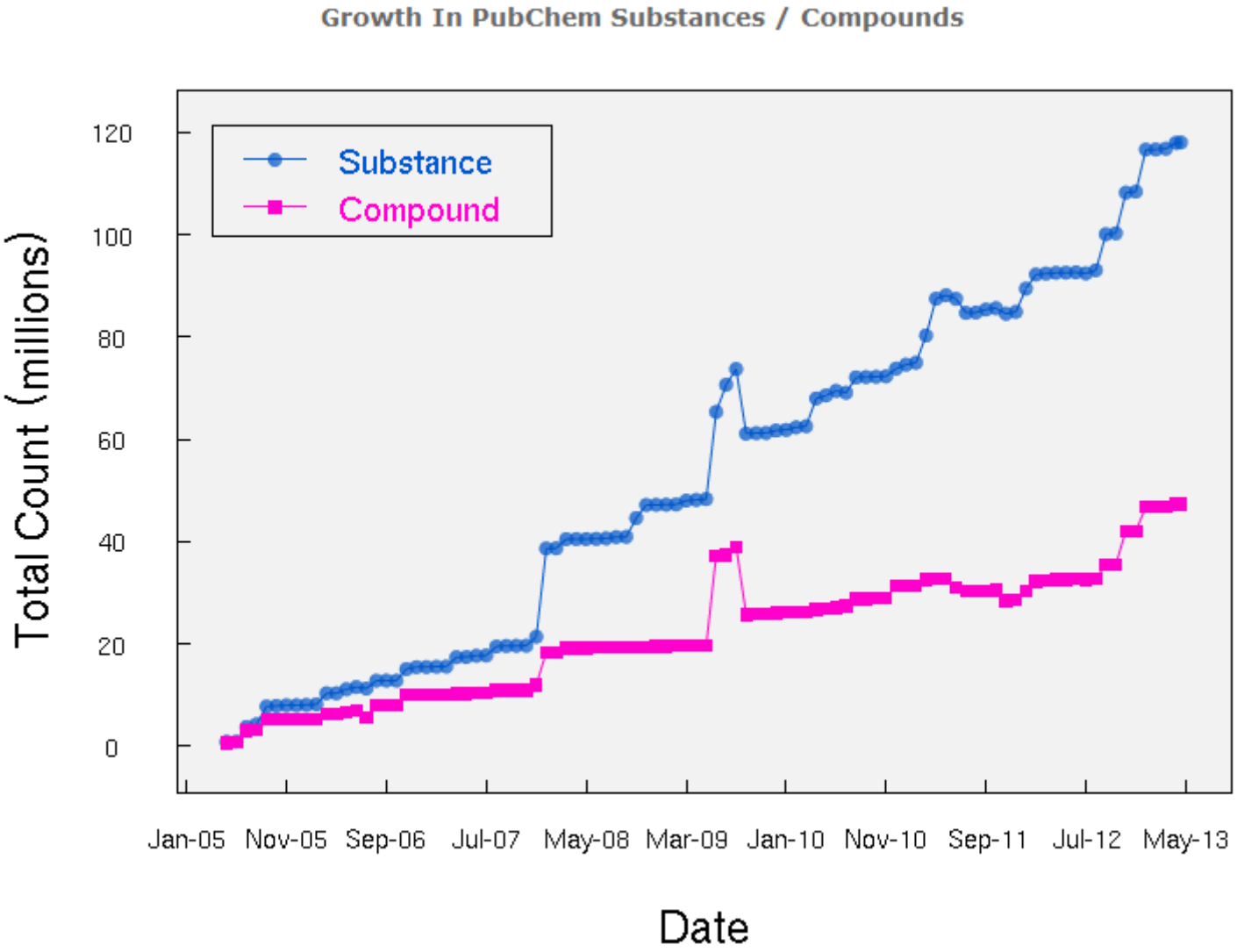
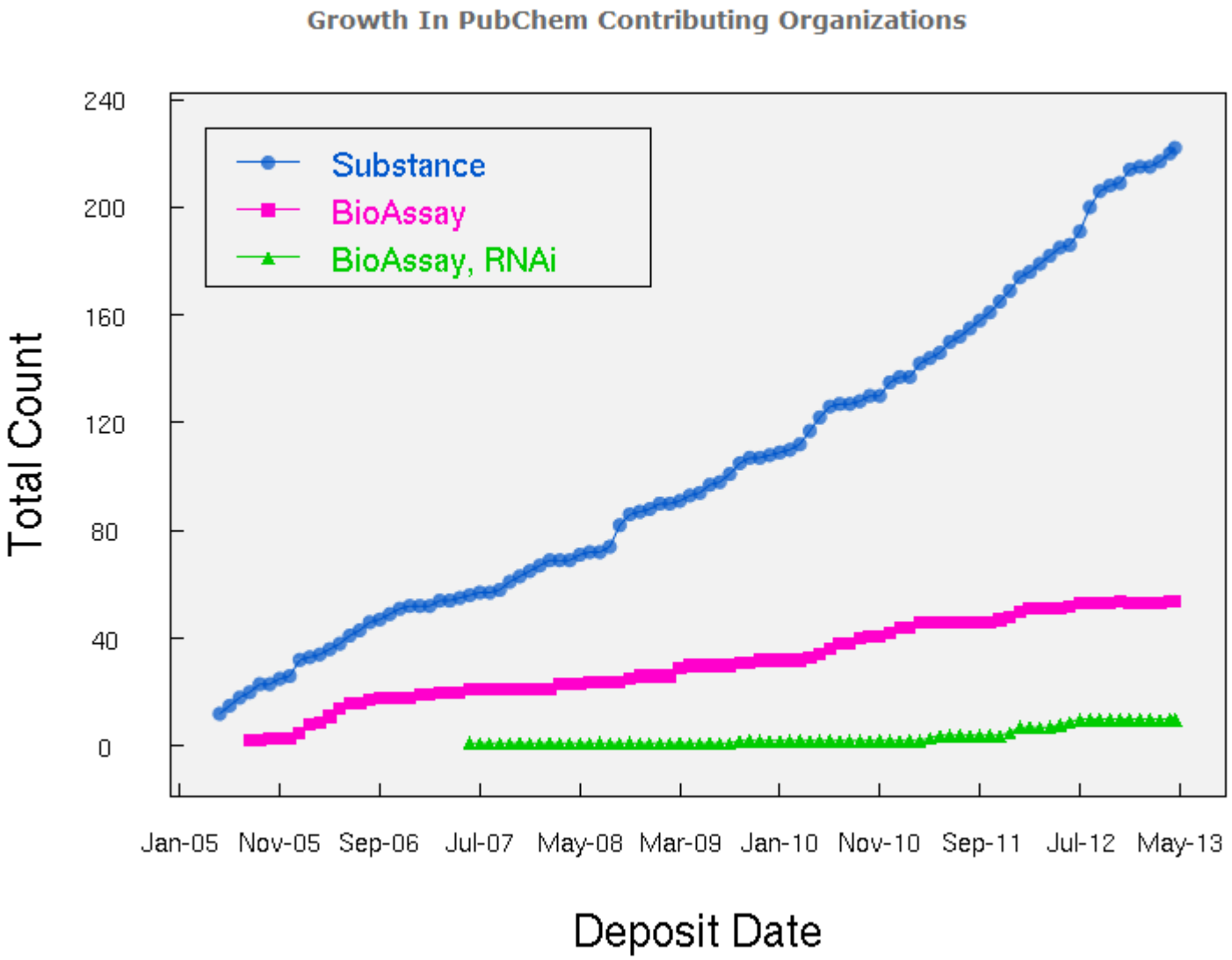
PUBCHEM UPLOAD: A STREAMLINED WAY TO SUBMIT CHEMICAL & BIOASSAY RESULTS

Benjamin A. Shoemaker

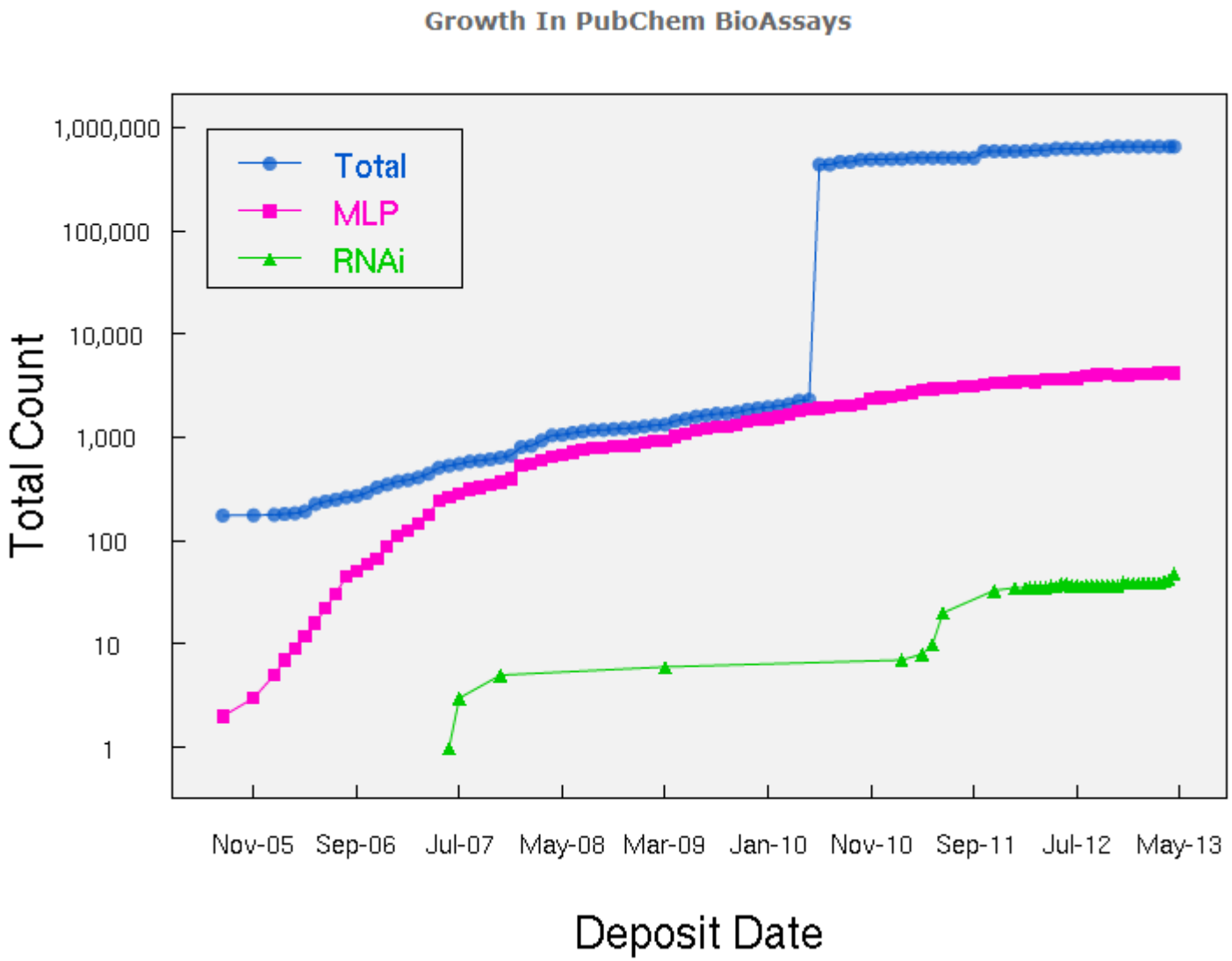
PubChem Data Size & Growth



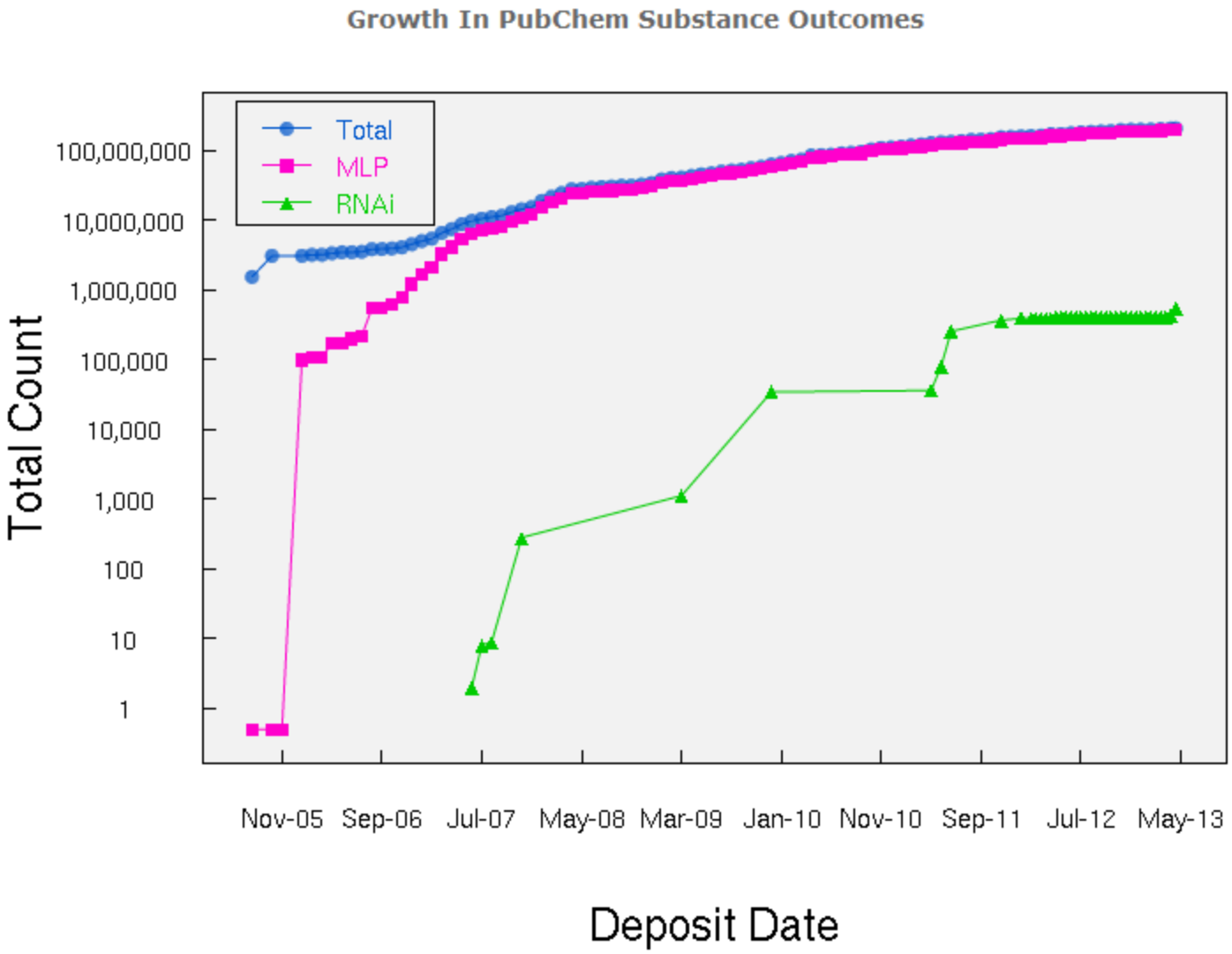
PubChem Data Size & Growth



PubChem Data Size & Growth



PubChem Data Size & Growth



Types of Experimental Data in PubChem

- PubChem Substance:
  - Chemical structures
  - Drug names/synonyms
  - Patents
- PubChem BioAssay:
  - 1 target, HTS screens
  - Dose-response, confirmatory
  - Summary, Probes
  - Counter screens

- Links to PubMed, Gene, Protein, OMIM, Biosystems
- Annotations/Ontologies

- ChEMBL
- siRNA screens
- Multi-target profiles
- Tox screens
- Curated (PDB, annotations)

Types of Submitters to PubChem

- Chemical supply companies
- Automated journal uploads (encourage assay journals)
- ChEMBL
- NIH Molecular Screening Centers
- siRNA screening consortium
- Database collections (gov’t, public, private)
- Individual research labs

PubChem Upload: Efficient Web Interface

https://pubchem.ncbi.nlm.nih.gov/upload/

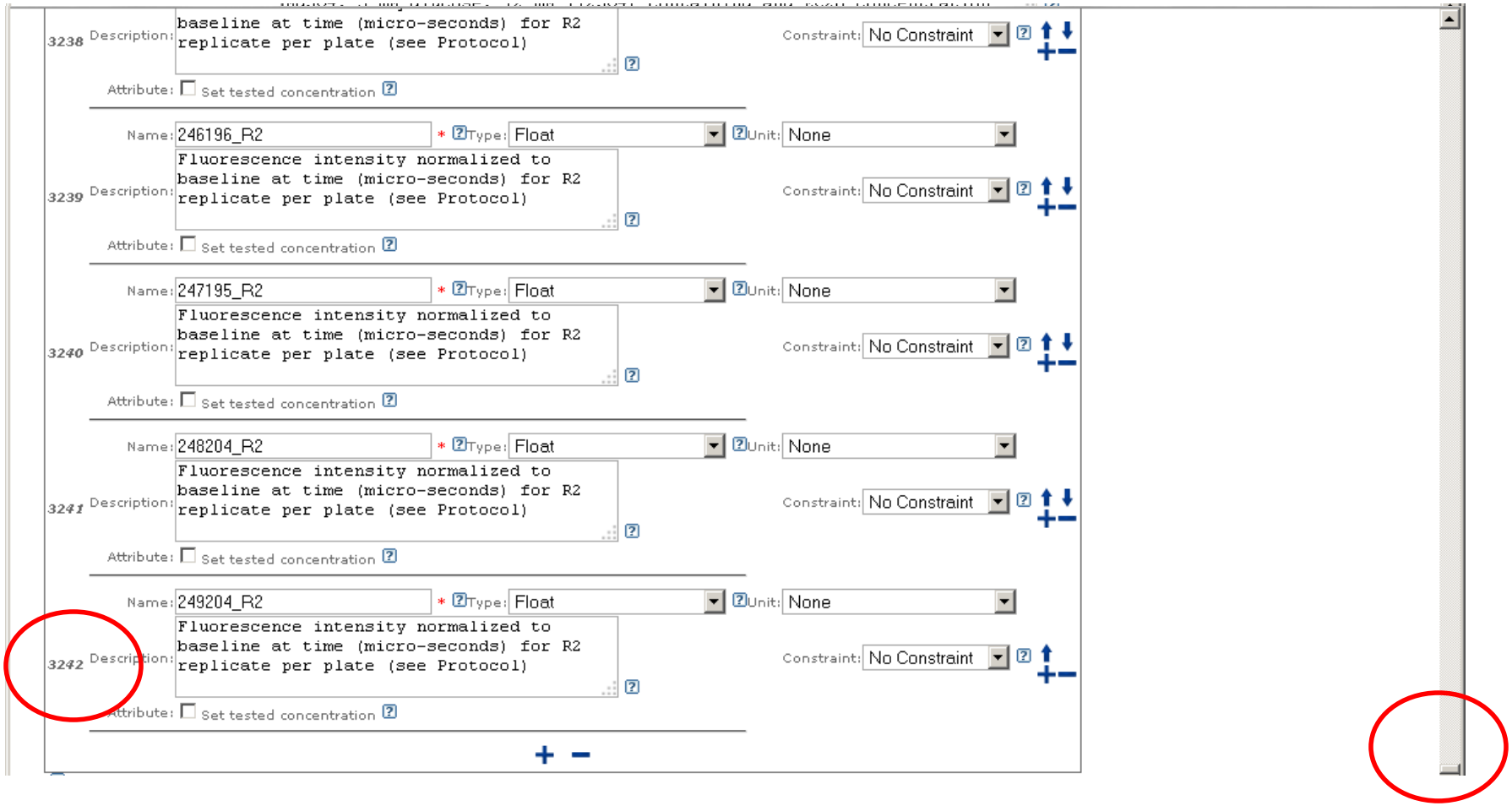
- Support wide range user-defined data
- Useful to the submitter:
  - Take everything they have
  - Minimize hassle
- Useful to the PubChem user:
  - Make it easy to find relevant data
  - Make it possible to aggregate & compare results

Goals / Features for New Interface

- Fewer time-outs for complicated forms
- Form data saved more robustly
- Less scrolling
- Page reloads minimized
- Extensible interface
  - Easy to modify
  - Data access independent
- In-place edit without file reload
- Uniform spreadsheet use

Previous Web Interface Issues

- Web controls: HTML sent, page size, reload



Security needs

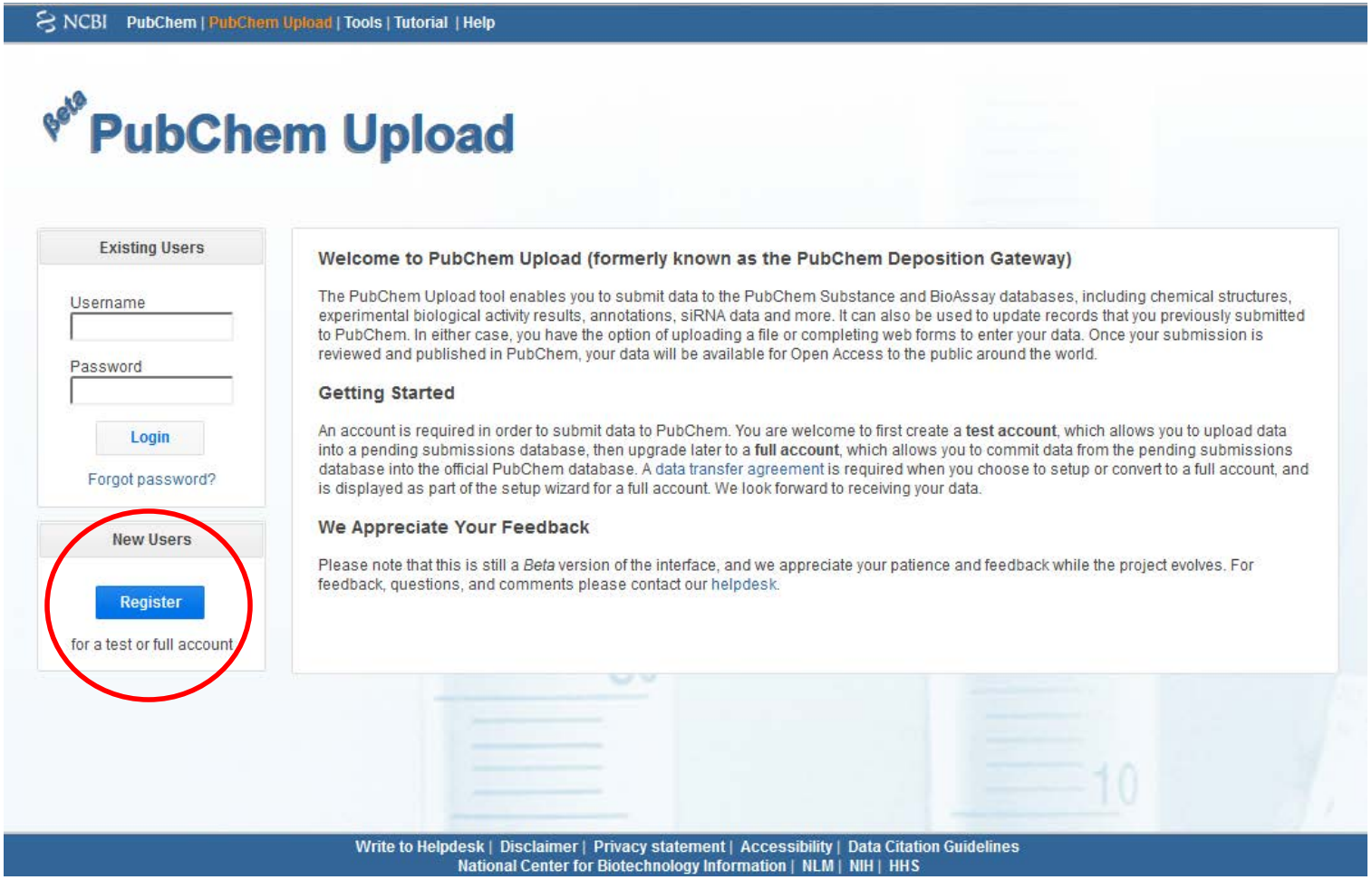
- Initial curator check of new submitter
- Login authentication
- Accredited updates/new additions per data source
- Multiple users on one submission account
- On-hold data up to one year

New Submitters: Make it easy!

- Get minimal information
- Convenient to start submission
- Get in and out quickly

- Challenges:
  - Want to verify identity
  - Get good source keywords for PubChem search
  - Sign Data Transfer Agreement
  - Quickly transition from test to production
  - Keep track of test submissions

New Submitter Info



New Submitter Info

New Submitter Info

Starting a submission

PubChem Upload Wizard

Substance Upload: Fill in Form

Do you have an SID (PubChem Substance ID) or a CID (PubChem Compound ID) that you would like to start from?

- (●) **No**
- ( ) **PubChem SID**
- ( ) **PubChem CID**

Hint

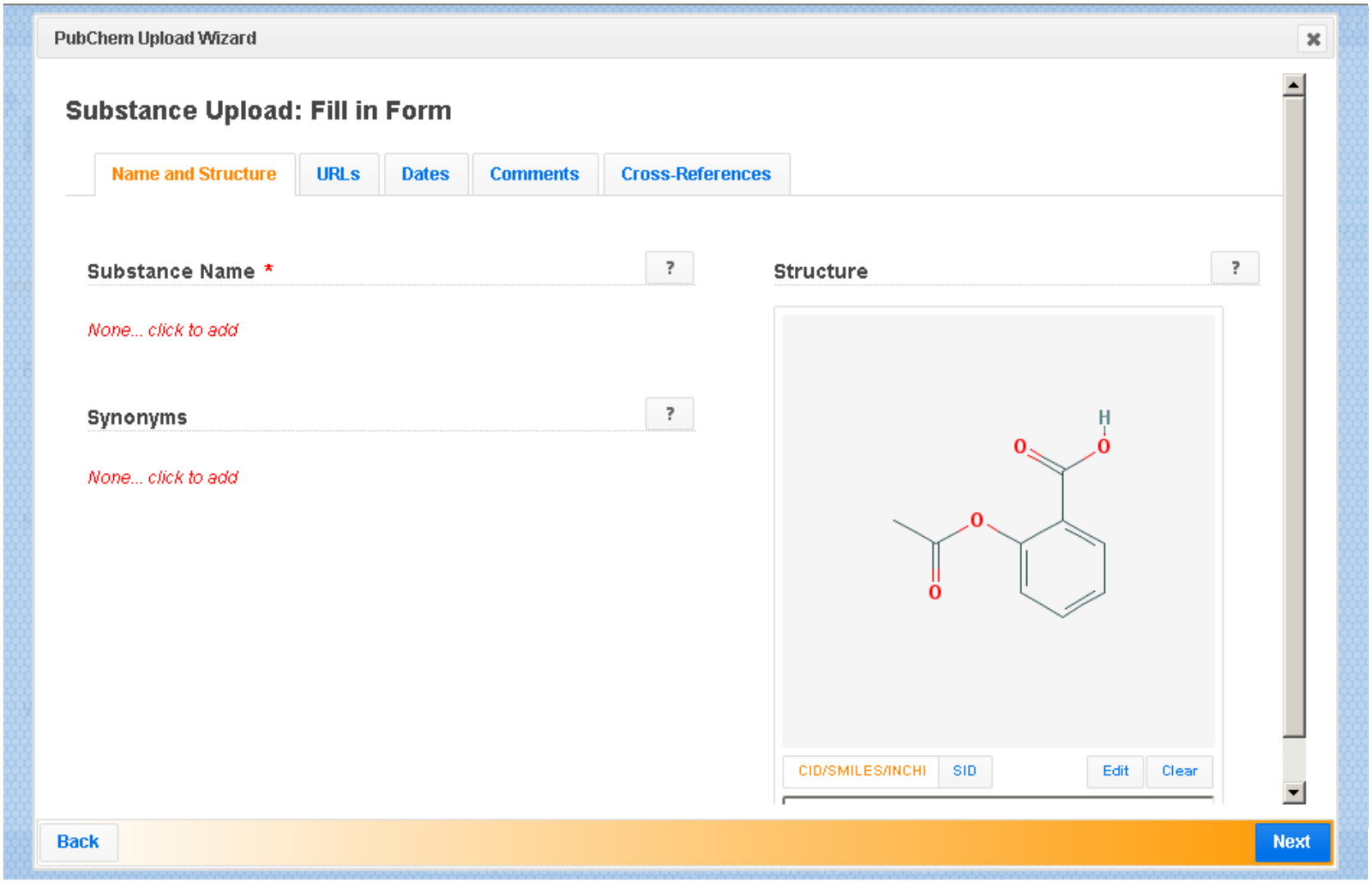
PubChem most likely already contains a substance with an exactly the same or similar structure to the one you are looking to upload. If you want to use an existing substance as a template, you can search PubChem Substance and then enter an SID here. Or, if you prefer, you can search PubChem Compound and then enter CID here.

If you enter an SID of the substance you own, you will also be given options to update it.

For more info, please refer to our brief substance upload tutorial.

Back | Next

Substance Input Options



Substance Input Options

PubChem Upload Wizard

Substance Upload: Modify Substance (SID 131485344)

Name and Structure | URLs | Dates | Comments | Cross-References

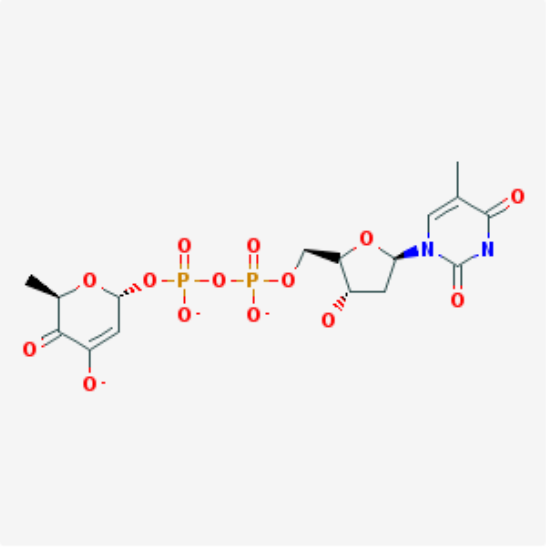
Substance Name * *cannot be changed in modify mode* ?

CPD-13380

Synonyms ?

CPD-13380
dTDP-2,6-dideoxy-D-glycero-hex-2-enos-4-ulose

Structure ?



CID/SMILES/INCHI | SID | Edit | Clear

Input from PubChem List

NCBI PubChem | PubChem Upload | Tools | Tutorial | Help IMPERSONATED as Peter Karp (BioCyc) | Logout

Beta **PubChem Upload**

New Submission

Welcome | Substances | Assays | Account Settings

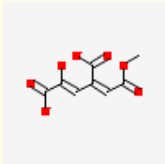
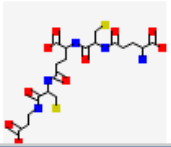
Pending | In PubChem

These substances have been previously uploaded to PubChem by you

Select a row for further options

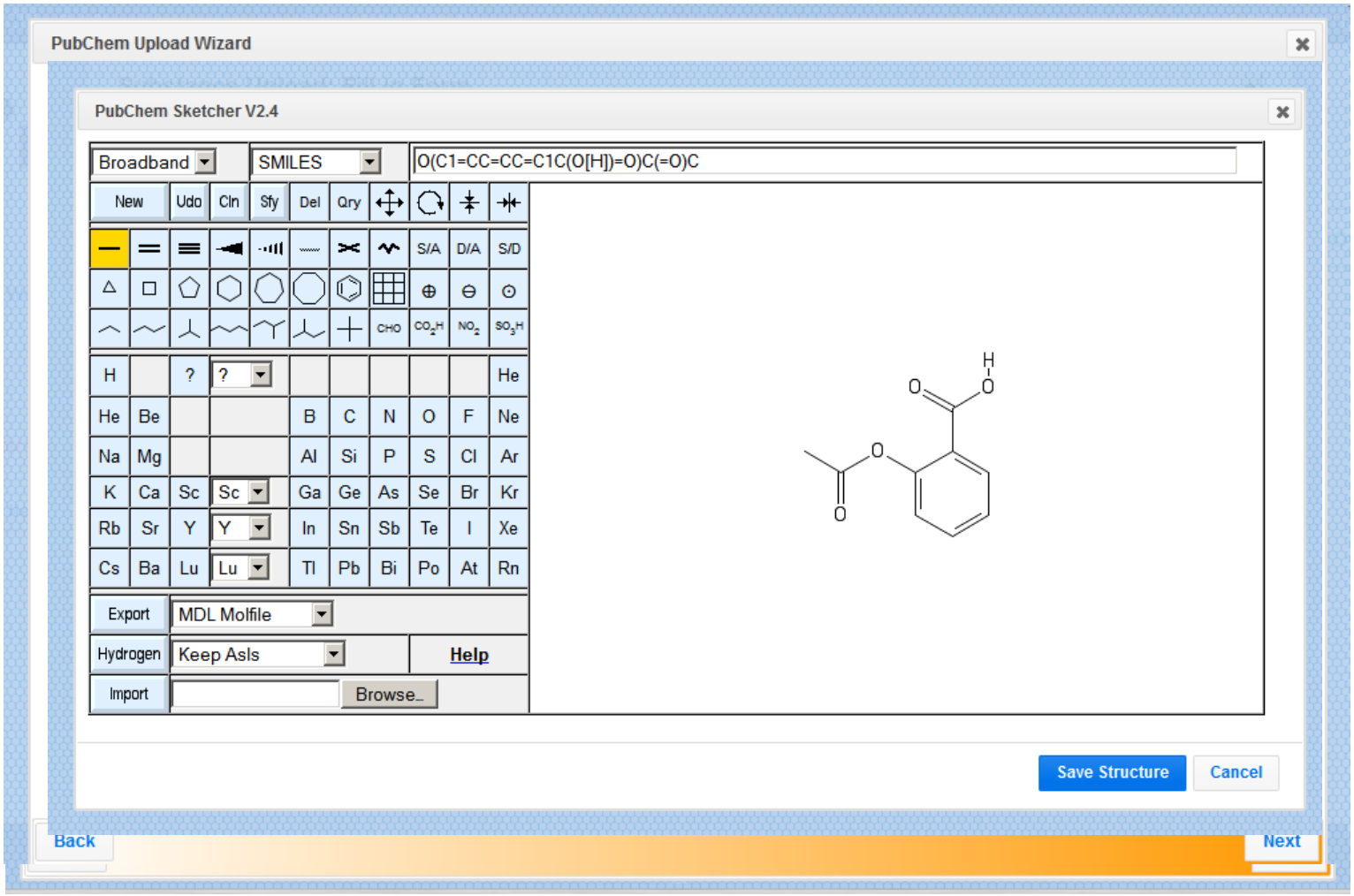
Showing rows 1 to 10 of 9270.

1 2 3 4 5 6 ... 927

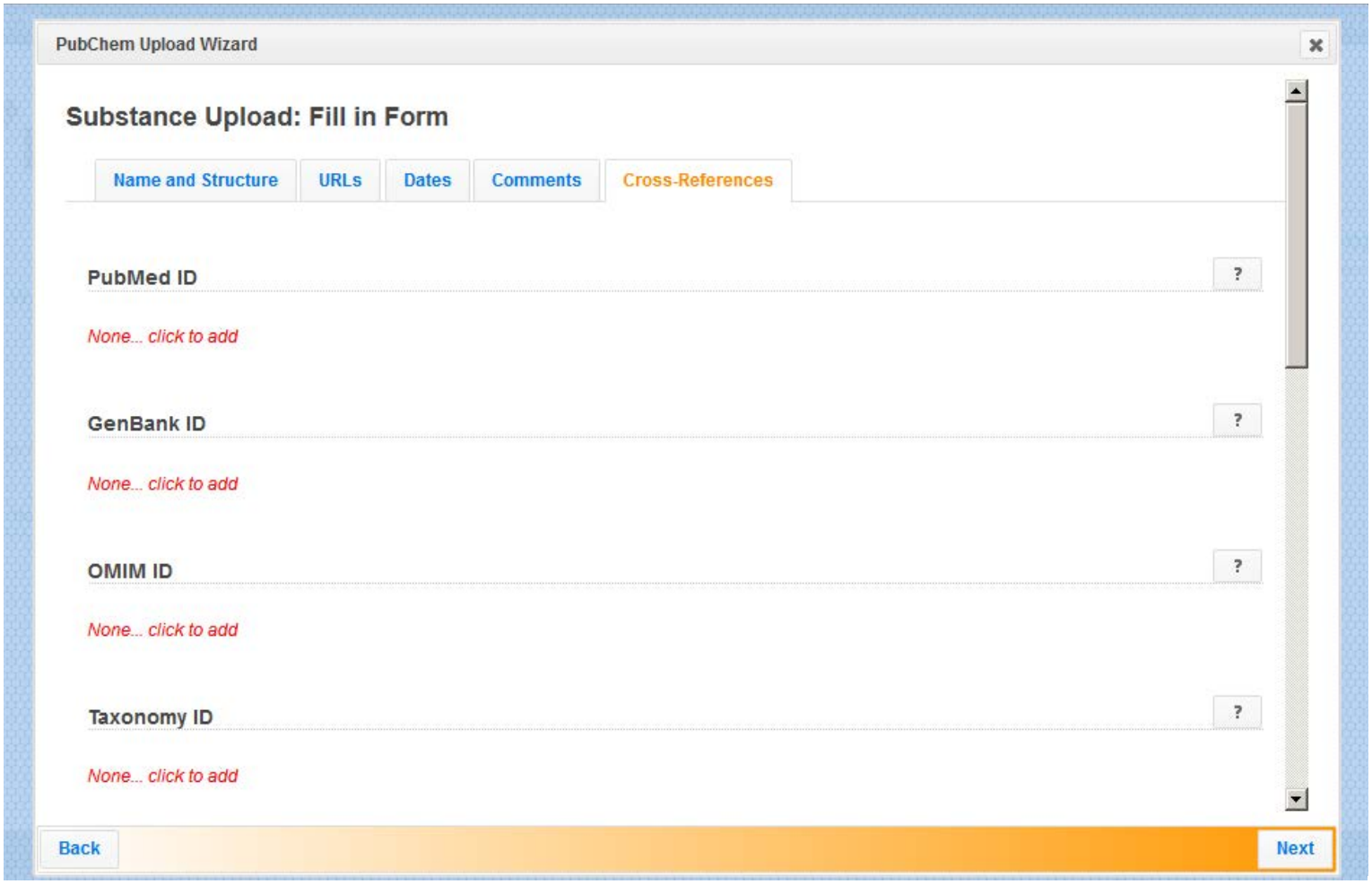
N	Depiction	SID	REGID	SYNONYM	Creation Date
1		131485348	CPD-13530	4-carboxy-2-hydroxy-6-methoxy-6-oxohexa-2,4-dienoate CHMOD View in PubChem | Use as Template | Modify | Revoke	2012/01/10
2		131485347	CPD-13498	gamma-Glu-Cys-gamma-Glu-Cys-beta-Ala CPD-13498	2012/01/10

Write to Helpdesk | Disclaimer | Privacy statement | Accessibility | Data Citation Guidelines
National Center for Biotechnology Information | NLM | NIH | HHS

Substance Form



Substance Tags



Assay Wizard

PubChem Upload Wizard

Assay Upload: Form

Do you have an AID (PubChem Assay ID) that you would like to start from?

- ○ No
- ● PubChem Assay ID 652068

Hint

PubChem might already contain an assay similar to an assay you are looking to upload. If you would like to use an existing assay as a template, you can search PubChem Assay for a suitable assay and then enter the AID here.

If you enter an AID of the assay you own, you will also be given options to update it.

For more info, please refer to our brief assay upload tutorial.

Back | Next

New Assay Submission

NCBI PubChem | PubChem Upload | Tools | Tutorial | Help Logged in as Linus Pauling (1084) | Upgrade to Full Account | Logout

Beta PubChem Upload

ASSAY SUBMISSION 15311 (Created)

New Assay: AUTO:name 20130426143214
DSN: 1084
Submitted: 04/26/2013 14:32:14

Please use the form below to enter/edit assay description (annotations) and data (test results), and then click **Validate** button when ready. You can also use **File Upload** button to upload all or part of the assay.

Save | Validate | Preview in PubChem | File Upload | File Export | Delete

Description | Data | Options | History

External Assay Registry ID (a unique assay identifier in your database) *

AUTO:20130426143214

Assay Name (for display purposes) *

AUTO:name 20130426143214

Assay Description

None... click to add

Assay Protocol (procedure used to generate the assay)

None... click to add

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National Center for Biotechnology Information | NLM | NIH | HHS

Input from PubChem List

NCBI PubChem | PubChem Upload | Tools | Tutorial | Help IMPERSONATED as Kashif Hoda (The Scripps Research Institute Molecular Screening Center) | Logout

Beta PubChem Upload

New Submission

Welcome | Substances | Assays | Account Settings

Pending | In PubChem

These assays have been previously uploaded to PubChem by you

Select a row for further options

Showing rows 1 to 10 of 1386.

1 2 3 4 5 6 ... 139

N	AID	Name	Creation Date	Hold Until Date
1	686953	Summary of a probe development effort to identify inhibitors of COUP-TFII (NR2F2)	2013/04/24	
2	652068	Counterscreen for molecules that bind rCAG RNA repeats: fluorescent based biochemical counterscreen assay for inhibitors of the DNA-based (5'CAG/3'GTC) TO-PRO-1 dye complex View in PubChem | Use as Template | Modify | Revoke	2013/02/28	
3	651821	Fluorescence-based biochemical primary high throughput screening assay to identify molecules that bind r(CAG) RNA repeats	2012/11/28	

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New Assay Submission

NCBI PubChem | PubChem Upload | Tools | Tutorial | Help Logged in as Linus Pauling (1084) | Upgrade to Full Account | Logout

ASSAY SUBMISSION 15311 (Created)

New Assay: AUTO:name 20130426143214
DSN: 1084
Submitted: 04/26/2013 14:32:14

Please use the form below to enter/edit assay description (annotations) and data (test results), and then click **Validate** button when ready. You can also use **File Upload** button to upload all or part of the assay.

Save | Revert to Saved | Validate | Preview in PubChem | File Upload | File Export | Delete

Description | Data | Options | History

External Assay Registry ID (a unique assay identifier in your database) *

AUTO:20130426143214

Assay Name (for display purposes) *

AUTO:name 20130426143214

Assay Description

Here is the complete description of my assay. . .

Assay Protocol (procedure used to generate the assay)

None... click to add

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Edit Multi-Value Fields

NCBI PubChem | PubChem Upload | Tools | Tutorial | Help Logged in as Linus Pauling (1084) | Upgrade to Full Account | Logout

Assay Cross-References: please use the spreadsheet below to type, paste (Ctrl-v), or upload a file, and then close...

Save | Revert to Saved | Clear | Import File | Export File

See Example

PUBCHEM_AID

XREF_TYPE

PubChem BioAssay Id (AID)

The database type of XRef identifier supplied. This type column must appear as the first column of the spreadsheet.

	A	B	C	Add Column
REQUIRED HEADER	XREF_TYPE	XREF_VALUE	XREF_ANNOTATION	
1	PUBCHEM_AID	651821	Primary screen (r(CAG) inhibitors in singlicate)	
2	PUBCHEM_AID	651825	Summary (r(CAG) inhibitors)	
3	PUBCHEM_NCBI_GENE_ID	3064	HTT huntingtin	
4	PUBCHEM_EXT_DATASOURCE_URL	http://mlpcn.florida.scripps.edu		
5	PUBCHEM_NCBI_OMIM_ID	143100		
6	PUBCHEM_NCBI_TAXONOMY_ID	9606		
7	PUBCHEM_NCBI_PUBMED_ID	17417937	Reference 1	
8	PUBCHEM_NCBI_PUBMED_ID	8937828	Reference 2	
9	PUBCHEM_NCBI_PUBMED_ID	12747895	Reference 3	
10	PUBCHEM_NCBI_PUBMED_ID	15223312	Reference 4	

Add More Rows Displaying rows 1 to 10 of 20 rows total

Show More

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Context-dependent Help

Assay Cross-References: please use the spreadsheet below to type, paste (Ctrl-v), or upload a file, and then close...

Save | Revert to Saved | Clear | Import File | Export File

See Example

Summary (r(CAG) inhibitors)

XREF_ANNOTATION

An explanatory text describing the relevance of this cross-referenced item to the assay.

	A	B	C	Add Column
REQUIRED HEADER	XREF_TYPE	XREF_VALUE	XREF_ANNOTATION	
1	PUBCHEM_AID	651821	Primary screen (r(CAG) inhibitors in singlicate)	
2	PUBCHEM_AID	651825	Summary (r(CAG) inhibitors)	
3	PUBCHEM_NCBI_GENE_ID	3064	HTT huntingtin	
4	PUBCHEM_EXT_DATASOURCE_URL	http://mlpcn.florida.scripps.edu		
5	PUBCHEM_NCBI_OMIM_ID	143100		
6	PUBCHEM_NCBI_TAXONOMY_ID	9606		
7	PUBCHEM_NCBI_PUBMED_ID	17417937	Reference 1	
8	PUBCHEM_NCBI_PUBMED_ID	8937828	Reference 2	
9	PUBCHEM_NCBI_PUBMED_ID	12747895	Reference 3	
10	PUBCHEM_NCBI_PUBMED_ID	15223312	Reference 4	

Add More Rows

Displaying rows 1 to 10 of 20 rows total

Assay Data: Result Definitions

NCBI PubChem | PubChem Upload | Tools | Tutorial | Help Logged in as Linus Pauling (1084) | Upgrade to Full Account | Logout

Please use the form below to enter/edit assay description (annotations) and data (test results), and then click **Validate** button when ready. You can also use **File Upload** button to upload all or part of the assay.

Save | Revert to Saved | Validate | Preview in PubChem | File Upload | File Export | Delete

Description | Data | Options | History

Assay Data ?

None... click to add

Result Column Definitions

Edit | Clear

PUBCHEM_RESULT_TAG	Average Inhibition at 3 uM	Standard Deviation	Inhibition at 3 uM [1]	Inhibition at 3 uM [2]	Inhibition at 3 uM [3]
RESULT_TYPE	FLOAT	FLOAT	FLOAT	FLOAT	FLOAT
RESULT_DESCR	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar.	Standard deviation of inhibition at 3 uM	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar, replicate [1]	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar, replicate [2]	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar, replicate [3]
RESULT_UNIT	PERCENT	NONE	PERCENT	PERCENT	PERCENT
RESULT_ATTR_CONC_MICROMOL	3		3	3	3

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National Center for Biotechnology Information | NLM | NIH | HHS

Assay Data: Result Definitions

Assay Data: please use the spreadsheet below to type, paste (Ctrl-v), or upload a file, and then close...

Save | Revert to Saved | Clear | Import File | Export File

See Example

PERCENT

This is not a standard P ovided by the assay submitter: Average Inhibition at 3 uM

Insert/Paste Data

RESULT_UNIT

Percent

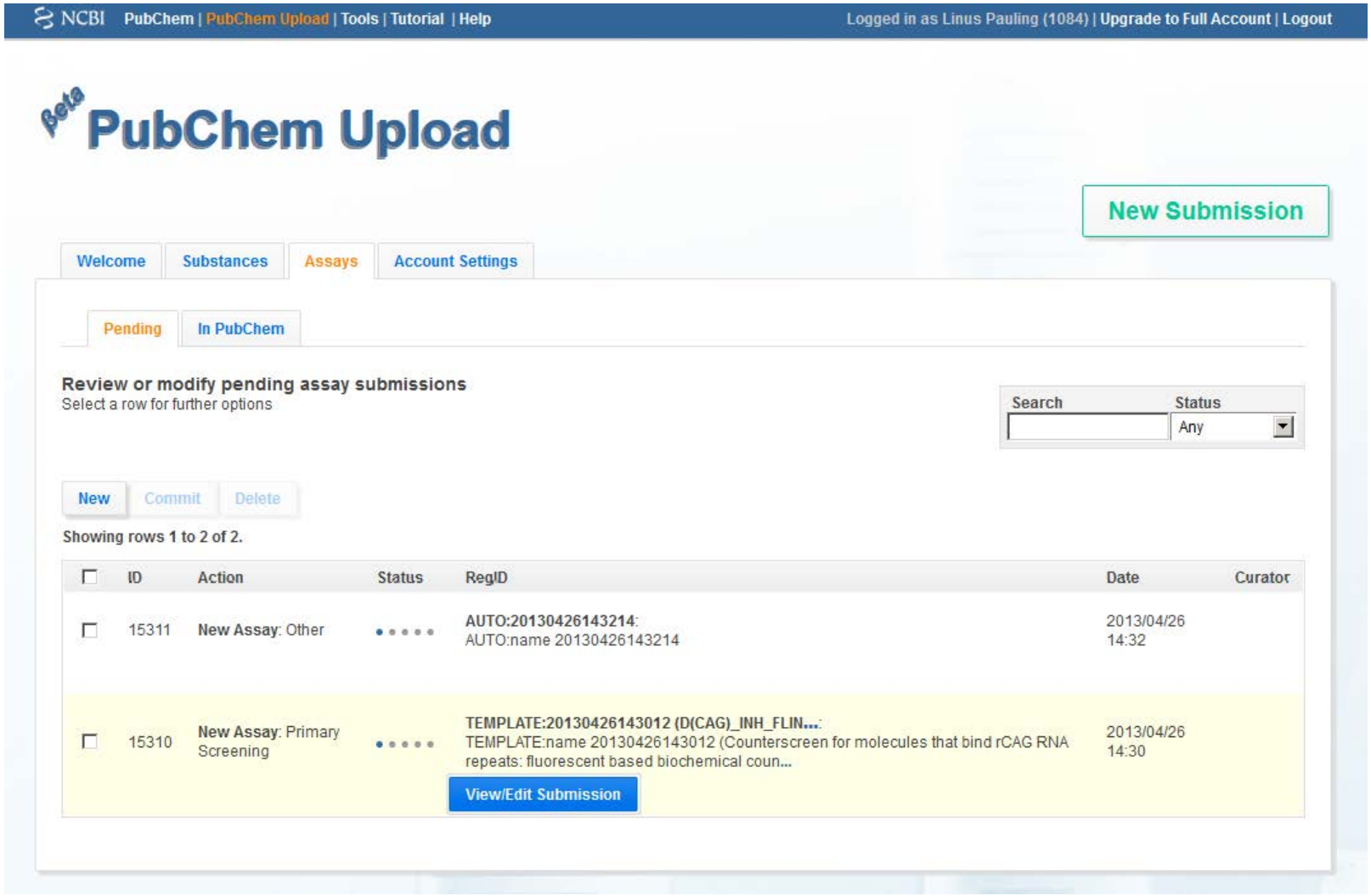
Various units are available to better define the measu ment of a given result column.

Hide Column Definitions	A	B	
PUBCHEM_RESULT_TAG	Average Inhibition t 3 uM	Standard Deviation	Inhibition at 3 uM [1]
RESULT_TYPE	FLOAT	FLOAT	FLOAT
RESULT_DESCR	Normalized percen inhibition of the primary screen at a compound concentration of 3.00 micromolar.	Standard deviation of inhibition at 3 uM	Normalized percent inhibition
RESULT_UNIT	PERCENT	NONE	PERCENT
RESULT_ATTR_CONC_MICROMOL	3		3
RESULT_CONC_RESPONSE_SERIES_ID			
RESULT_IS_ACTIVE_CONCENTRATION			
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

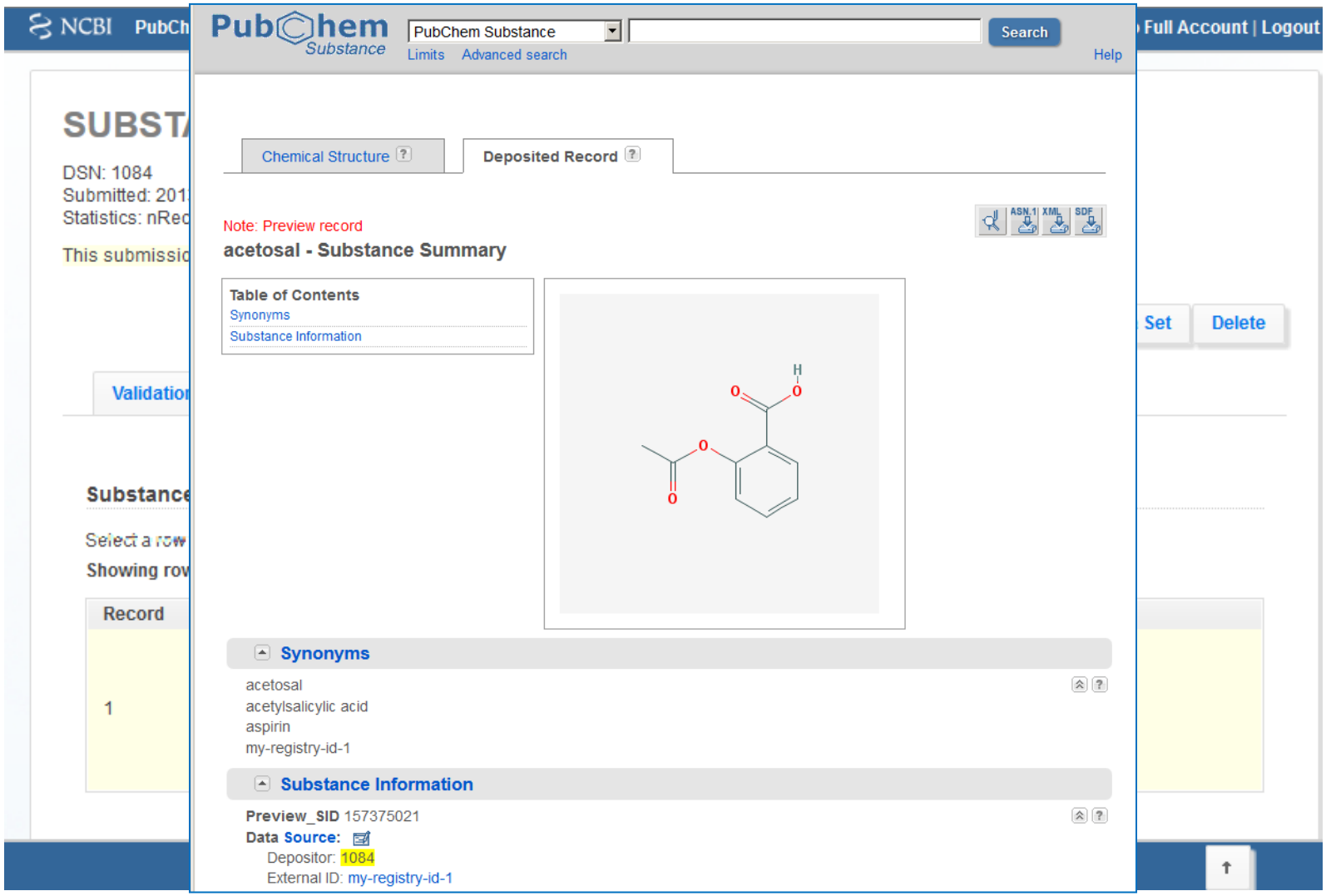
Add More Rows

Displaying rows 1 to 10 of 10 rows total

Review Pending Submissions



Preview in PubChem: Substance



Preview in PubChem: BioAssay

Short, yet infor
preview data)

Name: Countersc
for inhibitors of th

Table of Conten
- Target
- Description
- Protocol
- Comment
- Result Definitior
- Additional Inform

Target

Homo sapiens hu

Description:

Source (MLPCN C
Affiliation: The Sc
Assay Provider: M
Network: Molecula
Grant Proposal N
Grant Proposal P
External Assay ID

Name: Countersc

nt | Logout

an

lete

?

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Comment

Due to the increasing size of the MLPCN compound library, this assay may have been run as two or more separate campaigns, each campaign testing a unique set of compounds. All data reported were normalized on a per-plate basis. Possible artifacts of this assay can include, but are not limited to: dust or lint located in or on wells of the microtiter plate, and compounds that modulate well fluorescence. All test compound concentrations reported above and below are nominal; the specific test concentration(s) for a particular compound may vary based upon the actual sample provided by the MLSMR. The MLSMR was not able to provide all compounds selected for testing in this assay.

Result Definitions

TID	Name	Description	Histogram	Type	Unit
	Outcome	The BioAssay activity outcome		Outcome	
1	Average Inhibition at 3 uM (3μM**)	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar.		Float	%
2	Standard Deviation	Standard deviation of inhibition at 3 uM		Float	
3	Inhibition at 3 uM [1] (3μM**)	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar, replicate [1]		Float	%
4	Inhibition at 3 uM [2] (3μM**)	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar, replicate [2]		Float	%
5	Inhibition at 3 uM [3] (3μM**)	Normalized percent inhibition of the primary screen at a compound concentration of 3.00 micromolar, replicate [3]		Float	%

** Test Concentration.

Additional Information

Grant Number: 1 R03 DA033977-010

PubChem Upload Layout

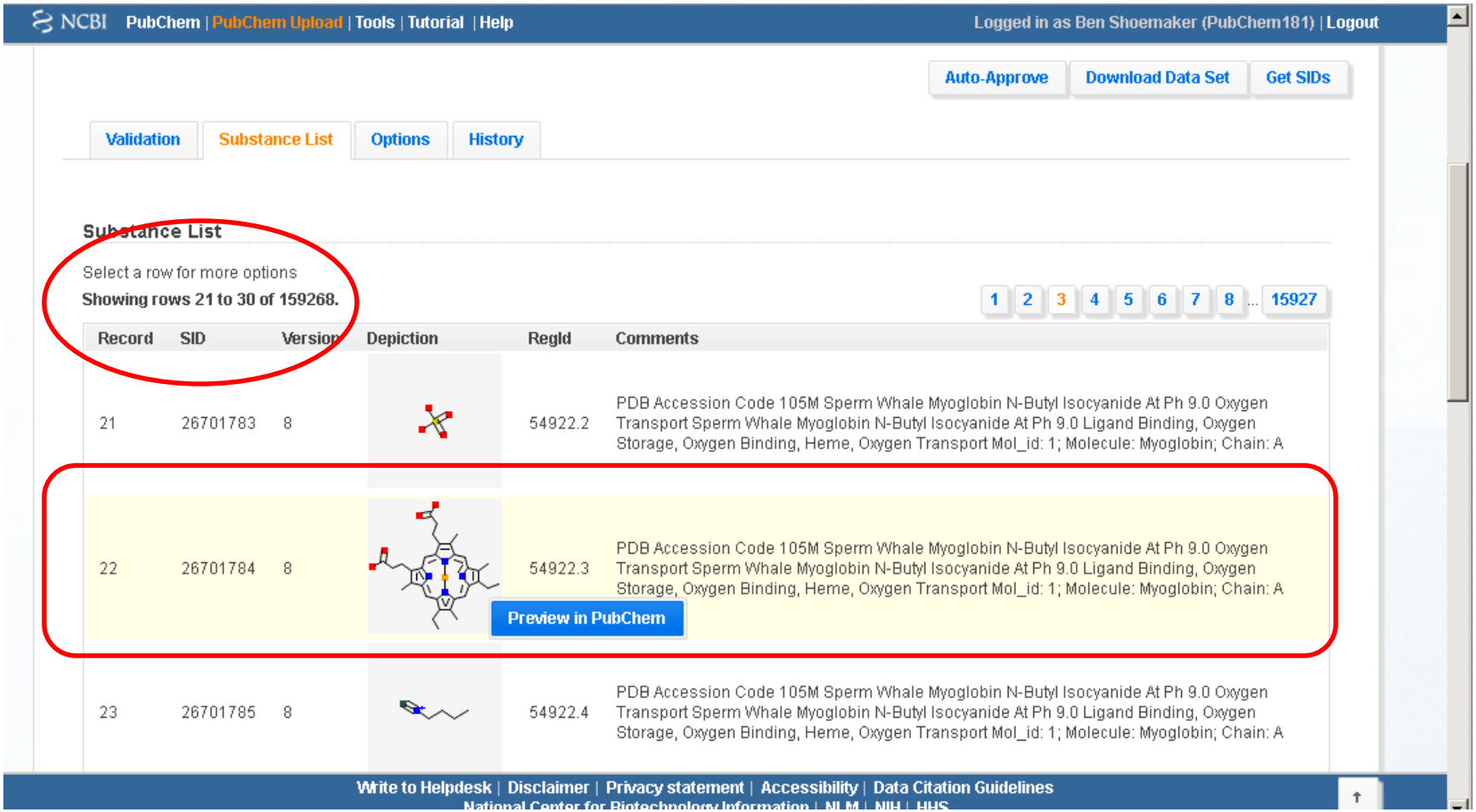
- jQuery JavaScript renders all web HTML on client side
- Server APIs (C++) send & receive data from/to the database
- Client (jQuery Ajax) calls ‘masked’ server cgi
- RESTful communication between client & server
- Security primarily handled by server cgi

- **Client responsible for web navigation, logic & state**
- **Server responsible for data queries, not state**

Example client/server exchanges

1. **Display table of user's pending submissions**
   - Send cookie, usr_id, request type to cgi
   - Receive status code, JSON table of data
   - Render display, make additional calls
2. Edit data within a submission
   - Send cookie, sub_id, request type, field, text
   - Receive status code
   - Render display (grey-out 'Save' button)

Client/Server: Page to Display



Read Data from Server

- Make request to server with arguments (& cookie):
  - action=get_subs
  - sub_id=16536, pgsize=10, startrec=21

- Receive response from server in JSON:

{"response":[{"name":"return","headers":["code"],"data":[["pass"]]},{"name":"subst_list","headers":["Record","SID","Version","tid","RegId","Comments"],"data":[["21","26701783","8","157215778","54922.2","PDB Accession Code 105M…”]]}

Read Data from Server

- Parsed data from JSON
- Server response includes error code

code
pass

Record	SID	Version	tid	RegId	Comments
21	26701783	8	157215778	54922.2	PDB Accession Code 105M Sperm Whale Myoglobin N-Butyl Isocyanide At Ph
22	26701784	8	157215781	54922.3	PDB Accession Code 105M Sperm Whale Myoglobin N-Butyl Isocyanide At Ph 9.0 Oxygen Transport
23	26701785	8	157215784	54922.4	PDB Accession Code 105M Sperm Whale Myoglobin N-Butyl Isocyanide At Ph 9.0 Oxygen

Read Data from Server

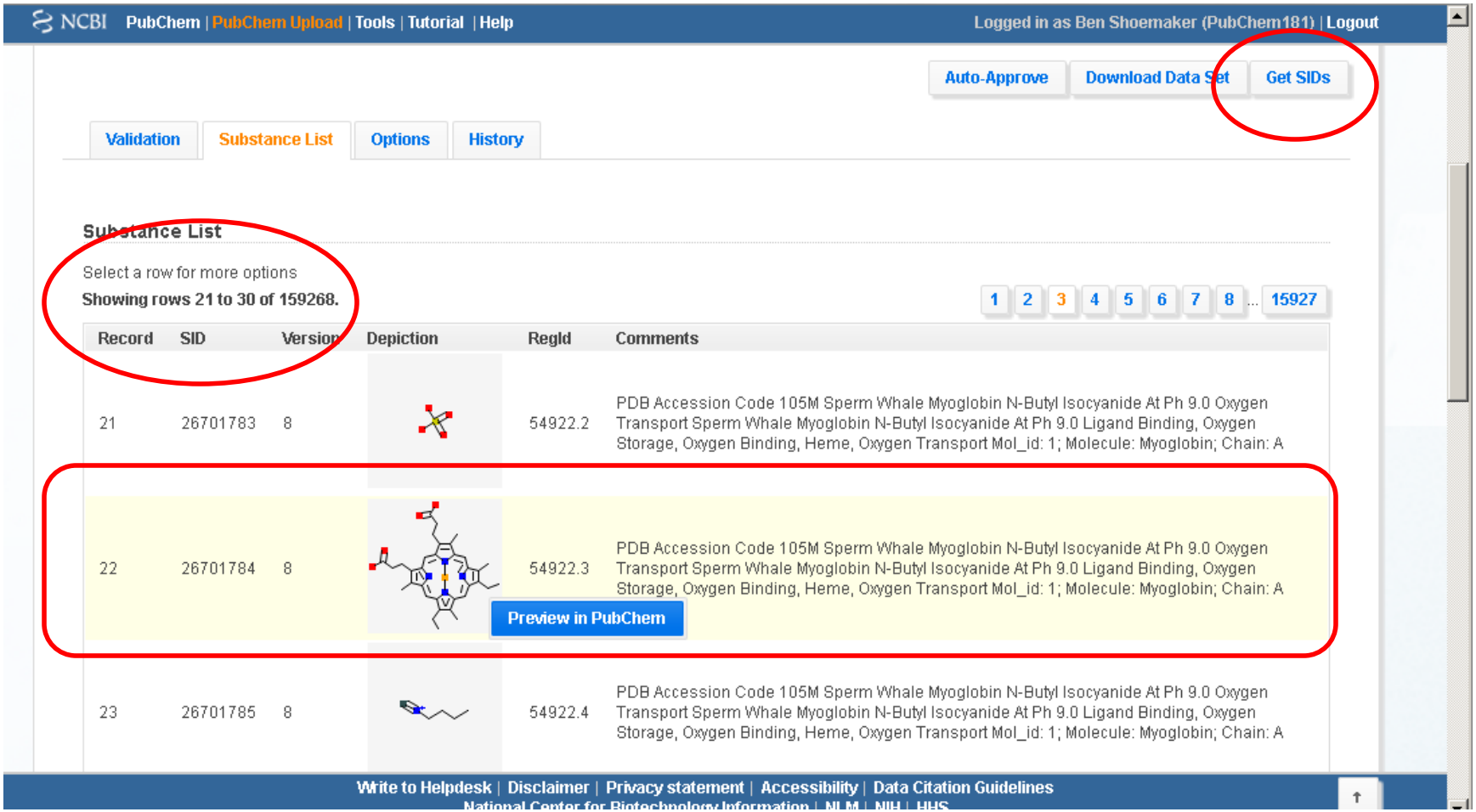
- Make request to server with arguments (& cookie):
  - action=get_subs
  - sub_id=16536, pgsize=10, startrec=21

- Receive response from server in JSON:

{"response":[{"name":"return","headers":["code"],"data":[["pass"]]},{"name":"subst_list","headers":["Record","SID","Version","tid","RegId","Comments"],"data":[["21","26701783","8","157215778","54922.2","PDB Accession Code 105M…”]]}

- Simple error code
- Data transfer is minimal
- Data on server can be arbitrarily large

Client/Server: Page to Display



Example client/server exchanges

1. Display table of user's pending submissions
   - Send cookie, usr_id, request type to cgi
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2. **Edit data within a submission**
   - Send cookie, sub_id, request type, field, text
   - Receive status code
   - Render display (grey-out 'Save' button)

Edit/Save Data to Server

Assay Data: please use the spreadsheet below to type, paste (Ctrl-v), or upload a file, and then close...

Save | Revert to Saved | Clear | Import File | Export File

See Example

23.1

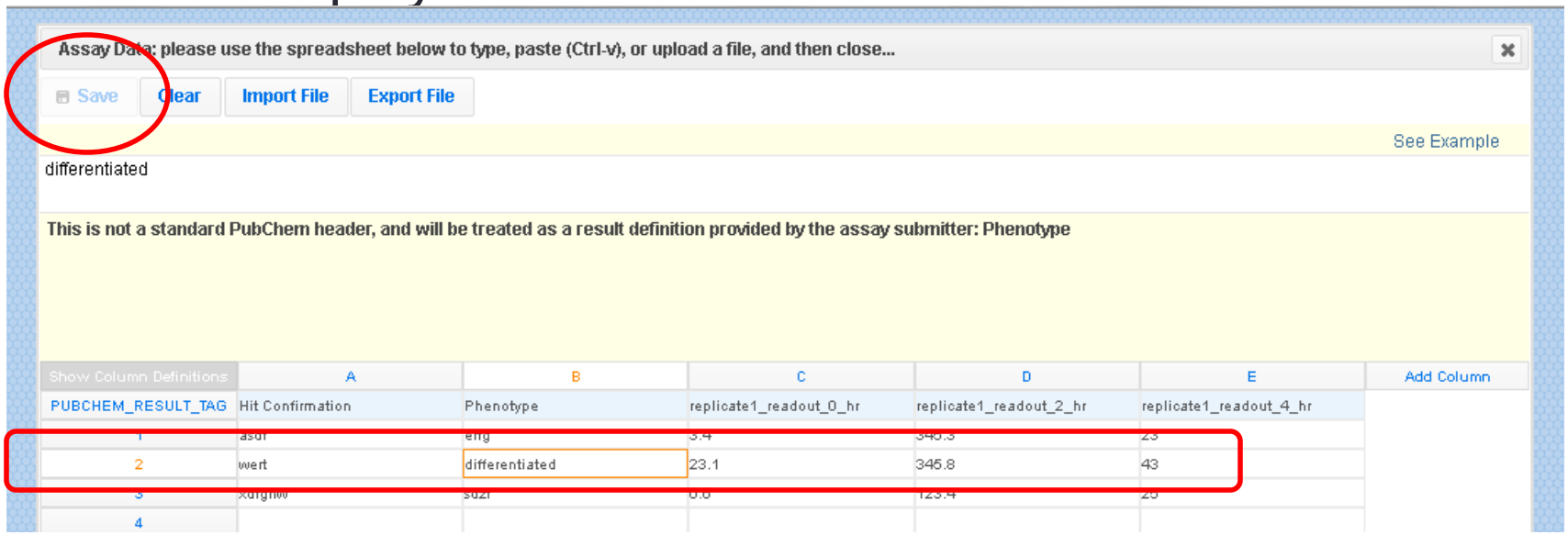
This is not a standard PubChem header, and will be treated as a result definition provided by the assay submitter: replicate1_readout_0_hr

Hide Column Definitions	A	B	C	D	E
PUBCHEM_RESULT_TAG	Hit Confirmation	Phenotype	replicate1_readout_0_hr	replicate1_readout_2_hr	replicate1_readout_4_hr
RESULT_TYPE	STRING	STRING	FLOAT	FLOAT	FLOAT
RESULT_DESCR	Confirmed by individial siRNA in Bmac1_dLuc	Biological effect type	bioluminescence measurement	bioluminescence measurement	bioluminescence measurem
RESULT_UNIT	NONE	NONE	PERCENT	PERCENT	PERCENT
RESULT_ATTR_CONC_MICROMOL					
RESULT_CONC_RESPONSE_SERIES_ID					
RESULT_IS_ACTIVE_CONCENTRATION					
1	asdf	afg	3.4	345.3	23
2	wert	differentiated	23.1	345.8	43
3	xdfghw	sdzf	0.6	123.4	25
4					
5					
6					
7					
8					
9					
10					

Edit/Save Data to Server

- Make request to server with args and data (& cookie):
  - action=replace_datarows
  - startrow=2, nrows=1
  - csv="2,wert,differentiated,23.1,345.8,43"
- Receive response from server in JSON:
- Render display

code
pass



Full Multi-Sheet Spreadsheet Support

- CSV (single sheet), Excel & OpenOffice
- Substance & BioAssay submissions
- Data upload & download
- Consistent with new web data editing

	A	B	C	D
1	PUBCHEM_EXT_DATASOURCE_REGID	PUBCHEM_SUBSTANCE_SYNONYM	PUBCHEM_EXT_DATASOURCE_SMILES	PUBCHEM_SUBSTANCE_COMMENT
2	my_sub1	GLUCOSE	C(C1C(C(C(C(O1)O)O)O)O)O	
3	my_sub2		CCOC1=CC=CC=C1NC(=O)C2=CC3=CC=CC=C3C	This is a comment.
4	my_sub3	benzene	C1=CC=CC=C1	
5				
6				
7				
8				
9				

Multi-Sheet Spreadsheet Example

	A	B	C	D	E
1	XREF_TYPE	XREF_VALUE	XREF_ANNOTATION		
2	PUBCHEM_AID	641	Screening assay		
3	PUBCHEM_AID	858	Confirmatory assay		
4	PUBCHEM_NCBI_TAXONOMY_ID	9606	human sequences		
5	PUBCHEM_EXT_DATASOURCE_URL	http://www.yoursite.com	My home page		
6	PUBCHEM_NCBI_GENE_ID	1812	DRD1 dopamine receptor D1 [Homo sapiens]		
7	PUBCHEM_NCBI_PUBMED_ID	15974933	Allosteric modulation of dopamine receptors, Schetz JA., Mini Rev Mec		
8	PUBCHEM_NCBI_PUBMED_ID	12021390	Dopamine receptor signaling, Neve KA, Seamans JK, J Recept Signal		

General | Results | Target | **Xrefs** | Categorized Comments

Large Submissions

- Substances
  - ~10s of millions per submission
  - Separate processing to SGE farm
  - Reworked database/backend handling with chunks of data

- Assays
  - Data rows often approach 500K in one assay
  - Result definitions (data columns) in the 1,000s
  - Panel Assays group columns per gene/protein target
  - Reworked access/update for preview, data table & download

Batch Id Lookup Tools

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Beta

PubChem Upload TOOLS

Gene Symbol to Gene ID | Nucleotide Accession to Gene ID

Gene Symbol to Gene ID Conversion Tool

Given a list of gene symbols, this tool will return a corresponding list of gene id's.

Note, however, that a gene symbol can be used to represent the same gene in several different species. Therefore, in order to make a unique mapping, we also require a taxonomy id. There are two ways to provide taxonomy ids:

1. Specify a single taxonomy id, in which case it will be assumed that all genes belong to the same species.
2. Specify a list of taxonomy ids - one for each gene symbol.

Gene Symbol (one per line)	Taxonomy ID (one per line)		Gene ID
CLOCK A2M CBL NFAT5	9606	Look Up	9575 2 867 10725

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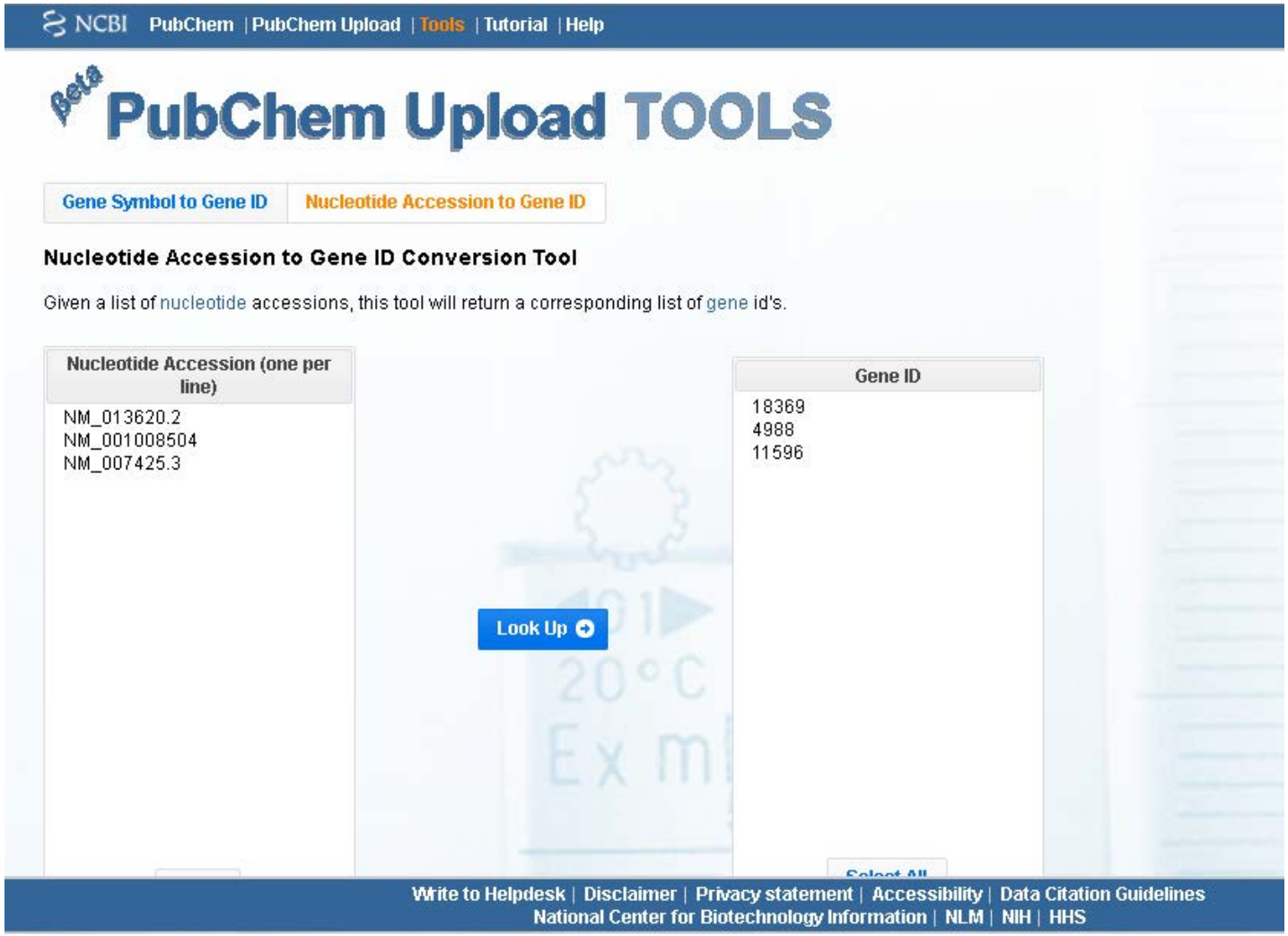
National Center for Biotechnology Information | NLM | NIH | HHS

Batch Id Lookup Tools



Curator/Power-user controls

NCBI PubChem | PubChem Upload | Tools | Tutorial | Help

Logged in as Ben Shoemaker (PubChem181) | Logout

New Submission

Welcome | Substances | Assays | Account Settings | Admin

Pending | Deleted

Review or modify pending assay submissions
Select a row for further options

Search	Submitter	Curator	Status
	Any	Ben Shoemaker	Any

Clear Filters

New | Commit | Delete | Check Out | Undo Check Out | Approve | Revise

Showing rows 1 to 2 of 2.

☐	ID	Submitter	Action	Status	RegID	Date	Curator	Is FTP	AutoOK
☑	15311	**Linus Pauling** (1084)	**New Assay**: Other	• • • • •	**My-Unique-Assay-Id-1...**: Allosteric Modulators of D1 Receptors	2013/04/27 11:10	Ben Shoemaker	No	
☐	15251	**Paul Kung** (Burnham Center for Chemical Ge...)	**New Assay**: Primary Screening 686954 (1.1)	• • • • •	**SBCCG-A991-Artemis-P...**: uHTS identification of small molecule inhibitors of Artemis ...	2013/04/27 07:50	Ben Shoemaker	No	

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PubChem Upload Feedback

- “I used it today and it looks really good. Works very smoothly and pages load a lot faster compared to the old one. And it’s great that the SD file can now be edited directly in the interface, saves me some downloading/deleting/re-uploading.” –PubChem Submitter/Journal Editor
- “By the way, tour new website looks great! Very clean look and feel.” –PubChem Submitter

- We welcome your feedback:
- pubchem-deposit-help@ncbi.nlm.nih.gov

Acknowledgments

- Asta Gindulyte

- Steve Bryant
- Yanli Wang
- Evan Bolton
- Paul Thiessen
- Siqian He
- Jeff Zhang
- Tugba Suzek
- Jiyao Wang
- PubChem Team

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