

## Release notes

**Date: 2018-03-13**

The Initial release of RSC APIs compounds V1

A swagger file describing the currently available APIs is available at:

<https://api.rsc.org/compounds/v1>

### Access

All API calls require an API key, which may be obtained by registering an account at <http://developer.rsc.org> and adding a key to your account, your API key (Consumer Key) is a 32-character string containing numbers, upper- and lower-case letters.

During the Open Developer preview, all tokens are limited to 1000 calls per month.

All our endpoints are listed here: <https://developer.rsc.org/compounds-v1/apis>

### What has changed?

Our APIs use https for secure data transfer. The new APIs expect request payloads as JSON and return JSON responses

APIs are classified into 4 groupings:

**Filtering** – these are all the APIs that provide functionality define a query and to obtain one or more record IDs as a result

**Records** – these APIs allow you to access information about a ChemSpider record

**Lookups** – This currently contains only one endpoint that returns a list of data sources

**Tools** – These APIs provide the operations that allow you transform data from one type to another

Our new APIs now have a more RESTful structure as compared to the SOAP APIs. However, for the Filter endpoints, obtaining a Record ID (a ChemSpider ID) still involves a stateful process whereby one call returns a queryId.

The queryId can be checked to see if the query has completed using the Status endpoint (/filter/{queryId}/status) and once complete the results can be obtained by using Result endpoint (/filter/{queryId}/results).

## Support for consuming APIs in toolkits and wrappers for programming languages

There are some tools and wrappers that provide access to the legacy SOAP ChemSpider APIs. We are reaching out to developers of tools that we are aware of, but if there are toolkits that you use please let us know.

Known toolkits that incorporate ChemSpider SOAP APIs:

- ChemSpiPy

There are number tools that provide the ability to generate a language specific client from a swagger file, e.g. Swagger Editor (<https://editor.swagger.io/>) which you may find useful.

### Known issues:

#### 1. InChI or InChIKey data, not available

We are actively looking at the best approach for making this data available; if you currently have a need of this data, please contact us, so that we can understand your use case.

#### 2. TooBigBody error from filter/mass/batch/{queryId}/results

<https://api.rsc.org/compounds/v1/filter/mass/batch/{queryId}/results>

In some cases, calls to this endpoint may return an error:

```
"errorcode": "protocol.http.TooBigBody"
```

This error arises when the result payload is greater than 10 MB. Investigation has shown that this arises when the queries in the previous batch search (<https://api.rsc.org/compounds/v1/filter/mass/batch>) return a very large number of results. Often as a result of using mass range parameters that are unsuitable (too wide).

Please notify us if you receive this error, if you are able to provide us with the details of the searches that triggered this issue it would help us to investigate the issue.

## Feedback

We welcome feedback about the APIs, please contact us by email at: [api-at-rsc.org](mailto:api-at-rsc.org) with any questions or comments that you may have about using these APIs and the developer portal.