

Chenomx NMR Suite identifies and quantifies a wide range of biologically and clinically relevant compounds. The lists below include all compounds available as Chenomx Reference Compounds.

## Alanine, Aspartate and Glutamate Metabolism

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

## Alcohols and Polyols

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

## Amides

1-Methylnicotinamide	Melatonin	NADH
Acetamide	N-Acetylglucosamine	NADP+
Acetaminophen	N-Acetylglutamine	NADPH
Allantoin	N-Acetylserotonin	Niacinamide
Biotin	N-Carbamoyl- $\beta$ -alanine	Nicotinamide N-oxide
Citrulline	N-Methylhydantoin	Riboflavin
Glycylproline	N6-Acetyllysine	UDP-N-Acetylglucosamine
Homocitrulline	NAD+	Urea

## Amido Acids

2-Furoylglycine	N-Acetylcysteine	Nicotinate
4-Aminohippurate	N-Acetylglutamate	N $\alpha$ -Acetyllysine
Anserine	N-Acetylglutamine	O-Acetylcarnitine
Asparagine	N-Acetyllysine	Pantothenate
Carnosine	N-Acetylornithine	Pyroglutamate
Glutamine	N-Acetyltyrosine	Salicylate
Glutathione	N-Carbamoylaspartate	Tiglylglycine
Glycylproline	N-Isovalerylglycine	$\gamma$ -Glutamylphenylalanine
Hippurate	N-Phenylacetyllysine	
N-Acetylaspartate	N-Phenylacetylphenylalanine	

## Amines

1,3-Diaminopropane	Creatinine	Nicotinic acid adenine dinucleotide
1-Methylnicotinamide	Dimethylamine	Nicotinate
3-Hydroxykynurenine	Ethanolamine	N $\alpha$ -Acetyllysine
4-Aminohippurate	Guanidinosuccinate	O-Acetylcholine
4-Guanidinobutanoate	Guanidoacetate	O-Phosphocholine
4-Pyridoxate	Histamine	O-Phosphoethanolamine
5-Aminolevulinate	Kynurenate	Ornithine
5-Aminopentanoate	Kynurenine	Putrescine
5-Hydroxylysine	Lysine	Pyridoxine
6-Hydroxynicotinate	Methylamine	Quinolate
Agmatine	Methylguanidine	Riboflavin
Anserine	N,N-Dimethylformamide	Serotonin
Anthranilate	N-Acetylornithine	Taurine
Arginine	N-Nitrosodimethylamine	Trigonelline
Cadaverine	NAD <sup>+</sup>	Trimethylamine
Carnitine	NADH	Tyramine
Carnosine	NADP <sup>+</sup>	Xanthurenate
Choline	NADPH	sn-Glycero-3-phosphocholine
Creatine	Niacinamide	
Creatine phosphate	Nicotinate	

## Amino Acids

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

## Arginine and Proline Metabolism

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

## Aromatics

1-Methylnicotinamide	Histamine	Nicotinic acid adenine dinucleotide
2-Furoate	Histidine	Nicotinate
2-Phenylpropionate	Ibuprofen	Phenylacetate
3-Indoxylsulfate	Imidazole	Phenylalanine
3-Phenyllactate	Indole-3-acetate	Phthalate

3-Phenylpropionate	Indole-3-lactate	Pyridoxine
4-Aminohippurate	Kynurenate	Quinolate
4-Pyridoxate	Kynurenine	Riboflavin
5-Hydroxyindole-3-acetate	Mandelate	Serotonin
5-Hydroxytryptophan	Melatonin	Trigonelline
6-Hydroxynicotinate	N-Acetylserotonin	Tropate
Acetylsalicylate	N-Phenylacetylglycine	Tryptophan
Anserine	N-Phenylacetylphenylalanine	Urocanate
Anthranilate	NAD+	Xanthurenate
Benzoate	NADP+	$\gamma$ -Glutamylphenylalanine
Carnosine	Niacinamide	$\pi$ -Methylhistidine
Cinnamate	Nicotinamide N-oxide	$\tau$ -Methylhistidine
Hippurate	Nicotinate	

## Bile Acid Biosynthesis

Cholate	Isocaproate
Glycocholate	Taurine

## Bile Acids

Cholate	Glycocholate
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## Carbohydrate Metabolism

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

## Carboxylic Acids

2,3,4-Trihydroxybenzoate	Azelate	Malonate
2,6-Dihydroxybenzoate	Benzoate	Methylmalonate
2-Aminoadipate	Biotin	Methylsuccinate
2-Ethylacrylate	Cinnamate	N-Acetylaspartate
2-Furoate	Citraconate	N-Acetylglutamate
2-Hydroxyglutarate	Citrate	N-Acetylglutamine
2-Hydroxyphenylacetate	Desaminotyrosine	N-Carbamoyl- $\beta$ -alanine
2-Methylglutarate	Ethylmalonate	N-Carbamoylaspartate
2-Oxoglutarate	Ferulate	Nicotinate
2-Phenylpropionate	Formate	Nicotinic acid adenine dinucleotide
2-Phosphoglycerate	Fumarate	Phenylacetate
3,4-Dihydroxybenzeneacetate	Galactarate	Phenylglyoxylate
3-Hydromuconate	Gentisate	Phthalate
3-Hydroxy-3-methylglutarate	Glucarate	Pimelate
3-Hydroxyphenylacetate	Gluconate	Protocatechuate
3-Methyladipate	Glutamate	Quinolate
3-Methylglutarate	Glutarate	Saccharopine
3-Phenylpropionate	Glutaric acid monomethyl ester	Salicylate
4-Carboxyglutamate	Guanidinosuccinate	Sebacate
4-Guanidinobutanoate	Guanidoacetate	Suberate
4-Hydroxybenzoate	Homogentisate	Succinate
4-Hydroxyphenylacetate	Homovanillate	Syringate
4-Pyridoxate	Ibuprofen	Tartrate
5-Hydroxyindole-3-acetate	Indole-3-acetate	Trigonelline
5-Methoxysalicylate	Isobutyrate	Urocanate
6-Hydroxynicotinate	Isocaproate	Vanillate
Acetylsalicylate	Isocitrate	Xanthurenate
Adipate	Kynurenate	cis,cis-Muconate
Anthranilate	Malate	cis-Aconitate
Aspartate	Maleate	trans-Aconitate

## Cysteine and Methionine Metabolism

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

## D-xylose Metabolism

D-Threitol
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## Drug Components

2,3,4-Trihydroxybenzoate	Azelate	Oxypurinol
2,6-Dihydroxybenzoate	Ibuprofen	Salicylate
3,5-Dibromotyrosine	Imidazole	Salicylurate
5-Methoxysalicylate	Lactulose	Thymol
Acetaminophen	Levulinate	Valproate
Acetylsalicylate	N-Phenylacetylphenylalanine	

## Environmental Pollutants

1,6-Anhydro- $\beta$ -D-glucose	2-Phenylpropionate	Mandelate
2-Furoate	Acetamide	N,N-Dimethylformamide
2-Hydroxyisobutyrate	Butanone	N-Nitrosodimethylamine
2-Hydroxyvalerate	Isoeugenol	Phthalate

## Fatty Acids

2-Octenoate	Caprate	Propionate
Acetate	Caprylate	Valerate
Butyrate	Isovalerate	Valproate

## Food Components

1,3-Dimethylurate	Chlorogenate	Isobutyrate
1,7-Dimethylxanthine	Dimethyl sulfone	Pyrocatechol
2-Furoylglycine	Epicatechin	Syringate
3-Methylxanthine	Erythritol	Theophylline

Acetoin	Ferulate	Trigonelline
Adipate	Gallate	Vanillate
Caffeine	Glutaric acid monomethyl ester	

## Glycine, Serine and Threonine Metabolism

2-Oxobutyrate	Homoserine	O-Phosphoserine
5-Aminolevulinate	Hydroxyacetone	Sarcosine
Betaine	N,N-Dimethylglycine	Serine
Glycine	N-Acetylglycine	Threonine
Guanidoacetate	N-Isovaleroylglycine	

## Histidine Metabolism

Anserine	Histidine	$\pi$ -Methylhistidine
Carnosine	Urocanate	$\tau$ -Methylhistidine
Histamine	$\beta$ -Alanine	

## Hydroxy Acids

2-Hydroxy-3-methylvalerate	3-Hydroxymandelate	Homoserine
2-Hydroxybutyrate	3-Phenyllactate	Indole-3-lactate
2-Hydroxyglutarate	4-Hydroxy-3-methoxymandelate	Isocitrate
2-Hydroxyisobutyrate	4-Hydroxybutyrate	Lactate
2-Hydroxyisocaproate	4-Hydroxyphenyllactate	Malate
2-Hydroxyisovalerate	Carnitine	Mandelate
2-Hydroxyvalerate	Chlorogenate	Serine
3,4-Dihydroxymandelate	Citrate	Tartrate
3-Hydroxy-3-methylglutarate	Galactonate	Threonate
3-Hydroxybutyrate	Gallate	Threonine
3-Hydroxyisobutyrate	Glycerate	Tropate
3-Hydroxyisovalerate	Glycolate	trans-4-Hydroxy-L-proline

## Internal Standards

DSS (Chemical Shape Indicator)	DSS-d6 (Chemical Shape Indicator)
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## Keto Acids

2-Oxobutyrate	3-Hydroxykynurenine	Levulinate
2-Oxocaproate	3-Methyl-2-oxovalerate	Pyruvate
2-Oxoglutarate	5-Aminolevulinate	Succinylacetone
2-Oxoisocaproate	Acetoacetate	
2-Oxovalerate	Kynurenine	

## Ketone Body Metabolism

3-Hydroxy-3-methylglutarate	Acetoacetate
3-Hydroxybutyrate	Acetone

## Ketones

Acetoacetate	Butanone	Phenylglyoxylate
Acetoin	Creatinine	Succinylacetone
Acetone	Hydroxyacetone	

## Lipid Metabolism

1,3-Dihydroxyacetone	Caprylate	Methylsuccinate
2-Hydroxybutyrate	Carnitine	O-Acetylcarnitine
2-Hydroxyglutarate	Choline	O-Acetylcholine
2-Methylglutarate	Ethanolamine	O-Phosphocholine
2-Octenoate	Ethylmalonate	O-Phosphoethanolamine
3-Hydroxymuconate	Glutarate	Propionate
3-Methyladipate	Glycerate	Propylene glycol
4-Aminohippurate	Glycerol	Sebacate
4-Hydroxybutyrate	Isopropanol	Suberate
Butyrate	Maleate	Valerate
Caprate	Malonate	sn-Glycero-3-phosphocholine

## Lysine Metabolism

2-Amino adipate	Lysine	Pipecolate
5-Aminopentanoate	N <sup>6</sup> -Acetyllysine	Saccharopine
5-Hydroxylysine	N $\alpha$ -Acetyllysine	
Homocitrulline	Pimelate	



## Methane Metabolism

Dimethylamine	Methylamine	Trimethylamine N-oxide
Methanol	Trimethylamine	

## Monosaccharides and Disaccharides

1,6-Anhydro- $\beta$ -D-glucose	Lactose	Ribose
Arabinose	Lactulose	Sucrose
Cellobiose	Maltose	Trehalose
Fructose	Mannose	UDP-N-Acetylglucosamine
Fucose	N-Acetylglucosamine	UDP-galactose
Galactose	NAD <sup>+</sup>	UDP-glucose
Glucose	NADH	UDP-glucuronate
Glucose-1-phosphate	NADP <sup>+</sup>	Xylose
Glucose-6-phosphate	NADPH	
Glucuronate	Nicotinic acid adenine dinucleotide	

## N-oxides

Nicotinamide N-oxide	Trimethylamine N-oxide
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## Nucleotides and Nucleosides

2'-Deoxyadenosine	Guanosine	UDP-N-Acetylglucosamine
2'-Deoxyguanosine	IMP	UDP-galactose
2'-Deoxyinosine	Inosine	UDP-glucose
2'-Deoxyuridine	NAD <sup>+</sup>	UDP-glucuronate
ADP	NADH	Uridine
AMP	NADP <sup>+</sup>	Xanthosine
ATP	NADPH	dCTP
Adenosine	Nicotinic acid adenine dinucleotide	dTTP
Cytidine	S-Adenosylhomocysteine	
GTP	Thymidine	

## Organohalides

3,5-Dibromotyrosine	3-Chlorotyrosine
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## Phenols

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

## Phenylalanine and Tyrosine Metabolism

2-Hydroxyphenylacetate	Benzoate	Phenylalanine
3,4-Dihydroxybenzeneacetate	Catechol	Phenylglyoxylate
3,4-Dihydroxymandelate	Cinnamate	Protocatechuate
3-Chlorotyrosine	Desaminotyrosine	Succinylacetone
3-Hydroxymandelate	Gentisate	Tropate
3-Hydroxyphenylacetate	Hippurate	Tyramine
3-Phenyllactate	Homogentisate	Tyrosine
3-Phenylpropionate	Homovanillate	cis,cis-Muconate
4-Hydroxy-3-methoxymandelate	N-Acetyltyrosine	o-Cresol
4-Hydroxybenzoate	N-Phenylacetyl glycine	p-Cresol
4-Hydroxyphenylacetate	Phenol	$\gamma$ -Glutamylphenylalanine
4-Hydroxyphenyllactate	Phenylacetate	

## Phosphates

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

## Purine and Pyrimidine Metabolism

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

## Purines and Pyrimidines

1,3-Dimethylurate	Caffeine	Thymine
1,7-Dimethylxanthine	Cytosine	UMP
3-Methylxanthine	Hypoxanthine	Uracil
5,6-Dihydrothymine	Oxypurinol	Xanthine
5,6-Dihydrouracil	Pyrimidine	
Adenine	Theophylline	

## Putrefaction

Cadaverine	Methylguanidine	Putrescine
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## Pyruvate and Tricarboxylate Metabolism

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

## Sulfur Compounds

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

## Tryptophan Metabolism

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

## Urea Cycle

Arginine	Ornithine
Citrulline	Urea

## Valine, Leucine and Isoleucine Metabolism

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

## Vitamins and Cofactors

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

## Xenobiotics

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