

# Open PHACTS Component Collection

## Version 1.4 Release Notes

The Open PHACTS collection enables protocol developers and users to access Open PHACTS data through easy-to-use components. Open PHACTS (<https://www.openphacts.org/>) is part of the Innovative Medicines Initiative (IMI), an EU-driven public-private partnership. It aggregates data from different sources and domains like compound, target, pathway, tissue and disease to enable scientists to address complex research questions under one roof, using one API.

The component collection facilitates access to the Open PHACTS API, with the following key features:

- Full API coverage: One component per API call, featuring all of the API call's parameters
- 69 components, organized in 11 groups
- Additional enhanced components for smooth chemistry searches (exact, substructure and similarity search)
- Results returned exactly as received from the API
- Component parameters available for result data manipulation like data extraction and flattening
- Example and Tutorial protocols provided to demonstrate how to generate solutions from component combinations
- Components generated automatically from the Open PHACTS documentation interface (Swagger) for stable future sustainability

### Prerequisites

This package requires an AEP server version 9.0 or above, and the following component collections:

- Integration Collection
- Reporting Collection
- Chemistry Collection

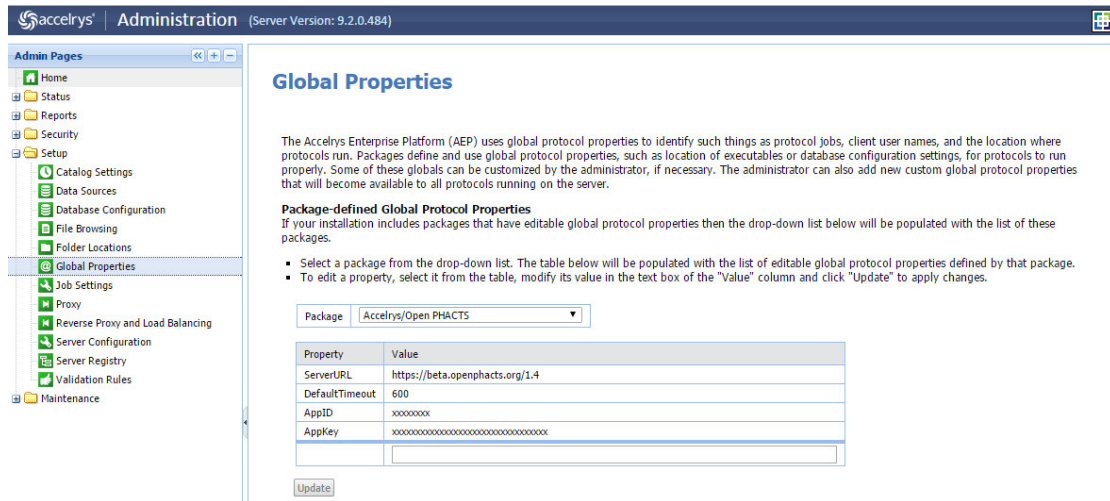
### Installation

It is recommended that this package is installed on the server using the pkgutil utility. You will need to have remote client access to the machine where AEP is installed. To install the package using pkgutil:

- %SCITEGIC\_ROOT% is the AEP installation directory on the server (typically C:\Program Files\Accelrys\AEP)
- First uninstall any previous version of this collection, if installed on your server:  
`%SCITEGIC_ROOT%/bin/pkgutil -u accelrys/openphacts`
- Delete any old collections from the %SCITEGIC\_ROOT%/apps/accelrys directory
- If you have ever imported any components from this collection to your server manually, you will need to delete them all using the Pipeline Pilot client before you install the package. Otherwise, the package will not install and you will see errors about components being already present on your server.
- Extract the contents of the accelrys\_openphacts.zip to your %SCITEGIC\_ROOT%/apps directory.
- You should now see a folder called openphacts inside the accelrys folder.
- Run the pkgutil utility:  
`%SCITEGIC_ROOT%/bin/pkgutil -i accelrys/openphacts`

The components connect to the Open PHACTS API using the credentials of a registered Open PHACTS API user. After registering at <https://dev.openphacts.org/signup> and obtaining an Open PHACTS application ID and key, some globals need to be configured using the Pipeline Pilot administration portal. Open the AEP server administration portal page, navigate to the Setup/Global Properties section, select the Accelrys/OpenPHACTS package from the drop-down menu and enter the values for the parameters shown below:

- **AppKey** : The Open PHACTS application key
- **AppID** : The Open PHACTS application ID
- **ServerURL**: Please set this to <https://beta.openphacts.org/1.4>
- **DefaultTimeout**: Leave as the default value (90) unless you are experiencing timeout errors when using the components. This value represents the time, in seconds, after which the HTTP call will time out if it doesn't receive a response from the remote API server. Some API calls (like compound similarity, for example) tend to take a long time to return, so increasing the time out value will give them a chance to finish.



If you don't have access to the AEP server, you can install these components manually using the Pipeline Pilot client. Just unpack the archive into a temporary location and import the folder `accelrys/openphacts/xml/Components/Open PHACTS` into your Components tab. However, please make sure to uninstall/remove any previous versions of the components from your system before importing the new ones, otherwise you might get unexpected results.

If the components & protocols have been copied into Pipeline Pilot manually, you will need to use the *OpenPHACTS Configuration* component (found under Utilities) to set the values for the globals indicated above. This component will have to be used in every single protocol you build using these components. Please note that you can also use this component to override any values set through the administration portal in case you want to use a different timeout or application key and ID.