



MOLINSTINCTS Database Products Guide **For Subscription Plan A**

Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
Enterprise	All compounds available in MOLINSTINCTS	0 – 57		2,512,391
DB #01	• Free Radicals*	1 – 23	Compounds in DB #02 and #03 (= DB #02 + DB #03)	384,565
DB #02	▶ Hydrocarbon Radicals	1 – 23	Hydrocarbon radicals	284,033
DB #03	▶ Hetero Radicals	1 – 10	Hetero Radicals 1 - 10 Hetero (including atoms other than C and H) radicals	100,532
DB #04	• Hydrocarbons	1 – 57	Compounds in DB #05 – #09 (= DB #05 + DB #06 + DB #07 + DB #08 + DB #09)	949,509
DB #05	▶ Alkane	1 – 57	Alkane (Paraffin)	212,173
DB #06	▶ Alkene	2 – 30	Alkene (Olefin)	246,612
DB #07	▶ Alkyne	2 – 28	Alkyne	77,499
DB #08	▶ Cyclo-Hydrocarbons	3 – 57	Cycloalkane(Cycloparaffins, Naphthenes), Cycloalkene(Cycloolefins), Cycloalkylene	165,406
DB #09	▶ Aromatics	4 – 57	Aromatics	247,819
DB #10	• Hetero Compounds	0 – 57	Compounds in DB #11 – #17 (= DB #11 + DB #12 + DB #13 + DB #14 + DB #15 + DB #16 + DB #17)	1,178,318
DB #11	▶ O-Hetero Compounds	0 – 57	O-heterocyclic, carbonyl compound, aldehyde, ketone, ketene, carbonyl hydrate, hemiacetal, acetal, enol, enoether, hydroxy compound, alcohol, prim. alcohol, sec. alcohol, tert. alcohol, 1,2-diol, phenol, 1,2-diphenol, enediol, ether, dialkylether, alkylarylether, diarylether, peroxide, hydroperoxide, carboxylic acid, carboxylic acid ester, lactone, carboxylic acid anhydride, carbonic acid monoester, carbonic acid diester, alpha-hydroxyacid, carboxylic acid deriv., carbonic acid deriv.	172,417
DB #12	▶ N-Hetero Compounds	0 – 54	N-heterocyclic, imine, hydrazone, aminal, enamine, hydrazine derivative, amine, prim. amine, prim. aliphatic amine, prim. aromatic amine, sec. amine, sec. aliphatic amine, sec. mixed amine (aryl alkyl), sec. aromatic amine, tert. amine, tert. aliphatic amine, tert.	100,541

* Note: Due to the unstable nature of radical compounds, some thermo-physico-chemical properties and molecular information are unavailable. Total number of sets of information per radical compound is around 380.



Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
			mixed amine, tert. aromat. amine, carboxylic acid amidine, carboxylic acid amidrazone, nitrile, guanidine, azide, azo compound, cyanate, carbodiimide	
DB #13	▶ S-Hetero Compounds	0 – 56	S-heterocyclic, thiocarbonyl compound, thioacetal, thioether, disulfide, thiocarboxylic acid deriv., thiol, alkylthiol, arylthiol, thiocarbonic acid deriv., sulfenic acid deriv., thiocarboxylic acid, thiocarboxylic acid ester, thiolactone	57,560
DB #14	▶ O/N-Hetero Compounds	0 – 38	semicarbazone, oxime, oxime ether, oxime ether, hemiaminal, 1,2-aminoalcohol, hydroxylamine, carboxylic acid amide, carboxylic acid prim. amide, carboxylic acid sec. amide, carboxylic acid tert. amide, lactam, carboxylic acid hydrazide, carboxylic acid azide, hydroxamic acid, acyl cyanide, imido ester, oxohetarene, carboxylic acid amide acetal, carboxylic acid imide, carboxylic acid unsubst. imide, carboxylic acid subst. imide, urea, isourea, semicarbazide, isocyanate, nitroso compound, nitro compound, nitrite, nitrate, alpha-aminoacid	374,423
DB #15	▶ O/S-Hetero Compounds	0 – 36	thiocarbonic acid monoester, thiocarbonic acid diester, sulfuric acid monoester, sulfuric acid diester, sulfonic acid, sulfonic acid ester, sulfone, sulfoxide, sulfinic acid, sulfinic acid ester, sulfinic acid ester, sulfuric acid deriv., sulfonic acid deriv., sulfinic acid deriv.	76,083
DB #16	▶ N/S-Hetero Compounds	0 – 25	thiosemicarbazone, thiohemiaminal, thiolactam, imidothioester, thioxohetarene, thiourea, isothiourea, thiosemicarbazide, thiocyanate, isothiocyanate, thiocarbamic acid deriv.	112,136
DB #17	▶ N/O/S-Hetero Compounds	0 – 32	thiocarbamic acid, thiocarbamic acid ester, sulfuric acid amide ester, sulfuric acid amide, sulfuric acid diamide, sulfonamide, sulfinic acid amide	285,158
DB #18	Gasoline	5 – 12	Alkane, Cycloalkane	104,681
DB #19	Jet-fuel	10 – 15	Alkane, Aromatics	170,810
DB #20	Diesel	12 – 25	Alkane, Alkene, Cycloalkane, Aromatics	731,935



Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
DB #21	Bio-Diesel	12 – 19	Alkane, Alkene, Cycloalkane, Aromatics	669,038
DB #22	Thermal Cracking	1 – 15	Alkane, Alkene, Alkyne, Aromatics, Hydrocarbon radicals	488,997
DB #23	Catalytic Cracking	1 – 40	Alkane, Alkene, Aromatics, Cycloalkane	791,485
DB #24	Hydro Cracking	5 – 19	Alkane, Cycloalkane, Aromatics, Hydrocarbon radicals	764,759
DB #25	Desulfurization	1 – 20	Alkane, Alkene, Alkyne, Cycloalkane, Aromatics, alcohol, ether, ketone, aldehyde, carboxylic acid, carboxylic acid ester, N-heterocyclic, S-heterocyclic, Hetero radicals	984,196
DB #26	Isomerization	4 – 15	Alkane, Alkene, Aromatics	230,014
DB #27	Catalytic Reforming	6 – 15	Alkane, Alkene, Alkyne, Cycloalkane, Aromatics	404,641
DB #28	Combustion	1 – 24	Alkane, Alkene, Alkyne, Cycloalkane, Aromatics, Hydrocarbon radicals, Hetero radicals, alcohol, ether, ketone, aldehyde, carboxylic acid, carboxylic acid ester, N-heterocyclic, S-heterocyclic	1,298,757
DB #29	Soot	13 – 24	Aromatics	245,098
DB #30	Naphtha	1 – 15	Alkane, Alkene, Alkyne, Aromatics	271,238
DB #31	Gas-To-Liquid (GTL, CH4 Reforming + Fischer-Tropsch)	1 – 57	Parafin, Cyclo-parafin, Olefin, Cyclo-olefin, Diene, Aromatics, Alcohol, Phenol, Aldehyde, Carboxylic acid, Ester, Ketone, Acetal, Ether, Furan	843,809
DB #32	Coal-To-Liquid (CTL, Coal Gasification + Fischer-Tropsch)	1 – 57	Parafin, Cyclo-parafin, Olefin, Cyclo-olefin, Diene, Aromatics, Alcohol, Phenol, Aldehyde, Carboxylic acid, Ester, Ketone, Acetal, Ether, Furan, Pyran, Pridine, Indole, Quinoline, Aniline, Nitrile, Phenazine, Carbazole, Thiophene, Hydrocarbon Radicals, Hetero Radicals	1,234,093



Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
DB #33	Methanol-To-Olefin (MTO) / Methanol-To-Gasoline (MTG)	1 – 57	Parafin, Olefin, Aromatics, Methanol, Dimethyl Ether, Water	682,041
DB #34	Drug-like Compounds	1 - 57	aldehyde, ketone, oxime, oxime ether, ketene acetal derivative, carbonyl hydrate, hemiacetal, acetal, enol, enolether, alcohol, prim. alcohol, sec. alcohol, tert. alcohol, phenol, enediol, ether, dialkylether, alkylarylether, diarylether, peroxide, hydroperoxide, carboxylic acid, carboxylic acid ester, lactone, orthocarboxylic acid deriv., carboxylic acid orthoester, carboxylic acid anhydride, carbonic acid deriv., carbonic acid monoester, carbonic acid diester, alpha-hydroxyacid, imine, hydrazone, semicarbazone, thiosemicarbazone, aminal, enamine, hydrazine derivative, amine, prim. amine, prim. aliphatic amine, prim. aromatic amine, sec. amine, sec. aliphatic amine, sec. mixed amine (aryl alkyl), sec. aromatic amine, tert. amine, tert. aliphatic amine, tert. mixed amine, tert. aromatic amine, nitrile, acyl cyanide, iminoheterene, guanidine, thiosemicarbazide, azide, azo compound, carbodiimide, thioaldehyde, thioketone, thioacetal, thioether, disulfide, alkylthiol, arylthiol, sulfurous acid deriv, hemiaminal, hydroxylamine, carboxylic acid prim. amide, carboxylic acid sec. amide, carboxylic acid tert. amide, lactam, carboxylic acid hydrazide, hydroxamic acid, carboxylic acid amidine, carboxylic acid amidrazone, imido ester, oxoheterene, carboxylic acid amide acetal, carboxylic acid unsubst. imide, carboxylic acid subst. imide, carbamic acid deriv, carbamic acid, carbamic acid ester (urethane), urea, isourea, semicarbazide, cyanate, isocyanate, nitroso compound, nitro compound, nitrite, nitrate, alpha-aminoacid, thiohemiaminal, imidothioester, thioxoheterene, thiocyanate, isothiocyanate, thiocarboxylic acid, thiocarboxylic acid ester, thiolactone, thiocarboxylic acid amide, thiolactam, thiocarbonic acid deriv., thiocarbonic acid monoester, thiocarbonic acid diester, thiourea, isothiurea, sulfuric acid deriv., sulfuric acid monoester, sulfuric acid diester, sulfonic acid deriv., sulfonic acid, sulfonic acid ester, sulfone, sulfoxide, sulfinic acid deriv., sulfinic acid, sulfinic acid ester, sulfenic acid deriv., sulfenic acid, sulfenic acid ester, thiocarbamic acid deriv., thiocarbamic acid, thiocarbamic acid ester, sulfuric acid amide ester, sulfuric acid amide, sulfuric acid diamide, sulfonamide, sulfinic acid amide, sulfinic acid amide	1,050,384