

Supplementary Table S1. List of metabolites identified using 2D-GC-TOF-MS platform. HMDB, PubChem, ChEBI, KEGG and METLIN identifiers are provided with the raw unprocessed peak abundance data. Derivatized metabolites are highlighted in yellow.

Metabolites Groups	Derivatized	MSI Matching Lev	MSI Matching Lev Match	HMDB	PubChem PubChem	ChEBI ChEBI	KEGG KEGG	METLIN METLIN	S1C S1	S1D S1	S1E S1	S2A S2	S2B S2	S2C S2	S3A S3	S3B S3	S3C S3
Butanoic acid	Yes	Level 2	Butyric acid	HMDB0000039	264		30772 C00246	107	614169	661804	724580	566986	132738	684411	1151271	1154392	1187018
Acetic acid	Yes	Level 2	Acetic acid	HMDB0000042	176		15366 C00033	3206	2896922 NA	11057002	1039731	952564	1071585	972112	28711		37148
Cholesterol	Yes	Level 2	Cholesterol	HMDB0000067	11025495		1370929 C00187	163	1011009	1710691	1676832	1636837	1613140	1625919	1985389	1103624	2737914
2-Piperidinecarboxylic acid	Yes	Level 2	Pipecolic acid	HMDB0000070	849		17964 C00408	50	20788	19236 NA		90375	60944	37140	34371	30420	26074
Ethanol	Yes	Level 2	Ethanol	HMDB0000108	702		16236 C00469	3203	79095	93402	11913	34949	27343	16680	97325	18141	13212
D-Glucose	Yes	Level 2	D-Glucose	HMDB0000122	5793		4167 C00013	133	893936 NA			63693	348350	3716354	667283	6701342	1095528
Glycerol	Yes	Level 2	Glycerol	HMDB0000131	753		17522 C00116	105	1605184	6906127	8548479 NA		2037477	1785064	2499252	23182	11048885
D-Galactose	Yes	Level 2	D-Galactose	HMDB0000143	438357		195215 C00518	134	195215	605618	19058	13993	38717 NA	NA	NA	68092	7650
L-Tyrosine	Yes	Level 2	L-Tyrosine	HMDB0000158	6057		17895 C00082	34	51274	48884	53998 NA		33552 NA	NA	38209	51412	87372
L-Phenylalanine	Yes	Level 2	L-Phenylalanine	HMDB0000159	6140		17285 C00079	28	24266	35062	51037	50044	56789	52290	68811	51410	151549
L-Proline	Yes	Level 2	L-Proline	HMDB0000162	145742		17203 C00148	29	720238	653250	697368	2167181	1672147	12477	2192473	1434060	1293554
L-Threonine	Yes	Level 2	L-Threonine	HMDB0000167	6288		16857 C00188	32	2591886	2849667	2901038	3900295	3704968	3625549	4590806	4933638	4267054
D-Mannose	Yes	Level 2	D-Mannose	HMDB0000169	18950		1817673 C00519	NA	1817673	5885421	78257	3157631	2851067	3990551	3635727	1150688	9571425
L-Aspartic acid	Yes	Level 2	L-Aspartic acid	HMDB0000191	5960		17053 C00049	5206	2148	25246	14394	58080	60378	50592	65512	58191	55118
Benzeneacetic acid	Yes	Level 2	Phenylacetic acid	HMDB0000209	999		30745 C00708	129	87392	98459	18592	11925	26415 NA	NA	37781	44044	26915
Myo-Inositol	Yes	Level 2	myo-Inositol	HMDB0000211	NA		17268 C00137	5221	3702529	3886817	3738657	3753812	3944842	3710460	4938069	4533095	4315292
Hexadecanoic acid	Yes	Level 2	Palmitic acid	HMDB0000220	985		15756 C00249	187	1004605	3905809	5340097	3197963	306253	3586072	2724810	2716872	3172045
Propanoic acid	Yes	Level 2	Propionic acid	HMDB0000237	1032		30768 C00163	3215	2810125	738055	11377821	91110	3957301	10976746	1050171	6867255	34136433
Pyridoxine	Yes	Level 2	Pyridoxine	HMDB0000239	1054		16709 C00314	5245 NA	NA	2443423	276897	1218567	1231021	1240947	3630736	3448188	3193249
Urea	Yes	Level 2	Urea	HMDB0000294	1176		16169 C00086	6	1198881	36344697	10742612	21312202	2056071	43119005	20459674	49672100	16159624
trans-3-Hexenedioic acid	Yes	Level 2	3-Hexenedioic acid	HMDB0000393	5351896		86952	5382 NA	NA	NA	49978 NA	NA	24622	24221 NA	NA	56148	11884
N-alpha-Acetyl-L-Lysine	Yes	Level 2	N-(alpha-acetyl)lysine	HMDB0000446	192596		35704 C12899	51	21052	69718 NA	NA	47731	178011 NA	NA	NA	25203 NA	NA
Hexadecanoic acid	Yes	Level 2	Adipic acid	HMDB0000448	196		30832 C00104	115	2205	11705	19602	37584	18088	8	213622	20628	20262
Decanoic acid	Yes	Level 2	Capric acid	HMDB0000511	2969		30813 C01571	336	30108	25942	13320	17865	15950	15723 NA	NA	17730	30045
Hexanoic acid	Yes	Level 2	Caproic acid	HMDB0000535	8892		30776 C01585	550	663198	1367826	1409116	17978	10242	55378	45303	1336927	NA
9-Octadecenoic acid	Yes	Level 2	Elaidic acid	HMDB0000573	446399		27997 C00722	3406	1620899	883176	691106	607319	621445	54884	751069	69145	727997
Methylmalonic acid	Yes	Level 2	Citric acid	HMDB0000634	643798		17626 C00226	5607	38661 NA	NA	28488	52068	57527	46831	46259	53652	64984
Dodecanoic acid	Yes	Level 2	Dodecanoic acid	HMDB0000638	3893		30805 C02679	5611	146405	59667	51053	33583	39905	40393	60784	58852	68977
Pentadecanoic acid	Yes	Level 2	Glutaric acid	HMDB0000661	743		17859 C00489	3254 NA	NA	44398 NA	NA	NA	35636	4457	23289	28134	49654
Heptanoic acid	Yes	Level 2	Heptanoic acid	HMDB0000666	8094		45571 C01744	5636	31773	29248	29364	20266	18132	22228	34910	34371	33955
4-Methylvaleric acid	Yes	Level 2	Isocaproic acid	HMDB0000689	12587		74903	4191	16409	12429 NA	NA	14561	12985	53129	298227	NA	51373
Malonic acid	Yes	Level 2	Malonic acid	HMDB0000691	867		30794 C00383	3237	28651	19703	37870	23628	10474	27215	2741228	53259	29765
Pseudouridine	Yes	Level 2	Pseudouridine	HMDB0000767	15047		17802 C02067	5734	569616	64404 NA	NA	NA	NA	79142	11574	1670	96035
Acetic acid	Yes	Level 2	Acetic acid	HMDB0000784	2266		48131 C08261	5750	10282	13555	13513	66444	77301	83597	14458	16345	17123
2-Pyrrolidone-5-carboxylic acid	Yes	Level 2	Pyrrrolidonecarboxylic acid	HMDB0000805	499		16010 C02237	5769	290840	137238	142493	139866	145799	199990	194818	183171	NA
Tetradecanoic acid	Yes	Level 2	Myristic acid	HMDB0000806	11005		28875 C06424	196	38582	57753	17601	15339	31613	4427 NA	NA	77162	36285
n-Pentadecanoic acid	Yes	Level 2	Pentadecanoic acid	HMDB0000826	13849 NA		C16537	5789	79196	48143	48260 NA	34097	19836	45082	52577	61301	NA
Octadecanoic acid	Yes	Level 2	Stearic acid	HMDB0000827	5281		28842 C01530	189	50401	47979	48897	46101	49916	41927	61931	67127	59334
Nonadecanoic acid	Yes	Level 2	Nonadecanoic acid	HMDB0000847	8158		29019 C01601	5010	36826	119496	119110	10544	19711	153734	10711	132738	NA
Ribonic acid	Yes	Level 2	Ribonic acid	HMDB0000867	5466977		21077 C01685	3290	67036	70962	51382	542576	626399	626239	723031	131273	591679
L-Valine	Yes	Level 2	L-Valine	HMDB0000883	6287		16144 C00183	5842	2484629	5851378	3084136	255091	4065316	8025858	4241	4454399	4581361
N-Trimethylamine	Yes	Level 2	Trimethylamine	HMDB0000906	1126		18319 C00565	3772	2897643	3182055	4068571	9036	18952	3625166	1267240	3832695	4427866
L-Tryptophan	Yes	Level 2	L-Tryptophan	HMDB0000929	6305		16828 C00078	5879	29122	292864	364014	98855	322011	366515	313471	105211	320949
Arachidonic acid	Yes	Level 2	Arachidonic acid	HMDB0001043	444899		15843 C00219	193	24810	59902	68042	50608	25742	53615	62356	62512	67206
Phenylethanolamine	Yes	Level 2	Phenylethanolamine	HMDB001085	1000		16344 C00175	59	697867 NA	680042	NA	13852	71167	15857	NA	57683	NA
Aminomalonic acid	Yes	Level 2	Aminomalonic acid	HMDB0001147	100714		17475 C00872	NA	165300	188613	207714	109118	288347	306621	364260	367248	381356
3-penten-2-one	Yes	Level 2	Methyl propenyl ketone	HMDB0001184	637920 NA		NA	NA	2227055	282412	2070074	93044	1055152	141295	368965	1877706	NA
7H-purine	Yes	Level 2	Purine	HMDB0001366	1044		17258 C15687	6193 NA	NA	91631 NA	NA	58594	44031	91025	67363	86227	68649
Alpha-Linolenic acid	Yes	Level 2	Alpha-Linolenic acid	HMDB0001388	5280934		27432 C06427	6208 NA	NA	14199	39930	92918	6174	13176	96485	78775	19566
1,4-Butanediamine	Yes	Level 2	Putrescine	HMDB0001414	1045		17144 C00130	NA	28509	37919	11545 NA	NA	NA	1991 NA	NA	NA	NA
Gamma-Tocopherol	Yes	Level 2	Gamma-Tocopherol	HMDB0001492	14986		298402	1276	18048 NA	17074	16226	17243	16403	21604	21052	21158	NA
Benzoic acid	Yes	Level 2	Benzoic acid	HMDB0001870	243		30746 C00184	6297	2554319	3259762	3730575	1148045	1822245	2636649	3263961	3835589	NA
1,2-Benzendicarboxylic acid	Yes	Level 2	2-Pyrrolidone	HMDB0002039	12025		30692 C11118	6452 NA	NA	NA	NA	77196	98327 NA	NA	17491	53567	75483
1,2-Benzene dicarboxylic acid	Yes	Level 2	Phthalic acid	HMDB002107	1017		29569 C01606	6489	195939	201025	212176	251255	247304	239786	303962	287007	275253
Phosphoric acid	Yes	Level 2	Phosphoric acid	HMDB0002142	1004		26078 C00009	NA	3457	55146 NA	NA	NA	15862	18312	46081	51412	NA
Docosahexanoic acid	Yes	Level 2	Docosahexanoic acid	HMDB0002183	445580		445580	NA	82476	16458	538332	77768	39586	79374	62431	69344	76377
Heptadecanoic acid	Yes	Level 2	Heptadecanoic acid	HMDB0002259	10045		32365	6578	20895 NA	NA	56212 NA	NA	42079 NA	NA	78407	45849 NA	NA
Cadaverine	Yes	Level 2	Cadaverine	HMDB0002322	273		18127 C01622	3236	37927	10317 NA	NA	NA	16380	20080	70394	87500	NA
Ethanedioic acid	Yes	Level 2	Oxalic acid	HMDB0002329	971		16995 C00209	113	3912236	3757020	1378698	5152022	4578014	4374286	6158487	36446124	3758781
1,4-Benzendicarboxylic acid	Yes	Level 2	Terephthalic acid	HMDB0002428	7489		15710 C08337	6676	50003	59407 NA	NA	70289	34134	37278	30979	29439	2678
1,5-Anhydro-D-sorbitol	Yes	Level 2	1,5-Anhydro-D-sorbitol	HMDB0002712	64960		16070 C01026	3775	291767	304847	306027	332771	200688	327671	440967	397432	495953
Erythritol	Yes	Level 2	Erythritol	HMDB0002994	222285		17113 C00503	140	63824	17888 NA	NA	NA	15011 NA	NA	24202	37377	6
Propanal	Yes	Level 2	Propanal	HMDB0003366	277		11573 C00494	6906 NA	NA	94247	63935 NA	NA	53722	47215 NA	NA	16495	92877
Carbamate	Yes	Level 2	Carbamic acid	HMDB0003551	527		28616 C01563	6950 NA	NA	15677 NA	NA	17997	15154	11651	57022	22506 NA	NA
Arabinofuranose	Yes	Level 2	Arabinofuranose	HMDB0013225	440921		6178 C08115	NA	NA	NA	80514	2363 NA	15727	31827 NA	NA	50194	NA
Palmitoleic acid	Yes	Level 2	Palmitoleic acid	HMDB0013238	5282745		59265	NA	57613	53783	96242	44310	52061 NA	NA	73571	71035	67419
Cyclohexanol	Yes	Level 2	Cyclohexanol	HMDB001414	1045		17144 C00130	NA	228	NA	19175 NA	NA	15687	16616	NA	NA	NA

4-Ethoxybenzhydrazide	No	Level 3	NA	NA	NA	NA	NA	NA	17055	70101	NA	NA	110199	6995	51003	NA	33296	NA
4-Ethoxyphenethyl alcohol	No	Level 3	NA	NA	NA	NA	NA	NA	96850	93385	89290	110199	102860	99884	122426	111402	138772	NA
4-Methoxy-7-methylindan-1-one	No	Level 3	NA	NA	NA	NA	NA	NA	215108	13560	220589	42074	NA	209561	16443	NA	247732	NA
4-Morpholinethanethiol	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	53463	20053	8475.5	31233	181841	20487	6062.7	NA
4-Morpholinethanol	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	3028	1823.4	NA	57122	15904	NA	48476	NA
4-Nonene, 2,3,3-trimethyl-, (Z)-	No	Level 3	NA	NA	NA	NA	NA	NA	18650	13123	37128	NA	NA	10454	48974	NA	16246	NA
4-Octene, 2,3,6-trimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	117852	67751	681004	57837	190620	2465.1	168813	284133	328579	NA
4-Piperidinone, 2,2,6,6-tetramethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	35155	NA	44023	NA	44183	58240	46915	50869
4-Undecane, 10-methyl-, (E)-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	NA	20883	NA	15881	46472	9874.2	18295	1351.7
5H-1,4-Diazepin-5-one, hexahydro-	No	Level 3	NA	NA	NA	NA	NA	NA	3993.4	7703.9	7827.8	12432	NA	NA	NA	NA	17822	NA
5-Hydroxytryptamine	No	Level 3	NA	NA	NA	NA	NA	NA	9961.4	NA	12034	NA	9513.4	9418.2	14114	12698	11538	NA
5-O-Methyl-D-gluconic acid dime	No	Level 3	NA	NA	NA	NA	NA	NA	14322	NA	NA	28752	31365	11223	NA	NA	487044	NA
6-tert-Butyl-4-methylcoumarin	No	Level 3	NA	NA	NA	NA	NA	NA	64804	63253	7453.9	NA	NA	11638	NA	10108	2481.8	NA
Acetic acid, oxo-, methyl ester	No	Level 3	NA	NA	NA	NA	NA	NA	NA	90478	NA	100848	NA	13779	NA	18745	17656	NA
ACETONITRILE	No	Level 3	NA	NA	NA	NA	NA	NA	NA	8233.4	9035.6	NA	3066	5213.8	NA	3292.9	NA	NA
Altrose	No	Level 3	NA	NA	NA	NA	NA	NA	51187	10210	224428	NA	93120	11361	117442	NA	202739	NA
Articaine	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	36909	43340	9119.5	48559	57307	54582	NA	NA
Benzene, (1,1-dimethyl-2-butynyl)	No	Level 3	NA	NA	NA	NA	NA	NA	20877	21574	30109	NA	17660	NA	NA	23003	NA	NA
Benzene, (1-ethyl-1-propenyl)-	No	Level 3	NA	NA	NA	NA	NA	NA	10224	NA	NA	14362	12813	14685	9101.3	20441	NA	NA
Benzenebutanoic acid, 4-methoxy-	No	Level 3	NA	NA	NA	NA	NA	NA	19045	21192	NA	NA	12813	25909	23318	NA	30395	27077
Benzoic acid, 3,5-bis(1,1-dimethyl-2-propenyl)-	No	Level 3	NA	NA	NA	NA	NA	NA	209699	194877	103595	225053	210573	203974	250707	231882	212502	NA
Benzoic acid, 4-ethoxy-, ethyl ester	No	Level 3	NA	NA	NA	NA	NA	NA	3307607	3498393	6638088	23567968	25025693	5571453	29450015	29837703	4326386	NA
Benzoic acid, 4-ethoxy-, ethyl ester	No	Level 3	NA	NA	NA	NA	NA	NA	6286.3	11386	199515	NA	NA	15998	42622	NA	NA	NA
Benzoic acid, 2-	No	Level 3	NA	NA	NA	NA	NA	NA	468048	21857	8244.7	2364.6	53673	5275.5	15971	NA	3988.3	NA
Carbonyl sulfide	No	Level 3	NA	NA	NA	NA	NA	NA	14219	17124	12009	19856	NA	17235	NA	1849.8	NA	NA
Cetene	No	Level 3	NA	NA	NA	NA	NA	NA	107393	302161	26829	NA	2560138	271377	1795799	333489	2002054	NA
Cetizine N-Oxide	No	Level 3	NA	NA	NA	NA	NA	NA	46612	37758	30909	39986	37747	78372	4048844	41050	35306	NA
cis-2-Methylcyclohexanol	No	Level 3	NA	NA	NA	NA	NA	NA	25679	8997.1	NA	118668	2159.5	3981.3	NA	19150	1474.8	NA
Cyclohexane, (2-methylpropyl)-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	6895.5	11291	9514.1	9075.1	NA	2923.1	2684.3	NA
Cyclohexane, 1-ethyl-1,3-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	1299	NA	11513	4824.2	3268.8	207435	1732.3	9556.1	21900	NA
Cyclohexane, 1-ethyl-2-propyl-	No	Level 3	NA	NA	NA	NA	NA	NA	194770	151626	550242	536033	221573	235656	192417	504988	176227	NA
Cyclohexane, 2-ethyl-1,3-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	4476	11197	NA	NA	11375	17819	NA	10629	NA	NA
Cyclohexane, ethoxycarbonyl-	No	Level 3	NA	NA	NA	NA	NA	NA	19762	18201	22500	6001.7	11576	10256	4570.2	5829	12565	NA
Cyclohexane, nonadecyl-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	20936	NA	4906.6	8843.3	4556.8	NA	5425.6	NA	NA
Cyclohexane, undecyl-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Cyclooctane, (1-methylpropyl)-	No	Level 3	NA	NA	NA	NA	NA	NA	345895	14813	14000	289422	242124	24752	54171	161438	NA	NA
Cyclooctane, 1,4-dimethyl-, cis-	No	Level 3	NA	NA	NA	NA	NA	NA	298818	1335023	306302	499665	340331	34379	33489	558462	1560706	NA
Cyclooctane, 1,4-dimethyl-, trans-	No	Level 3	NA	NA	NA	NA	NA	NA	310758	103706	129397	11378	447357	440251	1873.1	97244	8199.1	NA
Cyclopentane, 1-butyl-2-ethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	162511	234500	29730	139119	NA	248303	157606	NA
Cyclopentane, 1-hydroxymethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	6245.1	6427.8	6795.1	NA	3826.6	6216.4	NA	6592.6	NA	NA
Cyclopentane, 1-pentyl-2-propyl-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	13060	NA	NA	27792	5336.3	NA	63076	NA	NA
Cyclopentane, hexoxycarbonyl-	No	Level 3	NA	NA	NA	NA	NA	NA	17164	13963	13026	5615.1	1902.2	13506	4444.2	5694.9	3799.7	NA
Cyclopentane, hexyl-	No	Level 3	NA	NA	NA	NA	NA	NA	4175	44100	NA	101350	19191	15929	NA	10436	110754	NA
Decanal, O-methylxime	No	Level 3	NA	NA	NA	NA	NA	NA	505433	489329	520587	507332	515168	486407	716928	865343	656545	NA
Decane, 2,3,5,8-tetramethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	1988020	1591719	606076	363358	517496	2444447	844678	534248	155624	NA
Decane, 2,5,9-trimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	NA	7885.8	13950	13775	11621	NA	NA	9269	NA	NA
Decane, 2,9-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	107853	448671	681293	777992	3889114	10181	54640	32043	2527858	NA
Decane, 3,7-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	42368	NA	12594	34538	NA	18893	40485	NA	NA	NA
Dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	591992	289463	598157	508258	40944	48141	42888	65991	70228	NA
Disulfide, di-tert-dodecyl-	No	Level 3	NA	NA	NA	NA	NA	NA	259371	2509009	2534126	2533609	2486500	4652345	4145164	3596616	2595452	NA
Docosane	No	Level 3	NA	NA	NA	NA	NA	NA	22959	32623	NA	2897.3	6592.7	NA	8606.7	31014	NA	NA
Dodecanal	No	Level 3	NA	NA	NA	NA	NA	NA	NA	33495	NA	6309.6	5422.2	22435	26188	NA	NA	NA
Dodecane, 2,6,10-trimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	4173	44100	11743	152075	NA	19191	15929	20576	8468.4	NA
Dodecane, 2,7,10-trimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	4494329	3705040	6723065	8670784	7006069	5759409	5749768	7817054	3357548	NA
Dodecane, 4,6-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	2455555	2628590	2515370	3547280	2781910	2762955	3403987	2995020	2909536	NA
Dodecanenitrile	No	Level 3	NA	NA	NA	NA	NA	NA	NA	14647	NA	36844	13830	NA	14633	15244	15914	NA
D-Trehalose	No	Level 3	NA	NA	NA	NA	NA	NA	62622	78642	NA	71932	82511	71386	76578	80438	76302	NA
Eicosane	No	Level 3	NA	NA	NA	NA	NA	NA	7458790	3837567	971816	NA	16570	313962	NA	NA	NA	NA
Ethanone, 1-(4-ethoxyphenyl)-	No	Level 3	NA	NA	NA	NA	NA	NA	5102	83887	2402.4	35640	34755	NA	16672	9302.2	7436.3	NA
Ethanone, 1-(2,3-dihydro-2,3-dihydro-6-methylheptyl vinyl)	No	Level 3	NA	NA	NA	NA	NA	NA	300847	235360	187805	304715	314013	228841	308453	283959	318591	NA
Fumaric acid, 2-(diethylamino)ethyl	No	Level 3	NA	NA	NA	NA	NA	NA	32316	38570	9948	7839.3	NA	NA	NA	NA	46275	NA
heptacosane	No	Level 3	NA	NA	NA	NA	NA	NA	1496348	1547247	1562531	569283	972515	1366146	171574	531695	860899	NA
Heptadecane, 2,6,10,14-tetramethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	4175	44100	11743	152075	NA	19191	15929	20576	8468.4	NA
Heptadecane, 2,6-dimethyl-	No	Level 3	NA	NA	NA	NA	NA	NA	113046	2968.8	NA	NA	186009	1648053	245269	2805977	NA	NA
Heptadecane, 2-methyl-	No	Level 3	NA	NA	NA	NA	NA	NA	14052	11202	NA	4220209	12650	NA	NA	14259	NA	NA
HEPTANAL ETHYLENE GLYCOL	No	Level 3	NA	NA	NA	NA	NA	NA	NA	5165.6	33653	NA	10976	30320	5508.2	28991	4709	NA
hexacosane	No	Level 3	NA	NA	NA	NA	NA	NA	2799252	1370281	1683318	525324	841813	1303284	48279	6151326	63104	NA
Hexanedioic acid, bis(2-ethylhexyl)	No	Level 3	NA	NA	NA	NA	NA	NA	28255	28384	27300	24979	24174	25279	28261	26477	27170	NA
Hydroxylamine, O-methyl-	No	Level 3	NA	NA	NA	NA	NA	NA	31296	368871	147620	345841	17811	405005	283292	21039	NA	NA
L-Glycine	No	Level 3	NA	NA	NA	NA	NA	NA	3062.1	NA	16485	NA	17864	17268	4736.8	NA	NA	NA
L-GLYCINE	No	Level 3	NA	NA	NA	NA	NA	NA	5903151	6127278	3647715	1223544	1263073	6933374	4788524	1363807	7154159	NA
L-Methionine sulfone	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	NA	9225.6	3821.5	9875.3	24049	19017	13864	NA
Megastigma-4,6(E),8(Z)-triene	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	13949	NA	NA	12383	28559	18444	14669	NA
methanalphosphate	No	Level 3	NA	NA	NA	NA	NA	NA	NA	NA	8235.1	12611	8559.9	NA	6586.3	9465.2	NA	NA
Methyl (2Z)-dec-2-en-4,6-diminoate	No	Level 3	NA	NA	NA	NA	NA	NA	39226	38287	15846	NA	15735	38776	NA	48077	44372	NA
Methyl formate	No	Level 3	NA	NA	NA	NA	NA	NA	16004	12990	16191	18059	12450	14710	128731	22122	21043	NA
METHYL VINYL KETONE	No	Level 3	NA	NA	NA	NA	NA	NA	NA	37								