HUMAN HEALTH

ENVIRONMENTAL HEALTH

# **ChemDraw Web Service**

## Installation Guide





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#### Overview

The ChemDraw Web Service (CDWS) provides chemistry services for ChemDraw JS and other PerkinElmer applications. This guide explains how CDWS is delivered and how it should be installed. It also provides some suggestions on how to deploy it in production.

### Installing the ChemDraw Web Service

CDWS is delivered as a Docker image. It should run on any platform that can support Intel x64 Docker images. If the image is provided as a .tar file, you need to first import it into Docker using the command docker load. For example:

docker load --input chemdraw-web-service-x.y.z-release-latest.tar

To start CDWS, use the command docker run. CDWS will serve on port 80, you should map this to the desired host port using --publish.

For example, to map CDWS port 80 to host port 8080:

docker run --publish 8080:80 pkiinformatics/chemdraw-web-service:x.y.z-release-latest

### Testing

You can check if the service is running correctly by getting the /1.0/health-full resource. For example:

http://localhost:8080/1.0/health-full

This checks if the server is running and if it is, returns status: "OK" and some other information. You can obtain the version information from the /1.0/version endpoint. For example:

http://localhost:8080/1.0/version

You may need to provide this version information to PerkinElmer when technical support is required.

### **Production Deployment**

#### Load Balancing

Each CDWS instance is capable of handling multiple requests on multiple threads simultaneously, and multiple CPU cores/threads will be used if available. When deploying CDWS in production, it would be common to also deploy multiple instances behind a load balancer to provide scalable performance and fault tolerance.



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You can either use /1.0/health-full or /1.0/health-light endpoints for server monitoring. If the status returned by either of the endpoints is not status: "OK", then recycle that instance. CDWS is stateless and can be recycled at any time.

#### Encryption

CDWS does not support HTTPS directly. If encryption is needed, a typical approach would be to use <u>HTTPS</u> <u>termination in the load balancer</u>, <u>NGINX as a reverse proxy</u> or a similar solution in front of CDWS to terminate HTTPS and provide encryption to downstream clients.