

# Bioconda Recipes

meta.yaml build.sh post-link.sh

<https://bioconda.github.io/contributor/guidelines.html>

<https://docs.conda.io/projects/conda-build/en/latest/resources/define-metadata.html>

# Limitations

Supported OSs:

- Linux & MacOS

Supported Repositories:

- as-yet-unbuilt recipes in the repo but that will be included in the PR
- conda-forge channel
- bioconda channel
- default Anaconda channel

# Limitations

Supported Python versions:

- 2.7, 3.6, 3.7, 3.8 (development)

Supported Languages (other than Python):

- R
- Java
- Perl
- C/C++
- Haskell
- Fortran (**Not listed**)

# meta.yaml

- Template Jinja2 template language over yaml
- Preprocessing selectors are also replaced before installation

# meta.yaml: Jinja2

```
{% set name = "biobb_md" %}
{% set version = "3.5.1" %}
{% set file_ext = "tar.gz" %}
{% set hash_type = "sha256" %}
{% set hash_value = "20112124ccda9f95f708bd98a8b34b539b0390778b07adfcf93d59655340706e" %}

package:
  name: '{{ name|lower }}'
  version: '{{ version }}'

source:
  url: https://pypi.io/packages/source/{{ name[0] }}/{{ name }}/{{ name }}-{{ version }}.{{ file_ext }}
  '{{ hash_type }}': '{{ hash_value }}'
```

# meta.yaml: Preprocessing Selectors

```
source:
- url: http://packages.sequan.de/yara/yara-{{ version }}-Mac-x86_64.zip      # [osx]
  sha256: d519e797c1c66252331146b63f0cb6edba9c1a6a9e7b342fd60e7344b29baf36 # [osx]
- url: http://packages.sequan.de/yara/yara-{{ version }}-Linux-x86_64_sse4.tar.bz2 # [linux]
  sha256: 4f68552fbb4e4002fc4320bdd60b76c678e17d087bd3f893bf179387b1668b40    # [linux]
```

```
requirements:
  host:
    - python ==3.7.*
    - setuptools
    - tensorflow ==2.3.0 # [linux]
    - tensorflow ==2.0.0 # [osx]
  run:
    - python ==3.7.*
    - tensorflow ==2.3.0 # [linux]
    - tensorflow ==2.0.0 # [osx]
```

# meta.yaml: Sections

- package
- source
- build
- requirements
- test
- outputs
- about
- app
- extra

# meta.yaml: package section

package:

name: *name\_of\_your\_project* (no quotes needed, no spaces)

version: "x.x.x" (ie. "3.5.1")

```
{% set name = "biobb_md" %}  
{% set version = "3.5.1" %}  
{% set file_ext = "tar.gz" %}  
{% set hash_type = "sha256" %}  
{% set hash_value = "20112124ccda9f95f7081" %}  
  
package:  
  name: '{{ name|lower }}'  
  version: '{{ version }}'
```



# meta.yaml: source section

source:

url: *https://...* (it can be a git repo, pypi or file in server)  
md5: xxxxxxxxxxx (use one of the following: md5, sha1, sha256)

```
source:
- url: http://packages.seqan.de/yara/yara-{{ version }}-Mac-x86_64.zip      # [osx]
  sha256: d519e797c1c66252331146b63f0cb6edba9c1a6a9e7b342fd60e7344b29baf36 # [osx]
- url: http://packages.seqan.de/yara/yara-{{ version }}-Linux-x86_64_sse4.tar.bz2 # [linux]
  sha256: 4f68552fbb4e4002fc4320bdd60b76c678e17d087bd3f893bf179387b1668b40    # [linux]
```

# meta.yaml: build section

build:

number: X (integer 0, 1, 2... it's like a version of the recipe)

noarch: python (for pure python and platform independent packages)

skip: True # [osx] (conda will skip the build of this recipe, for platform dependent)

```
build:  
  number: 0  
  noarch: python
```

```
build:  
  number: 4
```

# meta.yaml: requirements section

requirements:

build: *build from build.sh dependencies (compilers not listed anywhere)*

host: same as build section in case the build and the host platform are not the same

run: packages required in runtime

```
requirements:
  build:
    - {{ compiler('c') }}
    - {{ compiler('cxx') }}
    - {{ compiler('fortran') }}
    - make
  host:
  run:
```

```
requirements:
  host:
    - python ==3.7.*
    - setuptools
    - biobb_common ==3.5.1
    - gromacs ==2019.1
  run:
    - python ==3.7.*
    - biobb_common ==3.5.1
    - gromacs ==2019.1
```

# meta.yaml: test section

test:

commands: *for command line tools tests if exit code is 0.*

import: *for python packages tests if it is possible to import a package*

```
test:
  imports:
    - biobb_md
    - biobb_md.gromacs
    - biobb_md.gromacs_extra
```

```
test:
  commands:
    - cmip -h
```

# meta.yaml: about section

about:

```
home: ...  
license: ...  
license_family: ...  
license_file: ...  
summary: ...  
description: ...
```

```
about:  
  home: https://github.com/bioexcel/biobb_md  
  license: Apache Software License  
  license_family: APACHE  
  license_file: LICENSE  
  summary: Biobb_md is the Biobb module collection to perfo  
  description: "Biobb_md is the Biobb module collection to  
  doc_url: http://biobb_md.readthedocs.io/en/latest/  
  dev_url: https://github.com/bioexcel/biobb_md
```

```
about:  
  home: http://mmb.irbbarcelona.org/gitlab/gelipi/CMIP  
  license: Apache Software License  
  license_family: APACHE  
  summary: CMIP Classical Molecular Interaction Potentials  
  description: "The latest version of the classical molecula
```

# meta.yaml: about section

about:

```
home: ...  
license: ...  
license_family: ...  
license_file: ...  
summary: ...  
description: ...
```

```
about:  
  home: https://github.com/bioexcel/biobb_md  
  license: Apache Software License  
  license_family: APACHE  
  license_file: LICENSE  
  summary: Biobb_md is the Biobb module collection to perfo  
  description: "Biobb_md is the Biobb module collection to  
  doc_url: http://biobb_md.readthedocs.io/en/latest/  
  dev_url: https://github.com/bioexcel/biobb_md
```

```
about:  
  home: http://mmb.irbbarcelona.org/gitlab/gelipi/CMIP  
  license: Apache Software License  
  license_family: APACHE  
  summary: CMIP Classical Molecular Interaction Potentials  
  description: "The latest version of the classical molecula
```

# meta.yaml: extra section

Schema-free section

```
extra:  
  any kind: ...  
  of: ...  
  extra information: ...
```

```
extra:  
  recipe-maintainers: PauAndrio
```

# build.sh: Bash style installation script

Provided env vars:

- `$PREFIX` The install prefix (the root directory of the new environment)
- `$PKG_NAME` The name of the package
- `$PKG_VERSION` The version of the package
- `$PKG_BUILDNUM` The build number of the package
- `$SP_DIR` Site-packages directory of the new environment (**not listed**)

Provided compiler vars:

- `${FC}` Fortran 77 compiler (not listed)
- `${CXX}` C++ compiler (not listed)
- `${C}` C compiler (not listed)



# post-link.sh: Print messages after installation

- Not working for messages (does not respect break lines)
- Everything done here is not translated to the container