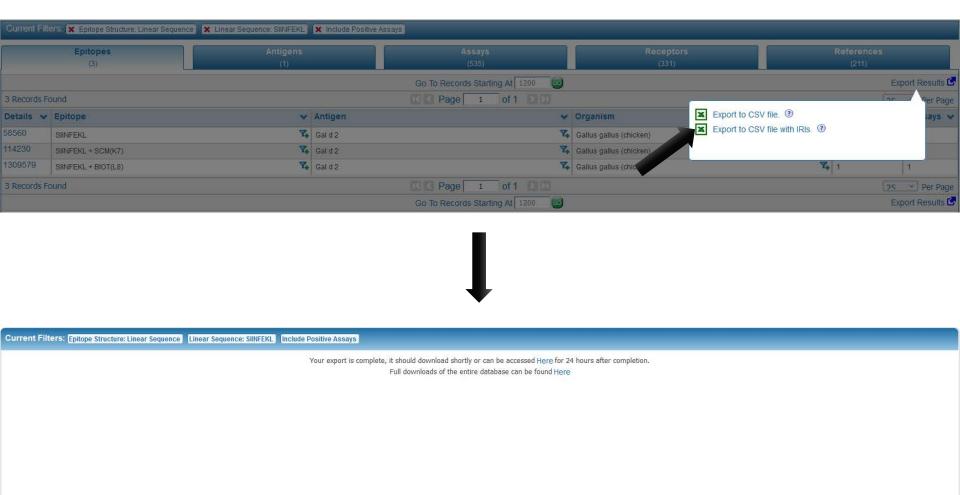


# **IEDB Customized Data Exports**

Presented by: Kelly Wheeler, Senior Software Engineer

### What was the previous export?



### .csv only with dual headers

4	Α	В	С	D	E	F	G	Н	1	J	K	L	M	N	0	Р	Q	R	S	Т
1	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Related O	Related O	Related
2	Epitope ID	Object Type	Description	Epitope N	Epitope Modification(s)	Starting P	Ending Po	Non-pept	Epitope S	Antigen Name	Antigen Accession	Parent Protein	Parent Protein Accession	Organism Name	Parent Organism	Parent Organism ID	Epitope C	Epitope R	Object Ty	Descrip
3	58560	Linear peptide	SIINFEKL			258	265			ovalbumin	AAA48998.1	Gal d 2	P01012	Gallus gallus	Gallus gallus	9031				
4	114230	Linear peptide	SIINFEKL + SCM(K7)	K7	Side chain modification	258	265			ovalbumin	AAA48998.1	Gal d 2	P01012	Gallus gallus	Gallus gallus	9031	The epito	pe is modif	fied with t	rinitropl
5	1309579	Linear peptide	SIINFEKL + BIOT(L8)	L8	Biotin BIOT	257	264			ovalbumin	0705172A	Gal d 2	P01012	Gallus gallus	Gallus gallus	9031				
6																				
7																				
8																				

Epitope, Epi

"11230", "Linear peptide", "Slinear, "Gallus gallus", "In epicope is modified with trinitrophenyl on Lys "1309579", "Linear peptide", "Slinear peptide", "Slinear peptide", "Slinear peptide", "Slinear peptide", "Gallus gallus", "Gallus gallus",

### Why Change?

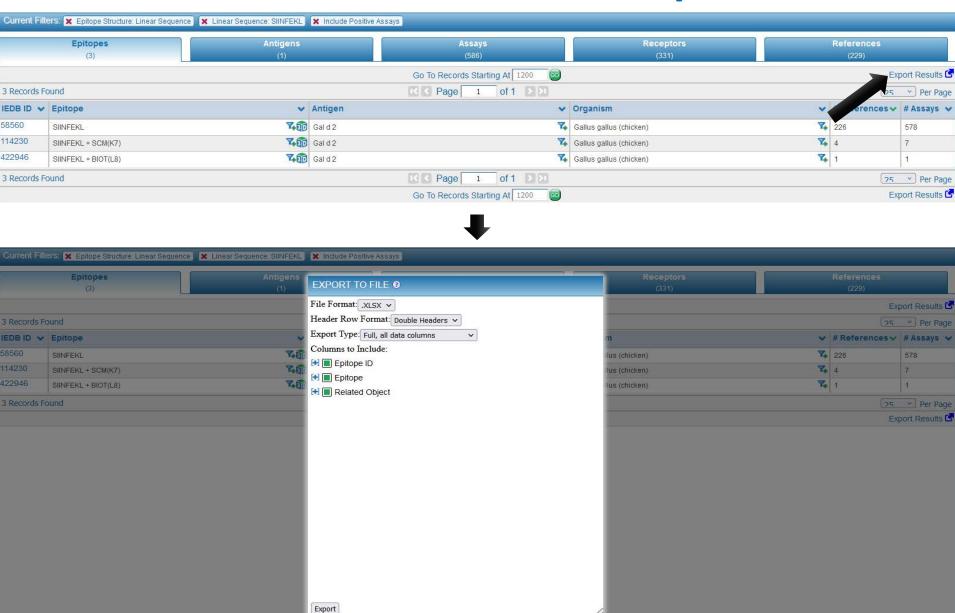
- Limited to .csv file format
- Fixed set of export fields
- Dual headers only
- Limited explanation of what each field means
- Limited information on the query performed
- Lack of information on when the query was performed

### **Introducing the New Customized Data Exports**

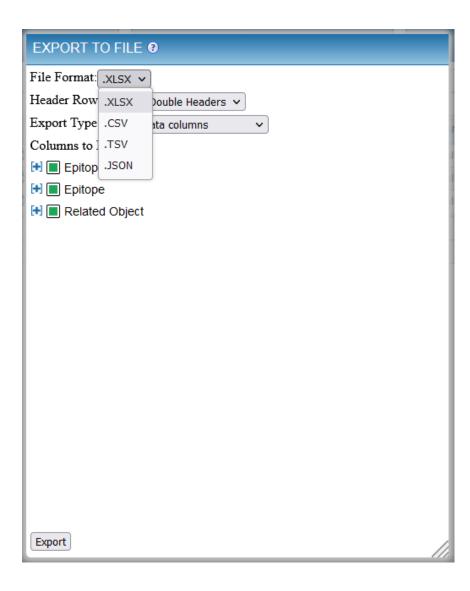
#### **Goals:**

- Expand the usability of the exports
- Provide more information on each field
- Allow more customization to the user
- Provide more information linking the exported data to the query

### **New Customized Data Exports**



### **Multiple File Formats**



#### .XLS - Excel format - Most user friendly

4	Α	В	С	D	E	F	G	Н	1	J	K	L
<b>1</b> E	itope ID	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope
2 II	DB IRI	Object Type	Name	Modified Residue(s)	Modifications	Starting Position	Ending Position	IRI	Synonyms	Source Molecule	Source Molecule IRI	Molecule Parent
3 h	tps://www.iedb.org/er	Linear peptide	SIINFEKL			258	265			ovalbumin	http://www.ncbi.nlm.nih	Gal d 2
4 h	tps://www.iedb.org/er	Linear peptide	SIINFEKL + SCM(K7)	K7	Side chain modification	258	265			ovalbumin	http://www.ncbi.nlm.nih	Gal d 2
5 h	tps://www.iedb.org/er	Linear peptide	SIINFEKL + BIOT(L8)	L8	Biotin   BIOT	257	264			ovalbumin	http://www.ncbi.nlm.nih	Gal d 2

#### .CSV – Comma Separated Values – Current format – Programmer friendly

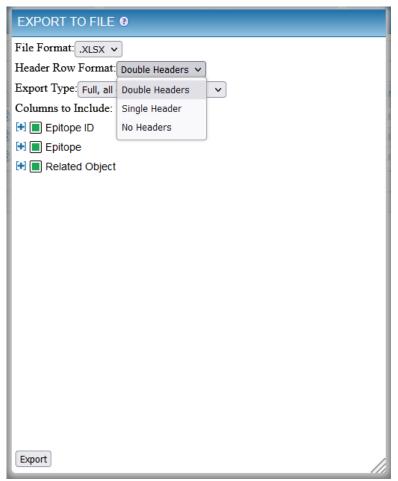
#### .TSV – Tab Separated Values – Similar to CSV but with tabs – Programmer friendly

```
Epitope Epitop
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   "Related Object"
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     "Related Object
  'Epitope ID'
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     "Related Object
                                                                                                                                                                                                                                                                                                                                                            "Ending Position"
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             "Source Molecule"
                                                      "Object Type" Name
                                                                                                                                     "Modified Residue(s)" Modifications "Starting Position"
                                                                                                                                                                                                                                                                                                                                                                                                                                                                    Synonyms
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              "Source Molecule IRI"
https://www.iedb.org/epitope/58560
                                                                                                                                      "Linear peptide"
                                                                                                                                                                                                                     SIINFEKL
                                                                                                                                                                                                                                                                                                                                                                                                                                            ovalbumin
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  http://www.ncbi.nlm.nih.gov/protein/AAA48998.1 "Gal d 2"
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        http://www.uniprot.org/unipro
https://www.iedb.org/epitope/114230
                                                                                                                                     "Linear peptide"
                                                                                                                                                                                                                     "SIINFEKL + SCM(K7)" K7
                                                                                                                                                                                                                                                                                                                                  "Side chain modification"
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            http://www.ncbi.nlm.nih.gov/protein/AAA48998.1 "Gal d 2"
                                                                                                                                                                                                                     "SIINFEKL + BIOT(L8)"
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      http://www.ncbi.nlm.nih.gov/protein/0705172A
https://www.iedb.org/epitope/422946
                                                                                                                                     "Linear peptide"
                                                                                                                                                                                                                                                                                                                                Biotin BIOT
                                                                                                                                                                                                                                                                                                                                                                                    257
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  ovalbumin
```

#### **.JSON** – JavaScript Object Notation – A programming friendly format used to transport data

```
"Search Parameters": [
    "Epitope Structure: Linear Sequence".
    "Linear Sequence: SIINFEKL",
    "Include Positive Assays",
    "Export Type: Full, all data columns"
"Export Date": "October 26, 2023",
"Data":
        "Epitope ID - IEDB IRI": "https://www.iedb.org/epitope/58560",
        "Epitope - Object Type": "Linear peptide",
        "Epitope - Name": "SIINFEKL"
        "Epitope - Modified Residue(s)": ""
        "Epitope - Modifications":
        "Epitope - Starting Position": "258"
        "Epitope - Ending Position": "265",
        "Epitope - IRI": ""
        "Epitope - Synonyms": ""
        "Epitope - Source Molecule": "ovalbumin"
        "Epitope - Source Molecule IRI": "http://www.ncbi.nlm.nih.gov/protein/AAA48998.1",
        "Epitope - Molecule Parent IRI": "http://www.uniprot.org/uniprot/P01012"
```

### **Multiple Header Formats**



**Double Headers:** Two header rows with a section and field row

<b>⊿</b> A	В	С	D	Ε	F	G	н
1 Epitope ID	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope
2 IEDB IRI	Object Type	Name	Modified Residue(s)	Modifications	Starting Position	Ending Position	IRI
https://www.ledb.org	g/er Linear peptide	SIINFEKL			258	265	
https://www.iedb.org	g/er Linear peptide	SIINFEKL + SCM(K7)	K7	Side chain modification	258	265	
https://www.iedb.org	g/er Linear peptide	SIINFEKL + BIOT(L8)	L8	Biotin BIOT	257	264	

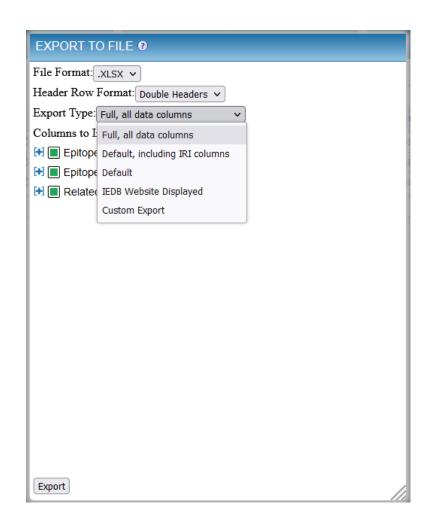
Single Header: Single header row with section and field merged



No Headers: Simple data centric format with no headers



### **Export Types**

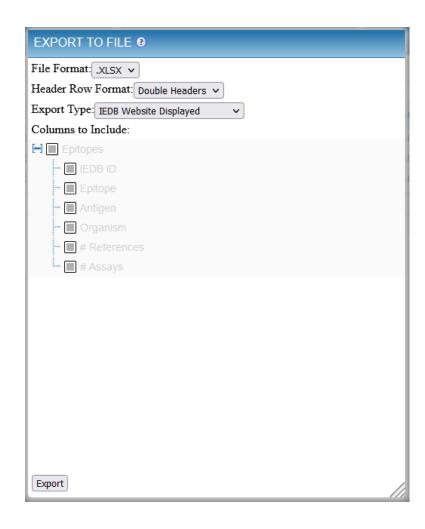


Export types are preselected subsets of fields to be exported

#### **Available Export Types:**

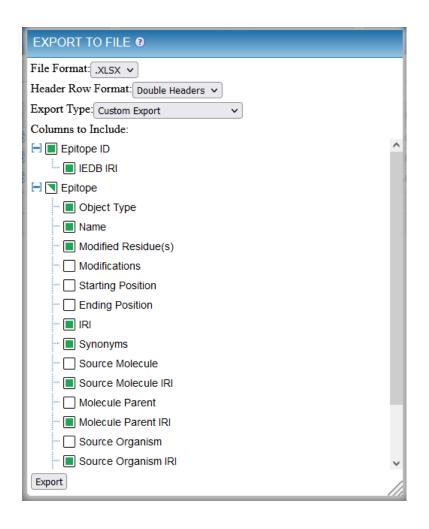
- <u>Full, all data columns</u>: All the available columns available for that export
- <u>Default</u>: A preselected 'default' set of columns selected by the IEDB team
- <u>Default, including IRI columns</u>: An expanded set of the Default column set with IRIs included where available
- <u>IEDB Website Displayed</u>: A set of columns that match what is shown in the tab being exported
- Custom Export: User selected set of columns

### **IEDB** Website Displayed



- IEDB Website Displayed is a special Export Type.
   It directly reflects the fields shown on the selected results page tab
- Due to it's unique nature it's fields can't be modified or added to other exports

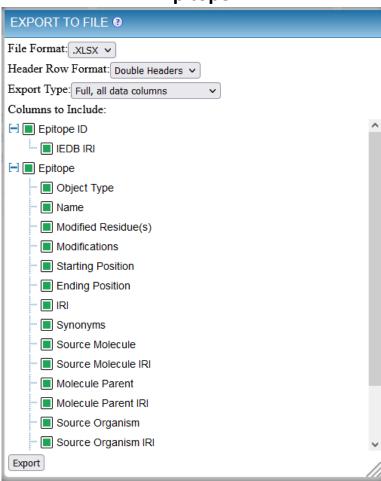
### **Custom Export**



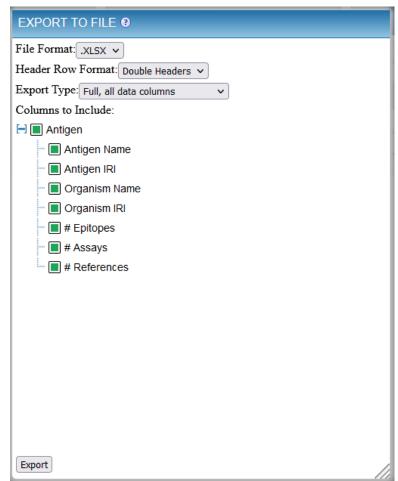
- Allows for fine grain customization of your export set of columns
- Section headers are shown with a [+] icon that can be expanded to show the individual columns beneath. Similar functionality to the trees in the finders
- Full sections can be selected or removed by clicking on the box next to the section header
- Full green boxes indicate a selected column/section. Half green boxes indicate that at least 1 column under that section is selected

### **Field Selection Examples**



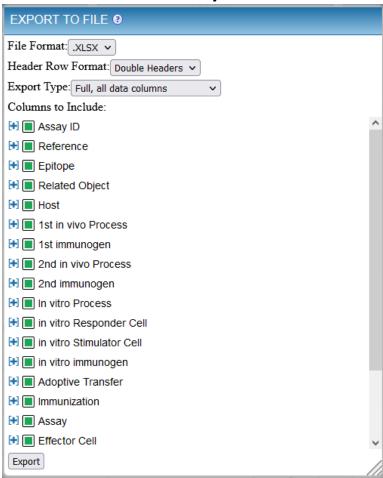


#### **Antigen**

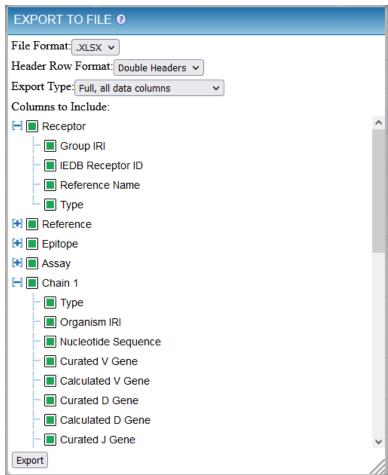


### **Field Selection Examples**

#### **Assay**

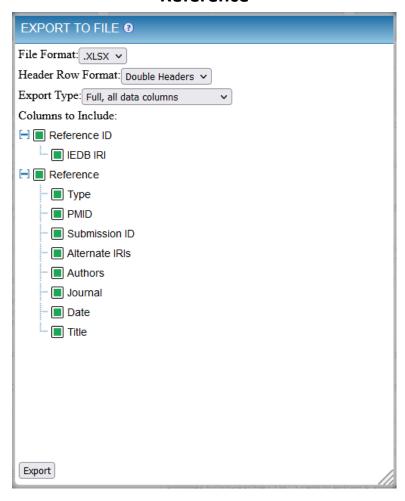


#### Receptor



## **Field Selection Examples**

#### Reference



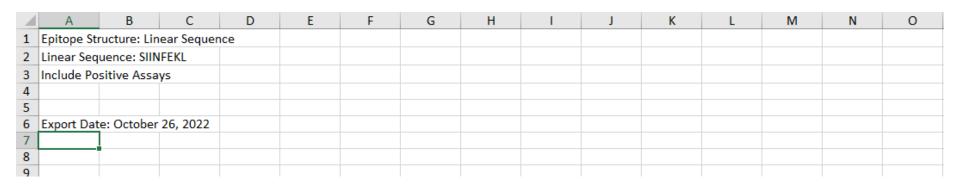
### **Additional Improvements**

 Inclusion of query parameters in the Excel export via a new sheet, and the JSON export

Inclusion of export date in the Excel and JSON exports

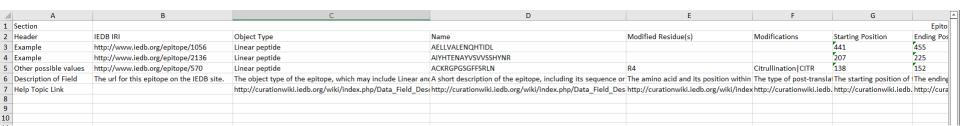
 Inclusion of field descriptions in the Excel export via a new sheet

### **Export Parameters Example**



- Includes the full list of the parameters used on the IEDB website to generate this export
- Also will include the date the export was ran for future use
- Available in the Excel and JSON formats

### Field Help Tab Example



- A new tab in the Excel export that offers information on each field selected and exported
- Each field has the section and header name matching the header format selected
- Below this are 2 pre-selected examples chosen by our team to demonstrate what is in the IEDB
- After this is another possible value to show what that field could include in case our above examples are blank or we want to show other possible values
- Next is a brief description of what that field represents
- Finally, there is a link to an IEDB help article for that field if available