

MS search for 80.963292 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34829	Sulfurous acid	M-H	80,9651890	81,9724646	0,001897

MS search for 85.077752 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB14730	Piperazine	M-H	85,0771220	86,0843983	0,00063
HMDB61949	(2-Aziridinyethyl)amine	M-H	85,0771220	86,0843983	0,00063

MS search for 87.008761 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00243	Pyruvic acid	M-H	87,0087680	88,0160440	0,000007
HMDB11111	Malonic semialdehyde	M-H	87,0087680	88,0160440	0,000007
HMDB40261	Glucosereductone	M-H	87,0087680	88,0160440	0,000007

MS search for 87.020427 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB31653	3-(Methylthio)-1-propene	M-H	87,0273950	88,0346709	0,006968
HMDB39807	cis-2,3-Dimethylthiirane	M-H	87,0273950	88,0346709	0,006968
HMDB59843	(1E)-1-(methylthio)prop-1-ene	M-H	87,0273950	88,0346709	0,006968
HMDB61876	(Z)-1-(Methylthio)-1-propene	M-H	87,0273950	88,0346709	0,006968

MS search for 88.040393 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00161	L-Alanine	M-H	88,0404020	89,0476785	0,000009
HMDB61370	L-amino acid	M-H	88,0404020	89,0476785	0,000009
HMDB01310	D-Alanine	M-H	88,0404020	89,0476785	0,000009

HMDB00271	Sarcosine	M-H	88,0404020	89,0476785	0,000009
HMDB31219	Ethyl carbamate	M-H	88,0404020	89,0476785	0,000009
HMDB00056	Beta-Alanine	M-H	88,0404020	89,0476785	0,000009

MS search for 89.024421 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB01882	Dihydroxyacetone	M-H	89,0244180	90,0316941	0,000003
HMDB31232	Monoethyl carbonate	M-H	89,0244180	90,0316941	0,000003
HMDB29580	Dimethyl carbonate	M-H	89,0244180	90,0316941	0,000003
HMDB01051	Glyceraldehyde	M-H	89,0244180	90,0316941	0,000003
HMDB00190	L-Lactic acid	M-H	89,0244180	90,0316941	0,000003
HMDB00700	Hydroxypropionic acid	M-H	89,0244180	90,0316941	0,000003
HMDB01311	D-Lactic acid	M-H	89,0244180	90,0316941	0,000003
HMDB41929	Methoxyacetic acid	M-H	89,0244180	90,0316941	0,000003

MS search for 90.991372 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34232	(Chloromethyl)oxirane	M-H	90,9956160	92,0028925	0,004244
HMDB60456	cis-3-Chloro-2-propene-1-ol	M-H	90,9956160	92,0028925	0,004244
HMDB60514	trans-3-Chloro-2-propene-1-ol	M-H	90,9956160	92,0028925	0,004244

MS search for 91.957133 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB61934	Thiocarbamic acid	M-H	91,9634140	92,9706905	0,006281

MS search for 92.928021 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB31524	Bromomethane	M-H	92,9345370	93,9418127	0,006516

MS search for 94.980606 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB31436	Silicic acid	M-H	94,9806090	95,9878851	0,000003

MS search for 96.969675 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB02142	Phosphoric acid	M-H	96,9696190	97,9768951	0,000056

MS search for 97.00434 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
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HMDB33119	3-Methylthiophene	M-H	97,0117450	98,0190209	0,007405
HMDB33118	2-Methylthiophene	M-H	97,0117450	98,0190209	0,007405

MS search for 98.024735 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB30276	(R)-Dihydromaleimide	M-H	98,0247520	99,0320284	0,000017

MS search for 99.008773 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB32523	Succinic anhydride	M-H	99,0087680	100,016043994	0,000005
HMDB59596	ETF	M-H	99,0063230	100,013599333	0,00245

MS search for 99.019992 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB33565	2,3-Dihydro-5-methylthiophene	M-H	99,0273950	100,034670946	0,007403
HMDB33564	2,3-Dihydro-2-methylthiophene	M-H	99,0273950	100,034670946	0,007403

MS search for 100.0404 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB36458	1-Aminocyclopropanecarboxylic acid	M-H	100,040402	101,047678473	0,000002
HMDB29615	(S)-2-Azetidinecarboxylic acid	M-H	100,040402	101,047678473	0,000002
HMDB29387	L-3-Aminodihydro-2(3H)-furanone	M-H	100,040402	101,047678473	0,000002

MS search for 101.0244 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00060	Acetoacetic acid	M-H	101,024418	102,031694058	0,000018
HMDB31646	Acetic anhydride	M-H	101,024418	102,031694058	0,000018
HMDB03381	4-Hydroxycrotonic acid	M-H	101,024418	102,031694058	0,000018
HMDB02217	(S)-Methylmalonic acid semialdehyde	M-H	101,024418	102,031694058	0,000018

HMDB01259	Succinic acid semialdehyde	M-H	101,024418	102,031694 058	0,000018
HMDB01172	2-Methyl-3-oxopropanoic acid	M-H	101,024418	102,031694 058	0,000018
HMDB00005	2-Ketobutyric acid	M-H	101,024418	102,031694 058	0,000018

MS search for 102.05605 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00092	Dimethylglycine	M-H	102,056053	103,063328 537	0,000003
HMDB41945	N-Ethylglycine	M-H	102,056053	103,063328 537	0,000003
HMDB31654	3-Aminobutanoic acid	M-H	102,056053	103,063328 537	0,000003
HMDB31329	Butyl nitrite	M-H	102,056053	103,063328 537	0,000003
HMDB00112	Gamma-Aminobutyric acid	M-H	102,056053	103,063328 537	0,000003
HMDB01906	2-Aminoisobutyric acid	M-H	102,056053	103,063328 537	0,000003
HMDB00650	D-Alpha-aminobutyric acid	M-H	102,056053	103,063328 537	0,000003
HMDB61050	Unknown	M-H	102,056053	103,063328 537	0,000003
HMDB00452	L-Alpha-aminobutyric acid	M-H	102,056053	103,063328 537	0,000003
HMDB02166	(S)-b-aminoisobutyric acid	M-H	102,056053	103,063328 537	0,000003
HMDB02299	(R)-b-aminoisobutyric acid	M-H	102,056053	103,063328 537	0,000003
HMDB03911	3-Aminoisobutanoic acid	M-H	102,056053	103,063328 537	0,000003
HMDB38394	O-Acetyethanolamine	M-H	102,056053	103,063328 537	0,000003

MS search for 103.04005 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB59748	2-Methyl-3-hydroxypropanoate	M-H	103,040068	104,047344 122	0,000018
HMDB31212	Ethoxyacetic acid	M-H	103,040068	104,047344 122	0,000018
HMDB00729	Alpha-Hydroxyisobutyric acid	M-H	103,040068	104,047344 122	0,000018
HMDB00710	4-Hydroxybutyric acid	M-H	103,040068	104,047344 122	0,000018
HMDB00442	(S)-3-Hydroxybutyric acid	M-H	103,040068	104,047344 122	0,000018
HMDB00008	2-Hydroxybutyric acid	M-H	103,040068	104,047344 122	0,000018

HMDB00011	(R)-3-Hydroxybutyric acid	M-H	103,040068	104,047344 122	0,000018
HMDB00023	(S)-3-Hydroxyisobutyric acid	M-H	103,040068	104,047344 122	0,000018
HMDB00336	(R)-3-Hydroxyisobutyric acid	M-H	103,040068	104,047344 122	0,000018
HMDB00357	3-Hydroxybutyric acid	M-H	103,040068	104,047344 122	0,000018
HMDB62027	3-Cyanopyridine	M-H	103,030172	104,037448 138	0,009878

MS search for 104.03532 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00187	L-Serine	M-H	104,035317	105,042593 095	0,000003
HMDB03406	D-Serine	M-H	104,035317	105,042593 095	0,000003

MS search for 106.02849 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60434	alpha-Fluoro-beta-alanine	M-H	106,030981	107,038256 646	0,002491

MS search for 107.03632 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34260	2,2-Dihydroperoxypropane	M-H	107,034983	108,042258 744	0,001337

MS search for 108.02169 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00965	Hypotaurine	M-H	108,012473	109,019749 163	0,009217

MS search for 110.98526 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB61711	Methylphosphate	M-H	110,985269	111,992545 16	0,000009
HMDB29717	2-Thiophenecarboxaldehyde	M-H	110,991009	111,998285 44	0,005749

MS search for 112.05163 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
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HMDB00562	Creatinine	M-H	112,051636	113,058911 861	0,000006
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MS search for 113.03564 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60245	L-3-Cyanoalanine	M-H	113,035651	114,042927 446	0,000011
HMDB03646	N-Methylhydantoin	M-H	113,035651	114,042927 446	0,000011
HMDB00076	Dihydrouracil	M-H	113,035651	114,042927 446	0,000011
HMDB40234	Di-1-propenyl sulfide	M-H	113,043045	114,050321 01	0,007405
HMDB36491	Di-2-propenyl sulfide	M-H	113,043045	114,050321 01	0,007405
HMDB31859	Norfuraneol	M-H	113,024418	114,031694 058	0,011222
HMDB60461	cis-Acetylacrylate	M-H	113,024418	114,031694 058	0,011222

MS search for 117.02067 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00254	Succinic acid	M-H	117,019333	118,026608 68	0,001337
HMDB31204	4-Hydroxy-2-oxobutanoic acid	M-H	117,019333	118,026608 68	0,001337
HMDB39324	xi-3-Hydroxy-2-oxobutanoic acid	M-H	117,019333	118,026608 68	0,001337
HMDB00202	Methylmalonic acid	M-H	117,019333	118,026608 68	0,001337
HMDB00940	Threonolactone	M-H	117,019333	118,026608 68	0,001337
HMDB00349	Erythrono-1,4-lactone	M-H	117,019333	118,026608 68	0,001337

MS search for 118.05096 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00167	L-Threonine	M-H	118,050967	119,058243 159	0,000007
HMDB61148	Hydroxyethyl glycine	M-H	118,050967	119,058243 159	0,000007

HMDB61877	4-Amino-3-hydroxybutyrate	M-H	118,050967	119,058243 159	0,000007
HMDB00719	L-Homoserine	M-H	118,050967	119,058243 159	0,000007
HMDB04041	L-Allothreonine	M-H	118,050967	119,058243 159	0,000007

MS search for 122.98525 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB15677	Dimercaprol	M-H	122,99438	124,001656 258	0,00913

MS search for 124.00737 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00251	Taurine	M-H	124,007388	125,014663 785	0,000018
HMDB11747	Ciliatine	M-H	124,016904	125,024179 639	0,009534

MS search for 125.02442 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB13675	1,3,5-Trihydroxybenzene	M-H	125,024418	126,031694 058	0,000002
HMDB59735	5-Methylfuran-2-carboxylic acid	M-H	125,024418	126,031694 058	0,000002
HMDB34355	5-Hydroxymethyl-2-furancarboxaldehyde	M-H	125,024418	126,031694 058	0,000002
HMDB32651	(Z)-Tamarindial	M-H	125,024418	126,031694 058	0,000002
HMDB31256	4-Hydroxy-2H-pyran-3-carboxaldehyde	M-H	125,024418	126,031694 058	0,000002
HMDB29750	Methyl 2-furoate	M-H	125,024418	126,031694 058	0,000002
HMDB30776	Maltol	M-H	125,024418	126,031694 058	0,000002
HMDB13674	1,2,3-Trihydroxybenzene	M-H	125,024418	126,031694 058	0,000002
HMDB36186	Pyrazinemethanethiol	M-H	125,017893	126,025168 892	0,006527
HMDB33152	2-(Methylthio)pyrazine	M-H	125,017893	126,025168 892	0,006527
HMDB59882	Benzyl chloride	M-H	125,016352	126,023627 931	0,008068
HMDB02024	Imidazoleacetic acid	M-H	125,035651	126,042927 446	0,011231
HMDB60261	Imidazol-4-ylacetate	M-H	125,035651	126,042927 446	0,011231
HMDB00262	Thymine	M-H	125,035651	126,042927 446	0,011231

HMDB29736	1H-Imidazole-1-acetic acid	M-H	125,035651	126,042927 446	0,011231
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MS search for 127.05131 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00079	Dihydrothymine	M-H	127,051302	128,058577 51	0,000008
HMDB31547	L-Cyclo(alanylglycyl)	M-H	127,051302	128,058577 51	0,000008
HMDB29874	Squamolone	M-H	127,051302	128,058577 51	0,000008
HMDB29751	Naphthalene	M-H	127,055324	128,062600 256	0,004014
HMDB31303	Osmundalactone	M-H	127,040068	128,047344 122	0,011242
HMDB38072	xi-5-Acetyltetrahydro-2(3H)-furanone	M-H	127,040068	128,047344 122	0,011242
HMDB33285	L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone	M-H	127,040068	128,047344 122	0,011242
HMDB40594	(±)-Furaneol	M-H	127,040068	128,047344 122	0,011242
HMDB31306	3-Hydroxy-4,5-dimethyl-2(5H)-furanone	M-H	127,040068	128,047344 122	0,011242
HMDB31847	2-Ethyl-3,4-dihydroxyfuran	M-H	127,040068	128,047344 122	0,011242
HMDB40732	2,7-Oxepanedione	M-H	127,040068	128,047344 122	0,011242
HMDB62047	3,4-Dimethyldihydrofuran-2,5-dione	M-H	127,040068	128,047344 118	0,011242
HMDB33517	5,6-Dihydro-4-methoxy-2H-pyran-2-one	M-H	127,040068	128,047344 122	0,011242

MS search for 128.0353 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB61093	dimethadione	M-H	128,035317	129,042593 095	0,000017
HMDB02234	1-Pyrroline-4-hydroxy-2-carboxylate	M-H	128,035317	129,042593 095	0,000017
HMDB01843	N-Acryloylglycine	M-H	128,035317	129,042593 095	0,000017
HMDB01369	Pyrroline hydroxycarboxylic acid	M-H	128,035317	129,042593 095	0,000017
HMDB00267	Pyroglutamic acid	M-H	128,035317	129,042593 095	0,000017
HMDB00805	Pyrrolidonecarboxylic acid	M-H	128,035317	129,042593 095	0,000017
HMDB60262	5-Oxoprolinate	M-H	128,035317	129,042593 095	0,000017

HMDB15231	Flucytosine	M-H	128,026564	129,033839 97	0,008736
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MS search for 129.01933 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60365	2,5-Dioxopentanoate	M-H	129,019333	130,026608 68	0,000003
HMDB13233	Gamma-delta-Dioxovaleric acid	M-H	129,019333	130,026608 68	0,000003
HMDB33809	Methyl hydrogen fumarate	M-H	129,019333	130,026608 68	0,000003
HMDB02092	Itaconic acid	M-H	129,019333	130,026608 68	0,000003
HMDB00749	Mesaconic acid	M-H	129,019333	130,026608 68	0,000003
HMDB00620	Glutaconic acid	M-H	129,019333	130,026608 68	0,000003
HMDB61185	2-Pentendioate	M-H	129,019333	130,026608 68	0,000003
HMDB00634	Citraconic acid	M-H	129,019333	130,026608 68	0,000003
HMDB59743	2-Hydroxyglutaric acid lactone	M-H	129,019333	130,026608 68	0,000003
HMDB14684	Fluorouracil	M-H	129,01058	130,017855 555	0,00875

MS search for 130.0622 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00064	Creatine	M-H	130,062201	131,069476 547	0,000001
HMDB13222	Beta-Guanidinopropionic acid	M-H	130,062201	131,069476 547	0,000001
HMDB62060	4-Methylindole	M-H	130,066223	131,073499 294	0,004023
HMDB34236	Benzenepropanenitrile	M-H	130,066223	131,073499 293	0,004023
HMDB00466	3-Methylindole	M-H	130,066223	131,073499 293	0,004023
HMDB40058	(±)-2-Propylthiazolidine	M-H	130,069594	131,076870 111	0,007394
HMDB02104	L-Glutamic gamma-semialdehyde	M-H	130,050967	131,058243 159	0,011233
HMDB00725	4-Hydroxyproline	M-H	130,050967	131,058243 159	0,011233
HMDB00766	N-Acetyl-L-alanine	M-H	130,050967	131,058243 159	0,011233
HMDB00783	Propionylglycine	M-H	130,050967	131,058243 159	0,011233

HMDB01149	5-Aminolevulinic acid	M-H	130,050967	131,058243 159	0,011233
HMDB02113	3-Hydroxy-L-proline	M-H	130,050967	131,058243 159	0,011233
HMDB59659	Trans-3-hydroxy-L-proline	M-H	130,050967	131,058243 159	0,011233
HMDB60460	cis-4-Hydroxy-D-proline	M-H	130,050967	131,058243 159	0,011233
HMDB36576	4-Hydroxy-2-pyrrolidinecarboxylic acid	M-H	130,050967	131,058243 159	0,011233
HMDB06272	5-Amino-2-oxopentanoic acid	M-H	130,050967	131,058243 159	0,011233
HMDB61880	N-Acetyl-beta-alanine	M-H	130,050967	131,058243 159	0,011233
HMDB06055	4-Hydroxy-L-proline	M-H	130,050967	131,058243 159	0,011233

MS search for 131.02373 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34799	Diammonium hydrogen phosphate ((NH ₄) ₂ HPO ₄)	M-H	131,022717	132,029993 298	0,001013
HMDB60402	5,6-Dihydro-5-fluorouracil	M-H	131,02623	132,033505 619	0,0025
HMDB59667	3-Methyl sulfolene	M-H	131,017224	132,024500 19	0,006506
HMDB30967	2,4,6-Octatriynoic acid	M-H	131,013853	132,021129 372	0,009877
HMDB37237	Ammonium sulfate	M-H	131,013201	132,020477 444	0,010529
HMDB06855	(S)-2-Acetolactate	M-H	131,034983	132,042258 744	0,011253
HMDB61879	(S)-Methylbutanethioic acid	M-H	131,034983	132,042258 744	0,011253
HMDB00661	Glutaric acid	M-H	131,034983	132,042258 744	0,011253
HMDB00576	Monoethyl malonic acid	M-H	131,034983	132,042258 744	0,011253
HMDB00622	Ethylmalonic acid	M-H	131,034983	132,042258 744	0,011253
HMDB29884	2-C-Methyl-1,4-erythrono-D-lactone	M-H	131,034983	132,042258 744	0,011253
HMDB33958	2-Deoxy-L-ribo-1,4-lactone	M-H	131,034983	132,042258 744	0,011253
HMDB40531	2-Hydroxy-4-oxopentanoic acid	M-H	131,034983	132,042258 744	0,011253
HMDB06833	2-Acetolactate	M-H	131,034983	132,042258 744	0,011253
HMDB02001	Dimethylmalonic acid	M-H	131,034983	132,042258 744	0,011253

HMDB01844	Methylsuccinic acid	M-H	131,034983	132,042258 744	0,011253
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MS search for 132.03156 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00191	L-Aspartic acid	M-H	132,030232	133,037507 717	0,001328
HMDB11753	Iminodiacetic acid	M-H	132,030232	133,037507 717	0,001328
HMDB06483	D-Aspartic acid	M-H	132,030232	133,037507 717	0,001328

MS search for 133.0394 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB32409	Methyl 3-mercaptoputanoate	M-H	133,032874	134,040150 254	0,006526
HMDB40263	Ethyl 2-(methylthio)acetate	M-H	133,032874	134,040150 254	0,006526
HMDB31521	Ethyl 2-mercaptopropionate	M-H	133,032874	134,040150 254	0,006526
HMDB34377	Methyl 3-(methylthio)propanoate	M-H	133,032874	134,040150 254	0,006526
HMDB40410	Ethyl 3-mercaptopropanoic acid	M-H	133,032874	134,040150 254	0,006526
HMDB62159	Terephthalaldehydefrom	M-H	133,029503	134,036779 433	0,009897
HMDB61916	Phenylglyoxal	M-H	133,029503	134,036779 436	0,009897
HMDB32469	Phthalide	M-H	133,029503	134,036779 436	0,009897
HMDB12141	(R)-2,3-Dihydroxy-isovalerate	M-H	133,050633	134,057908 808	0,011233
HMDB00421	2,3-Dihydroxyvaleric acid	M-H	133,050633	134,057908 808	0,011233
HMDB01292	1-Deoxy-D-xylulose	M-H	133,050633	134,057908 808	0,011233
HMDB03224	Deoxyribose	M-H	133,050633	134,057908 808	0,011233
HMDB29576	2,3-Dihydroxy-2-methylbutanoic acid	M-H	133,050633	134,057908 808	0,011233
HMDB12485	(R)-glycerol 1-acetate	M-H	133,050633	134,057908 808	0,011233
HMDB01441	Dihydropteridine	M-H	133,05197	134,059246 212	0,01257

MS search for 134.03598 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
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HMDB02108	Methylcysteine	M-H	134,028123	135,035399 227	0,007857
HMDB00742	Homocysteine	M-H	134,028123	135,035399 227	0,007857
HMDB29389	(+)-threo-2-Amino-3,4-dihydroxybutanoic acid	M-H	134,045882	135,053157 781	0,009902
HMDB32931	2-Benzoxazolol	M-H	134,024752	135,032028 409	0,011228
HMDB00034	Adenine	M-H	134,047219	135,054495 185	0,011239
HMDB32593	4-(Hydroxymethyl)benzene diazonium(1+)	M-H	134,048562	135,055837 856	0,012582

MS search for 135.02988 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00613	Erythronic acid	M-H	135,029897	136,037173 366	0,000017
HMDB00943	Threonic acid	M-H	135,029897	136,037173 366	0,000017
HMDB33054	Ethyl isopropyl disulfide	M-H	135,030766	136,038041 764	0,000886
HMDB31160	1-Pentanesulfenothioic acid	M-H	135,030766	136,038041 764	0,000886
HMDB33053	Ethyl propyl disulfide	M-H	135,030766	136,038041 764	0,000886
HMDB14581	Allopurinol	M-H	135,031235	136,038510 77	0,001355
HMDB00157	Hypoxanthine	M-H	135,031235	136,038510 77	0,001355
HMDB31825	Phenyl vinyl sulfide	M-H	135,027395	136,034670 946	0,002485

MS search for 135.03124 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB14581	Allopurinol	M-H	135,031235	136,038510 77	0,000005
HMDB00157	Hypoxanthine	M-H	135,031235	136,038510 77	0,000005
HMDB31160	1-Pentanesulfenothioic acid	M-H	135,030766	136,038041 764	0,000474
HMDB33054	Ethyl isopropyl disulfide	M-H	135,030766	136,038041 764	0,000474
HMDB33053	Ethyl propyl disulfide	M-H	135,030766	136,038041 764	0,000474
HMDB00943	Threonic acid	M-H	135,029897	136,037173 366	0,001343
HMDB00613	Erythronic acid	M-H	135,029897	136,037173 366	0,001343

HMDB31825	Phenyl vinyl sulfide	M-H	135,027395	136,034670 946	0,003845
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MS search for 137.00091 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB14966	Fosfomycin	M-H	137,000919	138,008195 224	0,000009

MS search for 138.05608 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB12153	3,4-Dihydroxybenzylamine	M-H	138,056053	139,063328 537	0,000027
HMDB38174	5-Acetyl-2,4-dimethyloxazole	M-H	138,056053	139,063328 537	0,000027
HMDB33388	Ammonium benzoate	M-H	138,056053	139,063328 537	0,000027
HMDB59856	Ethyl 2-pyrrolicarboxylate	M-H	138,056053	139,063328 537	0,000027
HMDB12234	Histidinal	M-H	138,067286	139,074561 925	0,011206
HMDB29558	Choline chloride	M-H	138,069116	139,076391 782	0,013036

MS search for 139.0513 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB04988	Pi-Methylimidazoleacetic acid	M-H	139,051302	140,058577 51	0,000002
HMDB02820	Methylimidazoleacetic acid	M-H	139,051302	140,058577 51	0,000002
HMDB02271	Imidazolepropionic acid	M-H	139,051302	140,058577 51	0,000002
HMDB02144	1,3-Dimethyluracil	M-H	139,051302	140,058577 51	0,000002
HMDB32948	5-Phenyl-1,3-pentadiyne	M-H	139,055324	140,062600 256	0,004024

MS search for 140.01181 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00224	O-Phosphoethanolamine	M-H	140,011818	141,019094 261	0,000008
HMDB60151	O-Phosphonatoethanaminium	M-H	140,011818	141,019094 261	0,000008

HMDB60152	Ethamp	M-H	140,011818	141,019094 261	0,000008
HMDB29188	5-Hydroxymethyl-2-furanoate	M-H	140,011508	141,018783 648	0,000302
HMDB37168	2-Propanoylthiazole	M-H	140,017559	141,024834 541	0,005749
HMDB60688	Nornitrogen mustard	M-H	140,003929	141,011204 707	0,007881

MS search for 141.06695 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB62000	2-Methylnaphthalene	M-H	141,070974	142,078250 32	0,004024
HMDB32860	1-Methylnaphthalene	M-H	141,070974	142,078250 32	0,004024
HMDB34230	Mesifurane	M-H	141,055718	142,062994 186	0,011232
HMDB33551	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	M-H	141,055718	142,062994 186	0,011232
HMDB41427	Erinapyrone B	M-H	141,055718	142,062994 186	0,011232
HMDB41426	Erinapyrone A	M-H	141,055718	142,062994 186	0,011232
HMDB33736	Homofureanol	M-H	141,055718	142,062994 186	0,011232

MS search for 144.04549 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB29737	1H-Indole-3-carboxaldehyde	M-H	144,045488	145,052763 851	0,000002

MS search for 145.04418 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB06900	(S)-2-Aceto-2-hydroxybutanoic acid	M-H	145,050633	146,057908 808	0,006453
HMDB02173	Solerol	M-H	145,050633	146,057908 808	0,006453
HMDB00858	Monomethyl glutaric acid	M-H	145,050633	146,057908 808	0,006453
HMDB00752	Methylglutaric acid	M-H	145,050633	146,057908 808	0,006453
HMDB00448	Adipic acid	M-H	145,050633	146,057908 808	0,006453
HMDB00422	2-Methylglutaric acid	M-H	145,050633	146,057908 808	0,006453

HMDB33837	Dimethyl succinate	M-H	145,050633	146,057908 808	0,006453
HMDB02074	2,2-Dimethylsuccinic acid	M-H	145,050633	146,057908 808	0,006453
HMDB61930	4-Ethoxy-4-oxobutanoic acid	M-H	145,050633	146,057908 808	0,006453

MS search for 145.06186 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB06899	Alanylglycine	M-H	145,061866	146,069142 196	0,000006
HMDB28687	Alanyl-Glycine	M-H	145,061866	146,069142 196	0,000006
HMDB00641	L-Glutamine	M-H	145,061866	146,069142 196	0,000006
HMDB03423	D-Glutamine	M-H	145,061866	146,069142 196	0,000006
HMDB02031	Ureidoisobutyric acid	M-H	145,061866	146,069142 196	0,000006
HMDB29640	3-(4-Methylphenyl)-2-propenal	M-H	145,065889	146,073164 942	0,004029
HMDB31617	Benzylideneacetone	M-H	145,065889	146,073164 942	0,004029
HMDB33176	2,3-Dimethylbenzofuran	M-H	145,065889	146,073164 942	0,004029
HMDB31619	2-Phenyl-2-butenal	M-H	145,065889	146,073164 942	0,004029
HMDB29602	4-Phenyl-2-butenal	M-H	145,065889	146,073164 942	0,004029
HMDB31566	2-Methyl-3-phenyl-2-propenal	M-H	145,065889	146,073164 942	0,004029
HMDB35925	4-(1-Methylethenyl)benzaldehyde	M-H	145,065889	146,073164 942	0,004029
HMDB59897	Benzofuran, 4,7-dimethyl-	M-H	145,065889	146,073164 942	0,004029
HMDB39465	S-Methyl hexanethioate	M-H	145,06926	146,076535 76	0,0074
HMDB39468	S-Methyl 4-methylpentanethioate	M-H	145,06926	146,076535 76	0,0074
HMDB37621	4-Methyl-4-(methylthio)-2-pentanone	M-H	145,06926	146,076535 76	0,0074
HMDB40186	3-(Methylthio)hexanal	M-H	145,06926	146,076535 76	0,0074
HMDB06900	(S)-2-Aceto-2-hydroxybutanoic acid	M-H	145,050633	146,057908 808	0,011227
HMDB02173	Solerol	M-H	145,050633	146,057908 808	0,011227
HMDB02074	2,2-Dimethylsuccinic acid	M-H	145,050633	146,057908 808	0,011227

HMDB00422	2-Methylglutaric acid	M-H	145,050633	146,057908 808	0,011227
HMDB00448	Adipic acid	M-H	145,050633	146,057908 808	0,011227
HMDB00752	Methylglutaric acid	M-H	145,050633	146,057908 808	0,011227
HMDB00858	Monomethyl glutaric acid	M-H	145,050633	146,057908 808	0,011227
HMDB33837	Dimethyl succinate	M-H	145,050633	146,057908 808	0,011227
HMDB61930	4-Ethoxy-4-oxobutanoic acid	M-H	145,050633	146,057908 808	0,011227

MS search for 146.04588 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00148	L-Glutamic acid	M-H	146,045882	147,053157 781	0,000002
HMDB33550	3-(Carboxymethylamino)propanoic acid	M-H	146,045882	147,053157 781	0,000002
HMDB02931	N-Acetylserine	M-H	146,045882	147,053157 781	0,000002
HMDB02393	N-Methyl-D-aspartic acid	M-H	146,045882	147,053157 781	0,000002
HMDB03011	O-Acetylserine	M-H	146,045882	147,053157 781	0,000002
HMDB03339	D-Glutamic acid	M-H	146,045882	147,053157 781	0,000002
HMDB06556	L-4-Hydroxyglutamate semialdehyde	M-H	146,045882	147,053157 781	0,000002
HMDB60475	DL-Glutamate	M-H	146,045882	147,053157 781	0,000002

MS search for 147.02989 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00428	3-Hydroxyglutaric acid	M-H	147,029897	148,037173 366	0,000007
HMDB00426	Citramalic acid	M-H	147,029897	148,037173 366	0,000007
HMDB00606	D-2-Hydroxyglutaric acid	M-H	147,029897	148,037173 366	0,000007
HMDB00694	L-2-Hydroxyglutaric acid	M-H	147,029897	148,037173 366	0,000007
HMDB01900	Ribonolactone	M-H	147,029897	148,037173 366	0,000007
HMDB11676	D-Xylono-1,5-lactone	M-H	147,029897	148,037173 366	0,000007
HMDB59655	2-Hydroxyglutarate	M-H	147,029897	148,037173 366	0,000007

HMDB61190	3-Methylmalic acid	M-H	147,029897	148,037173 366	0,000007
HMDB38890	Methyl 3-methyl-1-butenyl disulfide	M-H	147,030766	148,038041 764	0,000876
HMDB41392	1-Propenyl propyl disulfide	M-H	147,030766	148,038041 764	0,000876
HMDB33912	2-Propenyl propyl disulfide	M-H	147,030766	148,038041 764	0,000876

MS search for 156.93635 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB32554	Vinyl chloride-vinylidene chloride copolymer	M-H	156,938407	157,945683 281	0,002057
HMDB41065	Dimethyl tetrasulfide	M-H	156,927957	157,935232 952	0,008393

MS search for 163.0166 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB32749	R-Propyl 1-propenesulfinothioate	M-H	163,02568	164,032956 386	0,00908
HMDB39965	S-Propyl 2-propene-1-sulfinothioate	M-H	163,02568	164,032956 386	0,00908
HMDB32748	R-1-Propenyl 1-propanesulfinothioate	M-H	163,02568	164,032956 386	0,00908
HMDB32741	S-2-Propenyl 1-propanesulfinothioate	M-H	163,02568	164,032956 386	0,00908
HMDB61917	Terephthalate	M-H	163,00478	164,012055 776	0,01182

MS search for 165.04048 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB59750	2,3,4,5-Tetrahydroxypentanoic acid	M-H	165,040462	166,047738 052	0,000018
HMDB60255	L-Lyxonate	M-H	165,040462	166,047738 052	0,000018
HMDB00867	Ribonic acid	M-H	165,040462	166,047738 052	0,000018
HMDB00539	Arabinonic acid	M-H	165,040462	166,047738 052	0,000018
HMDB60256	L-Xylonate	M-H	165,040462	166,047738 052	0,000018
HMDB34394	S-Propyl 1-propanesulfinothioate	M-H	165,04133	166,048606 45	0,00085
HMDB59716	9-Methylxanthine	M-H	165,041799	166,049075 456	0,001319
HMDB10738	1-Methylxanthine	M-H	165,041799	166,049075 456	0,001319

HMDB01991	7-Methylxanthine	M-H	165,041799	166,049075 456	0,001319
HMDB01886	3-Methylxanthine	M-H	165,041799	166,049075 456	0,001319
HMDB62154	S-Methyl phenylethanethioate	M-H	165,03796	166,045236 116	0,00252
HMDB13029	Noradrenochrome o- semiquinone	M-H	165,043142	166,050418 127	0,002662
HMDB14747	Ethionamide	M-H	165,049193	166,056469 02	0,008713
HMDB02199	Desaminotyrosine	M-H	165,055718	166,062994 186	0,015238
HMDB32030	Guaicyl acetate	M-H	165,055718	166,062994 186	0,015238
HMDB40645	3-Hydroxy-1-(4- hydroxyphenyl)-1- propanone	M-H	165,055718	166,062994 186	0,015238
HMDB34243	Ipomeanine	M-H	165,055718	166,062994 186	0,015238
HMDB33752	3-(2- Hydroxyphenyl)propanoi c acid	M-H	165,055718	166,062994 186	0,015238
HMDB32605	Methyl 2- methoxybenzoate	M-H	165,055718	166,062994 186	0,015238
HMDB32573	Ethylparaben	M-H	165,055718	166,062994 186	0,015238
HMDB32639	Methyl 4- methoxybenzoate	M-H	165,055718	166,062994 186	0,015238
HMDB31132	3,4- Dihydroxyphenylacetone	M-H	165,055718	166,062994 186	0,015238
HMDB32138	3,4- Dimethoxybenzaldehyde	M-H	165,055718	166,062994 186	0,015238
HMDB29665	Ethyl vanillin	M-H	165,055718	166,062994 186	0,015238
HMDB34993	4-Methoxybenzyl formate	M-H	165,055718	166,062994 186	0,015238
HMDB00375	3-(3- Hydroxyphenyl)propanoi c acid	M-H	165,055718	166,062994 186	0,015238
HMDB00748	L-3-Phenyllactic acid	M-H	165,055718	166,062994 186	0,015238
HMDB00779	Phenyllactic acid	M-H	165,055718	166,062994 186	0,015238
HMDB02072	4-Methoxyphenylacetic acid	M-H	165,055718	166,062994 186	0,015238
HMDB02229	3-Phenoxypropionic acid	M-H	165,055718	166,062994 186	0,015238
HMDB05175	Homovanillin	M-H	165,055718	166,062994 186	0,015238

HMDB29817	Ethyl salicylate	M-H	165,055718	166,062994 186	0,015238
HMDB00563	D-Phenyllactic acid	M-H	165,055718	166,062994 186	0,015238
HMDB62026	2'-Hydroxy-6'-methoxyacetophenone	M-H	165,055718	166,062994 182	0,015238
HMDB41683	4-Hydroxyphenyl-2-propionic acid	M-H	165,055718	166,062994 186	0,015238
HMDB59969	3-Methoxyphenylacetic acid	M-H	165,055718	166,062994 186	0,015238
HMDB60412	6-Methylmercaptopurine	M-H	165,024041	166,031316 902	0,016439

MS search for 165.06694 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34294	1,3,11-Tridecatriene-5,7,9-triyn	M-H	165,070974	166,078250 32	0,004034
HMDB39104	(3E,5Z)-1,3,5-Tridecatriene-7,9,11-triyn	M-H	165,070974	166,078250 32	0,004034
HMDB38183	3-(4-Methyl-3-pentenyl)thiophene	M-H	165,074345	166,081621 138	0,007405
HMDB41500	1-Deoxy-D-glucitol	M-H	165,076848	166,084123 558	0,009908
HMDB00563	D-Phenyllactic acid	M-H	165,055718	166,062994 186	0,011222
HMDB32030	Guaicyl acetate	M-H	165,055718	166,062994 186	0,011222
HMDB40645	3-Hydroxy-1-(4-hydroxyphenyl)-1-propanone	M-H	165,055718	166,062994 186	0,011222
HMDB34243	Ipomeanine	M-H	165,055718	166,062994 186	0,011222
HMDB33752	3-(2-Hydroxyphenyl)propanoic acid	M-H	165,055718	166,062994 186	0,011222
HMDB32605	Methyl 2-methoxybenzoate	M-H	165,055718	166,062994 186	0,011222
HMDB32573	Ethylparaben	M-H	165,055718	166,062994 186	0,011222
HMDB32639	Methyl 4-methoxybenzoate	M-H	165,055718	166,062994 186	0,011222
HMDB31132	3,4-Dihydroxyphenylacetone	M-H	165,055718	166,062994 186	0,011222
HMDB32138	3,4-Dimethoxybenzaldehyde	M-H	165,055718	166,062994 186	0,011222
HMDB29665	Ethyl vanillin	M-H	165,055718	166,062994 186	0,011222

HMDB34993	4-Methoxybenzyl formate	M-H	165,055718	166,062994 186	0,011222
HMDB02199	Desaminotyrosine	M-H	165,055718	166,062994 186	0,011222
HMDB00375	3-(3-Hydroxyphenyl)propanoic acid	M-H	165,055718	166,062994 186	0,011222
HMDB00748	L-3-Phenyllactic acid	M-H	165,055718	166,062994 186	0,011222
HMDB00779	Phenyllactic acid	M-H	165,055718	166,062994 186	0,011222
HMDB02072	4-Methoxyphenylacetic acid	M-H	165,055718	166,062994 186	0,011222
HMDB02229	3-Phenoxypropionic acid	M-H	165,055718	166,062994 186	0,011222
HMDB05175	Homovanillin	M-H	165,055718	166,062994 186	0,011222
HMDB29817	Ethyl salicylate	M-H	165,055718	166,062994 186	0,011222
HMDB41683	4-Hydroxyphenyl-2-propionic acid	M-H	165,055718	166,062994 186	0,011222
HMDB59969	3-Methoxyphenylacetic acid	M-H	165,055718	166,062994 186	0,011222
HMDB62026	2'-Hydroxy-6'-methoxyacetophenone	M-H	165,055718	166,062994 182	0,011222

MS search for 166.08734 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB02182	Phenylephrine	M-H	166,087353	167,094628 665	0,000013
HMDB60807	a-Methyldopamine	M-H	166,087353	167,094628 665	0,000013
HMDB60592	4-Hydroxynorephedrine	M-H	166,087353	167,094628 665	0,000013
HMDB32020	4-(beta-Methylaminoethyl)catechol	M-H	166,087353	167,094628 665	0,000013
HMDB41888	Epinine	M-H	166,087353	167,094628 665	0,000013
HMDB14748	Metaraminol	M-H	166,087353	167,094628 665	0,000013
HMDB15165	Ethinamate	M-H	166,087353	167,094628 665	0,000013
HMDB00022	3-Methoxytyramine	M-H	166,087353	167,094628 665	0,000013
HMDB04826	p-Synephrine	M-H	166,087353	167,094628 665	0,000013
HMDB12162	4-Methoxytyramine	M-H	166,087353	167,094628 665	0,000013
HMDB38869	Norpandamarilactonine A	M-H	166,087353	167,094628 665	0,000013

HMDB39837	2-(2-Furanyl)-3-piperidinol	M-H	166,087353	167,094628 665	0,000013
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MS search for 167.08262 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB01431	Pyridoxamine	M-H	167,082602	168,089877 638	0,000018
HMDB38754	(E,E,E)-1,3,5,11-Tridecatetraene-7,9-diyne	M-H	167,086624	168,093900 384	0,004004
HMDB30929	2,4,6,8-Tridecatetrayne	M-H	167,086624	168,093900 384	0,004004
HMDB32610	4-Methylbiphenyl	M-H	167,086624	168,093900 384	0,004004
HMDB32329	2-Hexylthiophene	M-H	167,089995	168,097271 202	0,007375
HMDB59963	1,3,5-Trimethoxybenzene	M-H	167,071368	168,078644 25	0,011252
HMDB32252	Epoxyoxophorone	M-H	167,071368	168,078644 25	0,011252
HMDB30473	1-Ipomeanol	M-H	167,071368	168,078644 25	0,011252
HMDB38925	(4-Hydroxy-3-methoxyphenyl)ethanol	M-H	167,071368	168,078644 25	0,011252
HMDB30472	4-Ipomeanol	M-H	167,071368	168,078644 25	0,011252
HMDB29680	2,6-Dimethoxy-4-methylphenol	M-H	167,071368	168,078644 25	0,011252
HMDB37729	2-Furanylmethyl butanoate	M-H	167,071368	168,078644 25	0,011252
HMDB32921	Ethyl 2-furanpropionate	M-H	167,071368	168,078644 25	0,011252

MS search for 168.02778 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00439	2-Furoylglycine	M-H	168,030232	169,037507 717	0,002452
HMDB12247	L-2,3-Dihydrodipicolinate	M-H	168,030232	169,037507 717	0,002452
HMDB60244	Phosphodimethylethanol amine	M-H	168,043118	169,050394 389	0,015338

MS search for 168.04312 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60244	Phosphodimethylethanol amine	M-H	168,043118	169,050394 389	0,000002
HMDB12247	L-2,3-Dihydrodipicolinate	M-H	168,030232	169,037507 717	0,012888

HMDB00439	2-Furoylglycine	M-H	168,030232	169,037507 717	0,012888
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MS search for 168.99071 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB01112	D-Glyceraldehyde 3-phosphate	M-H	168,990748	169,998024 468	0,000038
HMDB01473	Dihydroxyacetone phosphate	M-H	168,990748	169,998024 468	0,000038
HMDB60176	(S)-3-Sulfonatolactate	M-H	168,981233	169,988508 614	0,009477

MS search for 169.01186 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB05807	Gallic acid	M-H	169,014247	170,021523 293	0,002387
HMDB29649	2,4,6-Trihydroxybenzoic acid	M-H	169,014247	170,021523 302	0,002387
HMDB59964	2,3,4-Trihydroxybenzoic acid	M-H	169,014247	170,021523 302	0,002387
HMDB01460	Diethylthiophosphate	M-H	169,009375	170,016651 42	0,002485
HMDB40590	Benzyl methyl disulfide	M-H	169,015116	170,022391 7	0,003256

MS search for 169.06188 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34446	Diphenyl ether	M-H	169,065889	170,073164 942	0,004009
HMDB32412	Methyl beta-naphthyl ketone	M-H	169,065889	170,073164 942	0,004009
HMDB32582	2-Biphenylol	M-H	169,065889	170,073164 942	0,004009
HMDB00318	3,4-Dihydroxyphenylglycol	M-H	169,050633	170,057908 808	0,011247
HMDB38761	Herierin IV	M-H	169,050633	170,057908 808	0,011247
HMDB38760	Herierin III	M-H	169,050633	170,057908 808	0,011247
HMDB59756	3,4-Methyleneadipic acid	M-H	169,050633	170,057908 808	0,011247

HMDB32966	Furaneol acetate	M-H	169,050633	170,057908 808	0,011247
HMDB29747	2-Amino-5-phenylpyridine	M-H	169,077122	170,084398 33	0,015242

MS search for 169.09826 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB15333	Levetiracetam	M-H	169,098252	170,105527 702	0,000008
HMDB33926	(3xi,6xi)-Cyclo(alanylvalyl)	M-H	169,098252	170,105527 702	0,000008
HMDB59701	1,6,7-Trimethylnaphthalene	M-H	169,102274	170,109550 448	0,004014
HMDB59733	1,4,5-Trimethylnaphtalene	M-H	169,102274	170,109550 448	0,004014
HMDB36106	Thiogeraniol	M-H	169,105645	170,112921 266	0,007385
HMDB32251	(+/-)-2,8-Epithio-cis-p-menthane	M-H	169,105645	170,112921 266	0,007385
HMDB32377	2,3 or 10-Mercaptopinane	M-H	169,105645	170,112921 266	0,007385
HMDB38192	p-Menth-3-ene-3-thiol	M-H	169,105645	170,112921 266	0,007385
HMDB35703	p-Menth-1-ene-8-thiol	M-H	169,105645	170,112921 266	0,007385
HMDB38276	cis-3-Hexenyl pyruvate	M-H	169,087018	170,094294 314	0,011242
HMDB30471	1,4-Ipomeadiol	M-H	169,087018	170,094294 314	0,011242

MS search for 170.05713 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB15052	Metronidazole	M-H	170,057115	171,064391 169	0,000015
HMDB12289	Tetrahydrodipicolinate	M-H	170,045882	171,053157 781	0,011248

MS search for 171.00639 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB02520	Beta-Glycerophosphoric acid	M-H	171,006399	172,013674 532	0,000009
HMDB00126	Glycerol 3-phosphate	M-H	171,006399	172,013674 532	0,000009

HMDB59933	p-Toluenesulfonic acid	M-H	171,012139	172,019414 812	0,005749
HMDB31868	Monomethyl phenylphosphonate	M-H	171,021655	172,028930 666	0,015265
HMDB14404	Sulfanilamide	M-H	171,023372	172,030648 2	0,016982

MS search for 171.0775 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB00721	Glycylproline	M-H	171,077516	172,084792 26	0,000016
HMDB11178	L-prolyl-L-glycine	M-H	171,077516	172,084792 26	0,000016
HMDB31621	Cinnamylideneacetone	M-H	171,081539	172,088815 006	0,004039
HMDB29688	2-Ethoxynaphthalene	M-H	171,081539	172,088815 006	0,004039
HMDB31699	S-(3-Methyl-2-butenyl) 2-methylpropanethioate	M-H	171,08491	172,092185 824	0,00741
HMDB39467	Allyl thiohexanoate	M-H	171,08491	172,092185 824	0,00741
HMDB13312	trans-3-Octenedioic acid	M-H	171,066283	172,073558 872	0,011217
HMDB32352	3-Isopropenylpentanedioic acid	M-H	171,066283	172,073558 872	0,011217
HMDB38601	Diethyl fumarate	M-H	171,066283	172,073558 872	0,011217
HMDB34851	Ethyl 2,4-dioxohexanoate	M-H	171,066283	172,073558 872	0,011217
HMDB04982	cis-4-Octenedioic acid	M-H	171,066283	172,073558 872	0,011217
HMDB00341	2-Octenedioic acid	M-H	171,066283	172,073558 872	0,011217
HMDB12488	1,2,3,4-Tetrahydro-beta-carboline	M-H	171,092772	172,100048 394	0,015272

MS search for 171.1139 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB40284	1,2-Dihydro-1,1,6-trimethylnaphthalene	M-H	171,117925	172,125200 512	0,004025
HMDB40202	Butyl 3-hydroxy-2-methylidenebutanoate	M-H	171,102668	172,109944 378	0,011232
HMDB40203	2-Methylpropyl 3-hydroxy-2-methylidenebutanoate	M-H	171,102668	172,109944 378	0,011232
HMDB36213	cis-3-Hexenyl lactate	M-H	171,102668	172,109944 378	0,011232

HMDB36188	Tetrahydrofurfuryl butyrate	M-H	171,102668	172,109944 378	0,011232
HMDB40165	Butyl levulinate	M-H	171,102668	172,109944 378	0,011232
HMDB36396	3-Methylbutyl 3-oxobutanoate	M-H	171,102668	172,109944 378	0,011232
HMDB59937	6-Pentyl-1,4-dioxan-2-one	M-H	171,102668	172,109944 378	0,011232
HMDB59936	5-Pentyl-1,4-dioxan-2-one	M-H	171,102668	172,109944 378	0,011232
HMDB60287	4-Hydroperoxy-2-nonenal	M-H	171,102668	172,109944 378	0,011232

MS search for 172.07277 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB04225	2-Oxoarginine	M-H	172,072765	173,080041 233	0,000005
HMDB37113	1,2,5,6-Tetrahydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one	M-H	172,076788	173,084063 979	0,004018
HMDB32887	4-Amino-2-methyl-1-naphthol	M-H	172,076788	173,084063 979	0,004018
HMDB06488	N-Acetyl-L-glutamate 5-semialdehyde	M-H	172,061532	173,068807 845	0,011238

MS search for 172.95794 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60455	cis-2-Chloro-4-carboxymethylenebut-2-en-1,4-olide	M-H	172,96471	173,971986 291	0,00677

MS search for 174.04082 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60273	2-Amino-3-oxoadipate	M-H	174,040796	175,048072 403	0,000024
HMDB39163	D-N-(Carboxyacetyl)alanine	M-H	174,040796	175,048072 403	0,000024
HMDB00812	N-Acetyl-L-aspartic acid	M-H	174,040796	175,048072 403	0,000024
HMDB03470	N-Formyl-L-glutamic acid	M-H	174,040796	175,048072 403	0,000024
HMDB31577	Berberoin	M-H	174,041665	175,048940 801	0,000845
HMDB03157	Guanidinosuccinic acid	M-H	174,05203	175,059305 791	0,01121

HMDB00197	Indoleacetic acid	M-H	174,056053	175,063328 537	0,015233
HMDB04073	5-Hydroxyindoleacetaldehyde	M-H	174,056053	175,063328 537	0,015233
HMDB40972	1-Methoxy-1H-indole-3-carboxaldehyde	M-H	174,056053	175,063328 537	0,015233
HMDB38628	Hydroxymethyl indol-3-yl ketone	M-H	174,056053	175,063328 537	0,015233

MS search for 181.02714 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB32825	Dipropyl trisulfide	M-H	181,018487	182,025762 518	0,008653
HMDB40235	1,1'-Thiobis-1-propanethiol	M-H	181,018487	182,025762 518	0,008653
HMDB33055	Ethyl 1-(ethylthio)ethyl disulfide	M-H	181,018487	182,025762 518	0,008653
HMDB39654	Ethyl 1-(methylthio)propyl disulfide	M-H	181,018487	182,025762 518	0,008653
HMDB01973	9-Methyluric acid	M-H	181,036714	182,043990 078	0,009574
HMDB01970	3-Methyluric acid	M-H	181,036714	182,043990 078	0,009574
HMDB03099	1-Methyluric acid	M-H	181,036714	182,043990 078	0,009574
HMDB11107	7-Methyluric acid	M-H	181,036714	182,043990 078	0,009574
HMDB60624	Ethionamide sulphoxide	M-H	181,044108	182,051383 642	0,016968

MS search for 183.11391 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB61384	N-(3-acetamidopropyl)pyrrolidin-2-one	M-H	183,113902	184,121177 766	0,000008
HMDB36470	1,4-Dimethyl-7-ethylazulene	M-H	183,117925	184,125200 512	0,004015
HMDB39052	(4S,8R)-8,9-Dihydroxy-p-menth-1(6)-en-2-one	M-H	183,102668	184,109944 375	0,011242
HMDB39710	1-Acetylcyclohexyl acetate	M-H	183,102668	184,109944 378	0,011242
HMDB36998	(S)-Oleuropeic acid	M-H	183,102668	184,109944 378	0,011242

HMDB36117	(1'R)-Nepetalic acid	M-H	183,102668	184,109944 378	0,011242
HMDB40883	(E)-10-Oxo-8-decenoic acid	M-H	183,102668	184,109944 378	0,011242

MS search for 184.07275 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34912	(S)-N-(4,5-Dihydro-1-methyl-4-oxo-1H-imidazol-2-yl)alanine	M-H	184,072765	185,080041 233	0,000015
HMDB32710	2-(1-Naphthyl)acetamide	M-H	184,076788	185,084063 979	0,004038
HMDB32597	4-Hydroxydiphenylamine	M-H	184,076788	185,084063 979	0,004038

MS search for 184.10918 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB32201	cis- and trans-5-Ethyl-4-methyl-2-(2-butyl)-thiazoline	M-H	184,116544	185,123820 303	0,007364
HMDB38437	9-(Methylthio)nonanenitrile	M-H	184,116544	185,123820 303	0,007364
HMDB32202	cis and trans-5-Ethyl-4-methyl-2-(2-methylpropyl)-thiazoline	M-H	184,116544	185,123820 303	0,007364
HMDB06548	Ecgonine	M-H	184,097917	185,105193 351	0,011263
HMDB06348	Pseudoecgonine	M-H	184,097917	185,105193 351	0,011263

MS search for 186.12483 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB15171	Selegiline	M-H	186,128824	187,136099 549	0,003994
HMDB13010	N-Heptanoylglycine	M-H	186,113567	187,120843 415	0,011263
HMDB37790	Polyethylene glycol	M-H	186,113567	187,120843 415	0,011263

MS search for 188.86625 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
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HMDB33208	Dimethyl diselenide	M-H	188,872718	189,879993 848	0,006468
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MS search for 189.06693 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB31173	6-Hydroxy-1H-indole-3-acetamide	M-H	189,066952	190,074227 574	0,000022
HMDB32259	Ethyl 4-(acetylthio)butyrate	M-H	189,059089	190,066365 004	0,007841
HMDB00325	3-Hydroxysuberic acid	M-H	189,076848	190,084123 558	0,009918
HMDB40220	Diethyl L-malate	M-H	189,076848	190,084123 558	0,009918
HMDB61681	6-(2-Hydroxyethoxy)-6-oxohexanoic acid	M-H	189,076848	190,084123 558	0,009918
HMDB40938	Coixinden A	M-H	189,055718	190,062994 186	0,011212
HMDB40326	7-Hydroxy-2,5-dimethyl-4H-1-benzopyran-4-one	M-H	189,055718	190,062994 186	0,011212
HMDB40731	Avenalunic acid	M-H	189,055718	190,062994 186	0,011212
HMDB32991	7-Methoxy-6-methyl-2H-1-benzopyran-2-one	M-H	189,055718	190,062994 186	0,011212
HMDB41122	(S)-2,3-Dihydro-5-hydroxy-2-methyl-1,4-naphthoquinone	M-H	189,055718	190,062994 186	0,011212
HMDB39359	Methyl (Z,Z)-10-hydroxy-2,8-decadiene-4,6-diyanoate	M-H	189,055718	190,062994 186	0,011212
HMDB11165	L-beta-aspartyl-L-glycine	M-H	189,051695	190,058971 44	0,015235
HMDB28837	Glycyl-Aspartate	M-H	189,051695	190,058971 44	0,015235
HMDB15673	Carglumic acid	M-H	189,051695	190,058971 44	0,015235
HMDB28753	Aspartyl-Glycine	M-H	189,051695	190,058971 44	0,015235

MS search for 194.09349 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60351	2-Phenyl-1,3-propanediol monocarbamate	M-H	194,082267	195,089543 287	0,011223
HMDB29217	Tyrosine methylester	M-H	194,082267	195,089543 287	0,011223
HMDB41943	N-Acetyldopamine	M-H	194,082267	195,089543 287	0,011223

HMDB60065	N-methyl-4,6,7-trihydroxy-1,2,3,4-tetrahydroisoquinoline	M-H	194,082267	195,089543 287	0,011223
HMDB14903	Metyrosine	M-H	194,082267	195,089543 287	0,011223

MS search for 196.07275 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB32055	N-Acetylhistidine	M-H	196,072765	197,080041 233	0,000015
HMDB33455	2-Hydroxy-3-methyl-9H-carbazole	M-H	196,076788	197,084063 979	0,004038
HMDB33487	1-Hydroxy-3-methyl-9H-carbazole	M-H	196,076788	197,084063 979	0,004038
HMDB00609	DL-Dopa	M-H	196,061532	197,068807 845	0,011218
HMDB38336	2-Hydroxy-3-(3,4-dihydroxyphenyl)propanamide	M-H	196,061532	197,068807 845	0,011218
HMDB00181	L-Dopa	M-H	196,061532	197,068807 845	0,011218
HMDB38750	N-Hydroxy-L-tyrosine	M-H	196,061532	197,068807 845	0,011218
HMDB33188	3-Amino-1-methyl-5H-pyrido[4,3-b]indole	M-H	196,088021	197,095297 367	0,015271

MS search for 197.02207 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB13858	3-Dechloroethylfosfamide	M-H	197,025216	198,032491 857	0,003146
HMDB60881	Dechloroethyl cyclophosphamide	M-H	197,025216	198,032491 857	0,003146
HMDB13859	2-Dechloroethylfosfamide	M-H	197,025216	198,032491 857	0,003146
HMDB14480	Nitrofurazone	M-H	197,031629	198,038904 7	0,009559

MS search for 197.12957 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB59698	Cadalene	M-H	197,133575	198,140850 576	0,004005
HMDB36648	7-Isopropyl-1,4-dimethylazulene	M-H	197,133575	198,140850 576	0,004005

MS search for 198.08842 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60477	gamma-Glutamyl-beta-aminopropionitrile	M-H	198,088415	199,095691297	0,000005
HMDB14331	Cevimeline	M-H	198,095809	199,103084861	0,007389
HMDB61079	cevimeline trans-sulfoxide	M-H	198,095809	199,103084861	0,007389
HMDB61081	cevimeline N-oxide	M-H	198,095809	199,103084861	0,007389
HMDB61080	cevimeline cis-sulfoxide	M-H	198,095809	199,103084861	0,007389
HMDB40443	3-Methyl-3H-imidazo[4,5-f]quinoxalin-2-amine	M-H	198,078519	199,085795313	0,009901
HMDB35177	2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-azepine-4-one	M-H	198,077182	199,084457909	0,011238
HMDB33135	Pyrimethanil	M-H	198,103671	199,110947431	0,015251

MS search for 200.10406 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB38835	(E)-1-Cinnamoylpyrrolidine	M-H	200,108088	201,115364107	0,004028
HMDB40007	2,3-Dihydro-6-methyl-5-(5-methyl-2-furanyl)-1H-pyrrolizine	M-H	200,108088	201,115364107	0,004028
HMDB35170	1',2'-Dihydro-1,1'-dimethyl-2'-oxo-4,4'-bipyridinium(1+)	M-H	200,095512	201,102788048	0,008548

MS search for 200.14047 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB59736	2-Hydroxyundecanoate	M-H	200,141794	201,149069538	0,001324
HMDB59745	N-Acetylaminooctanoic acid	M-H	200,129217	201,136493479	0,011253
HMDB13116	Valproylglycine	M-H	200,129217	201,136493479	0,011253
HMDB41540	N-(5-Methyl-3-oxohexyl)alanine	M-H	200,129217	201,136493479	0,011253

HMDB00832	Capryloylglycine	M-H	200,129217	201,136493 479	0,011253
MS search for 200.90484 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB39431	1,2,4,5,7-Pentathiocane	M-H	200,900028	201,907303 642	0,004812
MS search for 203.02048 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB31665	Daucic acid	M-H	203,019727	204,027002 61	0,000753
HMDB32026	Sinalexin	M-H	203,028458	204,035733 578	0,007978
HMDB60013	O-methoxycatechol-O-sulphate	M-H	203,001968	204,009244 056	0,018512
MS search for 204.98853 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB60369	3-Chloro-2-methylmaleylacetate	M-H	204,990925	205,998201 041	0,002395
HMDB60346	2-Chloro-5-methylmaleylacetate	M-H	204,990925	205,998201 041	0,002395
HMDB60018	Pyrogallol-2-O-sulphate	M-H	204,981233	205,988508 614	0,007297
HMDB60016	Pyrogallol-1-O-sulphate	M-H	204,981233	205,988508 614	0,007297
HMDB59752	5-Sulfoxymethylfurfural	M-H	204,981233	205,988508 614	0,007297
MS search for 212.1041 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB15506	Phenazopyridine	M-H	212,094169	213,101445 377	0,009931
HMDB29864	2-Amino-3,8-dimethyl-3H-imidazo[4,5-f]quinoxaline	M-H	212,094169	213,101445 377	0,009931
MS search for 214.04861 m/z					

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB59660	sn-glycero-3-Phosphoethanolamine	M-H	214,048598	215,055873 697	0,000012
HMDB00114	Glycerylphosphorylethanolamine	M-H	214,048598	215,055873 697	0,000012
HMDB01885	3-Chlorotyrosine	M-H	214,027645	215,034920 898	0,020965

MS search for 214.11974 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB13124	Propenoylcarnitine	M-H	214,108482	215,115758 037	0,011258

MS search for 214.92051 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB36351	Methyl 2-propenyl pentasulfide	M-H	214,915678	215,922953 706	0,004832
HMDB14470	Nitroprusside	M-H	214,941025	215,948300 785	0,020515

MS search for 215.03278 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB14693	Methoxsalen	M-H	215,034983	216,042258 738	0,002203
HMDB30637	Bergapten	M-H	215,034983	216,042258 738	0,002203
HMDB35190	Chlorohydrin	M-H	215,026917	216,034192 617	0,005863
HMDB04821	Bisnorbiotin	M-H	215,049587	216,056862 95	0,016807
HMDB60618	6-Aminopenicillanic acid	M-H	215,049587	216,056862 95	0,016807

MS search for 226.11972 m/z

Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB61302	N,N-Didesmethyldiphenhydramine	M-H	226,123738	227,131014 171	0,004018
HMDB40300	2-Amino-1,7,9-trimethylimidazo[4,5-g]quinoxaline	M-H	226,109819	227,117095 441	0,009901

HMDB32928	2-Amino-3,4,8-trimethyl-3H-imidazo[4,5-f]quinoxaline	M-H	226,109819	227,117095 441	0,009901
MS search for 226.92048 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB34831	Orthoperiodic acid	M-H	226,905805	227,913081 312	0,014675
MS search for 226.97047 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB37638	Ammonium peroxydisulfate	M-H	226,964931	227,972206 622	0,005539
MS search for 228.13541 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB39106	2,4-Undecadiene-8,10-diyonic acid isobutylamide	M-H	228,139388	229,146664 235	0,003978
HMDB37770	Neopellitorine A	M-H	228,139388	229,146664 235	0,003978
HMDB33531	2,4,6,8-Decatetraenoic acid dehydropiperidide	M-H	228,139388	229,146664 235	0,003978
HMDB13126	Butenylcarnitine	M-H	228,124132	229,131408 101	0,011278
MS search for 232.87675 m/z					
Compound	Name	Adduct	Adduct MW (Da)	Compound MW (Da)	Delta
HMDB39432	1,2,4,5,7,8-Hexathionane	M-H	232,872098	233,879374 332	0,004652
HMDB39648	1,2,3,5,6,8-Hexathionane	M-H	232,872098	233,879374 332	0,004652