

Metabolites	Derivatized	MSI Match	Match	HMDB	PubChen	CHEBI	KEGG	METLIN	S6	1_UF	S6	2_UF	S6	3_UF	4_UF	S7	5_UF	S7	6_UF	S8	7_UF	S8	8_UF	9_UF
Groups	Derivatized	MSI Match	Match	HMDB	PubChen	CHEBI	KEGG	METLIN	S6	S6	S6	S6	S7	S7	S7	S7	S8	S8	S8	S8	S8	S8	S8	S8
Cholesterol	Yes	Level 2	Cholesterol	HMDB00000067	1.1E+07	1307929	C00187	163	9.1E+08	9.1E+08	9.3E+08	8.9E+08	1.1E+09	1.0E+09	1.0E+09	9.9E+08	1.0E+09	9.9E+08	1.0E+09	9.9E+08	1.0E+09	9.9E+08	1.0E+09	9.9E+08
Adrenaline	Yes	Level 2	Epinephrine	HMDB00000068	5816	28918	C00788	5127	1.9E+08	2.3E+08	2.7E+08	NA	NA	5.1E+08	2.4E+08	2.3E+08	2.4E+08	2.3E+08	2.4E+08	2.3E+08	2.4E+08	2.3E+08	2.4E+08	2.3E+08
Citric acid	Yes	Level 2	Citric acid	HMDB00000094	311	30769	C00158	124	5.5E+08	5.2E+08	5.4E+08	5.1E+08	5.5E+08	5.5E+08	5.5E+08	5.1E+08	NA	NA	5.5E+08	5.5E+08	5.1E+08	NA	5E+08	5E+08
Glucose	Yes	Level 2	D-Glucose	HMDB00000122	5793	4167	C00031	133	1.4E+10	NA	NA	NA	1.9E+10	2.1E+10	2.1E+10	2.3E+10	NA	NA	2.1E+10	2.1E+10	2.3E+10	NA	2.1E+10	2.1E+10
L-Glutamic acid	Yes	Level 2	L-Glutamic acid	HMDB00000148	33032	16015	C00025	5174	1.3E+08	3.2E+08	3.4E+08	3.2E+08	3.5E+08	3.6E+08	3.6E+08	3.2E+08	3.5E+08	3.5E+08	3.6E+08	3.2E+08	3.5E+08	3.5E+08	3.6E+08	3.5E+08
Hypoxanthine	Yes	Level 2	Hypoxanthine	HMDB00000157	790	17368	C00262	83	NA	2.1E+07	2.4E+07	2.3E+07	2.6E+07	2.6E+07	2.4E+07	1.7E+07	1.9E+07	1.9E+07	1.7E+07	1.9E+07	1.9E+07	1.8E+07	1.8E+07	1.8E+07
L-Alanine	Yes	Level 2	L-Alanine	HMDB00000161	5950	16977	C00041	NA	1.5E+08	1.2E+08	1.1E+08	1.4E+08	1.6E+08	1.5E+08	1.5E+08	1.4E+08	1.6E+08	1.4E+08	1.6E+08	1.4E+08	1.6E+08	1.4E+08	1.6E+08	1.4E+08
Proline	Yes	Level 2	L-Proline	HMDB00000162	145742	17203	C00148	29	NA	NA	1.7E+07	1.8E+07	2.5E+07	NA	NA	5.8E+07	6.2E+07	NA	NA	5.8E+07	6.2E+07	NA	NA	5.8E+07
D-Mannose	Yes	Level 2	D-Mannose	HMDB00000169	18950	4208	C00159	NA	4.9E+10	2.8E+10	2.9E+10	2.8E+10	4.9E+10	4.9E+10	2.9E+10	2.9E+10	3E+10	2.9E+10	3E+10	2.9E+10	3E+10	2.9E+10	3E+10	2.9E+10
L-Lysine	Yes	Level 2	L-Lysine	HMDB00000182	5962	18019	C00047	5200	4.8E+09	5.2E+09	5.2E+09	5.2E+09	5.6E+09	6.3E+09	5.7E+09	6.3E+09	5.7E+09	6.3E+09	5.7E+09	6.3E+09	5.7E+09	6.3E+09	5.7E+09	6.3E+09
Serine	Yes	Level 2	L-Serine	HMDB00000187	5951	17115	C00065	5203	1.7E+09	1.7E+09	1.7E+09	1.7E+09	1.8E+09	1.8E+09	1.8E+09	1.6E+09	1.7E+09	1.7E+09	1.8E+09	1.6E+09	1.7E+09	1.7E+09	1.8E+09	1.7E+09
Lactic Acid	Yes	Level 2	L-Lactic acid	HMDB00000190	107689	422	C00186	5205	2.1E+10	2E+10	2E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10	2.1E+10
L-Aspartic acid	Yes	Level 2	L-Aspartic acid	HMDB00000191	5960	17053	C00049	5206	NA	1.3E+08	1.3E+08	1.3E+08	1.3E+08	1.3E+08	1.4E+08	1.2E+08	1.3E+08	1.3E+08	1.4E+08	1.2E+08	1.3E+08	1.3E+08	1.4E+08	1.3E+08
L-Cystine	Yes	Level 2	L-Cystine	HMDB00000192	67678	16283	C00491	5207	NA	8E+07	8.3E+07	8.9E+07	1E+08	1E+08	9.2E+07	9.9E+07	9.8E+07	9.9E+07	9.8E+07	9.9E+07	9.8E+07	9.9E+07	9.8E+07	9.9E+07
myo-Inositol	Yes																							

3,3-DIMETHYL-1-BUTENE	No	Level 3	NA	NA	NA	NA	NA	2.4E+08	1.1E+09	1.3E+09	8.6E+08	4.3E+08	3.6E+08	4.6E+08	1.4E+09	4.4E+08
3,4,5-TRIMETHYLPYRAZOLE	No	Level 3	NA	NA	NA	NA	NA	1.2E+07	4.5E+07	1.2E+07	1.2E+07	2.7E+07	1.1E+07	1.1E+07	1.1E+07	1.1E+07
3-Ethyl-3-methylheptane	No	Level 3	NA	NA	NA	NA	NA	2.5E+07	4.6E+07	4.2E+08	8005296	2.8E+07	1.6E+07	2.6E+07	2.7E+07	2.2E+08
3-ETHYLPENTANE	No	Level 3	NA	NA	NA	NA	NA	2.6E+08	3.1E+08	4E+07	4.8E+08	5.1E+07	4.1E+08	9.2E+07	5.1E+08	4E+07
4-Octene, 2,3,7-trimethyl-, [S-(E)]-	No	Level 3	NA	NA	NA	NA	NA	4.9E+07	4.2E+08	4.2E+08	4.7E+08	4.7E+08	4.6E+08	5.3E+08	5.3E+08	5.2E+08
8-benzyl-9,10-dimethoxy-5,8-dihydro	No	Level 3	NA	NA	NA	NA	NA	3659325	4002384	5221136	4104631	5093648	5511496	4066589	5469075	5485907
Acetyl-sulfamethoxazole	No	Level 3	NA	NA	NA	NA	NA	2.5E+08	2.3E+08	2.5E+08	2.6E+08	2.6E+08	2.2E+08	2.1E+08	2E+08	1.7E+08
Alloxyptopine	No	Level 3	NA	NA	NA	NA	NA	5.1E+07	5.5E+07	5.7E+07	5E+07	5.2E+07	5.5E+07	4.6E+07	1.1E+07	4.5E+07
Benthiaivalcarb-isopropyl	No	Level 3	NA	NA	NA	NA	NA	2.4E+07	2.2E+07	2.2E+07	3.8E+07	2.9E+07	3.2E+07	2.8E+07	2.8E+07	2.4E+07
Benzaldehyde, 2-ethyl-	No	Level 3	NA	NA	NA	NA	NA	3E+08	2.8E+08	2.8E+08	3.1E+08	3.1E+08	3.1E+08	3E+08	2.9E+08	2.9E+08
Benzene, 1,3-bis(benzoyloxy)-5-(2-nitr	No	Level 3	NA	NA	NA	NA	NA	1.7E+07	1.7E+07	1.7E+07	1.8E+07	2E+07	2E+07	1.8E+07	1.9E+07	1.7E+07
Butylphosphonic acid, decyl 4-(2-phe	No	Level 3	NA	NA	NA	NA	NA	9279463	8600716	8277948	7365887	9800902	9796740	7429372	7328448	7661905
CIS-2-HEXENE	No	Level 3	NA	NA	NA	NA	NA	1.1E+08	1.4E+08	1.4E+08	2.6E+07	2E+08	2.7E+07	2.9E+07	3E+07	1.7E+08
CIS-4-NONENE	No	Level 3	NA	NA	NA	NA	NA	2.2E+07	1E+08	2.3E+07	4.2E+07	2.4E+07	2.5E+07	1.8E+08	1.6E+08	2.4E+07
Cyclopropane, (1,2-dimethylpropyl)-	No	Level 3	NA	NA	NA	NA	NA	5.3E+08	5E+08	5.1E+08	5.8E+08	5.7E+08	5.7E+08	5.7E+08	5.7E+08	5.7E+08
Ethaneperoxoic acid, 1-cyano-1-[2-(2	No	Level 3	NA	NA	NA	NA	NA	4.8E+10	4.6E+10	4.8E+10	5.5E+10	4.5E+10	2E+08	2.2E+08	1.7E+08	2.3E+10
Man5GlcNAc-II	No	Level 3	NA	NA	NA	NA	NA	2E+07	1.8E+07	1.7E+07	1.5E+07	1.8E+07	1.7E+07	1.5E+07	1.4E+07	1.4E+07
N,N'-Dimethyl-N,N'-dioctadecyl-ethar	No	Level 3	NA	NA	NA	NA	NA	2.4E+08	3.1E+08	3E+08	2.4E+08	1.9E+08	3.4E+07	2E+08	4.4E+07	2.1E+08
N4-Acetylsulfadiazine	No	Level 3	NA	NA	NA	NA	NA	1.7E+08	1.6E+08	3.8E+08	1.4E+08	4.1E+08	3.7E+08	1.5E+08	3.3E+08	1.3E+08
Phosphatidylcholine 18:0-18:1	No	Level 3	NA	NA	NA	NA	NA	1.1E+08	1E+08	1E+08	1.1E+08	1E+08	9.9E+07	9.4E+07	9.3E+07	9E+07
Primiphos-methyl	No	Level 3	NA	NA	NA	NA	NA	4.1E+08	3.7E+08	3.7E+08	4.5E+08	4.5E+08	4.3E+08	4E+08	4.2E+08	3.8E+08
Thermoposide, crotonoyl	No	Level 3	NA	NA	NA	NA	NA	8.3E+07	7.5E+07	8.3E+07	7.1E+07	7.4E+07	7.6E+07	7.4E+07	7.2E+07	7.4E+07
trans-Zeatin	No	Level 3	NA	NA	NA	NA	NA	3.5E+09	2E+07	3.5E+09	3.7E+09	4E+09	4.3E+09	4.2E+09	4.4E+09	4.4E+09
(4-Methyl-piperidin-1-yl)-acetic acid, r	No	Level 3	NA	NA	NA	NA	NA	1.7E+07	4.6E+07	4.8E+07	NA	4.7E+07	4.7E+07	4.4E+07	4.4E+07	4.4E+07
2-METHYL-1-PENTENE	No	Level 3	NA	NA	NA	NA	NA	1.2E+08	1.5E+08	1.6E+08	5.4E+07	1.1E+08	8.3E+07	NA	2.6E+07	1.2E+08
4-Octene, 2,3,6-trimethyl-	No	Level 3	NA	NA	NA	NA	NA	5E+08	4.9E+08	4.9E+08	5.5E+08	5.5E+08	5.4E+08	5.1E+07	NA	5E+07
CIS-3-HEXENE	No	Level 3	NA	NA	NA	NA	NA	1.3E+08	1.1E+08	1.3E+08	1.6E+08	1.7E+08	1.5E+08	1.4E+08	1.6E+08	NA
Heptane, 4-methylene-	No	Level 3	NA	NA	NA	NA	NA	2.1E+07	6.3E+07	1.9E+07	6832074	1.8E+07	5.5E+07	1.9E+07	NA	5478675
Hexane, 3,3-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	6.6E+07	1.2E+08	4E+08	2.6E+08	NA	4.2E+08	3.1E+08	3E+08	9.4E+07
TERT-BUTANE	No	Level 3	NA	NA	NA	NA	NA	1.7E+08	NA	1.6E+08	1.8E+08	1.8E+08	1.8E+08	1.8E+08	1.8E+08	1.7E+08
1,4-DIMETHYLCYCLOHEXANE	No	Level 3	NA	NA	NA	NA	NA	7665236	1.6E+07	1.3E+07	4.2E+07	5957526	3.7E+07	NA	1E+08	NA
1,7-Dimethyl-4-(1-methylethyl)cyclod	No	Level 3	NA	NA	NA	NA	NA	1.1E+08	NA	1.5E+08	NA	1.1E+08	1.7E+08	7.5E+07	1.1E+08	2.5E+07
2,2,4-TRIMETHYLPENTANE	No	Level 3	NA	NA	NA	NA	NA	1.6E+07	NA	3.2E+08	3293851	4.5E+08	1.4E+07	6768687	NA	3029720
3-Stalylactose	No	Level 3	NA	NA	NA	NA	NA	9663412	NA	NA	1443082	1520589	1479618	1657694	1715479	1702627
4,4'-Methylen-bis(2-methyl aniline)	No	Level 3	NA	NA	NA	NA	NA	2.6E+07	2.3E+07	2.5E+07	1.8E+07	NA	1.9E+07	NA	1.4E+07	1.5E+07
5-TERT-BUTYL-3,3-DIMETHYL-1-IN	No	Level 3	NA	NA	NA	NA	NA	6.2E+07	6E+07	6.1E+07	5.6E+07	NA	5.8E+07	5.5E+07	NA	5.4E+07
9-Eicosene	No	Level 3	NA	NA	NA	NA	NA	4.1E+08	NA	4.1E+08	3.8E+08	4.1E+08	NA	4.2E+08	4.2E+08	4.2E+08
BENZALDEHYDE DIBUTYL ACETAL	No	Level 3	NA	NA	NA	NA	NA	1.3E+09	1.2E+09	3.3E+07	3E+07	NA	1.3E+09	2.9E+07	2.8E+07	NA
CIS-4-OCTENE	No	Level 3	NA	NA	NA	NA	NA	1E+08	NA	1.2E+07	3.2E+07	NA	2.3E+07	2.3E+07	2.6E+07	3.1E+07
CYCLOOCTENE	No	Level 3	NA	NA	NA	NA	NA	NA	NA	9.5E+07	9.4E+07	9.1E+07	2.2E+08	5.9E+07	1.9E+08	1.8E+08
Cyclopropane, (R,R)-1-(Z)-hex-1'-en	No	Level 3	NA	NA	NA	NA	NA	1.6E+07	1.7E+07	NA	NA	1.7E+07	1.7E+07	1.5E+07	1.6E+07	1.6E+07
Decane, 3-ethyl-3-methyl-	No	Level 3	NA	NA	NA	NA	NA	1.5E+07	4.5E+08	NA	NA	7.1E+07	1.6E+07	1.5E+07	2E+07	1.6E+07
ETHYLCYCLOHEXANE	No	Level 3	NA	NA	NA	NA	NA	7.8E+07	5.7E+07	NA	2.2E+08	1.6E+08	1.6E+08	2E+08	7680658	NA
Hexazinone	No	Level 3	NA	NA	NA	NA	NA	1.3E+07	1.3E+07	1E+07	1.1E+07	1.1E+07	NA	1.2E+07	1.1E+07	NA
l-Leucine, N-(2-methoxyethoxycarbon	No	Level 3	NA	NA	NA	NA	NA	1.3E+07	NA	1.3E+07	1.2E+07	1.4E+07	1.2E+07	1.2E+07	1.1E+07	NA
l-Norleucine, N-neopentylloxycarbony	No	Level 3	NA	NA	NA	NA	NA	6.3E+08	NA	4.3E+08	5.5E+08	6E+08	7E+08	NA	5.1E+09	6E+08
Mesotrione	No	Level 3	NA	NA	NA	NA	NA	2.5E+07	1.9E+07	NA	1.5E+08	1.6E+07	1.9E+07	NA	2.3E+07	1E+07
Nicosulfuron	No	Level 3	NA	NA	NA	NA	NA	1.3E+07	1.3E+07	5281677	4480822	5101759	5063212	NA	NA	1.2E+07
Phosphatidylcholine 17:1-22:6	No	Level 3	NA	NA	NA	NA	NA	1.4E+07	1.1E+07	1.3E+07	NA	1.6E+07	1.5E+07	2E+07	NA	5722174
Phosphatidylethanolamine 18:0-22:3	No	Level 3	NA	NA	NA	NA	NA	2.1E+08	NA	NA	2.2E+08	2.4E+08	2.4E+08	2.3E+08	2.3E+08	2.2E+08
Propanoic acid, dimethyl(isopropyl)sil	No	Level 3	NA	NA	NA	NA	NA	2.3E+07	7E+07	NA	NA	2E+07	3.2E+07	5E+07	4.8E+07	4.2E+07
Triadimefon	No	Level 3	NA	NA	NA	NA	NA	4213958	4112838	5501492	6250151	6969679	NA	9913231	NA	1.4E+07
(4S,5S)-4,5-BIS-(HYDROXYMETHYL)	No	Level 3	NA	NA	NA	NA	NA	3.2E+07	NA	2.8E+07	3.3E+07	NA	3.2E+07	3.4E+07	NA	3E+07
1,2-Dimethyl-4-tertbutyl-6-cyclopentyl	No	Level 3	NA	NA	NA	NA	NA	NA	5984629	NA	6352610	6460890	5228761	5178822	5238520	NA
1,5-Benzoxazepin-4(5H)-one, 2,3-di	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	5195999	5729162	6031727	4290732	4628333	5458843
1,5-Diphenylhex-3-ene	No	Level 3	NA	NA	NA	NA	NA	3800299	NA	NA	2894084	NA	4255880	3297998	3276160	3484142
1-Azetidinecarboxaldehyde, 2,2,4,4-t	No	Level 3	NA	NA	NA	NA	NA	NA	2.5E+07	NA	2.7E+07	2.5E+07	NA	2.7E+07	2.5E+07	2.4E+07
1H-Benzimidazole, 1-ethyl-	No	Level 3	NA	NA	NA	NA	NA	2.4E+07	NA	1.7E+07	NA	2.1E+07	2E+07	2.5E+07	2.1E+07	NA
2,2,4,4,6,8,8-HEPTAMETHYLNONANOL	No	Level 3	NA	NA	NA	NA	NA	5041600	NA	NA	1559520	2239877	1574529	1442539	NA	NA
2,2,5-TRIMETHYLHEXANE	No	Level 3	NA	NA	NA	NA	NA	2818708	NA	8082586	4533583	NA	NA	2675870	4477493	1.1E+07
2,3,4-TRIMETHYLPENTANE	No	Level 3	NA	NA	NA	NA	NA	3868407	9490173	NA	5.9E+07	NA	NA	3.3E+07	3022275	6008643
2-Methyl-N-(1-methylethylidene)-4-[(	No	Level 3	NA	NA	NA	NA	NA	NA	5914421	3386619	6803867	6488762	NA	NA	5261409	6416756
3,5-DIMETHYLPYRAZOLE	No	Level 3	NA	NA	NA	NA	NA	NA	1.1E+08	1.2E+08	8.6E+07	1E+08	NA	8.2E+07	NA	9.7E+07
3-Hexene, 2,2-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	4.8E+07	5.8E+07	NA	NA	4.5E+07	1.4E+07	7333685	4.7E+07
5-(2-Naphthylloxymethyl)-3-(O-tolyl)-2	No	Level 3	NA	NA	NA	NA	NA	7163367	NA	8402831	1.1E+07	1.2E+07	1.3E+07	NA	NA	3538166
6-AMINOFLAVANONE	No	Level 3	NA	NA	NA	NA	NA	2559305	2468503	NA	2593061	NA	2677037	1667311	2030048	NA
Alanine, N-methyl-N-(2-methoxyetho	No	Level 3	NA	NA	NA	NA	NA	NA	7925961	6593022	1.1E+07	NA	1E+07	1.1E+07	NA	8957817
Benzeneacetaldehyde, 1,2,5-trimeth	No	Level 3	NA	NA	NA	NA	NA	NA	4.7E+08	4.7E+08	4.9E+08	5E+08	4.9E+08	NA	4.8E+08	NA
Cyclopentane, 1-pentyl-2-propyl-	No	Level 3	NA	NA	NA	NA	NA	3.6E+07	3.5E+07	NA	NA	3.6E+07	3.5E+07	3.6E+07	3.6E+07	NA
Diglyme	No	Level 3	NA	NA	NA	NA	NA	2.2E+07	2E+07	NA	NA	2.2E+07	NA	2.2E+07	2.1E+07	2.1E+07
d-Proline, N-(2-methoxyethoxycarbon	No	Level 3	NA	NA	NA	NA	NA	NA	NA	1.2E+07	1.2E+07	1.5E+07	1.6E+07	NA	1.4E+07	1.4E+07
Hexane, 2,3,4-trimethyl-	No	Level 3	NA	NA	NA	NA	NA	3E+08	7.2E+08	NA	5.7E+08	NA	NA	5.5E+08	5.7E+08	2.2E+08
Kinetin-9-riboside	No	Level 3	NA	NA	NA	NA	NA	2.8E+07	2.7E+07	2.9E+07	NA	NA	2.6E+07	NA	3136071	2.6E+07
L-Alanine, N-[N-(3-pyridinyl)methyl]	No	Level 3	NA	NA	NA	NA	NA	1.3E+07	1.9E+07	NA	NA	1.4E+07	1.5E+07	NA	1E+07	1.6E+07
l-Alanine, N-ethoxycarbonyl-, undec-	No	Level 3	NA	NA	NA	NA	NA	1.3E+07	1.3E+07	1.3E+07	2.5E+07	NA	NA	1.7E+07	NA	1.7E+07
l-Leucine, n-butoxycarbonyl-N-methy	No	Level 3	NA	NA	NA	NA	NA	NA	4.7E+08	NA	5.1E+08	5.3E+08	5.2E+08	5.6E+08	NA	5.3E+08
Trientine	No	Level 3	NA	NA	NA	NA	NA									