thymine
UMP
Uracil
Uridine
Xanthine
Xanthosine
dCTP
dTTP

PURINES AND PYRIMIDINES

1,3-Dimethylurate
1,7-Dimethylxanthine
3-Methylxanthine
5,6-Dihydrothymine
5,6-Dihydrouracil
Adenine
Caffeine
Cytosine
Hypoxanthine

Oxypurinol
Pyrimidine
Theophylline
Thymine
UMP
Uracil
Xanthine

PUTREFACTION

Cadaverine
Methylguanidine
Putrescine

PYRUVATE AND TRICARBOXYLATE METABOLISM

2-Oxoglutarate
2-Oxovalerate
Acetate
Citrate
Ethylene glycol
Formate
Fumarate
Glycolate
Isocitrate
Lactate
Malate
Pyruvate
Succinate
Tartrate
cis-Aconitate
trans-Aconitate

SULFUR COMPOUNDS

3-Indoxylsulfate
Biotin
Cystathionine
Cysteine
Cystine
DSS (Chemical Shape Indicator)
DSS-d6 (Chemical Shape Indicator)
Dimethyl sulfone
Glutathione
Homocysteine
Homocystine
Methionine
N-Acetylcysteine
S-Adenosylhomocysteine
S-Sulfocysteine
Taurine

TRYPTOPHAN METABOLISM

3-Hydroxykynurenine
3-Indoxylsulfate
5-Hydroxyindole-3-acetate
5-Hydroxytryptophan
Anthranilate
Indole-3-acetate
Indole-3-lactate
Kynurenate
Kynurenine
Melatonin
N-Acetylserotonin
Nicotinic acid adenine dinucleotide
Nicotinurate
Serotonin
Tryptophan
Xanthurenate

UREA CYCLE

Arginine
Citrulline
Ornithine
Urea

VALINE, LEUCINE AND ISOLEUCINE METABOLISM

2-Ethylacrylate
2-Hydroxy-3-methylvalerate
2-Hydroxyisocaproate
2-Hydroxyisovalerate
2-Oxoisocaproate
3-Hydroxyisobutyrate
3-Hydroxyisovalerate
3-Methyl-2-oxovalerate
3-Methylglutarate
Alloisoleucine
Citraconate
Isoleucine
Isovalerate
Leucine
Tiglylglycine
Valine

VITAMINS AND COFACTORS

1-Methylnicotinamide
4-Pyridoxate
6-Hydroxynicotinate
Biotin
Glutathione
NAD+
NADH
NADP+
NADPH
Niacinamide
Nicotinamide N-oxide
Nicotinate
Pantothenate
Pyridoxine
Quinolate
Riboflavin

XENOBIOTICS

DSS (Chemical Shape Indicator)
DSS-d6 (Chemical Shape Indicator)

13C (Services Only)

13C6- Glucose
1,2- 13C2- Glucose
13C6- Glutamine
1,2- 13C2- Glutamine

Processor	The 'Processor' module imports a wide variety of NMR spectra into Chenomx NMR Suite and provides the standard processing tools needed to clean up and calibrate those spectra, for easy and accurate analysis in the Profiler.	STANDARD
Profiler	The 'Profiler' module identifies and quantifies the contents of the mixture spectrum by comparing it to a compound library with hundreds of reference spectra.	
Library Manager	The 'Library Manager' module manages the reference spectra in Chenomx NMR Suite, including custom compounds from the Compound Builder. Create new subset folders for faster reference.	
Spin Simulator	The 'Spin Simulator' module simulates an entire compound signature based on theoretical details. Set a magnet frequency, then start solving coupling relationships and measuring j-value constants while the simulation updates itself in real time.	
INCLUDES ALL STANDARD MODULES		PROFESSIONAL <i>(includes all Standard Modules)</i>
Compound Builder	The 'Compound Builder' module creates custom compound signatures, complete with full quantitative information. These signatures can then be used when analyzing samples in Profiler.	
Batch Import/Batch Process	Batch Import/Batch Process applies processing steps to groups of samples. Batching significantly reduces processing time for large sample sizes.	
Batch Fit/Batch Edit	Apply profiled compounds from a single spectra to an entire batch of spectra to reduce profiling time. Then, add stars, pins, and colors for labelling.	
Binning	Binning reduces the number of variables by dividing spectra into a series of ppm regions, or bins; subsequent analysis involves the integrated area of these bins instead of the raw spectral data.	
COMPLETE Autofit	A fully automated profile of your processed spectrum. COMPLETE Autofit performs numerous, parallel approaches to a complete autofit and generates multiple CNX files with a recommended 'Complete' fit.	

www.chenomx.com