

Guide to readJDX Vignettes

Bryan A. Hanson^a

^aDept. of Chemistry & Biochemistry, DePauw University; hanson@depauw.edu

This version was compiled on November 12, 2019

```
# readJDX is tested with > 100 files before release.  
# However, there are still challenging files out in the wild.  
# If you have trouble importing a file, please file an issue at  
# github.com/bryanhanson/readJDX/issues
```

This vignette is based on readJDX version 0.4.29.

The following vignettes are available, in addition to this one:

- *readJDX*, a general introduction and overview.
- The following vignettes will be useful for those wishing to contribute to the development of readJDX and those that are troubleshooting files:
 - *Program Flow*, a overview of how readJDX functions are organized and the input they require.
 - *MiniDIFDUP_1* is an annotated version of the MiniDIFDUP data set.
 - *MiniDIFDUP_2* is an expanded and annotated version of the MiniDIFDUP data set.