**MolPort Chemical Search**

**API v.3.0.**

11.10.2015

Revision

|  |  |  |  |
| --- | --- | --- | --- |
| **Version** | **Date** | **Author** | **Description** |
| 1.0 | 30-07-2015 | Normunds Kinne | Initial draft |

## 

Response structure

*MolPort JSON* response generic form is:

{

"Result": {

"Status": 1|2,

"Message": <message text>

},

"Data": {

"Version": <version number>,

… <Data Object> …

}

}

where:

Status – int; possible values:

1 – operation successful,

2 – operation was not successful;

Message – string; short informative, human readable message;

Version – string; version number of returned *MolPort JSON* data objects;

Data Object – json; *JSON* representation of returned data objects.

API Methods

## Load molecule

Method to load information about molecule from *MolPort* database if *MolPort ID* is known.

## Request

|  |  |
| --- | --- |
| **Method** | **URL** |
| **GET** | /api/molecule/load/{molecule id} |
| **JSON** | None |

## Example

|  |  |
| --- | --- |
| **Method** | **URL** |
| **GET** | http://www.molport.com/api/molecule/load/2325020 |

## Response

Method will return a Molecule object with data structure:

Id – int; molecule identifier in *MolPort* database;

MolPort Id – string, formatted molecule identifier in *MolPort* database;

SMILES – string; *SMILES* of molecule;

IUPAC – string; *IUPAC* of molecule;

Formula – string; molecular molecule;

Molecular Weight – string; molecular weight;

Status – string; status of availability;

Type – string; type of availability;

Largest Stock – string; maximum stock available in shop;

Largest Stock Measure – string; measure;

Largest Stock Measure Id – string; *MolPort* measure Id;

Synonyms – array of molecule names;

Catalogues – array of :

Screening Block Suppliers – array of suppliers;

Building Block Suppliers – array of suppliers;

Virtual Suppliers – array of suppliers.

Method will return a Supplier objects with data structure:

Supplier Name – string; supplier name;

Supplier Id – int; supplier Id;

Minimum Order – double; minimum order for supplier;

Currency – string; currency ISO code;

Currency Id – int; *MolPort* currency identifier;

Catalogues – array of supplier catalogues.

Method will return a Supplier objects with data structure:

Catalog Id – int; catalog Id in *MolPort* database;

Catalog Number – string; supplier catalog number;

Stock – double; amount in stock;

Stock Measure – string; amount measure;

Stock Measure Id – int; amount measure Id in *MolPort* database;

Last Update Date – string; last catalog update date in *MolPort* database;

Available Packings – array of packings.

Method will return a Packing objects with data structure:

Amount – string; amount;

Measure – string; amount measure;

Measure Id – int; amount measure Id in *MolPort* database;

Price – double; price;

Currency – string; currency;

Currency Id – int; currency Id in *MolPort* database;

Delivery Days – int; days in which supplier sends out requested molecules if payment was made.

Method will return a Synonym objects with data structure:

Value – string; name/MDL number of molecule.

Record was not found:

|  |  |
| --- | --- |
| **Status** | **Response** |
| 200 | {  "Result": {  "Status": 2,  "Message": "Molecule was not found!"  },  "Data": {  "Version": "v.1.0"  }  } |

Record found:

|  |  |
| --- | --- |
| **Status** | **Response** |
| 200 | {  "Result": {  "Status": 1,  "Message": "Molecule found!"  },  "Data": {  "Molecule": {  "Id": 2325020,  "MolPort Id": "MolPort-002-325-020",  "SMILES": "CCOC(\u003dO)c1[nH]c2ccc(C)cc2c1NC(\u003dO)CC",  "IUPAC": "ethyl 5-methyl-3-propanamido-1H-indole-2-carboxylate",  "Formula": "C15H18N2O3",  "Molecular Weight": 274.32,  "Status": "shop",  "Type": "stock",  "Largest Stock": "124",  "Largest Stock Measure": "mg",  "Largest Stock Measure Id": 234,  "Catalogues": {  "Screening Block Suppliers": [  {  "Supplier Name": "Specs",  "Supplier Id": 2070,  "Minimum Order": 200,  "Currency": "USD",  "Currency Id": 2,  "Catalogues": [  {  "Catalog Id": 84777984,  "Catalog Number": "AG-690/10530016",  "Stock": 2,  "Stock Measure": "mg",  "Stock Measure Id": 234,  "Last Update Date": "today",  "Available Packings": [  {  "Amount": 2,  "Measure": "mg",  "Measure Id": 234,  "Price": 32.20,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 7  }  ]  }  ],  "Shipment Costs": [  {  "Price": 50,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "EUROPE",  "Location Id": 1,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 50,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "USA",  "Location Id": 2,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 50,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "CANADA AND MEXICO",  "Location Id": 3,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 50,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "OTHER LOCATIONS",  "Location Id": 4,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  }  ]  },  {  "Supplier Name": "Vitas-M Laboratory, Ltd.",  "Supplier Id": 2077,  "Currency": "USD",  "Currency Id": 2,  "Catalogues": [  {  "Catalog Id": 191573558,  "Catalog Number": "STK374222",  "Stock": 124,  "Stock Measure": "mg",  "Stock Measure Id": 234,  "Purity": "\u003e90%",  "Last Update Date": "this week",  "Available Packings": [  {  "Amount": 1,  "Measure": "mg",  "Measure Id": 234,  "Price": 26.50,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 2,  "Measure": "mg",  "Measure Id": 234,  "Price": 28.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 3,  "Measure": "mg",  "Measure Id": 234,  "Price": 31.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 5,  "Measure": "mg",  "Measure Id": 234,  "Price": 38.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 10,  "Measure": "mg",  "Measure Id": 234,  "Price": 48.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 20,  "Measure": "mg",  "Measure Id": 234,  "Price": 68.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 30,  "Measure": "mg",  "Measure Id": 234,  "Price": 78.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 50,  "Measure": "mg",  "Measure Id": 234,  "Price": 97.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  },  {  "Amount": 100,  "Measure": "mg",  "Measure Id": 234,  "Price": 161.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 10  }  ]  }  ],  "Shipment Costs": [  {  "Price": 55,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "EUROPE",  "Location Id": 1,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 55,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "USA",  "Location Id": 2,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 55,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "CANADA AND MEXICO",  "Location Id": 3,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 55,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "OTHER LOCATIONS",  "Location Id": 4,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  }  ]  },  {  "Supplier Name": "Princeton BioMolecular Research, Inc.",  "Supplier Id": 2112,  "Minimum Order": 150,  "Currency": "USD",  "Currency Id": 2,  "Catalogues": [  {  "Catalog Id": 208007160,  "Catalog Number": "OSSL\_129598",  "Stock Measure Id": 0,  "Last Update Date": "last month",  "Available Packings": [  {  "Amount": 5,  "Measure": "µmol",  "Measure Id": 241,  "Price": 19.85,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 10,  "Measure": "µmol",  "Measure Id": 241,  "Price": 27.79,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 20,  "Measure": "µmol",  "Measure Id": 241,  "Price": 31.76,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 1,  "Measure": "mg",  "Measure Id": 234,  "Price": 15.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 2,  "Measure": "mg",  "Measure Id": 234,  "Price": 17.64,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 3,  "Measure": "mg",  "Measure Id": 234,  "Price": 19.85,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 5,  "Measure": "mg",  "Measure Id": 234,  "Price": 23.82,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 7,  "Measure": "mg",  "Measure Id": 234,  "Price": 27.79,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 10,  "Measure": "mg",  "Measure Id": 234,  "Price": 31.76,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 15,  "Measure": "mg",  "Measure Id": 234,  "Price": 35.73,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 20,  "Measure": "mg",  "Measure Id": 234,  "Price": 39.70,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 25,  "Measure": "mg",  "Measure Id": 234,  "Price": 49.50,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 30,  "Measure": "mg",  "Measure Id": 234,  "Price": 54.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 35,  "Measure": "mg",  "Measure Id": 234,  "Price": 58.50,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 40,  "Measure": "mg",  "Measure Id": 234,  "Price": 65.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 50,  "Measure": "mg",  "Measure Id": 234,  "Price": 80.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  },  {  "Amount": 100,  "Measure": "mg",  "Measure Id": 234,  "Price": 150.00,  "Currency": "USD",  "Currency Id": 2,  "Delivery Days": 25  }  ]  }  ],  "Shipment Costs": [  {  "Price": 110,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "EUROPE",  "Location Id": 1,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 60,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "USA",  "Location Id": 2,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 50,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "CANADA AND MEXICO",  "Location Id": 3,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  },  {  "Price": 120,  "Currency": "USD",  "Currency Id": 2,  "Location Type": "REGION",  "Location": "OTHER LOCATIONS",  "Location Id": 4,  "Shipment Type": "Basic Shipping",  "Shipment Type Id": 3  }  ]  }  ],  "Building Block Suppliers": [],  "Virtual Suppliers": []  },  "Synonyms": [  "ethyl",  "ethyl 5-methyl-3-(propanoylamino)-1H-indole-2-carboxylate"  ]  },  "Version": "v.1.0"  }  } |

## 2. Search molecules with chemical search

Method to search molecules with chemical search if *SMILES* is known. Currently supported chemical search types are:

1. exact search;
2. exact fragment search;
3. similarity search;
4. perfect search;
5. substructure search;
6. superstructure search;

## Request

|  |  |
| --- | --- |
| **Method** | **URL** |
| **GET** | /api/chemical-search/search |
| **JSON** | {  "Structure":"CC(C)(C)OC(=O)N1CCCCCC1C(O)=O",  "Search Type":4,  "Filter Id":0,  "Maximum Search Time":60000,  "Maximum Result Count":1000,  "Chemical Similarity Index":0.9  }  where:  Structure – string; SMILES of molecule;  Search Type – int, chemical search type with possible values:  CHEMICAL\_SEARCH\_TYPE\_\_SUBSTRUCTURE = 1  CHEMICAL\_SEARCH\_TYPE\_\_SUPERSTRUCTURE = 2  CHEMICAL\_SEARCH\_TYPE\_\_EXACT = 3  CHEMICAL\_SEARCH\_TYPE\_\_SIMILARITY = 4  CHEMICAL\_SEARCH\_TYPE\_\_PERFECT = 5  CHEMICAL\_SEARCH\_TYPE\_\_EXACT\_FRAGMENT = 6  Maximum Search Time – int; time in miliseconds - maximum search time to be spent on chemical search;  Maximum Result Count – int; maximum result count which must be returned as result; currently maximum allowed value is 1000; default value is 1000;  Chemical Similarity Index – double; if similarity search is made, it is possible to provide similarity index in range 0 – 1; default value is 0.9. |

## Response

Method will return a list of Molecule objects with data structure:

{

"Id": <MolPort molecule id>,

"MolPort Id": <formatted MolPort molecule id>,

"SMILES": <SMILES>,

"Similarity Index": <Similarity index>

}

where:

Id – int; molecule identifier in *MolPort* database;

MolPort Id – string, formatted molecule identifier in *MolPort* database;

SMILES – string; *SMILES* of molecule;

Similarity Index – double; if similarity search was made, will contain similarity index

to initially searched molecule.

Molecules were not found:

|  |  |
| --- | --- |
| **Status** | **Response** |
| 200 | {  "Result": {  "Status": 1,  "Message": "Chemical search completed!"  },  "Data": {  "Molecules": [],  "Version": "v.1.0"  }  } |

Molecules were found:

|  |  |
| --- | --- |
| **Status** | **Response** |
| 200 | {  "Result": {  "Status": 2,  "Message": "Index: 3, Size: 3"  },  "Data": {  "Molecules": [  {  "Id": 160,  "MolPort Id": "MolPort-000-000-160",  "SMILES": "CNC(\u003dO)CCCN[C@@H](C)c1ccccc1 |r|"  },  {  "Id": 20665883,  "MolPort Id": "MolPort-020-665-883",  "SMILES": "CC(\u003dO)c1ccc(OCC(\u003dO)c2cn(CCC#N)c3ccccc23)cc1"  },  {  "Id": 28065133,  "MolPort Id": "MolPort-028-065-133",  "SMILES": "CC(NC(\u003dO)COc1ccc(cc1)C(C)\u003dO)c1cccs1"  },  {  "Id": 28065134,  "MolPort Id": "MolPort-028-065-134"  }  ],  "Version": "v.1.0"  }  } |