

# Package ‘chromConverter’

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**Title** Chromatographic File Converter

**Version** 0.1.0

**Maintainer** Ethan Bass <ethanbass@gmail.com>

**Description** Reads chromatograms from binary formats into R objects. Currently supports conversion of Agilent ChemStation '.uv' and MassHunter '.sp', files using file parsers from the 'Aston' package <<https://github.com/bovee/aston>>.

**License** GPL (>= 3)

**URL** <https://github.com/ethanbass/chromConverter>

**BugReports** <https://github.com/ethanbass/chromConverter/issues>

**Imports** reticulate, utils

**Config/reticulate** list( packages = list( list(package = ``scipy",  
``numpy", ``pandas"), list(package=``aston", pip = TRUE) ) )

**Encoding** UTF-8

**Language** en-US

**RoxygenNote** 7.1.2

**Suggests** testthat (>= 3.0.0)

**Config/testthat/edition** 3

**NeedsCompilation** no

**Author** Ethan Bass [aut, cre] (<<https://orcid.org/0000-0002-6175-6739>>)

**Repository** CRAN

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read\_chroms

*Read Chromatograms***Description**

Reads chromatograms from specified folders or vector of paths using the [Aston](#) file parser.

**Usage**

```
read_chroms(
  paths,
  find_files = TRUE,
  format.in = c("chemstation.uv", "masshunter.dad"),
  pattern = NULL,
  parser = c("Aston"),
  R.format = c("matrix", "data.frame"),
  export = FALSE,
  path.out = NULL,
  format.out = "csv",
  dat = NULL
)
```

**Arguments**

paths	paths to files or folders containing files
find_files	TRUE
format.in	Format of files to be imported/converted.
pattern	pattern (e.g. a file extension). Defaults to NULL, in which case file extension will be deduced from format.in.
parser	= What parser to use. Currently, the only option is Aston.
R.format	R object format (i.e. data.frame or matrix).
export	Logical. If true, will export files as csvs.
path.out	Path for exporting files. If path not specified, files will export to current working directory.
format.out	Output format. Currently only .csv.
dat	Existing list of chromatograms to append results. (Defaults to NULL).

**Details**

Currently recognizes Agilent ChemStation '.uv' and MassHunter '.dad' files.

**Value**

A list of chromatograms in matrix or data.frame format, according to the value of 'R.format'.

**Author(s)**

Ethan Bass

**Examples**

```
path <- "tests/testthat/testdata/dad1.uv"  
chr <- read_chroms(path, find_files = FALSE, format.in = "chemstation.uv")
```

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`sp_converter`*Converter for Agilent MassHunter UV files*

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**Description**

Converts a single chromatogram from MassHunter .sp format to R data.frame.

**Usage**

```
sp_converter(file)
```

**Arguments**

file                    path to file

**Details**

Uses the [Aston](#) file parser.

**Value**

A data.frame object (retention time x wavelength).

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`uv_converter`*Converter for Agilent ChemStation UV files*

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**Description**

Converts a single chromatogram from ChemStation .uv format to R data.frame.

**Usage**

```
uv_converter(file)
```

**Arguments**

file                    path to file

**Details**

Uses the **Aston** file parser.

**Value**

A data.frame object (retention time x trace).

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