**HUMAN HEALTH** 

ENVIRONMENTAL HEALTH

PerkinElmer

# ChemDraw

JavaScript API Reference Guide 1.4

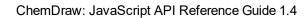


Last Updated: 31/12/2021



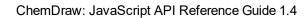
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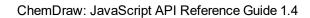


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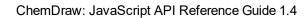


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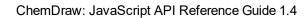


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# **ChemDraw JavaScript API Reference Guide**

This guide provides information about the ChemDraw JavaScript API.

The ChemDraw JavaScript API enables ChemDraw add-ins to access the various features of ChemDraw with JavaScript. With the latest version, the API can support limited access to the active document and the add-in container window.

To access the guide and tutorials for creating ChemDraw add-ins and using ChemDraw JavaScript API in ChemDraw add-ins, go to **Help>Contents>ChemDraw Add-ins**.

**Note:** The ChemDraw JavaScript API works only in ChemDraw add-ins. To access the add-in examples that demonstrate the usage of the API, go to ChemDraw Add-in Examples.



# **Global Objects**

## **ChemDrawAPI**

The singleton global object to access the active document, the add-in container window, etc.

## activeDocument : Document

Gets the active document that is currently open in ChemDraw.

#### **Example**

```
try {
    var activeDocument = ChemDrawAPI.activeDocument;
}
catch (err) {
    alert(err.message);
}
```

#### window: Window

Gets the add-in container window that contains the add-in that is currently running.

#### **Example**

```
try {
    var addinContainerWindow = ChemDrawAPI.window;
}
catch (err) {
    alert(err.message);
}
```

## version: string

Gets the version of the ChemDraw JavaScript API.

```
try {
    document.write(ChemDrawAPI.version);
}
catch (err) {
    alert(err.message);
}
```



**Note:** The add-in example **Hello World** demonstrates the usage of **ChemDrawAPI.version**. To access it, go to ChemDraw Add-in Examples.

## openURLInDefaultBrowser(url): void

Opens the specified URL in system's default browser. Only web URLs are supported i.e. The URL must start with an "http" or "https" otherwise an exception will be thrown.

#### **Parameters**

Name	Туре	Description
url	string	The URL to open in system's default browser

#### Returns

None

#### **Throws Exceptions**

Yes

#### **Example**

Note: The add-in example Open URL demonstrates the usage of

ChemDrawAPI.openURLInDefaultBrowser. To access it, go to ChemDraw Add-in Examples.

#### registerURLTriggeredCallback(callbackFunction): string

Registers a callback function with ChemDraw that will be called when ChemDraw is invoked by the URL handler. This API takes a callback function and returns a callback key that uniquely identifies this callback.

#### **Parameters**

Name	Туре	Description
callbackFunction	<u>Function</u>	The callback function that will be invoked

#### Returns

Return Type	Description
string	A callback key that uniquely identifies this callback

#### **Throws Exceptions**

Yes



## **Example**

```
try {
    const callbackKey = ChemDrawAPI.registerURLTriggeredCallback((arg) => {
        alert(arg);
    });
}
catch (err) {
    alert(err.message);
}
```

**Note:** The add-in example **ChemDrawOAuthExample** demonstrates the usage of **ChemDrawAPI.registerURLTriggeredCallback**. To access it, go to <u>ChemDraw Add-in Examples</u>. More information on the usage of this API can be found in the ChemDraw User Guide.

## copyToClipboard(text): void

Copies the specified text to the clipboard.

#### **Parameters**

Name	Туре	Description
text	string	The text to be copied

#### Returns

None

#### **Throws Exceptions**

Yes

```
try {
    ChemDrawAPI.copyToClipboard("Hello World");
}
catch (err) {
    alert(err.message);
}
```



## **Classes**

#### **Document**

Provides an API to add and get data in a ChemDraw document.

**Note:** The add-in example **Document Data Importer and Exporter** demonstrates the usage of the API for adding and getting data in the active document. To access it, go to ChemDraw Add-in Examples.

#### selection: Selection

Gets the selection in the document.

### **Example**

```
var selection = ChemDrawAPI.activeDocument.selection;
if (!selection.isEmpty()) {
    // Do something
}
```

#### addCDXML(cdxmlText): void

Adds a CDXML document to the active document. The active document honors the style and coordinates of the supplied CDXML document.

## **Parameters**

Name	Type	Description
cdxmlText	<u>string</u>	The CDXML document to add to the active document

## **Returns**

None

## **Throws Exceptions**

Yes

## **Example**

```
try {
    ChemDrawAPI.activeDocument.addCDXML(cdxmlText);
}
catch (err) {
    alert(err.message);
}
```

#### getCDXML(): string

Gets the contents of the active document as CDXML.



None

### **Returns**

Return Type	Description
string	The contents of the active document as a CDXML string

## **Throws Exceptions**

Yes

## **Example**

```
try {
    var cdxmlText = ChemDrawAPI.activeDocument.getCDXML();
}
catch (err) {
    alert(err.message);
}
```

## addCDXBase64Encoded(base64EncodedCDXText): void

Adds a CDX document, encoded as <u>Base64</u>, to the active document. The active document honors the style and coordinates of the supplied CDX document.

#### **Parameters**

Name	Туре	Description
base64EncodedCDXText	Istring	The CDX document to add to the active document.
		The string must be encoded as Base64

#### Returns

None

## **Throws Exceptions**

Yes

## **Example**

```
try {
    ChemDrawAPI.activeDocument.addCDXBase64Encoded(base64EncodedCDXText);
}
catch (err) {
    alert(err.message);
}
```

## getCDXBase64Encoded(): string

Gets the contents of the active document as Base64 encoded CDX.



None

### **Returns**

Return Type	Description
string	The contents of the active document as a Base64 encoded string

## **Throws Exceptions**

Yes

## **Example**

```
try {
    var base64EncodedCDXText = ChemDrawAPI.activeDocument.getCDXBase64Encoded();
}
catch (err) {
    alert(err.message);
}
```

## addSMILES(smilesText): void

Adds a structure, encoded in a <u>SMILES</u> string, to the active document. The document retains its original styling. The structure will be placed at the center of the currently visible view of the document.

#### **Parameters**

Name	Type	Description
smilesText	string	The SMILES encoded structure to add to the active document

#### **Returns**

None

## **Throws Exceptions**

Yes

```
try {
    ChemDrawAPI.activeDocument.addSMILES(smilesText);
}
catch (err) {
    alert(err.message);
}
```



## getSMILES(): string

Gets the contents of the active document as a <u>SMILES</u> string. If there is a mixture of structures and non-structures (e.g. clip-art, text etc), only the structures will be returned. If there are multiple structures, the <u>SMILES</u> string will be returned in dot-separated notation.

#### **Parameters**

None

#### **Returns**

Return Type	Description	
string	The contents of the active document as a SMILES string	

#### **Throws Exceptions**

Yes

## **Example**

```
try {
    var smilesText = ChemDrawAPI.activeDocument.getSMILES();
}
catch (err) {
    alert(err.message);
}
```

## addInChl(inChlText): void

Adds a structure, encoded in an <u>InChl</u> string, to the active document. The document retains its original styling. The structure will be placed at the center of the currently visible view of the document.

#### **Parameters**

Name	Туре	Description
inChIText	string	The InChI encoded structure to add to the active document

#### **Returns**

None

#### **Throws Exceptions**

Yes

```
try {
    ChemDrawAPI.activeDocument.addInChI(inChIText);
}
```



```
catch (err) {
   alert(err.message);
}
```

## getInChI(): string

Gets the contents of the active document as an <a href="InChl">InChl</a> string. If there is a mixture of structures and non-structures (e.g. clip-art, text etc), only the structures will be returned. If there are multiple structures, the <a href="InChl">InChl</a> string will return them in its native format.

#### **Parameters**

None

## **Returns**

Return Type	Description	
string	The contents of the active document as an InChl string	

#### **Throws Exceptions**

Yes

### **Example**

```
try {
    var inChIText = ChemDrawAPI.activeDocument.getInChI();
}
catch (err) {
    alert(err.message);
}
```

#### getInChlKey(): string

Gets the contents of the active document as an <u>InChlKey</u> string. If there is a mixture of structures and non-structures (e.g. clip-art, text etc), only the structures will be returned. If there are multiple structures, the <u>InChlKey</u> string will return them in its native format.

**Note:** The InChlKey is a one-way format. A key can be generated from a structure, but a structure cannot be generated from a key. Thus there is no Add method for InChlKey.

#### **Parameters**

None

#### **Returns**

Return Type	Description
string	The contents of the active document as an InChlKey string



## **Throws Exceptions**

Yes

## **Example**

```
try {
    var inChIKeyText = ChemDrawAPI.activeDocument.getInChIKey();
}
catch (err) {
    alert(err.message);
}
```

## addMolV2000(molV2000Text): void

Adds a structure, encoded in a MolV2000 string to the active document. The document retains its original styling. If present, 2D coordinates will be honored for the structure, otherwise the structure will be placed at the center of the currently visible view of the document.

#### **Parameters**

Name	Туре	Description
molV2000Text	string	The MolV2000 encoded structure to add to the active document

#### **Returns**

None

## **Throws Exceptions**

Yes

## **Example**

```
try {
    ChemDrawAPI.activeDocument.addMolV2000(molV2000Text);
}
catch (err) {
    alert(err.message);
}
```

## getMolV2000(): string

Gets the contents of the active document as a <u>MolV2000</u> string. If there is a mixture of structures and non-structures (e.g. clip-art, text etc), only the structures will be returned. If there are multiple structures, the <u>MolV2000</u> string will return them in its native format.



None

#### **Returns**

Return Type	Description
string	The contents of the active document as a MolV2000 string

## **Throws Exceptions**

Yes

## **Example**

```
try {
    var molV2000Text = ChemDrawAPI.activeDocument.getMolV2000();
}
catch (err) {
    alert(err.message);
}
```

## addMolV3000(molV3000Text): void

Adds a structure, encoded in a MolV3000 string to the active document. The document retains its original styling. If present, 2D coordinates will be honored for the structure, otherwise they will be placed at the center of the currently visible view of the document.

#### **Parameters**

Name	Туре	Description
molV3000Text	string	The MolV3000 encoded structure to add to the active document

#### **Returns**

None

## **Throws Exceptions**

Yes

```
try {
    ChemDrawAPI.activeDocument.addMolV3000(molV3000Text);
}
catch (err) {
    alert(err.message);
}
```



## getMoIV3000(): string

Gets the contents of the active document as a <u>MolV3000</u> string. If there is a mixture of structures and non-structures (e.g. clip-art, text etc), only the structures will be returned. If there are multiple structures, the <u>MolV3000</u> string will return them in its native format.

#### **Parameters**

None

#### **Returns**

Return Type	Description
string	The contents of the active document as a MolV3000 string

#### **Throws Exceptions**

Yes

### **Example**

```
try {
    var molV3000Text = ChemDrawAPI.activeDocument.getMolV3000();
}
catch (err) {
    alert(err.message);
}
```

#### addMol(molText): void

This is a convenience method that will automatically detect whether the string is in MolV2000 or MolV3000 format, and add the structure to the active document. The document retains its original styling. If present, 2D coordinates will be honored for the structure, otherwise the structure will be placed at the center of the currently visible view of the document. If the supplied string is in neither MolV2000 or MolV3000 format, an exception will be thrown.

**Note:** There is no equivalent getMol() method. Call the getMolV2000() or getMolV3000() methods instead.

#### **Parameters**

Name	Туре	Description
molText	string	The MolV2000 or MolV3000 encoded structure to add to the active document

#### **Returns**

None

#### **Throws Exceptions**

Yes



## **Example**

```
try {
    ChemDrawAPI.activeDocument.addMol(molText);
}
catch (err) {
    alert(err.message);
}
```

## addRXNV2000(rxnV2000Text): void

Adds a reaction, encoded in an RXNV2000 string, to the active document. The document retains its original styling. If present, 2D coordinates will be honored for the reaction, otherwise the reaction will be placed at the center of the currently visible view of the document.

#### **Parameters**

Name	Туре	Description
rxnV2000Text	string	The RXNV2000 encoded structure to add to the active document

#### **Returns**

None

## **Throws Exceptions**

Yes

## **Example**

```
try {
     ChemDrawAPI.activeDocument.addRXNV2000(rxnV2000Text);
}
catch (err) {
    alert(err.message);
}
```

## getRXNV2000(): string

Gets the contents of the active document as an <u>RXNV2000</u> string. If there is a mixture of reactions and non-reactions (e.g. clip-art, text etc), only the reactions will be returned. If there are multiple reactions, the <u>RXNV2000</u> string will return them in its native format.

#### **Parameters**

None



#### **Returns**

Return Type	Description
string	The contents of the active document as a RXNV2000 string

## **Throws Exceptions**

Yes

## **Example**

```
try {
    var rxnV2000Text = ChemDrawAPI.activeDocument.getRXNV2000();
}
catch (err) {
    alert(err.message);
}
```

## addRXNV3000(rxnV3000Text): void

Adds a reaction, encoded in an RXNV3000 string, to the active document. The document retains its original styling. If present, 2D coordinates will be honored for the reaction, otherwise the reaction will be placed at the center of the currently visible view of the document.

#### **Parameters**

Name	Type	Description
rxnV3000Text	string	The RXNV3000 encoded structure to add to the active document.

#### **Returns**

None

#### **Throws Exceptions**

Yes

```
try {
    ChemDrawAPI.activeDocument.addRXNV3000(rxnV3000Text);
}
catch (err) {
    alert(err.message);
}
```



## getRXNV3000(): string

Gets the contents of the active document as a <u>RXNV3000</u> string. If there is a mixture of reactions and non-reactions (e.g. clip-art, text etc), only the reactions will be returned. If there are multiple reactions, the <u>RXNV3000</u> string will return them in its native format.

#### **Parameters**

None

#### **Returns**

Return Type	Description
string	The contents of the active document as a RXNV3000 string

#### **Throws Exceptions**

Yes

## **Example**

```
try {
    var rxnV3000Text = ChemDrawAPI.activeDocument.getRXNV3000();
}
catch (err) {
    alert(err.message);
}
```

## getPNGBase64Encoded([options]): string

Gets the contents of the active document as a PNG image with the specified options. This can be used to generate a PNG image as a preview of the document.

#### **Parameters**

Name	Type	Description
options	Image options	Optional Options are for getting the PNG image.

## **Returns**

Return Type	Description
string	The contents of the active document as a Base64 encoded PNG string

#### **Throws Exceptions**

Yes

```
try {
    var pngBase64EncodedText = ChemDrawAPI.activeDocument.getPNGBase64Encoded({
         transparent: false,
```



```
scalePercent: 100,
    borderSizeInPixels: 100
});

catch (err) {
    alert(err.message);
}
```

## Window

## resizeTo(width, height): void

Resizes the window using the specified width and height.

This API is deprecated.

#### **Parameters**

Name	Туре	Description
width	integer	The new width of the window. A value greater than zero is expected, otherwise an exception will be thrown
height	integer	The new height of the window. A value greater than zero is expected, otherwise an exception will be thrown

#### Returns

None

## **Throws Exceptions**

Yes

## **Example**

```
try {
    ChemDrawAPI.window.resizeTo(width, height);
}
catch (err) {
    alert(err.message);
}
```

## setDefaultSize(width, height): void

Set default size for the window using the specified width and height.



Name	Туре	Description
width	integer	The new width of the window. A value greater than zero is expected, otherwise an exception will be thrown
height	integer	The new height of the window. A value greater than zero is expected, otherwise an exception will be thrown

#### Returns

None

## **Throws Exceptions**

Yes

## **Example**

```
try {
    ChemDrawAPI.window.setDefaultSize(width, height);
}
catch (err) {
    alert(err.message);
}
```

## close(): void

Closes the add-in container window.

#### **Parameters**

None

## **Returns**

None

## **Throws Exceptions**

Yes

## **Example**

```
try {
    ChemDrawAPI.window.close();
}
catch (err) {
    alert(err.message);
}
```

## onClose(callback): void

Registers a callback function which will be called when the add-in container window is about to close.



Name	Туре	Description
callback	tunction	( <b>Optional</b> ) The callback function which will called when the add-in container window is about to close.

#### **Returns**

None

## **Example**

```
ChemDrawAPI.window.onClose(function () {
      // Do clean up here when the add-in container window is about to close
});
```

#### Selection

Provides API to get the selected structures in a ChemDraw document.

**Note:** The add-in example Selection Monitor demonstrates the usage of the API for getting the preview image of the selected structures in the active document. To access it, go to ChemDraw Add-in Examples.

## containsPartialStructure(): boolean

Determines whether the selection contains partially selected structure.

#### **Parameters**

None

#### **Returns**

Return Type	Description
boolean	true if part of a single structure or grouped structures is selected, false otherwise

#### **Example**

```
if ChemDrawAPI.activeDocument.selection.containsPartialStructure()){
    // Do something
}
```

## getCDXML(): string

Gets the contents of the selection as a CDXML document.

#### **Parameters**

None



#### **Returns**

Return Type	Description
string	The contents of the selection as a CDXML document

## **Example**

```
var cdxmlText = ChemDrawAPI.activeDocument.selection.getCDXML();

// Do something with the CDXML text here
```

## getSVG([options]): string

Gets the contents of the selection as an SVG image with the specified options. This can be used to generate an SVG image as a preview of the selection.

#### **Parameters**

Name	Type	Description
options	Image options	Optional Options for getting the SVG image

#### **Returns**

Return Type	Description		
string	The contents of the selection as an SVG image		

## **Example**

```
var svg = ChemDrawAPI.activeDocument.selection.getSVG({
    transparent: false,
    scalePercent: 100,
    borderSizeInPixels: 20
});
// Do something with the svg image here
```

## getInChlKey(): string

Gets the contents of the selection as an InChlKey string.

#### **Parameters**

None

#### **Returns**

Return Type	Description		
string	The contents of the selection as an InChlKey string		

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## **Example**

```
var inChIKey = ChemDrawAPI.activeDocument.selection.getInChIKey();

// Do something with the inChIKey here
```

## getSMILES(): string

Gets the contents of the selection as a SMILES string.

#### **Parameters**

None

#### **Returns**

Return Type	Description		
string	The contents of the selection as a SMILES string		

## **Example**

```
var smilesText = ChemDrawAPI.activeDocument.selection.getSMILES();

// Do something with the SMILES here
```

## isEmpty(): boolean

Determines whether any object has been selected in the document.

#### **Parameters**

None

#### **Returns**

Return Type	Description	
boolean	true if nothing has been selected, false otherwise	

## **Example**

```
if (!ChemDrawAPI.activeDocument.selection.isEmpty()) {
    // Do something
}
```

## onChange(callback): void

Registers a callback function which will be called when the selection is changed in the document.

#### **Parameters**

Name	Туре	Description		
callback	function	The callback function which will called when the selection is		
Caliback		changed		

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#### **Returns**

None

## **Example**

```
// Set the callback (or handler) for the selection change event
ChemDrawAPI.activeDocument.selection.onChange(function () {
    if (!ChemDrawAPI.activeDocument.selection.isEmpty()) {
        cdxmlText = ChemDrawAPI.activeDocument.selection.getCDXML();
        svg = ChemDrawAPI.activeDocument.selection.getSVG();

        // Do something with the cdxmlText and the svg image here
    }
});
```

#### **JSON Structures**

## **ImageOption**

Options for getting an image. This can be used to specify the properties of the preview image for generating a preview of a document or a selection.

## **Properties**

Name	Туре	Default Value	Description
transparent	<u>boolean</u>	true	( <b>Optional</b> ) If true, the image will have a transparent background. If false, the background is generated along with the document contents
scalePercent	integer	100	( <b>Optional</b> ) The scaling applied to the image. 100% is the actual size. A value greater than zero is expected, otherwise an exception will be thrown
borderSizeInPixels	integer	0	( <b>Optional</b> ) The border (gap) to be placed around the image in pixels. A value of zero or greater is expected, otherwise an exception will be thrown