

MW0111075	4573.31676	5705.0455	5024.09486	4903.53648	4678.72489	4399.43893	4275.82568	5836.37379	4895.69633	4693.66653	4721.74548	4625.54506	4763.13496	4458.85484	5037.70172	C4H11NO3	Trometamol	Alcohol and amines	Alcohols	120.6645	121.0739	0.7802	M-H	0.26675	MSI	0.7434	rp	77.86-1	6503	HMDB006248	-	C07182	--	--	--	--	--	--					
MW0111124	12201.349	954.25189	1082.9893	451.57463	813.149153	1409.08336	4155.78147	1318.21599	1588.9022	1755.20988	1158.70999	1644.35173	1453.43879	1147.01454	1402.3582	CRH11NO3	N,N-Dimethyl-2-thiopyridinamine	Alcohol and amines	Amines	250.0382	169.9561	1.2202	M-CI+HCOOH	2.16325	MSI	0.6997	rp	51948-20	2408995	HMDB001111	-	C02846	--	--	--	--	--	--					
MW0111174	51452.9767	3173.468	4252.8582	2853.75017	8487.11121	8006.54141	4989.52725	3299.99001	4839.1318	3682.57428	6383.6668	438.50426	1996.14887	9807.89966	3663.92478	12607.6099	C3H4O3	Benzene and substituted derivatives	Alcohol and amines	Alcohols	218.2713	121.6819	7.8302	M-K	1.9174719	MSI	0.8508	rp	121.697	949	HMDB001020	64944	C02846	--	--	--	--	--	--				
MW0111225	176.64124	388.865441	259.150676	360.574886	190.959135	262.449219	361.686115	375.092545	494.381371	561.5412	236.977473	439.90122	411.497625	261.844253	348.300403	C2H6N2O	N-Tirosyldimethylamine	Alcohol and amines	Amines	82.9993	74.048	1.2	2M-Na+K	3.9679	MSI	0.66	rp	62-75.9	6124	HMDB0031419	-	C14704	ko05204	--	--	--	--	--	--				
MW0111256	15646.3469	15497.78	14896.3696	146418.818	15196.5516	14807.1404	15997.5648	15108.8824	15173.9524	14255.842	15648.8834	14720.8719	15298.3039	1255.2923	1341.0581	C5H11NO4P	Phosphocholine	Organic acid And Its derivatives	Phosphoric acids	184.0746	184.0739	8.6195	M-H	3.75811299	MSI	0.8919	rp	107-73.3	1014	HMDB001565	-	C05888	ko00564.ko01100.ko05231	--	--	--	--	--	--	--			
MW0111332	338.123407	110.47481	142.93461	111.34766	112.124	111.34766	112.124	111.34766	112.124	111.34766	112.124	111.34766	112.124	111.34766	112.124	C11H19NO2S	4-Amino-2-ethylamino-1,3-thiazol-5-yl-(4-chlorophenyl)methane	Aldehyde,Ketones,Esters	Ketones	208.0348	281.039	2.4502	M-H	3.7885	MSI	0.8891	rp	102-71.6	7638	HMDB003238	-	C06771	ko0564	--	--	--	--	--	--				
MW0111876	12043.4888	9176.63501	13024.546	11679.099	12696.6469	14983.2344	14526.1933	15600.9409	11815.7546	13182.7416	10888.6322	12979.0251	14538.3297	15155.582	14590.6728	C15H19BNOS2	2-(1,3-Benzothiazol-2-ylsulfanyl)-1-(4-chlorophenyl)ethane	Benzene and substituted derivatives	Benzene and substituted derivatives	363.2939	364.9366	6.8039	M-H	14.065	MSI	0.7475	rp	23384-65.8	990128	-	-	-	-	-	-	-	-	-	-				
MW0111890	956.761322	1443.30684	1075.81539	1372.189	639.862833	561.388206	565.584741	568.753476	155.814222	1536.00275	74.4166191	416.49172	721.650774	904.957329	393.85782	C5H13NO2	2,2-Dimethoxyethoxyethane	Alcohol and amines	Amines	120.1032	119.0946	11.6812	M-H	5.92825	MSI	0.6217	rp	31576-51.9	520530	-	-	-	-	-	-	-	-	-	-				
MW0111910	17006.2607	18118.321	21372.3234	26357.3273	28434.71	31736.544	36244.4874	45886.945	21065.3882	25906.0154	28459.2948	32376.6248	34354.1478	35148.1006	35148.1006	C10H16O6	2,3,4,5-Tetrahydroxyphenytoic acid	Organic acid And Its derivatives	Organic acid And Its derivatives	149.0087	166.4477	6.8039	M-H+CH4	0.65475	MSI	0.9839	rp	-	-	-	-	-	-	-	-	-	-	-	-				
MW0111943	62103.8899	2511.5939	2266611.14	22517597.7	20683180.9	22565622.6	22211032.4	22485076.7	21272539	21784.494	19885907.5	22046640	2425.4447	2131201.7	22139737.2	C4H6O2	2,3-Butanedione	Aldehyde,Ketones,Esters	Ketones	125.0012	86.0368	9.7246	M-K	3.198675	MSI	0.6761	rp	431-03.8	650	HMDB003040	-	C00741	ko0660	--	--	--	--	--	--	--			
MW0111948	25689.162	30972.6778	33015.817	29851.6173	29831.1697	29323.114	31325.390	37079.4683	28523.5193	33015.817	29586.5092	32405.6271	34925.9978	3196.924	3496.1998	C4H6O6	2,3-Dihydroxybutanedioic acid	Organic acid And Its derivatives	Organic acid And Its derivatives	149.0088	150.0688	4.3728	M-H	2.29414989	MSI	0.7605	rp	133-37.9	85	HMDB0093167	-	C02650	--	--	--	--	--	--	--	--	--		
MW0112231	604.31185	5627.8087	5286.25599	634.07733	5263.51038	5199.44004	5021.8122	4946.83152	4836.17649	5389.98704	4606.3131	4835.59805	4736.45413	4738.30614	4615.7053	C3H7O7P	2-Phosphoglyceric acid	Organic acid And Its derivatives	Organic acid And Its derivatives	186.9995	185.9929	12.134	M-H	7.34925	MSI	0.8462	rp	600-18.0	59	HMDB002005	-	C00109	ko00260.ko00270.ko00290.ko00640.ko01100.ko041720.ko01230	--	--	--	--	--	--	--	--	--	--
MW0112337	151678.317	145356.111	13682.174	14582.979	113669.979	121469.67	66465.611	117566.401	6005.36914	117566.401	6005.36914	117566.401	6005.36914	117566.401	6005.36914	C11H19NO2	4-Amino-2-ethylamino-1,3-thiazol-5-yl-(4-chlorophenyl)methane	Aldehyde,Ketones,Esters	Ketones	217.0628	224.117	5.6089	M-K+H2O	15.8131395	MSI	0.6625	rp	102-71.6	7638	HMDB006202	-	C01412	ko00564.ko01100.ko05231	--	--	--	--	--	--	--	--		
MW0112836	21030.7834	13594.8371	1409.4753	16131.7348	22899.7692	15528.9349	21253.8783	12533.0215	32336.3039	15148.0475	13652.9974	18980.723	16394.0719	15844.2667	19661.9495	C7H6O2	3-Hydroxybenzaldehyde	Benzene and substituted derivatives	Benzene and substituted derivatives	121.0292	122.0368	4.5606	M-H	1.94875	MSI	0.9536	rp	100-83.4	101	-	-	-	-	-	-	-	-	-	-	-			
MW0112868	3885.8271	3650.7514	3220.3428	3788.31216	3863.60804	3907.72446	3371.80089	3307.80024	3745.80742	4264.79346	4360.264	4394.00896	4354.19797	3922.02688	4028.4677	C5H10O	3-Methyl-2-buten-1-ol	Alcohol and amines	Alcohols	104.1084	86.0732	12.134	M+NH4	3.2765239	MSI	0.6364	rp	556-82.1	11373	HMDB0030124	-	C01390	--	--	--	--	--	--	--	--	--		
MW0113123	1621.74555	4622.4582	2853.75017	8487.11121	8006.54141	4989.52725	3299.99001	4839.1318	3682.57428	6383.6668	438.50426	1996.14887	9807.89966	3663.92478	12607.6099	C3H4O3	2,2-Dimethoxyethoxyethane	Organic acid And Its derivatives	Organic acid And Its derivatives	120.1032	119.0946	11.6812	M-H	5.92825	MSI	0.6217	rp	31576-51.9	520530	-	-	-	-	-	-	-	-	-	-				
MW0113190	17006.2607	18118.321	21372.3234	26357.3273	28434.71	31736.544	36244.4874	45886.945	21065.3882	25906.0154	28459.2948	32376.6248	34354.1478	35148.1006	35148.1006	C10H16O6	2,3,4,5-Tetrahydroxyphenytoic acid	Organic acid And Its derivatives	Organic acid And Its derivatives	149.0087	166.4477	6.8039	M-H+CH4	0.65475	MSI	0.9839	rp	-	-	-	-	-	-	-	-	-	-	-	-				
MW0113928	62103.8899	2511.5939	2266611.14	22517597.7	20683180.9	22565622.6	22211032.4	22485076.7	21272539	21784.494	19885907.5	22046640	2425.4447	2131201.7	22139737.2	C4H6O2	2,3-Butanedione	Aldehyde,Ketones,Esters	Ketones	125.0012	86.0368	9.7246	M-K	3.198675	MSI	0.6761	rp	431-03.8	650	HMDB003040	-	C00741	ko0660	--	--	--	--	--	--	--	--		
MW0113943	25689.162	30972.6778	33015.817	29851.6173	29831.1697	29323.114	31325.390	37079.4683	28523.5193	33015.817	29586.5092	32405.6271	34925.9978	3196.924	3496.1998	C4H6O6	2,3-Dihydroxybutanedioic acid	Organic acid And Its derivatives	Organic acid And Its derivatives	149.0088	150.0688	4.3728	M-H	2.29414989	MSI	0.7605	rp	133-37.9	85	HMDB0093167	-	C02650	--	--	--	--	--	--	--	--	--		
MW0114231	604.31185	5627.8087	5286.25599	634.07733	5263.51038	5199.44004	5021.8122	4946.83152	4836.17649	5389.98704	4606.3131	4835.59805	4736.45413	4738.30614	4615.7053	C3H7O7P	2-Phosphoglyceric acid	Organic acid And Its derivatives	Organic acid And Its derivatives	186.9995	185.9929	12.134	M-H	7.34925	MSI	0.8462	rp	600-18.0	59	HMDB002005	-	C00109	ko00260.ko00270.ko00290.ko00640.ko01100.ko041720.ko01230	--	--	--	--	--	--	--	--	--	
MW0114273	151678.317	145356.111	13682.174	14582.979	113669.979	121469.67	66465.611	117566.401	6005.36914	117566.401	6005.36914	117566.401	6005.36914	117566.401	6005.36914	C11H19NO2	4-Amino-2-ethylamino-1,3-thiazol-5-yl-(4-chlorophenyl)methane	Aldehyde,Ketones,Esters	Ketones	217.0628	224.117	5.6089	M-K+H2O	15.8131395	MSI	0.6625	rp	102-71.6	7638	HMDB006202	-	C01412	ko00564.ko01100.ko05231	--	--	--	--	--	--	--	--		
MW0114861	82078.812	67211.666	72183.268	56741.9344	66583.9365	67151.3754	67231.8108	64401.545	71180.285	68057.6496	37228.7376	70597.3412	75138.3148	70378.5173	69905.5519	C8H16O6	2-(2S,3R,4R,5R,2',3',4',5',6'-Pentahydroxyhexan-3-yl)-2,3,4,5,6-Pentahydroxyhexanol	Organic acid And Its derivatives	Organic acid And Its derivatives	217.0028	180.0634	3.3762	M-K+H2	18.5108994	MSI	0.7915	rp	3458-24.8	161658	HMDB0062473	-	-	-	-	-	-	-	-	-	-	-		
MW0114874	170355.74	200931.495	2051.4226	195644.226	21602.212	255343.493	194336.371	253823.119	235823.119	235823.119	235823.119	235823.119	235823.119	235823.119	235823.119	C5H10O6	3-Hydroxybenzaldehyde	Organic acid And Its derivatives	Organic acid And Its derivatives	165.0411	166.4477	4.3728	M-H	4.83440168	MSI	0.7057	rp	32609-14.6	122045	HMDB0060339	-	C00878	ko00053	--	--	--	--	--	--	--	--	--	
MW0114885	45075.4537	43655.1072	4219.8909	4100.6445	44888.0881	42000.5795	441301.4048	42648.6051	44473.1727	42332.3172	42941.4831	42044.9961	4251.7795	41930.809	42512.4233	C4H10O3	Diethylene glycol	Alcohol and amines	Alcohols	217.0707	106.063	4.4486	M-H	3.3803938	MSI	0.9278	rp	111-46.6	8117	-	-	-	-	-	-	-	-	-	-	-			
MW0114253	126125.385	66877.8099	117.026183	149897.673	111274.458	142129.244	22874.575	154448.933	183729.237	200480.113	134360.808	19466.525	C6H12O6	D																													

