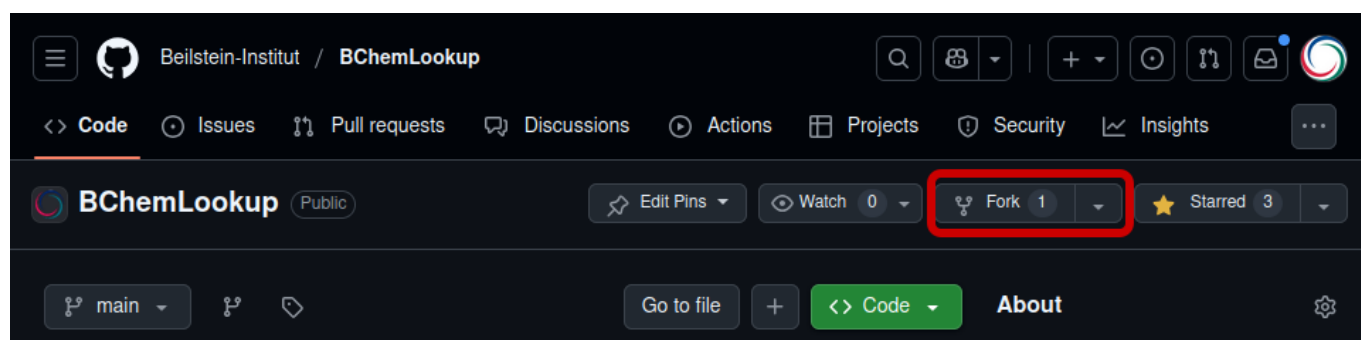


# How to create a Pull Request

This tutorial shows how to contribute to this project by creating a "Pull request".

## Fork the repository

- First you need a GitHub account, see [Creating an account on GitHub] (<https://docs.github.com/en/get-started/start-your-journey/creating-an-account-on-github>) for more details.
- On GitHub, navigate to the [ChemLookup](#) repository. Click the **Fork** button in the top right corner:




- Select an owner for the forked repository in the dropdown menu under "Owner" and type a name under "Repository name" if you do not wish to use the same name which is set by default, then click **Create fork** in the bottom right corner:

## Create a new fork

A *fork* is a copy of a repository. Forking a repository allows you to freely experiment with changes without affecting the original project. [View existing forks.](#)

Required fields are marked with an asterisk (\*).

**Owner \*** **Repository name \***

 fbaensch-beilstein / BChemLookup


✔ BChemLookup is available.

By default, forks are named the same as their upstream repository. You can customize the name to distinguish it further.

**Description (optional)**

An Open Science Initiative for Mapping Common Chemical Abbreviations

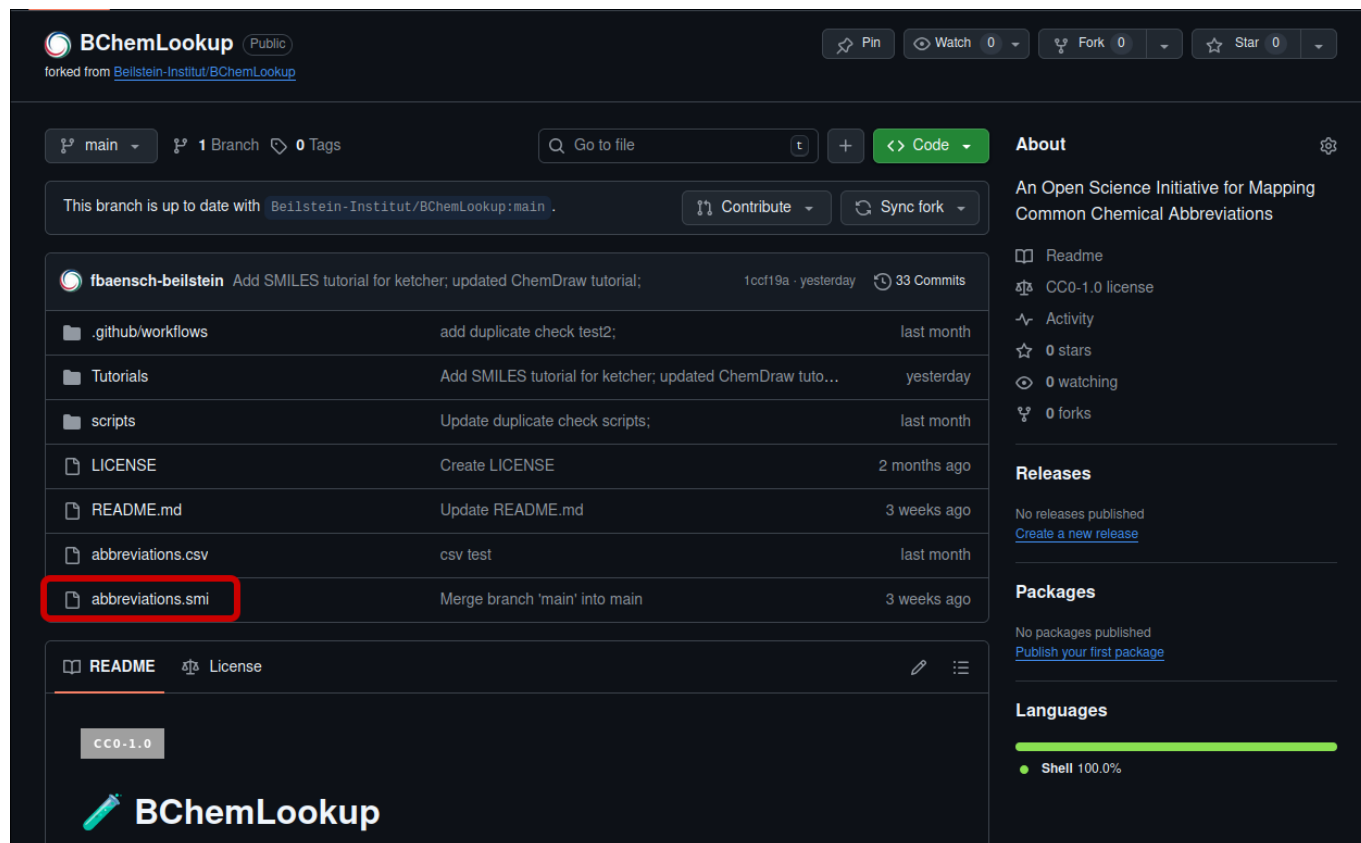
☒ Copy the `main` branch only  
Contribute back to Beilstein-Institut/BChemLookup by adding your own branch. [Learn more.](#)

 You are creating a fork in your personal account.

Create fork

## Working in browser

- In the forked repository, select the list to which you wish to contribute, for example `abbreviations.smi`:



**BChemLookup** (Public)  
forked from Beilstein-Institut/BChemLookup

main 1 Branch 0 Tags

Go to file

This branch is up to date with Beilstein-Institut/BChemLookup:main. [Contribute](#) [Sync fork](#)

**faensch-beilstein** Add SMILES tutorial for ketcher; updated ChemDraw tutorial; 1ccf19a · yesterday 33 Commits

File	Commit	Time
.github/workflows	add duplicate check test2;	last month
Tutorials	Add SMILES tutorial for ketcher; updated ChemDraw tuto...	yesterday
scripts	Update duplicate check scripts;	last month
LICENSE	Create LICENSE	2 months ago
README.md	Update README.md	3 weeks ago
abbreviations.csv	csv test	last month
abbreviations.smi	Merge branch 'main' into main	3 weeks ago

**README** License

CC0-1.0

**BChemLookup**

**About**  
An Open Science Initiative for Mapping Common Chemical Abbreviations

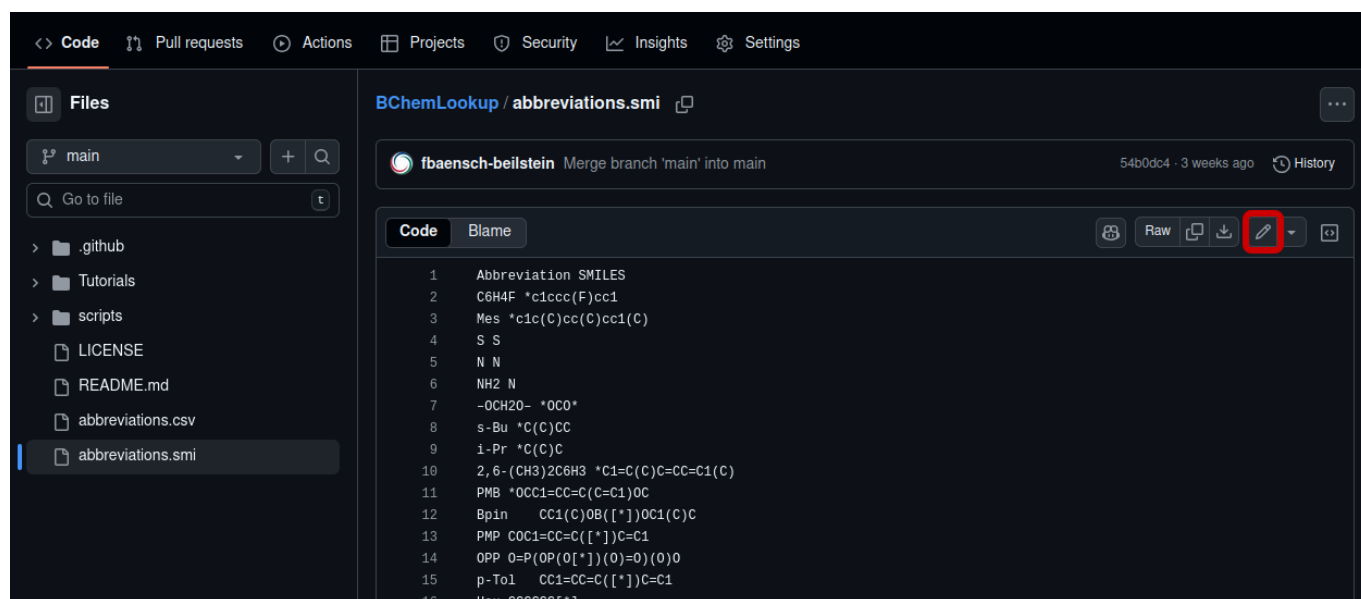
Readme  
CC0-1.0 license  
Activity  
0 stars  
0 watching  
0 forks

**Releases**  
No releases published  
[Create a new release](#)

**Packages**  
No packages published  
[Publish your first package](#)

**Languages**  
Shell 100.0%

- Click on **Edit this file** (small pen icon) in the top right corner:



**BChemLookup / abbreviations.smi**

**faensch-beilstein** Merge branch 'main' into main 54b0dc4 · 3 weeks ago History

**Code** Blame

Raw Download Edit

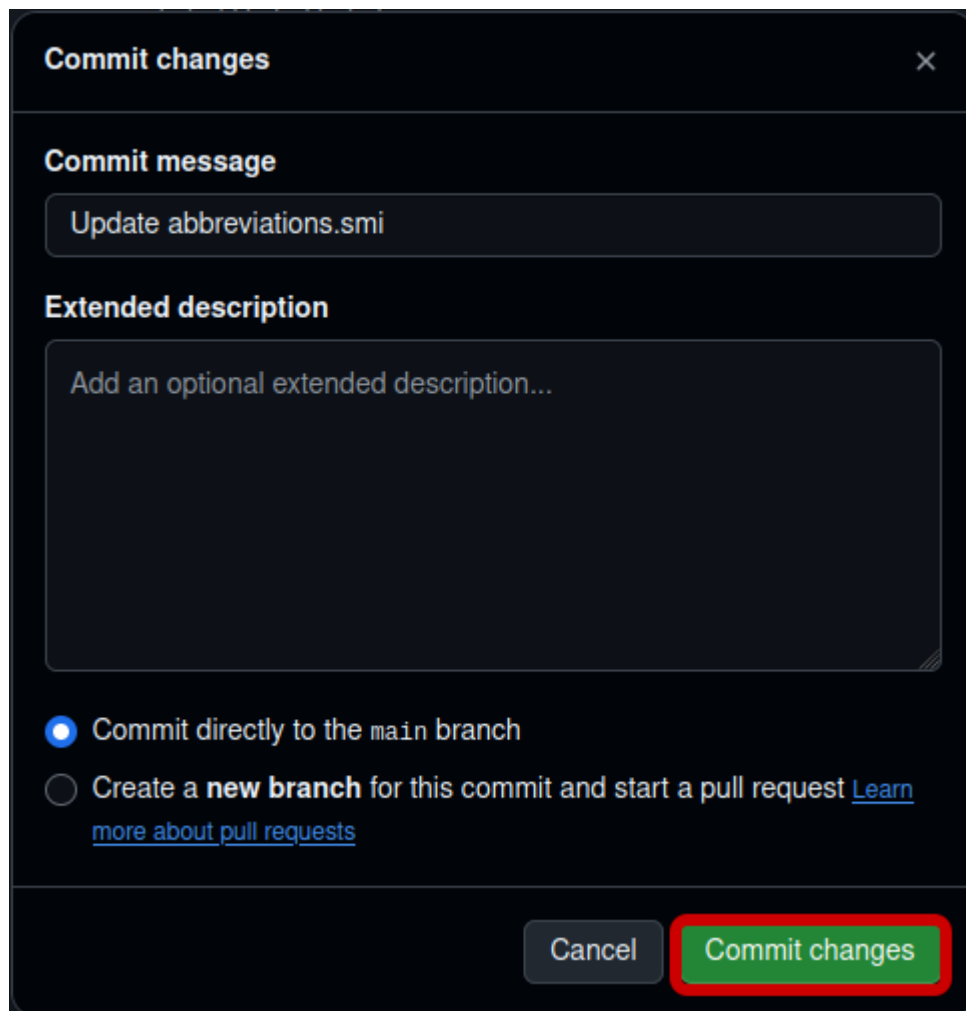
```
1 Abbreviation SMILES
2 C6H4F *c1ccc(F)cc1
3 Mes *c1c(C)cc(C)cc1(C)
4 S S
5 N N
6 NH2 N
7 -OCH2O- *OCO*
8 s-Bu *C(C)CC
9 i-Pr *C(C)C
10 2,6-(CH3)2C6H3 *C1=C(C)C=CC=C1(C)
11 PMB *OCC1=CC=C(C=C1)OC
12 Bp1n CC1(C)OB([*])OC1(C)C
13 PMP COC1=CC=C([*])C=C1
14 OPP O=P(OP(O[*]))(O)=O(O)O
15 p-Tol CC1=CC=C([*])C=C1
16 Hex CCCCCC[*]
```

- Add a new abbreviation or multiple ones and click **Commit changes...** in the top right corner:

The screenshot shows a web-based code editor for BChemLookup. The file explorer on the left lists files including .github, Tutorials, scripts, LICENSE, README.md, abbreviations.csv, and abbreviations.smi. The main editor area displays a list of chemical abbreviations and their corresponding SMILES strings. The 'Piv0' entry is highlighted with a red box. At the top right, there are buttons for 'Cancel changes' and 'Commit changes...'. The bottom of the editor shows a status bar with keyboard shortcuts.

Use **Control + Shift + m** to toggle the **tab** key moving focus. Alternatively, use **esc** then **tab** to move to the next interactive element on the page.

- Type in a "commit message" and click **Commit changes**:



**Commit changes**

**Commit message**

Update abbreviations.smi

**Extended description**

Add an optional extended description...

☒ Commit directly to the main branch

☐ Create a **new branch** for this commit and start a pull request [Learn more about pull requests](#)

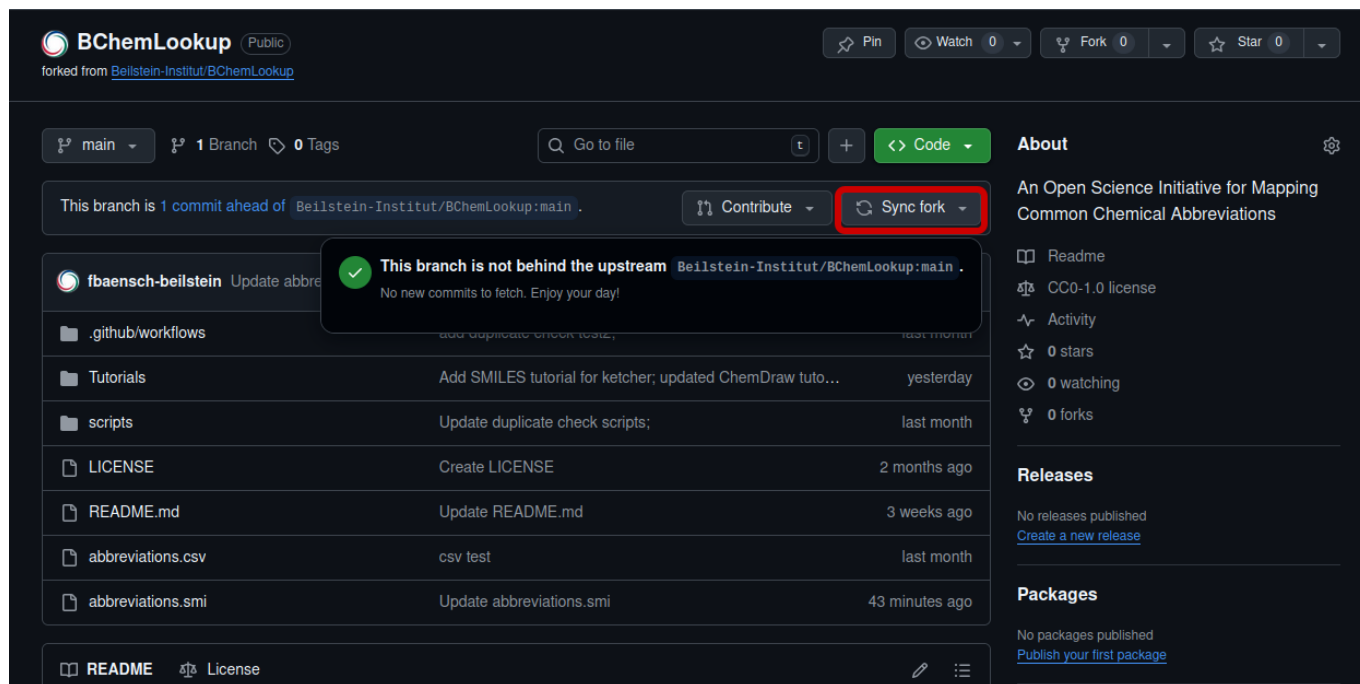
Cancel **Commit changes**

## Contribute or create a pull request

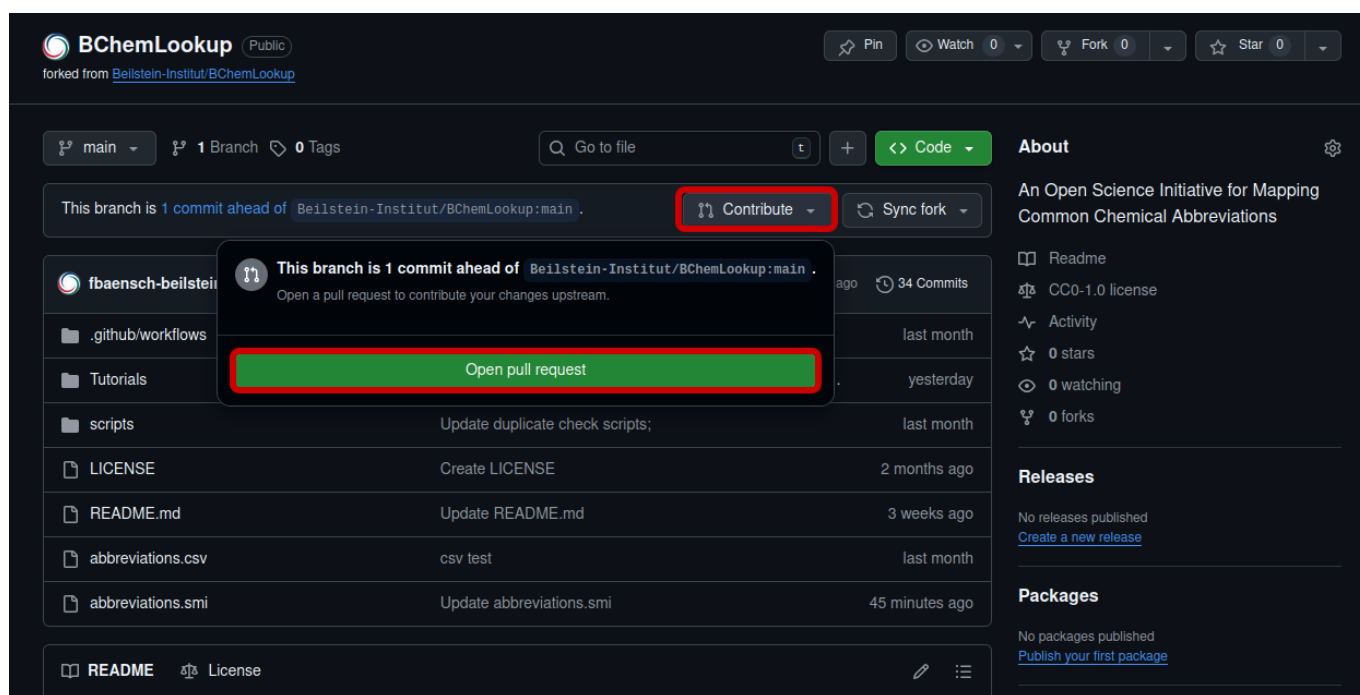
The branch of your forked repository is now ahead of the the branch of the origin repository. Now you can create pull request.

-First, make sure your branch is not behind the origin repository. Therefore click **Sync fork**. If everything is fine it will state:

"This branch is not behind the upstream Beilstein-Institut/BChemLookup:main":



- To contribute click **Contribute** and **Open pull request**:



- Add a title for your pull request and a description. In the description please include a short description or common use of your changes and state the source of the data. Then click **Create pull request**:

## Comparing changes


Choose two branches to see what's changed or to start a new pull request. If you need to, you can also [compare across forks](#) or [learn more about diff comparisons](#).

base repository: Beilstein-Institut/BChemLookup

base: main

head repository: fbaensch-beilstein/BChemLookup

compare: main













**Add a title**


Add pivalate ester as PivO


**Add a description**

WritePreview


H B I          


Add pivalate ester a carboxylic ester of pivalic acid.


Markdown is supported  Paste, drop, or click to add files


☒ Allow edits by maintainers 


Create pull request


 Remember, contributions to this repository should follow our [GitHub Community Guidelines](#).

**Reviewers**   
No reviews

**Assignees**   
No one—[assign yourself](#)


**Labels**   
None yet


**Projects**   
None yet


**Milestone**   
No milestone

**Development**  
Use [Closing keywords](#) in the description to automatically close issues

**Helpful resources**  
[GitHub Community Guidelines](#)

 1 commit

 1 file changed

 1 contributor

And you are done!