

List of **701** compounds currently contained in the COLMAR ^{13}C - ^1H HSQC database. For each compound, the number of their isomeric states recorded in the database is given in the “Number of isomers” column. (Updated May 18, 2016)

Number of isomers	Compound name
2	Acetaldehyde_oxime_mixture_of_syn_and_anti
1	Acetic_acid
1	Acetophenone
1	Kanamycin
1	N_Acetyl_L_Glutamine
1	5-(Acetylamino)-2-nitrobenzoic_acid
1	Acetylcarnitine
1	N_Acetyl_L_glutamic_acid
1	Nepsilon_Acetyl_L_Lysine
1	N_acetyl_L_aspartic_acid
1	N_(2_Acetamido)iminodiacetic_acid
1	Adenosine_3_monophosphate
1	Adipic_acid
1	Alanine
1	Alanine-Alanine
2	(1_Amino_1_phenylmethyl)phosphonic_acid
1	4_Aminoantipyrine
1	gamma_Aminobutyric_acid
1	Phosphoethanolamine
1	6_Aminohexanoic_acid
1	2_Aminophenol
1	AMP
1	1,6-anhydro_beta_d_glucose
1	L_Arabitol
1	D_Aspartate
1	Acetamide
1	Dihydroxyacetone
1	Acetyl_phosphate
1	Acetylcholine
1	N_Acetyl glycine
1	N_Acetylneuraminic_acid
1	dAMP_(from HMDB)
1	S_Adenosyl_L_homocysteine
1	Adonitol
1	Agmatine
1	Allantoin
1	alpha_Ketoglutaric_acid
1	alpha_((Methylamino)methyl)benzylalcohol
1	2_Amino_1_phenylethanol
2	2_Amino_3_phosphonopropionic_acid
1	4_Aminobenzoic_acid
1	2_Aminobutyric_acid
1	4_(2_Aminoethyl)morpholine
1	3_Aminoisobutyric_acid
1	4_Aminophenol
1	L_Anserine
1	Arbutin
1	L_Ascorbate

1	4_Acetamidobutyric_acid
1	Acetonitrile
1	N_Acetyl_L_alanine
1	N_alpha_Acetyl_L_Lysine
1	N_acetyl_D_Phenyl_alanine
1	Acrylamide
1	Adenosine
1	ADP
1	beta_Alanine
1	D_Allose
1	2_Amino_5_ethyl_1,3,4_thiadiazole
1	1_amino_1_cyclohexanecarboxylic_acid
2	2_Aminoadipic_acid
1	Methyl_4_aminobutyrate
1	2_Aminocaprylic_acid
2	2_Aminoethylphosphonic_acid
1	6_Aminopenicillanic_acid
1	1_Amino_2_propanol
1	p_Anisic_acid
1	Anthranilic_acid
2	L_Arabinose
1	L_Arginine
1	L_Aspargine
1	ATP
1	Benzoate
1	Betaine
1	Biotin
1	4_Hydroxy_benzoic_acid
1	Benzyl_alcohol
1	Betaine_aldehyde
1	3_Hydroxybutyrate
1	1,2,4_Benzenetriol
1	Benzonitrile
1	Butanol
1	Butyric_acid
1	cAMP
1	N_carbamyl_L_Glutamic_acid
1	L_Carnitine
1	Chlorogenic_acid
1	trans_Cinnamic_acid
1	R_Citramalic_acid
1	Creatinine
1	p_Cresol
1	Cyclohexanol
1	N_cyclohexylformamide
1	L_Cystathionine
1	L_Cysteine
1	CMP
1	Cadaverine
1	L_Canavanine
1	CDP
1	Choline
1	4_Hydroxycinnamic_acid
1	Citrate
2	CoA
1	Cotinine

1	Creatine
1	m_Cresol
1	CTP
1	cis_1,2_cyclohexanediol
1	Cyclohexanone
1	N_cyclohexylsulfamic_acid
2	Cysteamine
1	L_Cystine
1	Cytosine
1	epsilon_Caprolactam
1	3_Carboxypropyl_trimethyl_ammonium
1	L_Carnosine
1	Chorismic_acid
1	trans_3_Hydroxycinnamic_acid
1	cis_Aconitic_acid
1	Citraconic_acid
1	L_Citrulline
1	Creatine_phosphate
1	o_Cresol
1	Cyclohexylamine
1	L_Cysteic_acid
1	Cytidine
1	dADP
1	dGTP
1	dGMP
1	1,3_Diaminopropane
1	Diethanolamine
1	2,5_Dihydroxybenzoic_acid
1	3,4_Dihydroxyphenylacetic_acid
1	1,3_Dimethylurea
1	DSS
1	dAMP
1	3_Deazauridine
1	2_Deoxycytidine
1	2_Deoxyuridine
1	Dihydrocoumarin
1	cis_1,2_dihydronaphthalene_1,2_diol
1	Dihydrouracil
1	3,4_Dihydroxybenzoic_acid
1	3,4_Dihydroxy_L_phenylalanine
1	N,N_Dimethylglycine
1	dTMP
1	Decamethonium
1	2_Deoxyguanosine
1	d_Desthiobiotin
2	alpha,epsilon_Diaminopimelic_acid
1	2,3_Dideoxycytidine
1	O,O_diethyl_thiophosphate
1	L_Dihydroorotic_acid
1	trans_2,3_Dimethylacrylic_acid
1	2,2_Dimethylsuccinic_acid
1	meso_Erythritol
1	Ethanol
1	Ethanolamine
1	Ethylmalonic_acid
1	2_Ethylpiperidine

1	Epinephrine
1	Ethanesulfonic_acid
1	FAD
1	Ferulic_acid
1	Folate
1	Formate
2	Fructose_1,6_bisphosphate
2	L_Fucose
1	Formaldehyde
3	D_Fructose
1	D_Fructose_1_phosphate
1	Fumaric_acid
1	2_Furoylglycine
1	FMN
1	Formamide
1	D_Fructose_2,6_bisphosphate
2	D_Fructose_6_phosphate
1	2_Furoic_acid
1	N_(2_furoyl)glycine_methylester
1	alpha_D_Galactose_1_phosphate
1	N_acetyl_tyrosine
2	D_Glucosamine_6_phosphate
1	D_Glucosaminic_acid
1	alpha_D_Glucose_1,6_bisphosphate
2	D_Glucuronate
1	L_Glutamine
1	L_Glutathione_reduced
1	2,3_Diphospho_D_glyceric_acid
1	Glycolate
1	Guaiacol
1	Guanidineacetic_acid
2	D_Galactono_1,4_lactone
2	D_Galacturonic_acid
2	D_Glucosamine
1	N_Acetyl_D_glucosamine_1_phosphate
1	Methyl_N_acetyl_alpha_D_glucosaminide
2	D_Glucose_6_phosphate
1	Glutaconic_acid
1	Glutaric_acid
1	Glyceraldehyde
1	Glycerol
1	Glycine
1	Glyoxylic_acid
1	4_Guanidinobutyric_acid
2	L_Gulonolactone
2	D_Galactose
1	Gallic_acid
1	GDP
1	Gluconic_acid
2	N_Acetyl_D_glucosamine
2	N_Acetyl_D_glucosamine_6_phosphate
2	D_Glucose
1	alpha_D_Glucose_1_phosphate
1	L_Glutamic_acid
1	L_Glutathione_oxidized
1	Orotic_acid

1 DL_alpha_Glycerol_phosphate
1 Glycolaldehyde
2 Gly_Pro
1 Hexanoic_acid
1 cis_3_hexen_1_ol
1 L_Histidine
1 L_Homocitrulline
1 L_Homoserine
1 3_Hydroxyanthranilic_acid
1 4_Hydroxybenzyl_alcohol
1 trans_2_Hydroxycinnamic_acid
1 2_Hydroxyisocaproic_acid
1 2_Hydroxy_3_methylbutyric_acid
1 5_(Hydroxymethyl)uracil
1 4_Hydroxyphenethyl_alcohol
1 2_Hydroxyphenylacetic_acid
1 3_(2_Hydroxyphenyl)propionic_acid
1 4_Hydroxy_3_methoxybenzyl_alcohol
1 HEPES
1 Hippuric_acid
1 L_Histidinol
1 Homocysteine
1 O_Succinyl_L_homoserine
1 4_Hydroxy_3_methoxymandelic_acid
1 4_Hydroxybenzaldehyde
1 2_Hydroxyhexanoic_acid
1 3_Hydroxymandelic_acid
1 3_Hydroxy_3_methylglutaric_acid
1 6_Hydroxynicotinic_acid
1 4_Hydroxyphenylacetic_acid
1 4_Hydroxy_3_methoxycinnamaldehyde
1 Hypotaurine
1 trans_3_Hexenedioic_acid
1 Histamine
1 Homoarginine
1 Homogentisic_acid
1 Homovanillic_acid
1 Hydroquinone
1 3_Hydroxybenzoic_acid
1 2_Hydroxybutyric_acid
1 3_Butyn_1_ol
1 5_Hydroxyindole_3_acetic_acid
1 3_Hydroxy_4_methoxycinnamic_acid
1 2_Hydroxyoctanoic_acid
1 3_Hydroxyphenylacetic_acid
1 4_Hydroxyphenylacetonitrile
1 4_Hydroxyphenylglycine
1 5_Hydroxy_L_tryptophan
1 Imidazole
1 Indole_3_lactic_acid
1 IMP
1 scyllo_Inositol
1 Isethionic_acid
1 Threo_isocitric_acid
1 L_Isoleucine
1 Itaconic_acid

1	Indole_3_acetic_acid
1	muco_Inositol
1	Isobutyric_acid
1	Isonicotinic_acid
1	ITP
1	Inosine
1	myo_Inositol
1	IPTG
1	Isovaleric_acid
1	Kynurenic_acid
1	2_Ketobutyric_acid
1	L_Kynurenine
1	beta_Leucine
1	Lactic_acid
1	Cysteinesulfinic_acid
1	Leucine
1	Lysine
1	Maleamic_acid
1	Malic_acid
2	Methionine_sulfoxide
1	4_Methylcatechol
1	5_Methylcytosine
1	3_Methylglutaric_acid
1	Methylmalonic_acid
1	4_Methyl_2_oxovaleric_acid
1	3_Methylphenylacetate
1	4_Methylsalicylic_acid
1	N_Methylurea
1	trans,trans_Muconic_acid
1	Maleic_acid
2	D_Mannose
1	MES
1	Methanol
1	3_Methyl_2_butenic_acid
1	3_Methyladipic_acid
1	1_Methyl_L_Histidine
1	3_Methyl_2_oxobutinoic_acid
1	4_Methyl_5_thiazoleethanol
1	5_Methyluridine
1	Monoethyl_malonate
1	D_Mannitol
1	Mesaconic_acid
1	L_Methionine
1	3_Methylcatechol
2	3_Methylcrotonaldehyde
1	2_Methylglutaric_acid
1	N_methyl_L_Aspartic_acid
1	3_Methyl_2_oxopentanoic_acid
1	3_Methylsalicylic_acid
1	MOPS
1	Nicotinamide
1	Nicotinuric_acid
1	N_acetyl_Histidine
1	Neostigmine
1	4_Nitrophenol
1	Norepinephrine

1	Nicotinic_acid
1	Nicotine
1	4_Nitrocatechol
1	4_Nitrophenyl_phosphate
1	L_Norleucine
1	L_Ornithine
1	Orthanilic_acid
1	2_Octenoic_acid
1	N(alpha)_Acetyl_ornithine
1	Pantolactone
1	Pantothenate
1	Phenol
2	Phenylacetylglycine
1	Phenylglyoxylic_acid
1	6_Phosphogluconic_acid
1	O_phospho_threonine
1	D_Pinitol
1	Pipecolic_acid
1	3,4_Dehydro_proline
1	1,3_Propanediol
1	Propionic_acid
1	Purine
1	3_Pyridine_aldoxime
2	Pyridoxal_5_phosphate
1	Pyridoxine
1	2_Pyrrolidinone_5_carboxylate
1	Panthenol
1	L_Phenylalanine
1	2_Phenylbutyric_acid
1	3_Phosphoglyceric_acid
1	O_Phospho_L_serine
1	Phthalic_acid
1	Polygalacturonic_acid
1	trans_4_Hydroxy_L_proline
1	Propanol
1	Putrescine
1	3_Pyridinecarbonitrile
1	Pyridoxamine
1	Pyrocatechol
2	Pyruvic_acid
1	Phenethylamine
1	Phenoxyacetic_acid
1	Phenylacetic_acid
1	2_Phenylethanol
1	Phosphoenolpyruvic_acid
2	Phosphonoacetic_acid
1	Phthalaldehydic_acid
1	Pimelic_acid
1	L_Proline
1	1,2_Propanediol
1	Pyridine
1	Pyridoxal
1	Pyridoxamine_5_phosphate
1	Quinaldic_acid
1	Quinolinic_acid
1	Quinic_acid

2	D_Ribose_5_phosphate
1	Resorcinol
1	D_Saccharate
1	Salicylate
1	Sarcosine
1	Selenomethionine
1	Serotonin
1	D_Sorbose
1	Spermine
1	D_Salicin
1	L_Serine
1	Shikimic_acid
1	Sinapic_acid
1	Suberic_acid
1	Sulfanilic_acid
1	Saligenin
1	D_Sorbitol
1	Spermidine
1	Succinic_acid
1	Sulfoacetic_acid
1	Thiamine_monophosphate
1	L_Threitol
1	Thymidine
1	Trigonelline
1	Trimethylamine_N_oxide
1	Tryptamine
1	L_Tyrosine
1	L_Tartaric_acid
1	Tetramethylammonium
1	Thioacetamide
1	Threo_beta_methylaspartate
1	p_Toluic_acid
1	Triethanolamine
2	Trimethyl_phosphate
1	L_Tryptophan
1	Taurine
1	Thiamin
1	L_Threonine
1	D_Trehalose
1	Triethylenetetramine
1	Trimethylamine
1	Tropic_acid
1	Tyramine
1	UDP
1	3_Ureidopropionic_acid
1	Uridine
1	UTP
1	UMP
1	Uracil
1	Urocanate
1	Ureidosuccinic_acid
1	UDP_GlcNAc
1	UDP_glucuronate
1	Valeric_acid
1	L_Valine
1	Vanillin

1	Vanillic_acid
1	Xylitol
2	D_Xylose
1	D_Xylonate
1	Caffeine
1	NADH
1	NAD
1	NADPH
1	NADP+
1	Nicotinamide_D_ribonucleotide_reduced
1	Nicotinamide_D_ribonucleotide_oxidized
1	Sucrose
2	Lactose
2	Maltose
4	D_Ribose
2	N_Acetylmannosamine_HMDB
2	Cellobiose
2	Dehydroascorbic_acid
2	delta_Hexanolactone
2	Glucosamine_6_sulfate
2	Isomaltose
1	Adenine
2	Mannose_6_phosphate
2	Melibiose
2	Muramic_acid
2	N_acetylgalactosamine
2	N_acetylgalactosamine_4_sulfate
2	Rhamnose
1	Acetoacetic_acid
1	Deoxyinosine
1	Galactitol
1	Guanine
1	Guanosine
1	Methylamine
1	Glycerophosphocholine
1	Thymine
1	2_Isopropylmalic_acid
1	Galactaric_acid
1	L_2_Hydroxyglutaric_acid
1	Cysteine_S_Sulfate
1	Trans_aconitic_acid
1	5_Aminolevulinic_acid
1	Allantoic_acid
1	Succinic_acid_semialdehyde
1	3_Mercaptopyruvic_acid
1	N_acetyl_putrescine
2	Butanediol
1	Acetoin
1	(S)_3_Hydroxyisobutyric_acid
1	Dimethylamine
1	Glyceric_acid
1	2_Methylacetoacetate
1	2_Hydroxyadipic_acid
1	3_Hydroxysuberic_acid
1	3_Deoxyarabinohexonic_acid
1	3_Oxoadipic_acid

1	2,3_Dihydroxyvaleric_acid
2	5_Hydroxylysine
1	Allocystathionine
1	Butanone
1	Alloisoleucine
1	DL_Homocystine
1	Glutaryl-glycine
1	Succinylacetone
1	Isovaleryl-glycine
1	Indoxyl_Sulfate
1	Isocaproic_acid
1	3_Hydroxypropionic_acid
1	Mandelic_acid
1	Levulinic_acid
1	Alpha_hydroxyisobutyric_acid
1	Isovalerylalanine
1	3_Hydroxyisovaleric_acid
1	Glycyl_L_Leucine
1	Propionyl-glycine
1	Monomethylglutaric_acid
1	Isopropyl_alcohol
1	N_Formyl_L_Methionine
1	Methyl_propenyl_ketone
1	Methylguanidine
1	Phosphorylcholine
1	Acetone
1	Methylsuccinic_acid
1	1,3_Dimethyluric_acid
1	2_Ethylacrylic_acid
1	2_Ketohexanoic_acid
1	N,N_Dimethylformamide
1	N_Acetylcysteine
1	Aminoisobutyric_acid
1	2_Ethyl_2_Hydroxybutyric_acid
1	2_Hydroxy_2_Methylbutyric_acid
1	Dimethylmalonic_acid
1	2,3_Diaminopropionic_acid
1	2_Pyrrolidinone
1	Methylcysteine
1	N_Methyl_aminoisobutyric_acid
1	2,4_Diaminobutyric_acid
1	Erythrose
1	Methyl_isobutyl_ketone
1	Aniline
1	Guanidinosuccinic_acid
1	Gulonic_acid
1	5_Aminopentanoic_acid
1	Pyrimidine
1	2_Heptanone
1	L_Allothreonine
1	4_Heptanone
1	FAPy_adenine
1	cis_4_Octenedioic_acid
1	Dimethyl_sulfone
1	alpha_Asparyl_lysin
1	2-Oxohexane

1	Isopropyl_ethyl_ketone
1	L_Iditol
1	Cysteine_glutathione_disulfide
1	Riboflavin
1	Xanthosine
1	UDP_galactose
1	3,4_Dihydroxyphenylglycol
1	2_Pyrocatechuic_acid
1	Homocarnosine
1	gamma_Glutamylcysteine
1	Dimethylallylpyrophosphate
1	FADH
1	dCMP
1	GTP
1	GMP
1	dTTP
1	Thiamine_pyrophosphate
1	dUMP
1	Pyridoxic_acid
1	3_Methoxytyramine
1	Argininosuccinic_acid
2	Mevalonic_acid
1	Tetrahydrofuran
1	Saccharopine
1	UDP_glucose
1	2_Methylbutyroylcarnitine
1	6_Dimethylaminopurine
1	3_Methylhistidine
1	Gamma_butylolactone
1	Heptanoic_acid
1	1_Methylnicotinamide
1	Aspartyl_phenylalanine
1	Isovalerylglutamic_acid
1	Orotidine
1	Capryloylglycine
1	Xanthurenic_acid
1	Suberylglycine
1	Tiglylglycine
1	5_Methylcytidine
1	N,N_Dimethylaniline
1	7_Methylguanosine
1	CDP_choline
1	3_Pyridylacetic_acid
1	1_Methylguanosine
1	Paraxanthine
1	4_Aminohippuric_acid
1	Valproic_acid
1	Ribonolactone
1	3_Nitrotyrosine
1	1,1_Dimethylbiguanide
1	3_Phenylbutyric_acid
1	Caffeic_acid
1	5_Methoxydimethyltryptamine
1	Imidazoleacetic_acid
1	1,9_Dimethyluric_acid
1	5_Phenylvaleric_acid

1 4_Methoxyphenylacetic_acid
1 Syringic_acid
1 4_Ethylbenzoic_acid
1 1,3,7_Trimethyluric_acid
1 2,4_Diamino_6_hydroxypyrimidine
1 1,3_Dimethyluracil
1 3_(4_Hydroxyphenyl)propionic_acid
1 2_Phenylglycine
1 Picolinic_acid
1 5_Methoxytryptophan
1 Alpha_hydroxyhippuric_acid
1 Pyruvatoxime
1 Alpha_ketoglutaric_acid_oxime
1 3,4,5_Trimethoxycinnamic_acid
1 Methylimidazoleacetic_acid
1 N_methylnicotinamide
1 Sedoheptulose
1 3_Methoxy_4_Hydroxyphenylglycol_sulfate
1 D_Tagatose
2 N_Methylhydantoin
1 Pantethine
1 Gamma_caprolactone
1 Indoxyl
1 5_Methoxytryptamine
1 Perillic_acid
1 4_Hydroxy_3_methylbenzoic_acid
1 o_Tyrosine
1 Benzaldehyde
1 D_Glucurono_6,3_lactone
1 1_Methyladenine
1 3_Methyladenine
1 Hydrocinnamic_acid
1 Homoveratric_acid
1 Hexadecanedioic_acid
1 Hydroxyphenylpyruvic_acid
1 L_3_Phenyllactic_acid
1 Isobutyryl_carnitine
1 Hydroxyphenyllactic_acid
1 Salicyluric_acid
1 1_Methylhistamine
1 Valerylglycine
1 Melatonin
1 Xylulose
1 3_Methylhistamine
1 3,4_Dihydroxymandelic_acid
1 2_Hydroxy_5_methoxybenzoic_acid
1 3_Aminobenzoic_acid
1 3,7_Dimethyluric_acid
1 Biocytin
1 Benzene
1 Malonic_acid
1 Indole
1 Terephthalic_acid
1 Normetanephine
1 Undecanedioic_acid
1 Deoxyadenosine

1	Dihydrothymine
1	Dopamine
1	Adenosine_3_5_diphosphate
1	2_Oxadipic_acid
1	3_Furoic_acid
1	3_Hydroxyglutaric_acid
1	3,4_Dihydroxyhydrocinnamic_acid
1	2_Methyl_3_ketovaleric_acid
1	Hexanoylcarnitine
1	Neopterin
1	N1_Acetylspermine
1	AMP_sulfate
1	Acetaminophen
1	N_Acryloylglycine
1	3_Methoxytyrosine
1	L_Homocysteic_acid
1	Phenylephrine
1	3_Aminosalicylic_acid
1	3_(3_Hydroxyphenyl)_3_hydroxypropanoic_acid
1	Chitosan
1	3_Phenoxypropionic_acid
1	1,11_Undecanedicarboxylic_acid
1	3_Methoxybenzenepropanoic_acid
1	2_Piperidinone
1	N_acetyl_methionine
1	Gly_gly
1	2_Methylhippuric_acid
1	Norspermidine
1	7_Methyladenine
1	Carvone
1	Selenocystine
1	Hydroxykynurenine
1	Ethenodeoxyadenosine
1	3_Methylxanthine
1	7_Methylxanthine
1	1_Methyluric_acid
1	Quinone