Supplementary Information: Goslin - A Grammar of Succinct Lipid Nomenclature

Dominik Kopczynski[1,*], Nils Hoffmann[1,*], Bing Peng[1,2] and Robert Ahrends[3,✉]

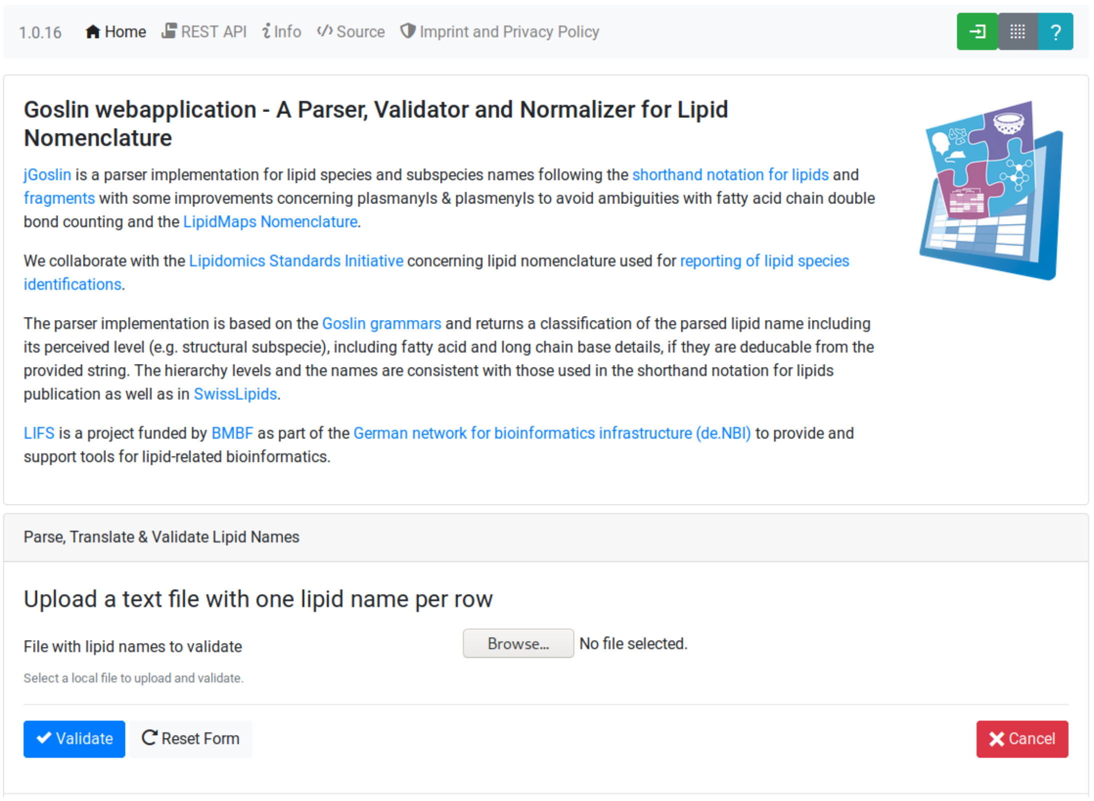
[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., 44139 Dortmund, Germany
[2]Division of Rheumatology, Department of Medicine, Solna, Karolinska Institutet and Karolinska University Hospital, 17176 Stockholm, Sweden
[3]University of Vienna, Department of Analytical Chemistry, 1090 Vienna, Austria
[*]Shared first authors
[✉]Robert.Ahrends@univie.ac.at

Contents

1 Web Application and REST API

Interactive Usage

The interactive grammar of succinct lipid nomenclatures (Goslin) web application is available at `https://apps.lifs.isas.de/goslin`. It provides two forms to i) upload a file containing one lipid name per line (see Supplementary Figure S1), or ii) upload a list of lipid names, defined by the user in an interactive form (see Supplementary Figure S2). The latter form also allows pasting lists of lipid names directly from the clipboard with `CTRL+V`. Both forms provide feedback for issues concerning every processed lipid, such as invalid names or typos (see Supplementary Figure S3), to allow the user to cross-check their data before proceeding.



Goslin webapplication - A Parser, Validator and Normalizer for Lipid Nomenclature

jGoslin is a parser implementation for lipid species and subspecies names following the shorthand notation for lipids and fragments with some improvements concerning plasmanyls & plasmenyls to avoid ambiguities with fatty acid chain double bond counting and the LipidMaps Nomenclature.

We collaborate with the Lipidomics Standards Initiative concerning lipid nomenclature used for reporting of lipid species identifications.

The parser implementation is based on the Goslin grammars and returns a classification of the parsed lipid name including its perceived level (e.g. structural subspecie), including fatty acid and long chain base details, if they are deducable from the provided string. The hierarchy levels and the names are consistent with those used in the shorthand notation for lipids publication as well as in SwissLipids.

LIFS is a project funded by BMBF as part of the German network for bioinformatics infrastructure (de.NBI) to provide and support tools for lipid-related bioinformatics.

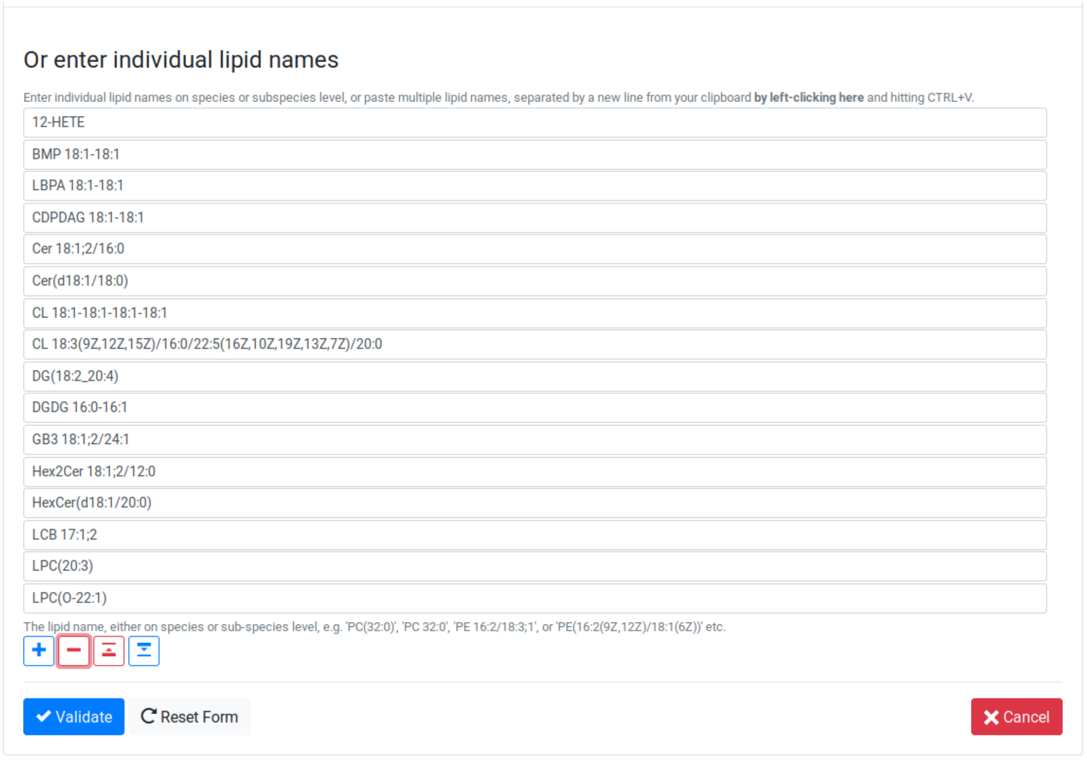
Parse, Translate & Validate Lipid Names

Upload a text file with one lipid name per row

File with lipid names to validate — Browse... No file selected.

Select a local file to upload and validate.

Figure S1: Goslin web application submission form for text files with one lipid name per row.



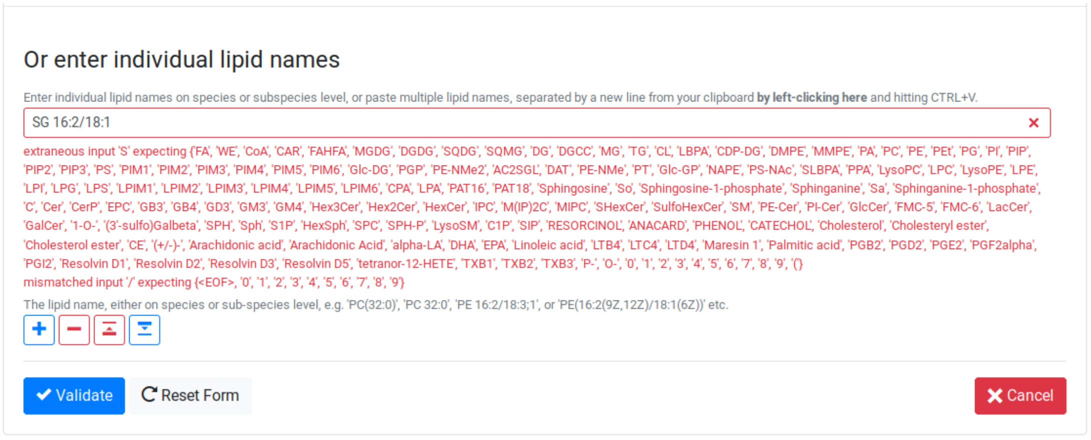
Or enter individual lipid names

Enter individual lipid names on species or subspecies level, or paste multiple lipid names, separated by a new line from your clipboard **by left-clicking here** and hitting CTRL+V.

12-HETE
BMP 18:1-18:1
LBPA 18:1-18:1
CDPDAG 18:1-18:1
Cer 18:1;2/16:0
Cer(d18:1/18:0)
CL 18:1-18:1-18:1-18:1
CL 18:3(9Z,12Z,15Z)/16:0/22:5(16Z,10Z,19Z,13Z,7Z)/20:0
DG(18:2_20:4)
DGDG 16:0-16:1
GB3 18:1;2/24:1
Hex2Cer 18:1;2/12:0
HexCer(d18:1/20:0)
LCB 17:1;2
LPC(20:3)
LPC(O-22:1)

The lipid name, either on species or sub-species level, e.g. 'PC(32:0)', 'PC 32:0', 'PE 16:2/18:3;1', or 'PE(16:2(9Z,12Z)/18:1(6Z))' etc.

Figure S2: Goslin web application submission form for user-defined lipid names.



Or enter individual lipid names

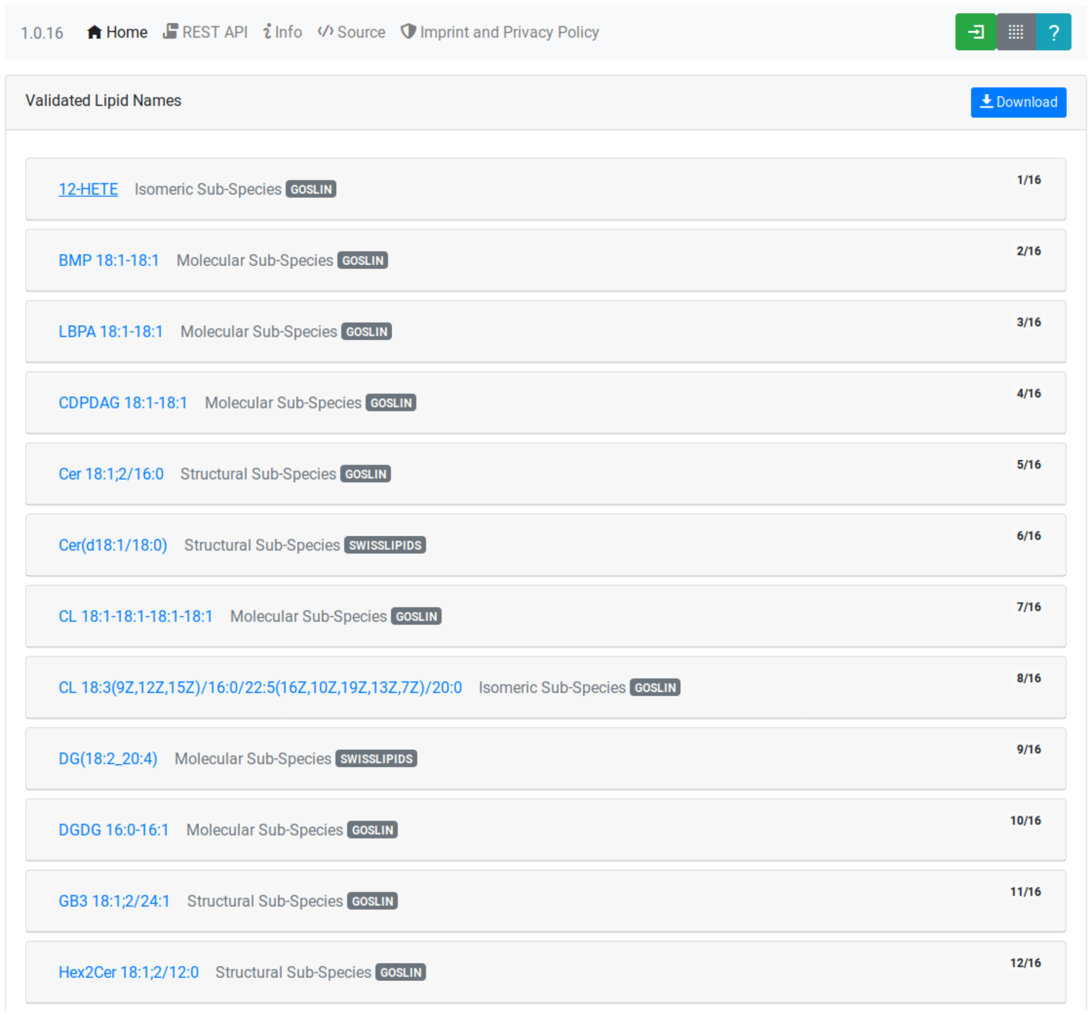
Enter individual lipid names on species or subspecies level, or paste multiple lipid names, separated by a new line from your clipboard **by left-clicking here** and hitting CTRL+V.

SG 16:2/18:1

extraneous input 'S' expecting {'FA', 'WE', 'CoA', 'CAR', 'FAHFA', 'MGDG', 'DGDG', 'SQDG', 'SQMG', 'DG', 'DGCC', 'MG', 'TG', 'CL', 'LBPA', 'CDP-DG', 'DMPE', 'MMPE', 'PA', 'PC', 'PE', 'PEt', 'PG', 'PI', 'PIP', 'PIP2', 'PIP3', 'PS', 'PIM1', 'PIM2', 'PIM3', 'PIM4', 'PIM5', 'PIM6', 'Glc-DG', 'PGP', 'PE-NMe2', 'AC2SGL', 'DAT', 'PE-NMe', 'PT', 'Glc-GP', 'NAPE', 'PS-NAc', 'SLBPA', 'PPA', 'LysoPC', 'LPC', 'LysoPE', 'LPE', 'LPI', 'LPG', 'LPS', 'LPIM1', 'LPIM2', 'LPIM3', 'LPIM4', 'LPIM5', 'LPIM6', 'CPA', 'LPA', 'PAT16', 'PAT18', 'Sphingosine', 'So', 'Sphingosine-1-phosphate', 'Sphinganine', 'Sa', 'Sphinganine-1-phosphate', 'C', 'Cer', 'CerP', 'EPC', 'GB3', 'GB4', 'GD3', 'GM3', 'GM4', 'Hex3Cer', 'Hex2Cer', 'HexCer', 'IPC', 'M(IP)2C', 'MIPC', 'SHexCer', 'SulfoHexCer', 'SM', 'PE-Cer', 'PI-Cer', 'GlcCer', 'FMC-5', 'FMC-6', 'LacCer', 'GalCer', '1-O-', '(3'-sulfo)Galbeta', 'SPH', 'Sph', 'S1P', 'HexSph', 'SPC', 'SPH-P', 'LysoSM', 'C1P', 'SIP', 'RESORCINOL', 'ANACARD', 'PHENOL', 'CATECHOL', 'Cholesterol', 'Cholesteryl ester', 'Cholesterol ester', 'CE', '(+/-)-', 'Arachidonic acid', 'Arachidonic Acid', 'alpha-LA', 'DHA', 'EPA', 'Linoleic acid', 'LTB4', 'LTC4', 'LTD4', 'Maresin 1', 'Palmitic acid', 'PGB2', 'PGD2', 'PGE2', 'PGF2alpha', 'PGI2', 'Resolvin D1', 'Resolvin D2', 'Resolvin D3', 'Resolvin D5', 'tetranor-12-HETE', 'TXB1', 'TXB2', 'TXB3', 'P-', 'O-', '0', '1', '2', '3', '4', '5', '6', '7', '8', '9', '('}
mismatched input '/' expecting {<EOF>, '0', '1', '2', '3', '4', '5', '6', '7', '8', '9'}

The lipid name, either on species or sub-species level, e.g. 'PC(32:0)', 'PC 32:0', 'PE 16:2/18:3;1', or 'PE(16:2(9Z,12Z)/18:1(6Z))' etc.

Figure S3: Goslin web application submission form for user-defined lipid names provides feedback for unknown or unsupported names and parts thereof.

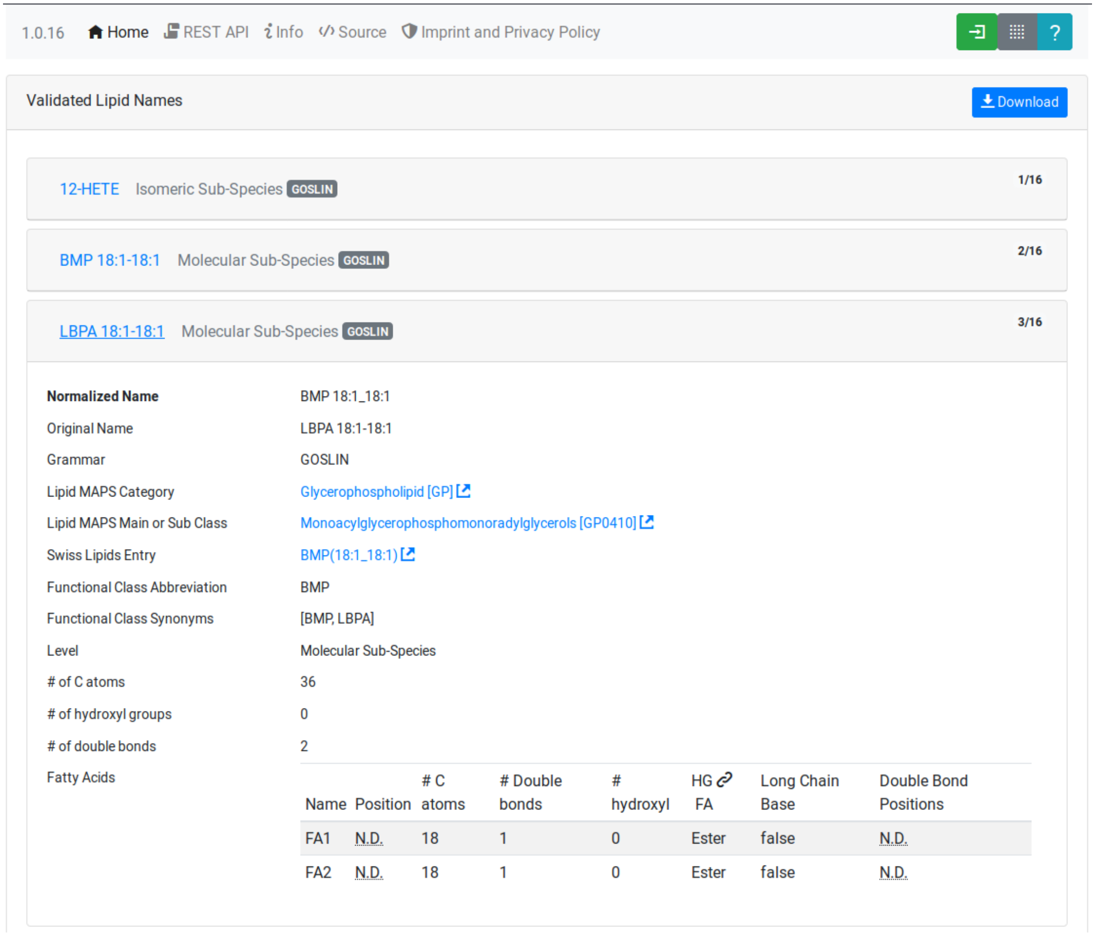


Validated Lipid Names

12-HETE Isomeric Sub-Species GOSLIN	1/16
BMP 18:1-18:1 Molecular Sub-Species GOSLIN	2/16
LBPA 18:1-18:1 Molecular Sub-Species GOSLIN	3/16
CDPDAG 18:1-18:1 Molecular Sub-Species GOSLIN	4/16
Cer 18:1;2/16:0 Structural Sub-Species GOSLIN	5/16
Cer(d18:1/18:0) Structural Sub-Species SWISSLIPIDS	6/16
CL 18:1-18:1-18:1-18:1 Molecular Sub-Species GOSLIN	7/16
CL 18:3(9Z,12Z,15Z)/16:0/22:5(16Z,10Z,19Z,13Z,7Z)/20:0 Isomeric Sub-Species GOSLIN	8/16
DG(18:2_20:4) Molecular Sub-Species SWISSLIPIDS	9/16
DGDG 16:0-16:1 Molecular Sub-Species GOSLIN	10/16
GB3 18:1;2/24:1 Structural Sub-Species GOSLIN	11/16
Hex2Cer 18:1;2/12:0 Structural Sub-Species GOSLIN	12/16

Figure S4: Parsing results are displayed as ’cards’ for every lipid name. Clicking on a card opens it and shows details of the according lipid.

After successful validation, the validated lipids are returned in overview cards (see Supplementary Figure S4), detailing their LipidMAPS classification[1], cross-links to SwissLipids[2] and/or LipidMAPS or HMDB[3]. Additionally, the cards show summary information about the number of carbon atoms, double bonds, hydroxylations and detailed information, such as double bond position, long-chain-base status, and the bond type of the fatty acyl to the head group for each fatty acyl, if available (see Supplementary Figure S5) .


1.0.16
Home
REST API
Info
Source
Imprint and Privacy Policy
?
Validated Lipid Names
Download
12-HETE Isomeric Sub-Species GOSLIN 1/16
BMP 18:1-18:1 Molecular Sub-Species GOSLIN 2/16
LBPA 18:1-18:1 Molecular Sub-Species GOSLIN 3/16

Normalized Name	BMP 18:1_18:1
Original Name	LBPA 18:1-18:1
Grammar	GOSLIN
Lipid MAPS Category	Glycerophospholipid [GP]
Lipid MAPS Main or Sub Class	Monoacylglycerophosphomonoradylglycerols [GP0410]
Swiss Lipids Entry	BMP(18:1_18:1)
Functional Class Abbreviation	BMP
Functional Class Synonyms	[BMP, LBPA]
Level	Molecular Sub-Species
# of C atoms	36
# of hydroxyl groups	0
# of double bonds	2
Fatty Acids	

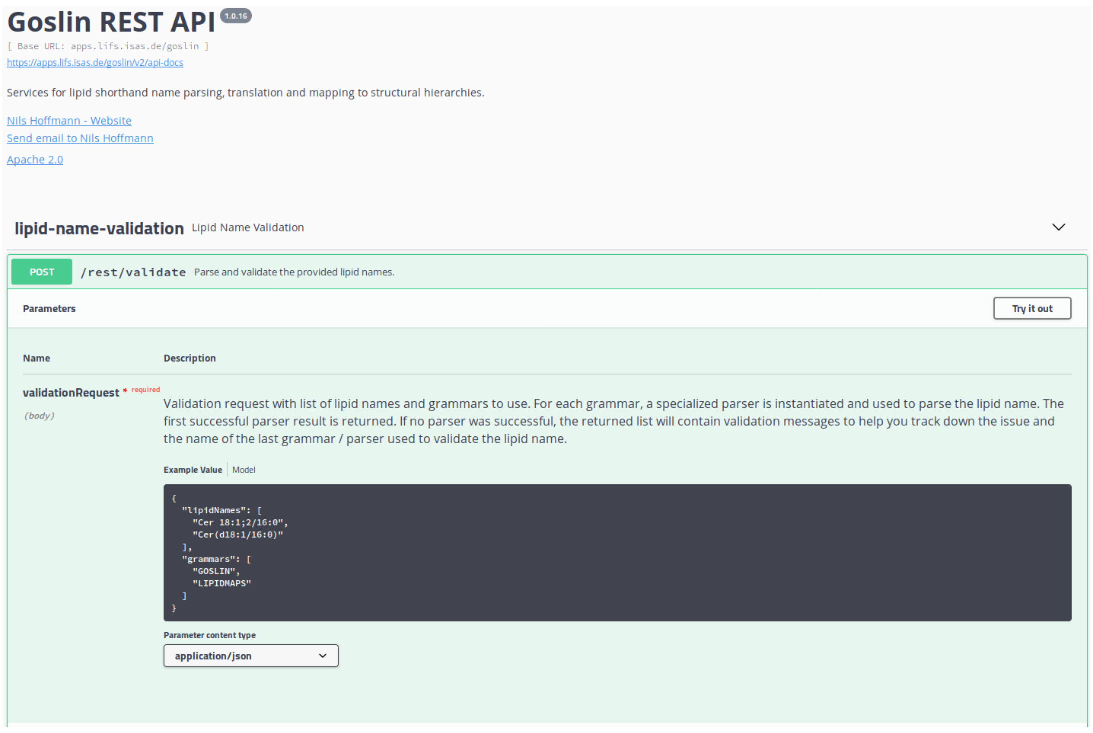
Name	Position	# C atoms	# Double bonds	# hydroxyl	HG FA	Long Chain Base	Double Bond Positions
FA1	N.D.	18	1	0	Ester	false	N.D.
FA2	N.D.	18	1	0	Ester	false	N.D.

Figure S5: Each result card displays summary and detail information about a lipid. Depending on the lipid level, this can include information about each individual fatty acyl. Cross-links to SwissLipids and LipidMAPS are shown where a normalized lipid name could be matched unambiguously against the normalized shorthand names of SwissLipids and / or LipidMAPS lipids.

The source code for the web application and instructions to build it as a Docker container are available at `https://github.com/lifs-tools/goslin-webapp` under the terms of the open source Apache license version 2.

Programmatic access via the REST API

An interactive documentation for the representational state transfer (REST) application programming interface (API) of the Goslin web application is available at `https://apps.lifs.isas.de/goslin/swagger-ui.html` (see Supplementary Figure S6). To illustrate its usage, we will briefly show a small example how a user can access the REST API with a standard hypertext transfer protocol (HTTP) client.



Goslin REST API 1.0.16

[Base URL: apps.lifs.isas.de/goslin]

https://apps.lifs.isas.de/goslin/v2/api-docs

Services for lipid shorthand name parsing, translation and mapping to structural hierarchies.

Nils Hoffmann - Website
Send email to Nils Hoffmann
Apache 2.0

lipid-name-validation Lipid Name Validation

POST /rest/validate Parse and validate the provided lipid names.

Parameters

Name	Description
validationRequest * required (body)	Validation request with list of lipid names and grammars to use. For each grammar, a specialized parser is instantiated and used to parse the lipid name. The first successful parser result is returned. If no parser was successful, the returned list will contain validation messages to help you track down the issue and the name of the last grammar / parser used to validate the lipid name.

Example Value | Model

```
{
  "lipidNames": [
    "Cer 18:1;2/16:0",
    "Cer(d18:1/16:0)"
  ],
  "grammars": [
    "GOSLIN",
    "LIPIDMAPS"
  ]
}
```

Parameter content type: application/json

Figure S6: The Goslin web application provides an interactive documentation for its REST API to simplify programmatic access.

The Structure for the request consists of a JavaScript object notation (JSON) object {} enclosing two lists, with the names `lipidNames` and `grammars`. Acceptable values for `grammars` are: LIPIDMAPS, GOSLIN, GOSLIN_FRAGMENTS, SWISSLIPIDS, and HMDB. A complete list is available from the interactive REST API documentation's `Models` section under `ValidationRequest`. Both fields in the `ValidationRequest` accept comma-separated entries, enclosed in double quotes:

```
{
    "lipidNames": [
      "Cer(d18:1/16:1(6Z))"
    ],
    "grammars": [
      "LIPIDMAPS"
    ]
}
```

Sending the HTTP POST request with `curl` as an HTTP client looks as follows:

```
curl -X POST "https://apps.lifs.isas.de/goslin/rest/validate" -H "accept: */*" -H
```

```
    "Content-Type: application/json" -d "{ \"lipidNames\": [
    \"Cer(d18:1/16:1(6Z))\" ], \"grammars\": [ \"LIPIDMAPS\" ]}"
```

The REST API will return the following result for the request, with a HTTP response code of 200 (OK). This result returns a map of properties for each lipid name that was parsed. If at least one name is not parseable, the REST API will return a response code of 400 (Client error), together with the same results reponse object. In that case, the `failedToParse` field in the response will contain the number of lipid names that could not be parsed. For those results where no grammar was applicable, the `grammar` field will contain the string `NOT_PARSEABLE`.¸In other cases, that field will contain the last grammar used to parse the lipid name and the `messages` field will contain a list of validation messages that help to narrow down the offending bits in the lipid name.

```
{
  "results": [
    {
      "lipidName": "Cer(d18:1/16:1(6Z))",
      "grammar": "LIPIDMAPS",
      "messages": [],
      "lipidAdduct": {
        "lipid": {
          "lipidCategory": "SP",
          "lipidClass": "CER",
          "headGroup": "Cer",
          "info": {
            "type": "STRUCTURAL",
            "name": "Cer",
            "position": -1,
            "lipidFaBondType": "ESTER",
            "lcb": false,
            "modifications": [],
            "doubleBondPositions": {},
            "level": "STRUCTURAL_SUBSPECIES",
            "ncarbon": 34,
            "nhydroxy": 2,
            "ndoubleBonds": 2
          },
```

The response part also reports the normalized name (`goslinName`), as well as classification information using the LipidMAPS category and class associated to the parsed lipid.

```
      },
      "goslinName": "Cer 18:1;2/16:1(6Z)",
      "lipidMapsCategory": "SP",
      "lipidMapsClass": "SP0203",
```

The response also reports information on the fatty acyls detected in the lipid name. In this case, a long chain base (LCB) (in the ceramide) has been detected. The name given here as an example was classified on structural subspecies level, since the LCB contains one double bond, but without positional E/Z information. The fatty acyl FA1 at the sn2 position does report E/Z information for its double bond, thus FA1 is an isomeric fatty acyl. Overall, the lipid can thus be classified as a structural subspecies.

```
      "fattyAcids": {
          "LCB": {
            "type": "STRUCTURAL",
            "name": "LCB",
            "position": 1,
            "lipidFaBondType": "ESTER",
            "lcb": true,
            "modifications": [],
            "doubleBondPositions": {},
            "ncarbon": 18,
            "nhydroxy": 2,
            "ndoubleBonds": 1
          },
          "FA1": {
            "type": "ISOMERIC",
            "name": "FA1",
            "position": 2,
            "lipidFaBondType": "ESTER",
            "lcb": false,
            "modifications": [],
            "doubleBondPositions": {
              "6": "Z"
            },
            "ncarbon": 16,
            "nhydroxy": 0,
            "ndoubleBonds": 1
          }
        }
```

Finally, the response reports the total number lipid names received, the total number parsed and the total number of parsing failures.

```
    ],
    "totalReceived": 1,
    "totalParsed": 1,
    "failedToParse": 0
  }
```

2 C++ Implementation

This is the documentation for the Goslin reference implementation for C++. Please be aware, that the documentation is dedicated to developers of tools for computational lipidomics who want to use cppgoslin within their project. If you are interested to run Goslin as a user, please read Supplementary Section 1. The cppgoslin implementation has been developed with the following objectives:

1. To ease the handling with lipid names for developers working on mass spectrometry-based lipidomics tools.
2. To offer a tool that unifies all existing dialects of lipid names.

It is an open-source package under the MIT License available via github[1]. For a detailed structure of the implementation, read Supplementary Section 6.

Prerequisites

The cppgoslin library needs a GNU g++ compiler version with support for the C++ 11 standard. It comes with simple makefiles for easy compilation and installation. You need the following packages:

```
$ g++ (compiler)
$ make
```

To install the library globally on your system, simply type:

```
$ [sudo] make install
```

Be sure that you have root permissions. Here, the library and headers are installed into the /usr directory. If you want to change that location, you have to edit the first line within the *makefile*.

Testing cppgoslin

We set up more than 150 000 single unit and integration tests, to ensure that cppgoslin is parsing correctly. To run the tests, please type:

```
$ make test
$ make runtests
```

If a test should fail, please contact the developers[2].

[1] https://github.com/lifs-tools/cppgoslin
[2] goslin@lipidomics.at

Using cppgoslin

The two major functions within cppgoslin are the parsing and printing of lipid names. A minimalistic example will demonstrate both functions the easiest way. In the examples folder, you will find the *lipid_name_parser.cpp* file. Compile it by typing:

```
$ cd examples
$ make
$ ./lipid_name_parser
```

Here is the minimalistic C++ code:

```
#include "cppgoslin/cppgoslin.h"
#include <iostream>
int main(){
    LipidParser parser;
    try {
        LipidAdduct* lipid = parser.parse("PA(12:0_14:0)");
        cout << lipid->get_lipid_string() << endl;
        delete lipid;
    }
    catch(LipidException& e){
        // handle the exception
        cout << e.what() << endl;
    }
    return 0;
}
```

To handle unexpected behavior, the parsing command should always be placed within a try/catch block and the `LipidAdduct` pointer should be deleted after usage to avoid memory leaks. Be aware when changing the installation directory, you also have to change the library directory within the examples *makefile*.

To retrieve a parsed lipid name on a higher hierarchy of lipid level, simply define the level when requesting the lipid name:

```
#include "cppgoslin/cppgoslin.h"
#include <iostream>
int main(){
    LipidParser parser;
    try {
        // providing a lipid name on isomeric subspecies level
        LipidAdduct* lipid = parser.parse("PA(12:1(5Z)/14:0)");
        cout << lipid->get_lipid_string(ISOMERIC_SUBSPECIES) << endl;
        cout << lipid->get_lipid_string(STRUCTURAL_SUBSPECIES) << endl;
        cout << lipid->get_lipid_string(MOLECULAR_SUBSPECIES) << endl;
        cout << lipid->get_lipid_string(SPECIES) << endl;
        cout << lipid->get_lipid_string(CLASS) << endl;
        cout << lipid->get_lipid_string(CATEGORY) << endl;
        delete lipid;
    }
    catch(LipidException& e){
        // handle the exception
        cout << e.what() << endl;
    }
    return 0;
}
```

Requesting a lipid name on a lower level than the provided will throw an exception. This functionality especially enables an easy way for computing data for histograms on lipid class or category level.

To increase the parsing performance, one can pick a parser for only one specific grammar:

```
GoslinParser goslin_parser;
GoslinFragmentParser goslin_fragment_parser;
LipidMapsParser lipid_maps_parser;
SwissLipidsParser swiss_lipids_parser;
HmdbParser hmdb_parser;
```

3 Python Implementation

This is the documentation for the Goslin reference implementation for Python 3. Please be aware, that the documentation is dedicated to developers of tools for computational lipidomics who want to insert pygoslin into their project. If you are interested to run Goslin as a user, please read Section 1. The pygoslin implementation has been developed with the following objectives:

1. To ease the handling with lipid names for developers working on mass spectrometrybased lipidomics tools.
2. To offer a tool that unifies all existing dialects of lipid names.

It is an open-source package under the MIT License available via github[3]. For a detailed structure of the implementation, read Supplementary Section 6.

Prerequisites

The pygoslin package uses Python's package management system *pip* to create an isolated and defined build environment. You need Python >=3.5 and the following packages to build the pygoslin package:

```
python3-pip
cython (module for Python 3)
make (optional)
```

To install the package globally in your Python distribution, simply type:

```
$ [sudo] make install
```

or

```
$ [sudo] python setup.py install
```

Be sure that you have root permissions.

Testing pygoslin

We set up more than 150 000 single unit and integration tests, to ensure that pygoslin is parsing correctly. To run the tests, please type:

```
$ make test
```

or

[3] https://github.com/lifs-tools/pygoslin

```
$ python3 -m unittest pygoslin.tests.FattyAcidTest
$ python3 -m unittest pygoslin.tests.ParserTest
$ python3 -m unittest pygoslin.tests.SwissLipidsTest
$ python3 -m unittest pygoslin.tests.GoslinTest
$ python3 -m unittest pygoslin.tests.LipidMapsTest
$ python3 -m unittest pygoslin.tests.HmdbTest
```

Using pygoslin

The two major functions within pygoslin are the parsing and printing of lipid names. You have several options, to access these functions. This example will demonstrate both functions the easiest way. Open a Python shell and type in:

```python
from pygoslin.parser.Parser import LipidParser

lipid_parser = LipidParser() # setup the parser
lipid_name = "PE 16:1-12:0"

try:
    lipid = lipid_parser.parse(lipid_name) # start parsing
    print(lipid.get_lipid_string())
except Exception as e:
    print(e) # handle the exception
```

For all unexpected states, an exception is being raised. Be aware, that this method uses all available grammars in turn until a lipid name can be parsed successfully by a parser. Currently, five grammars are available, namely: Goslin, GoslinFragment, LipidMaps, SwissLipids, HMDB. To use a specific grammar / parser, you can use the following code:

```python
# using solely the Goslin parser
from pygoslin.parser.Parser import GoslinParser
goslin_parser = GoslinParser()

lipid_name = "Cer 18:1;2/12:0"
try:
    lipid = goslin_parser.parse(lipid_name)
    print(lipid.get_lipid_string())
except Exception as e:
    print(e)
```

```python
# using solely the Goslin Fragment parser
from pygoslin.parser.Parser import GoslinFragmentParser
goslin_fragment_parser = GoslinFragmentParser()

lipid_name = "Cer 18:1;2/12:0"
try:
    lipid = goslin_fragment_parser.parse(lipid_name)
    print(lipid.get_lipid_string())
except Exception as e:
    print(e)
```

```python
# using solely the LipidMaps parser
from pygoslin.parser.Parser import LipidMapsParser
lipid_maps_parser = LipidMapsParser()

lipid_name = "Cer(d18:1/12:0)"
try:
    lipid = lipid_maps_parser.parse(lipid_name)
    print(lipid.get_lipid_string())
except Exception as e:
    print(e)
```

```python
# using solely the SwissLipids parser
from pygoslin.parser.Parser import SwissLipidsParser
swiss_lipids_parser = SwissLipidsParser()

lipid_name = "Cer(d18:1/12:0)"
try:
    lipid = swiss_lipids_parser.parse(lipid_name)
    print(lipid.get_lipid_string())
except Exception as e:
    print(e)
```

```python
# using solely the HMDB parser
from pygoslin.parser.Parser import HmdbParser
hmdb_parser = HmdbParser()

lipid_name = "Cer(d18:1/12:0)"
try:
    lipid = hmdb_parser.parse(lipid_name)
    print(lipid.get_lipid_string())
except Exception as e:
    print(e)
```

To be as generic as possible, no treatment of validation of the fragment is conducted within the GoslinFragmentParser.

To retrieve a parsed lipid name on a higher hierarchy of lipid level, simply define the level when requesting the lipid name:

```python
# report on different lipid hierarchies
from pygoslin.parser.Parser import *
from pygoslin.domain.LipidLevel import LipidLevel

parser = LipidParser()
# providing a lipid name on isomeric subspecies level
lipid_name = "PA 18:1(5Z)/12:0"
```

```
try:
    lipid = parser.parse(lipid_name)
    print(lipid.get_lipid_string(LipidLevel.ISOMERIC_SUBSPECIES))
    print(lipid.get_lipid_string(LipidLevel.STRUCTURAL_SUBSPECIES))
    print(lipid.get_lipid_string(LipidLevel.MOLECULAR_SUBSPECIES))
    print(lipid.get_lipid_string(LipidLevel.SPECIES))
    print(lipid.get_lipid_string(LipidLevel.CLASS))
    print(lipid.get_lipid_string(LipidLevel.CATEGORY))
except Exception as e:
    print(e)
```

This functionality especially enables an easy way for computing data for histograms on lipid class or category level. Requesting a lipid name on a lower level than the provided will raise an exception.

4 R Implementation

This project is a parser, validator and normalizer implementation for shorthand lipid nomenclatures, using the Grammar of Succinct Lipid Nomenclatures project for the R language [4].

Goslin defines multiple grammars compatible with ANTLRv4 for different sources of shorthand lipid nomenclature. This allows to generate parsers based on the defined grammars, which provide immediate feedback whether a processed lipid shorthand notation string is compliant with a particular grammar, or not.

rgoslin uses the Goslin grammars and the cppgoslin parser to support the following general tasks:

1. Facilitate the parsing of shorthand lipid names dialects.
2. Provide a structural representation of the shorthand lipid after parsing.
3. Use the structural representation to generate normalized names.

rgoslin is an open-source package available via github[5].

Prerequisites

This project uses the R programming language. To be able to use it, please install R[6] following the instructions for your particular operating system. rgoslin is based on native C++ code (via cppgoslin). It therefore requires additional tools on your system to compile and install it. Please see the Rcpp FAQ[7], question 1.3 for installation details for your specific operating system.

Install the ‘devtools‘ package with the following command.

```r
if(!require(devtools)) { install.packages("devtools") }
```

Run

```r
install_github("lifs-tools/rgoslin")
```

to install from the github repository.

This will install the latest, potentially unstable development version of the package with all required dependencies into your local R installation.

If you want to use a proper release version, referenced by a Git tag (here: v1.0.0) install the package as follows:

[4]https://www.r-project.org/
[5]https://github.com/lifs-tools/rgoslin
[6]https://cloud.r-project.org/
[7]https://cran.r-project.org/web/packages/Rcpp/vignettes/Rcpp-FAQ.pdf

```
install_github("lifs-tools/rgoslin", ref="v1.0.0")
```

If you have cloned the code locally, use devtools as follows. Make sure you set the working directory to where the API code is located. Then execute

```
library(devtools)
install(".")
```

Testing rgoslin

rgoslin uses the testthat R package to provide unit tests for the lipid name parsing methods. The tests are located in the `tests` folder. To run the tests, execute

```
library(devtools)
test()
```

Using rgoslin

To load the package, start an R session and type

```
library(rgoslin)
```

Type the following to see the package vignette / tutorial:

```
vignette('introduction', package = 'rgoslin')
```

In order to use the provided translation functions of rgoslin, you first need to load the library.

```
library(rgoslin)
```

To check, whether a given lipid name can be parsed by any of the parsers supplied by cppgoslin, you can use the `isValidLipidName` method. It will return `TRUE` if the given name can be parsed by any of the available parsers and `FALSE` if the name was not parseable.

```
isValidLipidName("PC 32:1")
```

Using `parseLipidName` with a lipid name returns a named vector of properties of the parsed lipid name.

```
pc32vector <- parseLipidName("PC 32:1")
pc32df <- as.data.frame(t(pc32vector))
```

If you want to set the grammar to parse against manually, this is also possible:

```
originalName <- "TG(16:1(5E)/18:0/20:2(3Z,6Z))"
tagVec <- rgoslin::parseLipidNameWithGrammar(originalName, "LipidMaps")
tagDf <- as.data.frame(t(tagVec))
```

Currently, the following grammars are available: LipidMaps, SwissLipids, Goslin, Goslin-Fragments, HMDB.

If you want to parse multiple lipid names, use the `parseLipidNames` method with a vector of lipid names. This returns a data frame of properties of the parsed lipid names with one row per lipid.

```
multipleLipidNames <- parseLipidNames(c("PC 32:1","LPC 34:1","TG(18:1_18:0_16:1)"))
```

Finally, if you want to parse multiple lipid names and want to use one particular grammar:

```
originalNames <- c("PC 32:1","LPC 34:1","TAG 18:1_18:0_16:1")
multipleLipidNamesWithGrammar <- parseLipidNamesWithGrammar(originalNames,
    "Goslin")
```

5 Java Implementation

This project is a parser, validator and normalizer implementation for shorthand lipid nomenclatures, based on Goslin for the Java programming language[8].

Goslin defines multiple grammars compatible with ANTLRv4 for different sources of shorthand lipid nomenclature. This allows to generate parsers based on the defined grammars, which provide immediate feedback whether a processed lipid shorthand notation string is compliant with a particular grammar, or not.

Here, jgoslin uses the Goslin grammars and the generated parsers to support the following general tasks:

1. Facilitate the parsing of shorthand lipid names dialects.
2. Provide a structural representation of the shorthand lipid after parsing.
3. Use the structural representation to generate normalized names.

Furthermore, jgoslin is an open-source package available via github[9].

Prerequisites

This project is based on Java 11. To use it, you need a Java Runtime Environment (JRE) installed on your system. If you want to use the library in your own Java projects, you need a Java Development Kit (JDK) installed on your system. Please consult `https://adoptopenjdk.net/installation.html` for installation options and instructions for your operating system.

Installation instructions

Building the project and generating client code from the command-line

In order to build the client code and run the unit tests, execute the following command from a terminal:

```
./mvnw install
```

or on Windows:

```
mvnw.bat install
```

This compiles and tests the Java library.

[8]`https://go.java/`

[9]`https://github.com/lifs-tools/jgoslin`

Testing jgoslin

Here, jgoslin comes with a comprehensive collection of unit (JUnit 5), integration (JUnit 5) and acceptance (Cucumber) tests. You can run all of them as follows:

```
./mvnw verify
```

Using the command-line interface

The `cli` sub-project provides a command line interface (CLI) for parsing of lipid names either from the command line or from a file with one lipid name per line.

After building the project as mentioned above with `./mvnw install`, the `cli/target` folder will contain the `jgoslin-cli-<VERSION>-bin.zip` file. Alternatively, you can download the latest cli zip file from Bintray: https://bintray.com/lifs/maven/jgoslin-cli[Search for latest jgoslin-cli-<VERSION>-bin.zip artefact] and click to download.

In order to run the validator, unzip that file, change into the unzipped folder and run

```
java -jar jgoslin-cli-<VERSION>.jar
```

to see the available options.

To parse a single lipid name from the command line using all available parsers, run

```
java -jar jgoslin-cli-<VERSION>.jar -n "Cer(d18:1/20:2)"
```

The output will tell you what is done and will echo a table of the results to the terminal:

```
Parsing lipid identifier: Cer(d18:1/20:2)
Parsing lipid identifier: Cer(d18:1/20:2)
Parsing lipid maps identifier: Cer(d18:1/20:2)
Parsing swiss lipids identifier: Cer(d18:1/20:2)
Parsing HMDB lipids identifier: Cer(d18:1/20:2)
Echoing output to stdout.
Normalized Name Original Name Grammar Message Lipid Maps Category Lipid Maps Main
    Class Functional Class Abbr Functional Class Synonyms Level Total #C Total #OH
    Total #DB LCB SN Position LCB #C LCB #OH LCB #DB LCB Bond Type FA1 SN Position
    FA1 #C FA1 #OH FA1 #DB FA1 Bond Type
Cer(d18:1/20:2) GOSLIN no viable alternative at input 'Cer('
Cer(d18:1/20:2) GOSLIN_FRAGMENTS no viable alternative at input 'Cer('

Cer 18:1;2/20:2 Cer(d18:1/20:2) LIPIDMAPS  Sphingolipid [SP]
    N-acyl-4-hydroxysphinganines (phytoceramides) [SP0203] [Cer] [Cer, Ceramide]
    STRUCTURAL_SUBSPECIES 38 2 3 1 18 2 1 ESTER 2 20 0 2 ESTER
Cer 18:1;2/20:2 Cer(d18:1/20:2) SWISSLIPIDS  Sphingolipid [SP]
    N-acyl-4-hydroxysphinganines (phytoceramides) [SP0203] [Cer] [Cer, Ceramide]
    STRUCTURAL_SUBSPECIES 38 2 3 1 18 2 1 ESTER 2 20 0 2 ESTER
Cer 18:1;2/20:2 Cer(d18:1/20:2) HMDB  Sphingolipid [SP]
    N-acyl-4-hydroxysphinganines (phytoceramides) [SP0203] [Cer] [Cer, Ceramide]
    STRUCTURAL_SUBSPECIES 38 2 3 1 1821 ESTER 2 20 0 2 ESTER
```

To parse multiple lipid names from a file via the commmand line, run

```
java -jar jgoslin-cli-<VERSION>.jar -f lipidNames.txt
```

To use a specific grammar, instead of trying all, run

```
java -jar jgoslin-cli-<VERSION>.jar -f lipidNames.txt -g GOSLIN
```

To write output to the tab-separated output file 'goslin-out.tsv' instead of to the terminal, run

```
java -jar jgoslin-cli-<VERSION>.jar -f lipidNames.txt -g GOSLIN -o
```

If you want to use all available grammars, simply omit the `-g GOSLIN` argument. Please note that you will then receive N times M lines in the output file, where N is the number of lipid names and M the number of grammars.

Using jgoslin

To integrate jgoslin in your own projects as a library, please see the README file at `https://github.com/lifs-tools/jgoslin` for more details.

The following snippet shows how to parse a shorthand lipid name with the different parsers:

```
import de.isas.lipidomics.domain.*; // contains Domain objects like LipidAdduct,
    LipidSpecies ...
import de.isas.lipidomics.palinom.*; // contains the parser implementations
...

String ref = "Cer(d18:1/20:2)";
try {
    // use the SwissLipids parser
    SwissLipidsVisitorParser slParser = new SwissLipidsVisitorParser();
    LipidAdduct sllipid = slParser.parse(ref);
    System.out.println(sllipid.getLipidString()); // to print the lipid name to
        the console
} catch (ParsingException pe) {
// catch this for any syntactical issues with the name during parsing with a
    particular parser
    pe.printStackTrace();
} catch (ParseTreeVisitorException ptve) {
// catch this for any structural issues with the name during parsing with a
    particular parser
    ptve.printStackTrace();
}

//alternatively, use the other parsers. Don't forget to place try catch blocks
    around the following lines, as for the SwissLipids parser example
    // use the LipidMAPS parser
    LipidMapsVisitorParser lmParser = new LipidMapsVisitorParser();
    LipidAdduct lmlipid = lmParser.parse(ref);
    // use the shorthand notation parser GOSLIN
    GoslinVisitorParser goslinParser = new GoslinVisitorParser();
    LipidAdduct golipid = goslinParser.parse(ref);
    // use the shorthand notation parser with support for fragments
        GOSLIN_FRAGMENTS
```

```
      GoslinFragmentsVisitorParser goslinFragmentsParser = new
          GoslinFragmentsVisitorParser();
      LipidAdduct gflipid = goslinFragmentsParser.parse(ref);
```

To retrieve a parsed lipid name on a higher hierarchy of lipid level, simply define the level when requesting the lipid name:

```
System.out.println(sllipid.getLipidString(LipidLevel.CATEGORY));
System.out.println(sllipid.getLipidString(LipidLevel.CLASS));
System.out.println(sllipid.getLipidString(LipidLevel.SPECIES));
System.out.println(sllipid.getLipidString(LipidLevel.MOLECULAR_SUBSPECIES));
System.out.println(sllipid.getLipidString(LipidLevel.STRUCTURAL_SUBSPECIES));
System.out.println(sllipid.getLipidString(LipidLevel.ISOMERIC_SUBSPECIES)); //
    will throw a ConstraintViolationException since this lipid is only on
    structural subspecies level
```

This functionality allows easy computation of aggregate statistics of lipids on lipid class, category or arbitrary levels. Requesting a lipid name on a lower level than the provided will raise an exception.

For an overview of the domain model used by jgoslin, please see Supplementary Section 6.

6 Goslin Object Model

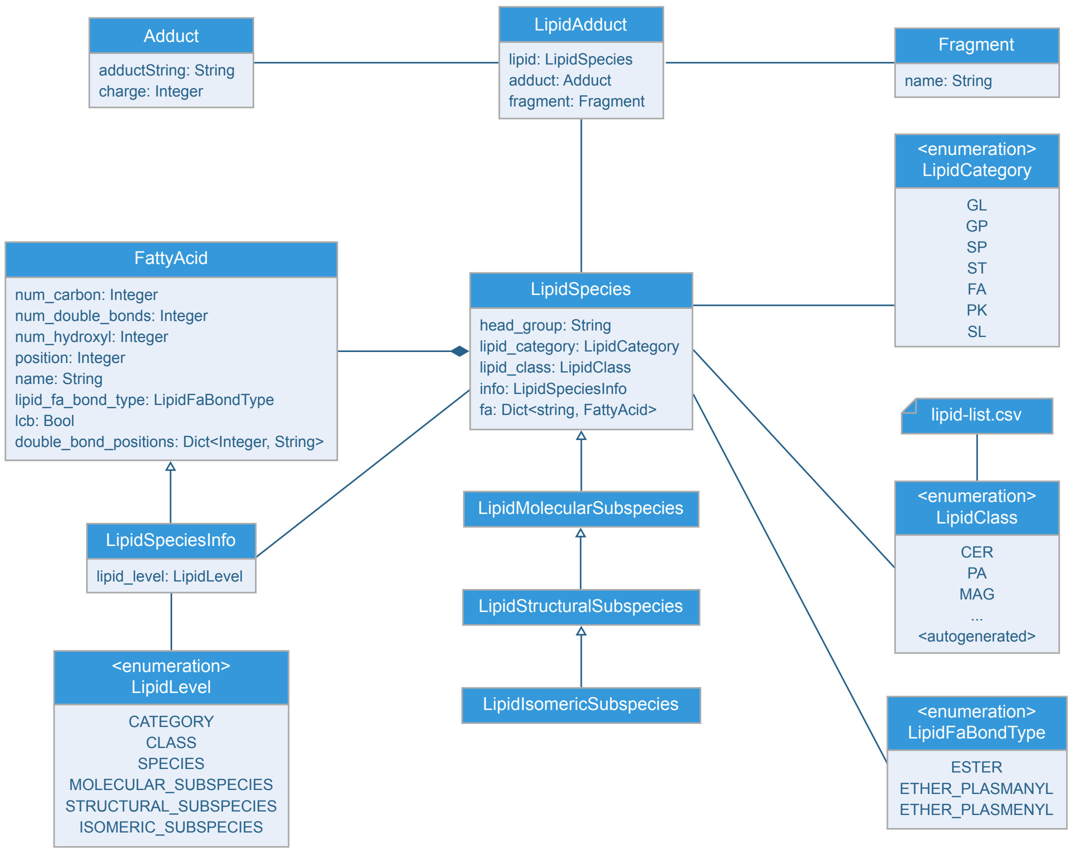


Figure S7: Goslin object model.

All goslin implementations are implementing the goslin object model as illustrated in Supplementary Figure S7. The classes `LipidCategory`, `LipidLevel`, `LipidClass`, and `LipidFaBondType` are predefined enumerations. Here, `LipidClass` is being generated automatically from a list containing lipid information (name, description, category, abbreviation, synonyms) for all implementations, see Supplementary Table S1 for details. This especially eases the maintenance and ensures that the goslin implementations have the same data base. The main class unifying all classes and being provided by the parsers is `LipidAdduct`. It contains information about the pure lipid, the adduct as well as the fragment (if defined). The different lipid classes inherit from each other in a hierarchical fashion as defined by Liebisch et al.[4]. A dictionary with the class `LipidSpecies` is storing all its associated fatty acyl chains which are defined within the class `FattyAcid`. For storing the cummulated information on species level for the carbon length, double bonds, etc, the class `LipidSpeciesInfo` is utilized.

7 List of Supported Lipids

Table S1: List of supported lipids, lipid classes and their normalized abbreviations

Category	Description	Abbreviation
Fatty acyls	Other Docosanoids	10-HDoHE
	Epoxyeicosatrienoic acids	11(12)-EET
	Hydroxy/hydroperoxyeicosatetraenoic acids	11,12-DHET
	Other Docosanoids	11-HDoHE
	Hydroxy/hydroperoxyeicosatetraenoic acids	11-HETE
	Other Octadecanoids	12(13)-EpOME
	Hydroxy/hydroperoxyeicosapentaenoic acids	12-HEPE
	Hydroxy/hydroperoxyeicosatetraenoic acids	12-HETE
	Hydroxy/hydroperoxyeicosatrienoic acids	12-HHTrE
	Fatty acids and conjugates	12-OxoETE
	Other Octadecanoids	13-HODE
	Other Octadecanoids	13-HOTrE
	Epoxyeicosatrienoic acids	14(15)-EET
	Other Eicosanoids	14(15)-EpETE
	Hydroxy/hydroperoxyeicosatetraenoic acids	14,15-DHET
	Hydroxy/hydroperoxyeicosapentaenoic acids	15-HEPE
	Hydroxy/hydroperoxyeicosatetraenoic acids	15-HETE
	Prostaglandins	15d-PGJ2
	Other Docosanoids	16-HDoHE
	Hydroxy/hydroperoxyeicosatetraenoic acids	16-HETE
	Hydroxy/hydroperoxyeicosapentaenoic acids	18-HEPE
	Epoxyeicosatrienoic acids	5(6)-EET
	Hydroxy/hydroperoxyeicosatetraenoic acids	5,12-DiHETE
	Lipoxins	5,6,15-LXA4
	Hydroxy/hydroperoxyeicosatetraenoic acids	5,6-DiHETE
	Hydroxy/hydroperoxyeicosapentaenoic acids	5-HEPE
	Hydroxy/hydroperoxyeicosatetraenoic acids	5-HETE
	Hydroxy/hydroperoxyeicosatetraenoic acids	5-HpETE
	Fatty acids and conjugates	5-OxoETE
	Epoxyeicosatrienoic acids	8(9)-EET
	Hydroxy/hydroperoxyeicosatetraenoic acids	8,9-DHET
	Other Docosanoids	8-HDoHE
	Hydroxy/hydroperoxyeicosatetraenoic acids	8-HETE
	Other Octadecanoids	9(10)-EpOME
	Hydroxy/hydroperoxyeicosapentaenoic acids	9-HEPE
	Hydroxy/hydroperoxyeicosatetraenoic acids	9-HETE
	Other Octadecanoids	9-HODE
	Other Octadecanoids	9-HOTrE
	Unsaturated fatty acids	AA
	Fatty acyl carnitines	CAR
	Fatty acyl CoAs	CoA
	Unsaturated fatty acids	DHA

Category	Description	Abbreviation
Fatty acyls	Unsaturated fatty acids	EPA
	Fatty acids and conjugates	FA
	Fatty acyl	FA
	Wax monoesters	FAHFA
	Glycerophosphoethanolamine	GP-NAE
	Leukotrienes	LTB4
	Eicosanoid derivatives	LTC4
	Leukotrienes	LTD4
	Unsaturated fatty acids	Linoleic acid
	Maresins	Maresin 1
	Fatty amides	NAE
	Prostaglandins	PGB2
	Prostaglandins	PGD2
	Prostaglandins	PGE2
	Prostaglandins	PGF2alpha
	Prostaglandins	PGI2
	Straight chain fatty acids	Palmitic acid
	Resolvin Ds	Resolvin D1
	Resolvin Ds	Resolvin D2
	Resolvin Ds	Resolvin D3
	Resolvin Ds	Resolvin D5
	Thromboxanes	TXB1
	Thromboxanes	TXB2
	Thromboxanes	TXB3
	Fatty esters	WE
	Fatty acids and conjugates	alpha-LA
	Hydroxy/hydroperoxyeicosatetraenoic acids	tetranor-12-HETE
Glycero-lipids	Diacylglycerols	DAG
	Other Glycerolipids	DGCC
	Glycosyldiradylglycerols	DGDG
	Dihexosyldiacylglycerol	DHDG
	Monoacylglycerols	MAG
	Glycosyldiacylglycerols	MGDG
	Monohexosyldiacylglycerol	MHDG
	Glycosyldiradylglycerols	SQDG
	Glycosylmonoacylglycerols	SQMG
	Triacylglycerols	TAG
Glycero-phospho-lipids	Glycosylglycerophospholipids	6-Ac-Glc-GP
	Monoacylglycerophosphomonoradylglycerols	BMP
	CDP-diacylglycerols	CDPDAG
	Cardiolipins	CL
	Glycerophosphoinositolglycans	CPA
	Glycerophosphoglycerophosphoglycerols	DLCL
	Dimethylphosphatidylethanolamine	DMPE
	Glycosyldiradylglycerols	Glc-DG
	Diacylglycosylglycerophospholipids	Glc-GP

Category	Description	Abbreviation
Glycero-phospho-lipids	Lyso-CDP-diacylglycerol	LCDPDAG
	Lysodimethylphosphatidylethanolamine	LDMPE
	Lysomonomethylphosphatidylethanolamine	LMMPE
	Monoacylglycerophosphates	LPA
	Monoacylglycerophosphocholines	LPC
	Monoacylglycerophosphoethanolamines	LPE
	1Z-alkenylglycerophosphoglycerols	LPG
	Monoacylglycerophosphoinositols	LPI
	Monoacylglycerophosphoinositolglycans	LPIM1
	Glycerophosphoinositolglycans	LPIM2
	Glycerophosphoinositolglycans	LPIM3
	Glycerophosphoinositolglycans	LPIM4
	Glycerophosphoinositolglycans	LPIM5
	Glycerophosphoinositolglycans	LPIM6
	Lysophosphatidylinositol- mannosideinositolphos-phate	LPIMIP
	Lysophosphatidylinositol-glucosamine	LPIN
	Monoacylglycerophosphoserines	LPS
	Glycerophosphoglycerophosphoglycerols	MLCL
	Monomethylphosphatidylethanolamine	MMPE
	Glycerophosphoethanolamine	NAPE
	Diacylglycerophosphates	PA
	Oxidized glycerophosphocholines	PC
	Oxidized glycerophosphoethanolamines	PE
	Glycerophosphoethanolamines	PE-NMe
	Glycerophosphoethanolamines	PE-NMe2
	Glycerophosphoethanolamines	PEt
	Diacylglycerophosphoglycerols	PG
	Diacylglycerophosphoglycerophosphates	PGP
	Diacylglycerophosphoinositols	PI
	Diacylglycerophosphoinositolglycans	PIM1
	Glycerophosphoinositolglycans	PIM2
	Glycerophosphoinositolglycans	PIM3
	Glycerophosphoinositolglycans	PIM4
	Glycerophosphoinositolglycans	PIM5
	Glycerophosphoinositolglycans	PIM6
	Phosphatidylinositol mannoside inositol phosphate	PIMIP
	Diacylglycerophosphoinositol monophosphates	PIP
	Diacylglycerophosphoinositol bisphosphates	PIP2
	Glycerophosphoinositolbisphosphates	PIP2[3',4']
	Glycerophosphoinositolbisphosphates	PIP2[3',5']
	Glycerophosphoinositolbisphosphates	PIP2[4',5']
	Diacylglycerophosphoinositol trisphosphates	PIP3
	Glycerophosphoinositoltrisphosphates	PIP3[3',4',5']
	Glycerophosphoinositolmonophosphates	PIP[3']
	Glycerophosphoinositolmonophosphates	PIP[4']

Category	Description	Abbreviation
	Glycerophosphoinositolmonophosphates	PIP[5']
	Diacylglyceropyrophosphates	PPA
	Diacylglycerophosphoserines	PS
	Diacylglycerophosphoserines	PS-NAc
	Other Glycerophospholipids	PT
	Glycerophosphonocholines	PnC
	Glycerophosphoinositolglycans	PnE
	Diacylglycerophosphomonoradylglycerols	SLBPA
Saccharo-lipids	Acyltrehaloses	AC2SGL
	Acyltrehaloses	DAT
	Acyltrehaloses	PAT16
	Acyltrehaloses	PAT18
Sphingo-lipids	Glycosphingolipids	(3'-sulfo)LacCer
	Glycosphingolipids	(Fuc)iGb3Cer
	Acylceramides	1-O-behenoyl-Cer
	Acylceramides	1-O-carboceroyl-Cer
	Acylceramides	1-O-cerotoyl-Cer
	Acylceramides	1-O-eicosanoyl-Cer
	Acylceramides	1-O-lignoceroyl-Cer
	Acylceramides	1-O-myristoyl-Cer
	Acylceramides	1-O-palmitoyl-Cer
	Acylceramides	1-O-stearoyl-Cer
	Acylceramides	1-O-tricosanoyl-Cer
	Globoside	Ac-O-9-GD1a
	Globoside	Ac-O-9-GT1b
	Globoside	Ac-O-9-GT3
	Glycosphingolipids	Branched-Forssman
	Ceramide-1-phosphates	C1P
	N-acylsphingosines (ceramides)	Cer
	Ceramide 1-phosphates	CerP
	Glycosphingolipids	DSGG
	Ceramide phosphoethanolamines	EPC
	Simple Glc series	FMC-5
	Neutral glycosphingolipids	FMC-6
	Glycosphingolipids	Forssman
	Acidic glycosphingolipids	Fuc(Gal)-GM1
	Glycosphingolipids	Fuc(Gal)Gal-iGb4Cer
	Glycosphingolipids	Fuc-Branched-Forssman
	Globoside	Fuc-GA1
	Globoside	Fuc-GD1b
	Globoside	Fuc-GM1
	Globoside	Fuc-GM1(NeuGc)
	Glycosphingolipids	Fuc-iGb3Cer
	Glycosphingolipids	FucGalGb3Cer

Category	Description	Abbreviation
	Glycosphingolipids	GA1
	Glycosphingolipids	GA2
	Neutral glycosphingolipids	GB4
	Glycosphingolipids	GD1
	Ganglioside GD1a(d18:1(4E))	GD1a
	Ganglioside GD1a alpha(d18:1(4E))	GD1a alpha
	Globoside	GD1a(NeuAc/NeuGc)
	Globoside	GD1a(NeuGc/NeuAc)
	Globoside	GD1a(NeuGc/NeuGc)
	Ganglioside GD1b(d18:1(4E))	GD1b
	Ganglioside GD1c(d18:1(4E))	GD1c
	Globoside	GD1c(NeuGc/NeuGc)
	Glycosphingolipids	GD2
	Glycosphingolipids	GD3
	Glycosphingolipids	GM1
	Globoside	GM1 alpha
	Globoside	GM1(NeuGc)
	Ganglioside GM1b(d18:1(4E))	GM1b
	Globoside	GM1b(NeuGc)
	Glycosphingolipids	GM2
	Globoside	GM2(NeuGc)
	Glycosphingolipids	GM3
	Gangliosides	GM4
	Glycosphingolipids	GP1
	Ganglioside GP1c(d18:1(4E))	GP1c
	Ganglioside GP1c alpha(d18:1(4E))	GP1c alpha
	Glycosphingolipids	GQ1
	Ganglioside GQ1b(d18:1(4E))	GQ1b
	Ganglioside GQ1b alpha(d18:1(4E))	GQ1b alpha
	Ganglioside GQ1c(d18:1(4E))	GQ1c
	Glycosphingolipids	GT1
	Ganglioside GT1a(d18:1(4E))	GT1a
	Ganglioside GT1a alpha(d18:1(4E))	GT1a alpha
	Ganglioside GT1b(d18:1(4E))	GT1b
	Globoside	GT1b alpha
	Globoside	GT1b alpha(NeuGc)
	Ganglioside GT1c(d18:1(4E))	GT1c
	Glycosphingolipids	GT2
	Glycosphingolipids	GT3
	Globoside	Gal(Fuc)-GA1
	Globoside	Gal(Fuc)-GD1b
	Globoside	Gal-GD1b
	Glycosphingolipids	Gal-iGb4Cer
	Globoside	GalGal-GD1b
	Glycosphingolipids	GalGalGalGb3Cer
	Glycosphingolipids	GalGalGb3Cer

Category	Description	Abbreviation
	Globoside	GalGalNAc-GM1b(NeuGc)
	Glycosphingolipids	GalGb3Cer
	Glycosphingolipids	GalGb4Cer
	Glycosphingolipids	GalGlcNAc-GalGb4Cer
	Globoside	GalNAc-GD1a
	Globoside	GalNAc-GD1a(NeuAc/NeuGc)
	Globoside	GalNAc-GD1a(NeuGc/NeuAc)
	Globoside	GalNAc-GM1
	Globoside	GalNAc-GM1b
	Globoside	GalNAc-GM1b(NeuGc)
	Globoside	GalNAcGal(Fuc)-GA1
	Glycosphingolipids	GalNAcGalGb3Cer
	Glycosphingolipids	Gb3
	Glycosphingolipids	Gb3Cer
	Glycosphingolipids	Gb4Cer
	Glycosphingolipids	GlcNAc-GalGb4Cer
	Glycosphingolipids	GlcNAcGb3Cer
	Glycosphingolipids	Globo-A
	Glycosphingolipids	Globo-B
	Glycosphingolipids	Globo-H
	Glycosphingolipids	Globo-Lex-9
	Glycosphingolipids	Hex2Cer
	Neutral glycosphingolipids	Hex3Cer
	Glycosphingolipids	HexCer
	Ceramide phosphoinositols	IPC
	Sphinganines	LCB
	Sphingoid base 1-phosphates	LCBP
	Hexosylsphingosine	LHexCer
	Ceramides	LSM
	Globoside	Lex-GM1
	Phosphosphingolipids	M(IP)2C
	Phosphosphingolipids	MIPC
	Glycosphingolipids	MSGG
	Glycosphingolipids	NOR1
	Glycosphingolipids	NOR2
	Glycosphingolipids	NORint
	Glycosphingolipids	NeuAc(alpha2-6)-MSGG
	Glycosphingolipids	NeuAc(alpha2-8)-MSGG

Category	Description	Abbreviation
Sphingo-lipids	Glycosphingolipids	NeuAcGal-iGb4Cer
	Glycosphingolipids	NeuGc-GalGb4Cer
	Globoside	NeuGc-LacNAc-GM1(NeuGc)
	Glycosphingolipids	NeuGcNeuGc-GalGb4Cer
	Glycosphingolipids	Para-Forssman
	Globoside	SB1a
	Glycosphingolipids	SHex2Cer
	Sulfoglycosphingolipids (sulfatides)	SHexCer
	Ceramide phosphocholines (sphingomyelins)	SM
	Globoside	SM1a
	Globoside	SM1b
	Globoside	SO3-GM1(NeuGc)
	Glycosphingolipids	SO3-Gal-iGb4Cer
	Glycosphingolipids	SO3-GalGb4Cer
	Glycosphingolipids	SO3-Gb4Cer
	Glycosphingolipids	SO3-iGb4Cer
	Glycosphingolipids	SulfoGalCer
	Glycosphingolipids	i-Forssman
	Glycosphingolipids	iGb3Cer
	Glycosphingolipids	iGb4Cer
Sterols	Sterol esters	SE
	Steryl esters	SE 27:1
	Desmosterol Ester	SE 27:2
	Ergostadienol Ester	SE 28:2
	Ergosterol Ester	SE 28:3
	Stigmasterol Ester	SE 29:2
	Lanosterol Ester	SE 30:2
	Sterols	ST
	Cholesterol and derivatives	ST 27:1;1
	Desmosterol	ST 27:2;1
	Ergostadienol	ST 28:2;1
	Ergosterol	ST 28:3;1
	Stigmasterol	ST 29:2;1
	Lanosterol	ST 30:2;1
Polyketides	Anacardic acids and derivatives	ANACARD
	Alkyl catechols and derivatives	CATECHOL
	Alkyl phenols and derivatives	PHENOL
	Alkyl resorcinols and derivatives	RESORCINOL

Acronyms

API application programming interface. 6, 7

CLI command line interface. 20

Goslin grammar of succinct lipid nomenclatures. 2, 3, 6, 9, 12, 16, 19, 23

HTTP hypertext transfer protocol. 6, 7

JDK Java Development Kit. 19

JRE Java Runtime Environment. 19

JSON JavaScript object notation. 6

LCB long chain base. 7

REST representational state transfer. 6, 7

References

[1] Fahy, E.; Subramaniam, S.; Murphy, R. C.; Nishijima, M.; Raetz, C. R. H.; Shimizu, T.; Spener, F.; van Meer, G.; Wakelam, M. J. O.; Dennis, E. A. Update of the LIPID MAPS comprehensive classification system for lipids. *Journal of Lipid Research* **2009**, *50*, S9–S14.

[2] Aimo, L.; Liechti, R.; Hyka-Nouspikel, N.; Niknejad, A.; Gleizes, A.; Götz, L.; Kuznetsov, D.; David, F. P.; van der Goot, F. G.; Riezman, H.; Bougueleret, L.; Xenarios, I.; Bridge, A. The SwissLipids knowledgebase for lipid biology. *Bioinformatics* **2015**, *31*, 2860–2866.

[3] Wishart, D. S. et al. HMDB: the Human Metabolome Database. *Nucleic Acids Research* **2007**, *35*, D521–D526.

[4] Liebisch, G.; Vizcaíno, J. A.; Köfeler, H.; Trötzmüller, M.; Griffiths, W. J.; Schmitz, G.; Spener, F.; Wakelam, M. J. O. Shorthand notation for lipid structures derived from mass spectrometry. *Journal of Lipid Research* **2013**, *54*, 1523–1530.