

Table S3

Usual name	Category	MetaCyc ID	References
dodecanoic acid	12:0 fatty acid	DODECANOATE	Santos et al., 2015 ; Robertson et al., 2015
Myristic acid	14:0 fatty acid	CPD-7836	Pettitt et al., 1989; Tasende, 2000; Van Ginneken et al., 2011; Robertson et al., 2015 ; Belghit et al., 2017
Pentadecanoic acid	15:0 fatty acid	CPD-8462	Santos et al., 2015. Belghit et al., 2017
Palmitic acid	16:0 fatty acid	PALMITATE	Pettitt et al., 1989; Tasende, 2000; Van Ginneken et al., 2011; Robertson et al., 2015 ; Belghit et al., 2017
Heptadecanoic acid	17:0 fatty acid	CPD-7830	Santos et al., 2015
Stearic acid	18:0 fatty acid	STEARIC_ACID	Tasende et al., 2000 ; Robertson et al., 2015
Eicosanoic acid	20:0 fatty acid	ARACHIDIC_ACID	Santos et al., 2015
Docosanoic acid	22:0 fatty acid	DOCOSANOATE	Santos et al., 2015
Tricosanoic acid	23:0 fatty acid	CPD-7834	Santos et al., 2015
Tetracosanoic acid	24:0 fatty acid	TETRACOSANOATE	Santos et al., 2015
Palmitoleic acid	16:1(n-7) fatty acid	CPD-9245	Pettitt et al., 1989; Tasende, 2000; Robertson et al., 2015 ; Belghit et al., 2017
Oleic acid	18:1(n-9) fatty acid	OLEATE-CPD	Tasende et al., 2000; Van Ginneken et al., 2011; Robertson et al., 2015 ; Belghit et al., 2017
Linoleic acid	18:2(n-6) fatty acid	LINOLEIC_ACID	Tasende et al., 2000 ; Robertson et al., 2015 ; Belghit et al., 2017
Alpha Linolenic acid	18:3(n-3) fatty acid	LINOLENIC_ACID	Tasende et al., 2000
γ-linolenic acid	18:3(n-6) fatty acid	CPD-8117	Robertson et al., 2015 ; Belghit et al., 2017
Octadecatetraenoic acid	18:4(n-3) fatty acid	CPD-12653	Tasende et al., 2000 ; Robertson et al., 2015 ; Belghit et al., 2017
Arachidonic acid	20:4(n-6) fatty acid	ARACHIDONIC_ACID	Tasende et al., 2000 ; Banskota et al., 2014 ; Robertson et al., 2015 ; Belghit et al., 2017
Eicosapentaenoic acid	20:5(n-3) fatty acid	5Z8Z11Z14Z17Z-EICOSAPENTAENOATE	Tasende et al., 2000 ; Banskota et al., 2014 ; Robertson et al., 2015 ; Belghit et al., 2017
Octanedioic acid	fatty acid	CPD0-1264	Santos et al., 2015
Nonanedioic acid	fatty acid	CPD0-1265	Santos et al., 2015
Cycloartenol	sterol	CYCLOARTENOL	Saito and Idler, 1966; Alcaide et al., 1968
Cholesterol	sterol	CHOLESTEROL	Saito and Idler, 1966; Tasende et al., 2000 ; Santos et al., 2015
7-Dehydrocholesterol	sterol	7-DEHYDROCHOLESTEROL	Tasende et al., 2000
Brassicasterol	sterol	BRASSICASTEROL	Saito and Idler, 1966 ; Tasende et al., 2000
Campesterol	sterol	CAMPESTEROL	Tasende et al., 2000 ; Santos et al., 2015
24-Methylenecholesterol	sterol	24-METHYLENECHOLESTEROL	Tasende et al., 2000
Sitosterol	sterol	SITOSTEROL	Saito and Idler, 1966; Tasende et al., 2000 ; Santos et al., 2015
Stigmasterol	sterol	STIGMASTEROL	Tasende et al., 2000
15-keto-prostaglandin E2	oxylipin	HYDROXY-915-DIOXOPROSTA-13-ENOATE	Gaquerel et al., 2007
lutein	carotenoid	LUTEIN	Banskota et al., 2014
Chlorophyll a	tetrapyrrole	CHLOROPHYLL-A	Melo et al., 2015 ; Robertson et al., 2015
all-trans-beta-carotene	carotenoid	CPD1F-129	Robertson et al., 2015
9-cis-beta-carotene	carotenoid	CPD-14646	Robertson et al., 2015 ; Belghit et al., 2017
zeaxanthin	carotenoid	CPD1F-130	Robertson et al., 2015
2,6,6-trimethyl-1,3-cyclohexadiene-1-carboxaldehyde (safranal)	carotenoid	CPD-8669	Pina et al., 2014
Alanine	aminoacid	L-ALPHA-ALANINE	Young et al., 1958, Belghit et al., 2017
Arginine	aminoacid	ARG	Young et al., 1958, Belghit et al., 2017
Aspartic acid	aminoacid	L-ASPARTATE	Young et al., 1958, Belghit et al., 2017
Citrulline	aminoacid	L-CITRULLINE	Young et al., 1958 ; Belghit et al., 2017
Cystine	aminoacid	CYSTINE	Young et al., 1958
Glutamic acid	aminoacid	GLT	Young et al., 1958 ; Belghit et al., 2017
Glycine	aminoacid	GLY	Young et al., 1958 ; Belghit et al., 2017
Histidine	aminoacid	HIS	Young et al., 1958 ; Belghit et al., 2017
Isoleucine	aminoacid	ILE	Young et al., 1958 ; Belghit et al., 2017
Leucine	aminoacid	LEU	Young et al., 1958 ; Belghit et al., 2017
Lysine	aminoacid	LYS	Young et al., 1958 ; Belghit et al., 2017
Methionine	aminoacid	MET	Young et al., 1958 ; Belghit et al., 2017
Ornithine	aminoacid	L-ORNITHINE	Young et al., 1958 ; Belghit et al., 2017
Phenylalanine	aminoacid	PHE	Young et al., 1958
Proline	aminoacid	PRO	Young et al., 1958 ; Belghit et al., 2017
Serine	aminoacid	SER	Young et al., 1958 ; Belghit et al., 2017
Threonine	aminoacid	THR	Young et al., 1958 ; Belghit et al., 2017
Tyrosine	aminoacid	TYR	Young et al., 1958 ; Belghit et al., 2017

Table S3

Valine	aminoacid	VAL	Young et al., 1958 ; Belghit et al., 2017
Shinorine	Mycosporine-like aminoacid	CPD-18778	Kräbs et al., 2004
UDP- α -D-galactose	nucleotide sugar	CPD-14553	Collén et al., 2014
i-carrageenose	carrageenan	Iota-Carrageenan	Matsuhira et al., 1992
v-carrageenan	carrageenan	Nu-Carrageenan	Matsuhira et al., 1992
Glycerol	polyol	GLYCEROL	Santos et al., 2015
Heptadecane	alcane	HEPTADECANE-CPD	Santos et al., 2015
6,10,14-Trimethyl-2-pentadecanone	methylketone	CPD-7875	Santos et al., 2015
Hexadecan-1-ol	Long chain aliphatic alcohol	CPD-348	Santos et al., 2015
9-Octadecan-1-ol	Long chain aliphatic alcohol	CPD-7873	Santos et al., 2015
Docosan-1-ol	Long chain aliphatic alcohol	CPD-7845	Santos et al., 2015
Octacosan-1-ol	Long chain aliphatic alcohol	CPD-7872	Santos et al., 2015
acetaldehyde	aldehyde	ACETALD	Pina et al., 2014
2-methylpropanal	aldehyde	BUTANAL	Pina et al., 2014
Butanal	aldehyde	CPD-7031	Pina et al., 2014
3-methylbutanal	aldehyde	METHYLBUT-CPD	Pina et al., 2014
Pentanal	aldehyde	CPD-9053	Pina et al., 2014
Hexanal	aldehyde	HEXANAL	Pina et al., 2014
Benzaldehyde	aldehyde	BENZALDEHYDE	Pina et al., 2014
Ethanol	short chain aliphatic alcohol	ETOH	Pina et al., 2014
1-butanol	short chain aliphatic alcohol	BUTANOL	Pina et al., 2014
1-pentanol	short chain aliphatic alcohol	PENTANOL	Pina et al., 2014
2-butanone	short chain ketone	ACETONE	Pina et al., 2014
3,5-octadien-2-one	short chain ketone	MEK	Pina et al., 2014
dichloromethane	halocarbon	CPD-681	Pina et al., 2014
chloroform	halocarbon	CPD-843	Pina et al., 2014
2-methylpropanoic acid	carboxylic acid	ACET	Pina et al., 2014
2-methylbutanoic acid	carboxylic acid	ISOBUTYRATE	Pina et al., 2014
hexane	alcane	CPD-9288	Pina et al., 2014
2,2,4-trimethylpentane	alcane	CPD-19039	Pina et al., 2014

Table S4

Usual name	Category	References
Heneicosanoic acid	21:0 fatty acid	Santos et al., 2015
N/A	15:1 fatty acid	Robertson et al., 2015
N/A	18:1(n-7) fatty acid	Robertson et al., 2015
10-nonadecenoate	19:1(n-9) fatty acid	Belghit et al., 2017
Eicosadienoic acid	20:2(n-6) fatty acid	Robertson et al., 2015
Eicosatrienoic acid	20:3(n-6) fatty acid	Robertson et al., 2015
Docosadienoate	22:2(n-6) fatty acid	Belghit et al., 2017
Octadeca-9-enoic acid	fatty acid	Santos et al., 2015
22-Dehydrocholesterol	sterol	Tasende et al., 2000
11-hydroxy-octadecadienoic acid (11-HODE)	oxylipin	Gaquereel et al., 2007
13-hydroxy-9Z,11E-octadecadienoic acid (13-HODE)	oxylipin	Gaquereel et al., 2007; Belghit et al., 2017
13S-hydroxy-9Z,11E,15Z-octadecatrienoic acid (13-HOTrE)	oxylipin	Belghit et al., 2017
13-oxo-9Z,11E-octadecadienoic acid (13-oxo-ODE)	oxylipin	Gaquereel et al., 2007
13-hydroxyeicosatrienoic acid (13-HETrE)	oxylipin	Gaquereel et al., 2007
13-hydroxyeicosatetraenoic acid (13-HETE)	oxylipin	Gaquereel et al., 2007
13-hydroxyeicosapentaenoic acid (13-HEPE)	oxylipin	Gaquereel et al., 2007
15-hydroxydocosahexaenoic acid (15-HDHE)	oxylipin	Gaquereel et al., 2007
11-hydroxyoctadecadienoic acid (11-HETE)	oxylipin	Gaquereel et al., 2007
Hydroxypheophytin a	tetrapyrrole	Melo et al., 2015
Pheophytin d	tetrapyrrole	Melo et al., 2015
Hydroxypheophytin d	tetrapyrrole	Melo et al., 2015
Monogalactosyldiacylglycerol 2 (MGDG2)	galactolipid	Pettitt et al., 1989
Digalactosyldiacylglycerols (DGDG)	galactolipid	Pettitt et al., 1989
Sulfoquinovosyldiacylglycerol 1 (SQDG1)	galactolipid	Pettitt et al., 1989
Sulfoquinovosyldiacylglycerol 2 (QDG2)	galactolipid	Pettitt et al., 1989
(2S)-1,2-bis-O-eicosapentaenoyl-3-O-β-D-galactopyranosylglycerol	galactolipid	Banskota et al., 2014
(2S)-1-O-eicosapentaenoyl-2-O-arachidonoyl-3-O-β-D-galactopyranosylglycerol	galactolipid	Banskota et al., 2014
(2S)-1-O-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-2-O-palmitoyl-3-O-β-D-galactopyranosylglycerol	galactolipid	Banskota et al., 2014
(2S)-1-O-eicosapentaenoyl-2-O-palmitoyl-3-O-β-D-galactopyranosylglycerol	galactolipid	Banskota et al., 2014
(2S)-1, 2-bis-O-arachidonoyl-3-O-β-D-galactopyranosylglycerol	galactolipid	Banskota et al., 2014
(2S)-1-O-arachidonoyl-2-O-palmitoyl-3-O-β-D-galactopyranosylglycerol	galactolipid	Banskota et al., 2014
(2S)-1-O-eicosapentaenoyl-2-O-palmitoyl-3-O-β-D-galactopyranosyl-6-1α-D-galactopyranosyl-glycerol	galactolipid	Banskota et al., 2014
(2S)-1-O-arachidonoyl-2-O-palmitoyl-3-O-β-D-galactopyranosyl-6-1α-D-galactopyranosyl-glycerol	galactolipid	Banskota et al., 2014
diphosphatidylglycerol, phosphatidic acid	DPG/PA	Pettitt et al., 1989
l-citrullinyl-l-arginine	aminoacid	Laycock et al., 1977
Gigartinine	aminoacid	Laycock et al., 1977
Amide N	aminoacid	Young et al., 1958
Asterina-330	Mycosporine-like aminoacid	Athukorala et al., 2016; Guihéneuf et al., 2018
MAA1	Mycosporine-like aminoacid	This study
MAA2	Mycosporine-like aminoacid	This study
Palythine	Mycosporine-like aminoacid	Karsten et al., 1998; Athukorala et al., 2016; Guihéneuf et al., 2018
Palythene	Mycosporine-like aminoacid	Karsten et al., 1998
Palythinol	Mycosporine-like aminoacid	Karsten et al., 1998; Athukorala et al., 2016
Isofloridoside	heteroside	Kremer et al., 1982
1-Monohexadecanoin	Long chain aliphatic alcohol	Santos et al., 2015
Tetradecan-1-ol	Long chain aliphatic alcohol	Santos et al., 2015
Octadecan-1-ol	Long chain aliphatic alcohol	Santos et al., 2015
1-penten-3-ol	short chain aliphatic alcohol	Pina et al., 2014
2(Z)-penten-1ol	short chain aliphatic alcohol	Pina et al., 2014
3-methylbutanoic acid	carboxylic acid	Pina et al., 2014
2-methylbutanal	aldehyde	Pina et al., 2014
1-octen-3-ol	short chain aliphatic alcohol	Pina et al., 2014

Table S4

2,6-dimethylpyrazine	short chain ketone	Pina et al., 2014
2-propanone	short chain ketone	Pina et al., 2014
acetic acid, anhydride	carboxylic acid	Pina et al., 2014
2,2,3-trimethylpentane	alcane	Pina et al., 2014
tetradecane	alcane	Pina et al., 2014