

## Release Notes - iCSS Chemical Dashboard - Version 3.0.1 – March 2019

### New Functionality

- [ICD-3789] - Download of filtered list of assays should download only the filtered list
- [ICD-3793] - GenRA should be enabled for all chemicals
- [ICD-3813] - Change the data on the Assay modal so it is coming from the database not Stored JSON
- [ICD-3814] - Add Active/Inactive Counts above ToxCast Summary Table
- [ICD-3818] - Add to Batch Search ability to include DTXCID identifiers in download
- [ICD-3822] - Add selection by Assay Vendor (ASID) to List of Assays
- [ICD-3843] - Label GenRA subtab as beta
- [ICD-3846] - Add information to the default hover for OPERA
- [ICD-3849] - Support MULTIPLE formats for MetFrag
- [ICD-3852] - Collapse all other tab accordions when a new accordion is opened
- [ICD-3862] - Add to batch search ability search by DTXCIDs
- [ICD-3866] - Add Ability to Copy Synonyms
- [ICD-3868] - Increase size of the Input box on home page for searching
- [ICD-3874] - Provide some indication that a file is downloading
- [ICD-3875] - TECH: File structure reorganization
- [ICD-3878] - TECH: Shore up Rails controller tests
- [ICD-3887] - Link out to the AOP from the Assay Modal and Include Author Status
- [ICD-3888] - Add Heading at the top of the page and associate Help Notifications
- [ICD-3894] - Make list name hyperlinked to list URL
- [ICD-3901] - Add Molecular Formula as an option to Show/Hide in the Chemical Results Page
- [ICD-3928] - Search all adducts based on Mass Search
- [ICD-3955] - Include cutoff in the ToxCast Summary table
- [ICD-3958] - Add to ToxCast Summary table ability to sort based on AOP, Event and SeqaPASS
- [ICD-3961] - Make List Details on List page collapsible
- [ICD-3967] - Set default sort of results page to be based on the GSID
- [ICD-3970] - Change operation of how select lists works
- [ICD-3972] - Add support for all ToxCast assays
- [ICD-3974] - Change all database queries using Invitrodb\_v2 to invitrodb\_v3
- [ICD-3979] - Executive Summary data moved off of Actor Web Services
- [ICD-3980] - Move remaining ACToR web services to InvitroDB\_v3
- [ICD-3983] - Allow a filter to be included for a list of lists
- [ICD-4006] - Update assay descriptions associated with all invitroDBv3 assays
- [ICD-4014] - Change order of subtabs under Bioactivity

### Bugs

- [ICD-3808] - Error detected by Excel with spreadsheet containing ToxPrint Chemotypes
- [ICD-3819] - Executive Summary error for chemical DTXSID60725828
- [ICD-3820] - Search on specific CAS Number causes error
- [ICD-3821] - Abstract Sifter finding odd MeSH synonym
- [ICD-3823] - Not possible to select queries via Abstract Sifter
- [ICD-3825] - Changes label on column headers
- [ICD-3826] - Images are missing from the downloads page
- [ICD-3828] - Data Quality INCOMPLETE level are being displayed
- [ICD-3832] - The popup image in OPERA model reports is small
- [ICD-3833] - No ability to select GoogleScholar query terms

[ICD-3834] - No images associated with External Links  
[ICD-3836] - Chemical Functional Use data never loads  
[ICD-3837] - NHANES Monitoring data sub-tab should gray out when no data available  
[ICD-3839] - Sets of chemicals associated with an assay do not load  
[ICD-3840] - Sorting on AC50 in Bioactivity Table doesn't seem to work  
[ICD-3841] - Cannot download SeqaPass reports  
[ICD-3850] - Missing MS-Ready structure under linked substances tab  
[ICD-3851] - Edit the query for advanced search MS-Ready formula  
[ICD-3855] - Search returns dashboard services error  
[ICD-3858] - Duplicates of MS-Ready structures  
[ICD-3863] - Edit the Case in InChI for a message  
[ICD-3867] - Toxcast Models subtab is listed twice  
[ICD-3871] - Executive Summary suggests PhysChem and Env Fate data available for UVCB  
[ICD-3872] - Presence in Lists not working  
[ICD-3873] - Improve layout of Predictions pages  
[ICD-3889] - Batch search fails when NHANES/Predicted Exposure is selected  
[ICD-3891] - Number of chemicals in List of Assays View differs from Assays page  
[ICD-3893] - Display of Production volume where there are no data or zero is of no value  
[ICD-3895] - The Data shown for CERAPP ToxCast Models is INCORRECT  
[ICD-3897] - Searched by details are not visible for some chemicals  
[ICD-3898] - Batch help notification for ToxPrint single fingerprints mismatched to QSAR-Ready SMILES  
[ICD-3899] - No ability to add help notifications to Batch Enhanced Data Sheets  
[ICD-3902] - Test Reports do not work on external production  
[ICD-3909] - Batch Search linkouts not using correct URLs  
[ICD-3910] - Google reCAPTCHA malformed JSON  
[ICD-3912] - Lost message for "Searched by Deleted CASRN"  
[ICD-3915] - Search on DTXSID80897718 has result but not in Batch Search  
[ICD-3923] - Cannot download SeqaPASS reports from Public Production  
[ICD-3927] - Stereochemistry images missing in Table View for Multiple chemicals  
[ICD-3929] - Change in URL for assay endpoints  
[ICD-3930] - EDSP21 charts not loading  
[ICD-3934] - Not all SeqaPASS reports are downloadable  
[ICD-3935] - Remove Zoom for structure zooming in production database  
[ICD-3951] - DTXSID5040752 error when selecting ToxPrints  
[ICD-3953] - Bioactivity ToxCast Summary and ToxCast Data should grey out when there is no data  
[ICD-3965] - Structure zoom functionality is not visible for a list of chemicals accessed via an assay  
[ICD-3975] - Sorting on Top doesn't work. Sorting on Scaled Top does work.  
[ICD-3981] - News Page Header and Name Issues  
[ICD-3986] - TOXCAST display of ZERO suggests not examined for bioactivity in assays  
[ICD-3992] - Chemicals associated with certain categories do not show up under exposure tab  
[ICD-3993] - Issues with displaying crowdsourced comments on dev  
[ICD-3995] - UVCB Chemicals display broken  
[ICD-3996] - Issues with displaying ToxVal table of data in the modal  
[ICD-4002] - Toxcast Models query not correct  
[ICD-4004] - Methods data shown in modal, plus citations and reagents added  
[ICD-4009] - Loading Executive Summary shows issue  
[ICD-4015] - Assays not linked to genes don't show up in Assay List  
[ICD-4018] - Fix no search result page style

- [ICD-4021] - Individual Properties don't load a second time
- [ICD-4024] - Assay Endpoint Multiple Results doesn't load
- [ICD-4048] - List link outs from Batch Search have wrong URL
- [ICD-4049] - No ability to add Informational Icon for DTXCID
- [ICD-4050] - No informational icon in -prod but available on public production
- [ICD-4052] - The information details on Public Production have not made it into internal production
- [ICD-4057] - Remove  $\leq 0$  values from Toxval
- [ICD-4058] - Clarity of meaning of ND in ToxVal
- [ICD-4060] - Lists are not properly associated with the type of list in Presence in lists
- [ICD-4061] - Remove specific assay vendor from the Filter by Vendor List

#### **Known Bugs at release**

- [ICD-4019] - Output file is out of order in terms of INPUT terms
- [ICD-4036] - Searching on block of InChIKeys for chemicals with known DTXCIDs produces no hits
- [ICD-4044] - Overflow text in similarity search results page for chemicals with superscripts in name
- [ICD-4042] - Search "selenocysteine" returns no hits & message "Searched by InChIKey skeleton"
- [ICD-4055] - Number of linked records shown does not match number in chemicals results page
- [ICD-4056] - GenRA issue - selecting Toxprints in the first frame leads to failure for some chemicals
- [ICD-4059] - Number of decimal places for the predicted logP values increased
- [ICD-4067] - Information Icon for "Retrieve Articles" for Abstract Sifter is wrapped
- [ICD-4068] - X-axis label for Histogram should say AC50 (uM) not LogAC50
- [ICD-4069] - Systematic Names not generated for the 130k chemical differential file for 3.01 release
- [ICD-4070] - OPERA reports for new calculations do not include full details of new predictions