HUMAN HEALTH

ENVIRONMENTAL HEALTH

PerkinElmer

ChemDraw

JavaScript API Reference Guide 1.1

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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.

Example

```
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.*

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	string	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.

Parameters
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 Base64, to the active document. The active document honors the style and coordinates of the supplied CDX document.

Parameters
Name	Type	Description
base64EncodedCDXText	string	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.

Parameters
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 SMILES 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

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

getSMILES() : string

Gets the contents of the active document as a SMILES 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 SMILES 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);
}
```

addInChI(inChIText) : void

Adds a structure, encoded in an InChI 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
inChIText	string	The InChI encoded structure to add to the active document

Returns
None

Throws Exceptions
Yes

Example

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

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

getInChI() : string

Gets the contents of the active document as an InChI 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 InChI string will return them in its native format.

Parameters
None

Returns

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

Throws Exceptions
Yes

Example

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

getInChIKey() : string

Gets the contents of the active document as an InChIKey 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 InChIKey string will return them in its native format.

> ***Note:*** *The InChIKey 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 InChIKey.*

Parameters
None

Returns

Return Type	Description
string	The contents of the active document as an InChIKey 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	Type	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 MolV2000 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 MolV2000 string will return them in its native format.

Parameters
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	Type	Description
molV3000Text	string	The MolV3000 encoded structure to add to the active document

Returns
None

Throws Exceptions
Yes

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

getMolV3000() : string

Gets the contents of the active document as a MolV3000 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 MolV3000 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	Type	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	Type	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 RXNV2000 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 RXNV2000 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

Example

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

getRXNV3000() : string

Gets the contents of the active document as a RXNV3000 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 RXNV3000 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

Example

```
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.

Parameters

Name	Type	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);
}
```

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.

Parameters

Name	Type	Description
callback	function	(**Optional**) 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
```

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	Type	Description
callback	function	The callback function which will called when the selection is changed

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	Type	Default Value	Description
transparent	boolean	true	(**Optional**) If true, the image will have a transparent background. If false, the background is generated along with the document contents
scalePercent	integer	100	(**Optional**) 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	(**Optional**) 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