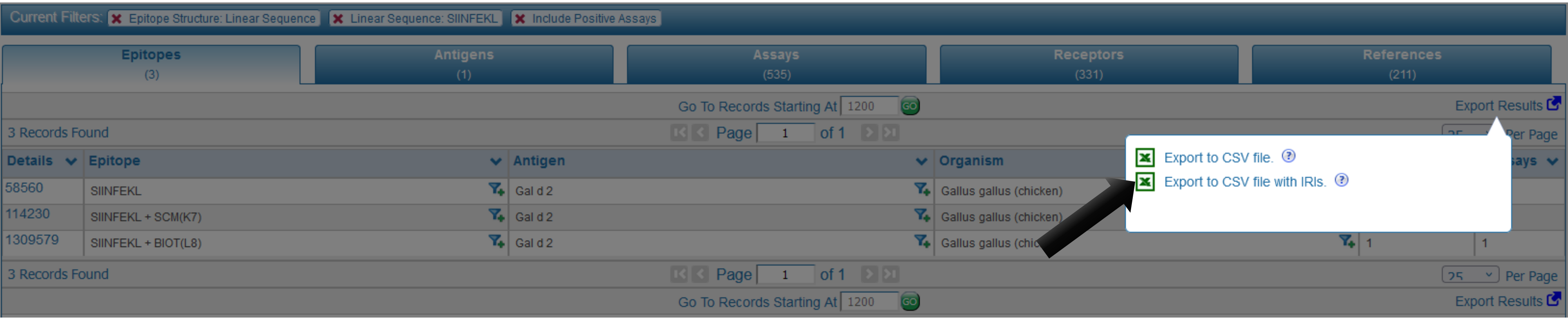
IMMUNE EPITOPE DATABASE
AND ANALYSIS RESOURCE

IEDB Custom Export Update

Presented by: Kelly Wheeler, Senior Software Engineer

What is the current export?

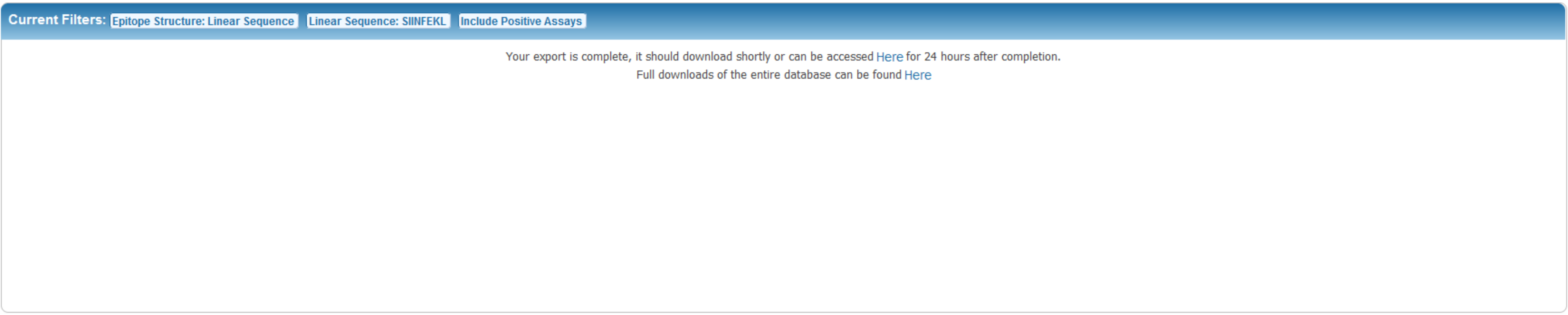


Current Filters: ✖ Epitope Structure: Linear Sequence ✖ Linear Sequence: SIINFEKL ✖ Include Positive Assays

3 Records Found

Details	Epitope	Antigen	Organism		
58560	SIINFEKL	Gal d 2	Gallus gallus (chicken)		
114230	SIINFEKL + SCM(K7)	Gal d 2	Gallus gallus (chicken)		
1309579	SIINFEKL + BIOT(L8)	Gal d 2	Gallus gallus (chic	1	1

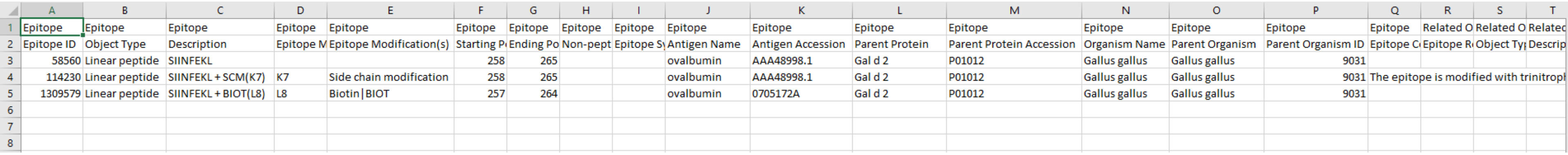
3 Records Found



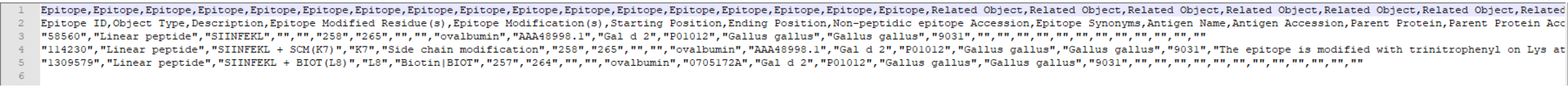
Current Filters: Epitope Structure: Linear Sequence Linear Sequence: SIINFEKL Include Positive Assays

Your export is complete, it should download shortly or can be accessed Here for 24 hours after completion.
Full downloads of the entire database can be found Here

Currently .csv only with dual headers



Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Epitope	Related O	Related O	Relatec
Epitope ID	Object Type	Description	Epitope M	Epitope Modification(s)	Starting P	Ending Po	Non-pept	Epitope Sy	Antigen Name	Antigen Accession	Parent Protein	Parent Protein Accession	Organism Name	Parent Organism	Parent Organism ID	Epitope C	Epitope R	Object Ty	Descrip
58560	Linear peptide	SIINFEKL			258	265			ovalbumin	AAA48998.1	Gal d 2	P01012	Gallus gallus	Gallus gallus	9031				
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 epitope is modified with trinitropl			
1309579	Linear peptide	SIINFEKL + BIOT(L8)	L8	Biotin|BIOT	257	264			ovalbumin	0705172A	Gal d 2	P01012	Gallus gallus	Gallus gallus	9031				



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Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Related Object,Related Object,Related Object,Related Object,Related Object,Related Object,Related
Epitope ID,Object Type,Description,Epitope Modified Residue(s),Epitope Modification(s),Starting Position,Ending Position,Non-peptidic epitope Accession,Epitope Synonyms,Antigen Name,Antigen Accession,Parent Protein,Parent Protein Acc
"58560","Linear peptide","SIINFEKL","","","258","265","","","ovalbumin","AAA48998.1","Gal d 2","P01012","Gallus gallus","Gallus gallus","9031","","","","","","","","","","","",""
"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 epitope is modified with trinitrophenyl on Lys at
"1309579","Linear peptide","SIINFEKL + BIOT(L8)","L8","Biotin|BIOT","257","264","","","ovalbumin","0705172A","Gal d 2","P01012","Gallus gallus","Gallus gallus","9031","","","","","","","","","","","",""
```

Why change?

- One of the most requested change to the IEDB!
- 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

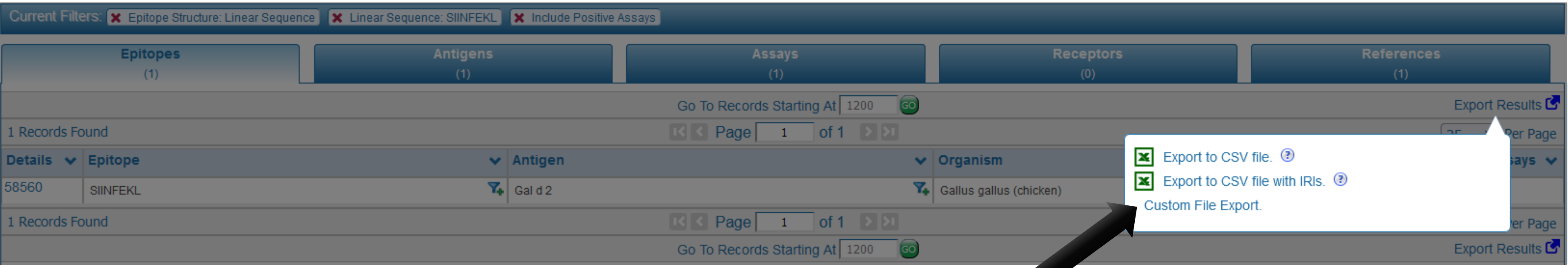
Introducing the new Custom Exports

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 ran

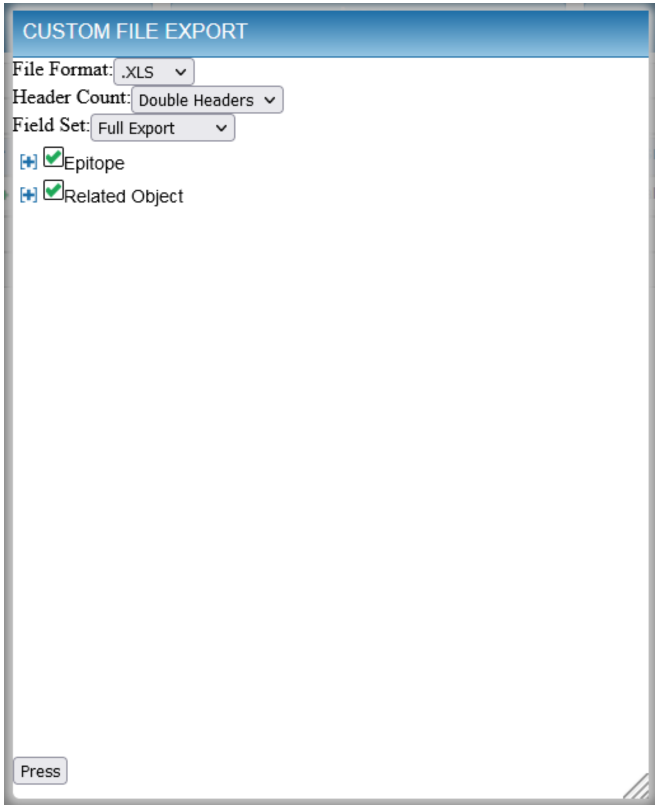
* All shown functionality is currently in development and subject to change

New Custom Exports



Current Filters: Epitope Structure: Linear Sequence; Linear Sequence: SIINFEKL; Include Positive Assays

Details	Epitope	Antigen	Organism
58560	SIINFEKL	Gal d 2	Gallus gallus (chicken)



CUSTOM FILE EXPORT

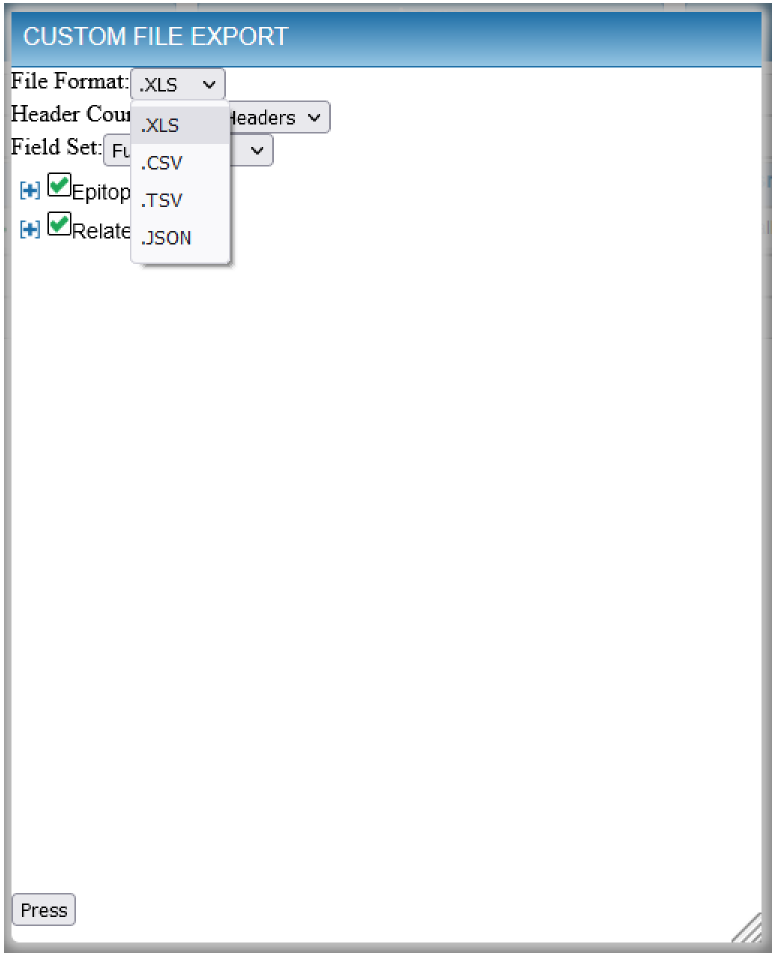
File Format: .XLS

Header Count: Double Headers

Field Set: Full Export

- ☑ Epitope
- ☑ Related Object

Multiple File Formats



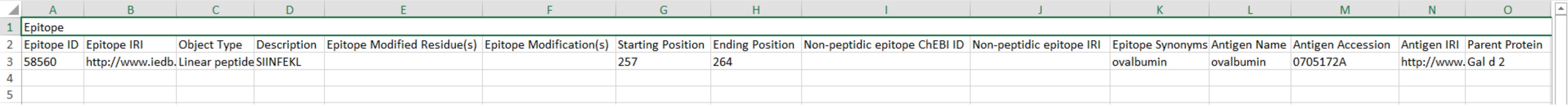
CUSTOM FILE EXPORT

File Format: .XLS

Header Coun

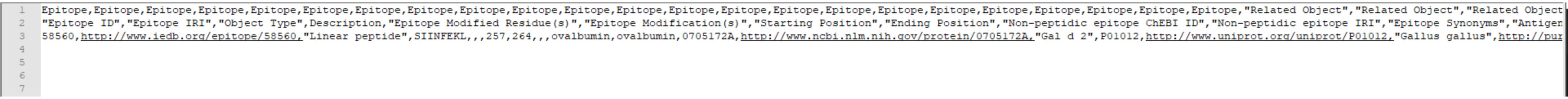
Field Set: Fu

.XLS – Excel format – Most user friendly



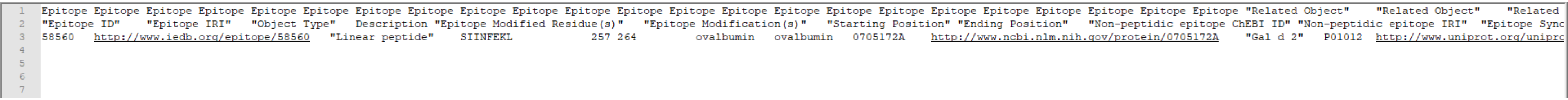
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Epitope														
2	Epitope ID	Epitope IRI	Object Type	Description	Epitope Modified Residue(s)	Epitope Modification(s)	Starting Position	Ending Position	Non-peptidic epitope ChEBI ID	Non-peptidic epitope IRI	Epitope Synonyms	Antigen Name	Antigen Accession	Antigen IRI	Parent Protein
3	58560	http://www.iedb.	Linear peptide	SIINFEKL			257	264			ovalbumin	ovalbumin	0705172A	http://www.	Gal d 2
4															
5															

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



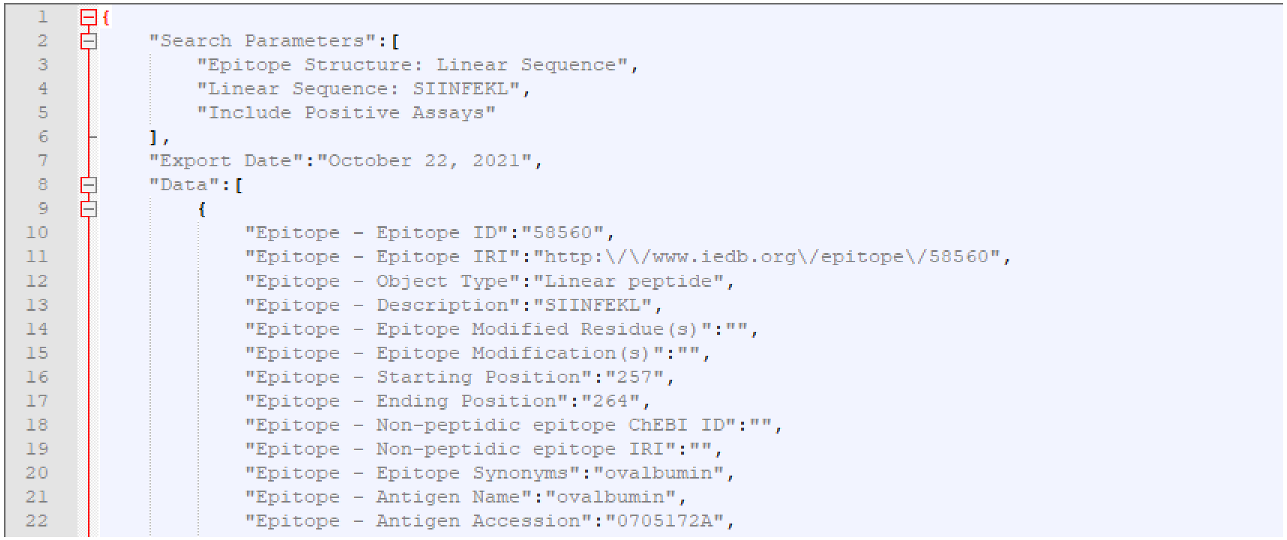
```
Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,Epitope,"Related Object","Related Object","Related Object
"Epitope ID","Epitope IRI","Object Type",Description,"Epitope Modified Residue(s)","Epitope Modification(s)","Starting Position","Ending Position","Non-peptidic epitope ChEBI ID","Non-peptidic epitope IRI","Epitope Synonyms","Antigen
58560,http://www.iedb.org/epitope/58560,"Linear peptide",SIINFEKL,,,257,264,,,ovalbumin,ovalbumin,0705172A,http://www.ncbi.nlm.nih.gov/protein/0705172A,"Gal d 2",P01012,http://www.uniprot.org/uniprot/P01012,"Gallus gallus",http://pur
```

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



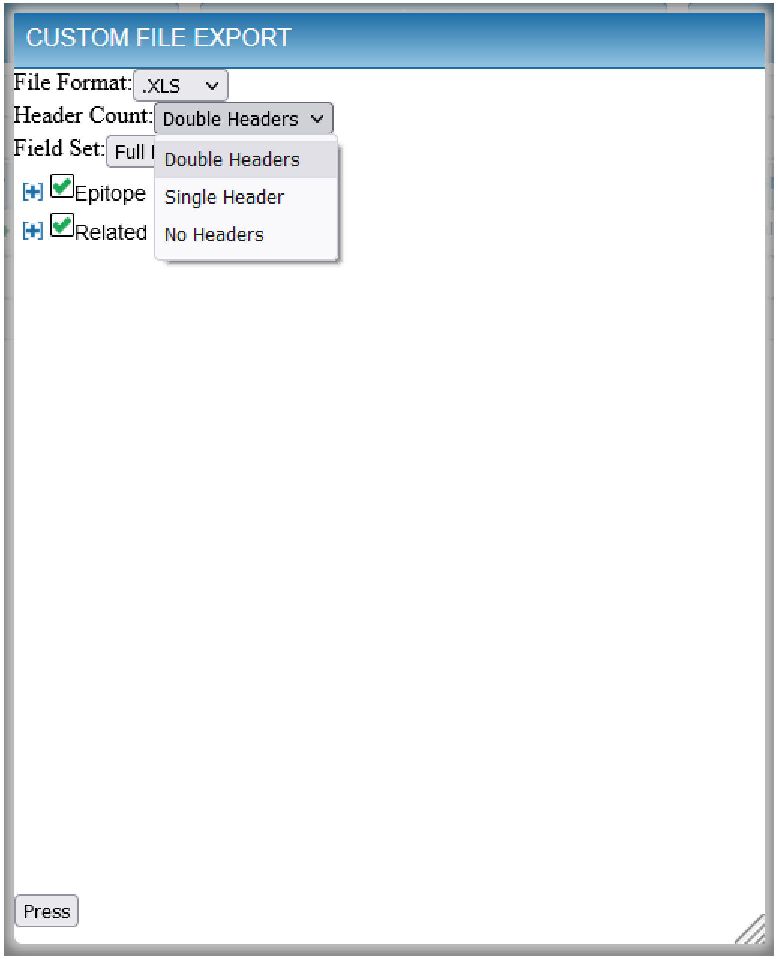
```
Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope Epitope "Related Object"    "Related Object"    "Related
"Epitope ID"    "Epitope IRI"   "Object Type"   Description "Epitope Modified Residue(s)"   "Epitope Modification(s)"   "Starting Position" "Ending Position"   "Non-peptidic epitope ChEBI ID" "Non-peptidic epitope IRI"  "Epitope Sync
58560   http://www.iedb.org/epitope/58560   "Linear peptide"    SIINFEKL            257 264         ovalbumin   ovalbumin   0705172A    http://www.ncbi.nlm.nih.gov/protein/0705172A    "Gal d 2"   P01012  http://www.uniprc
```

.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 Date":"October 22, 2021",
    "Data":[
        {
            "Epitope - Epitope ID":"58560",
            "Epitope - Epitope IRI":"http:\/\/www.iedb.org\/epitope\/58560",
            "Epitope - Object Type":"Linear peptide",
            "Epitope - Description":"SIINFEKL",
            "Epitope - Epitope Modified Residue(s)":"",
            "Epitope - Epitope Modification(s)":"",
            "Epitope - Starting Position":"257",
            "Epitope - Ending Position":"264",
            "Epitope - Non-peptidic epitope ChEBI ID":"",
            "Epitope - Non-peptidic epitope IRI":"",
            "Epitope - Epitope Synonyms":"ovalbumin",
            "Epitope - Antigen Name":"ovalbumin",
            "Epitope - Antigen Accession":"0705172A",
```

Multiple Header Formats



CUSTOM FILE EXPORT

File Format: .XLS

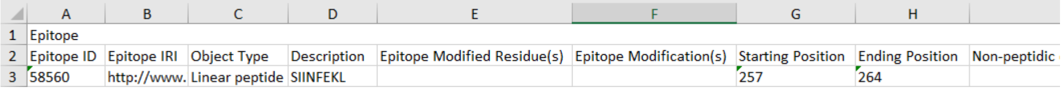
Header Count: Double Headers

Field Set: Full

☑ Epitope

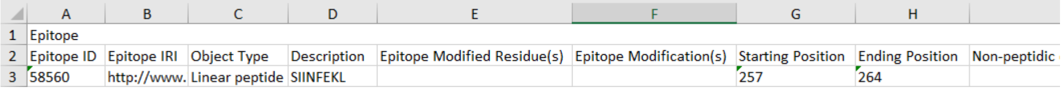
☑ Related

Double Headers – Current format with a section and field header row



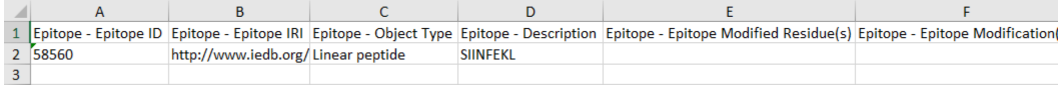
	A	B	C	D	E	F	G	H	
1	Epitope								
2	Epitope ID	Epitope IRI	Object Type	Description	Epitope Modified Residue(s)	Epitope Modification(s)	Starting Position	Ending Position	Non-peptidic
3	58560	http://www.	Linear peptide	SIINFEKL			257	264	

Single Header – Single header row with section and field merged



	A	B	C	D	E	F	G	H	
1	Epitope								
2	Epitope ID	Epitope IRI	Object Type	Description	Epitope Modified Residue(s)	Epitope Modification(s)	Starting Position	Ending Position	Non-peptidic
3	58560	http://www.	Linear peptide	SIINFEKL			257	264	

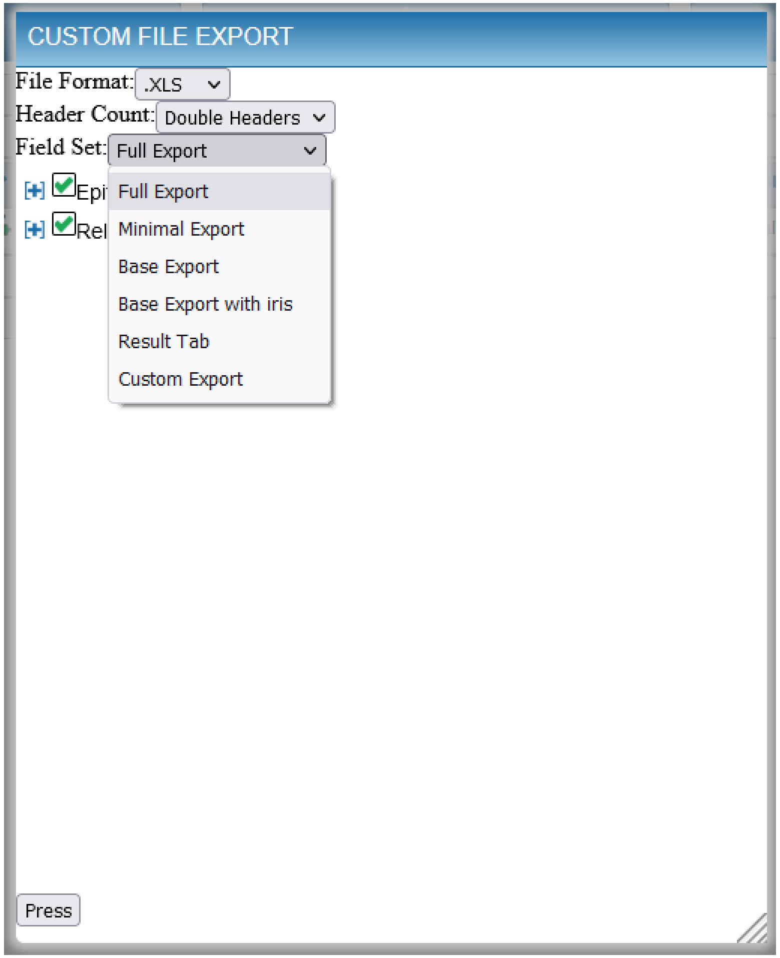
Double Headers – Current Format with a section and field header row



	A	B	C	D	E	F
1	Epitope - Epitope ID	Epitope - Epitope IRI	Epitope - Object Type	Epitope - Description	Epitope - Epitope Modified Residue(s)	Epitope - Epitope Modification(
2	58560	http://www.iedb.org/	Linear peptide	SIINFEKL		
3						

No Headers – Simple data centric format with no headers

Custom Field Selection and Field Sets



CUSTOM FILE EXPORT

File Format: .XLS

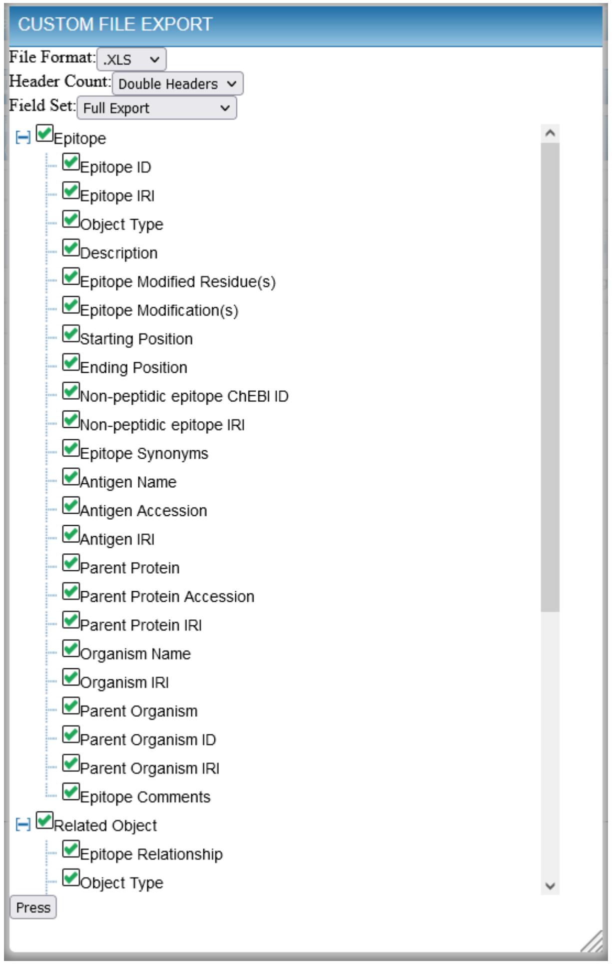
Header Count: Double Headers

Field Set: Full Export

- Field sets are preselected subsets of fields to be exported. These are currently examples only and will be further refined upon release.
- Custom field section shown in a similar structure as the finder trees.
- Fields shown under section headers that expand to show the individual field names that can also be selected separately.
- Allows for extremely fine grain customization of exports to fit each users needs.

Field Selection Examples

Epitope


CUSTOM FILE EXPORT

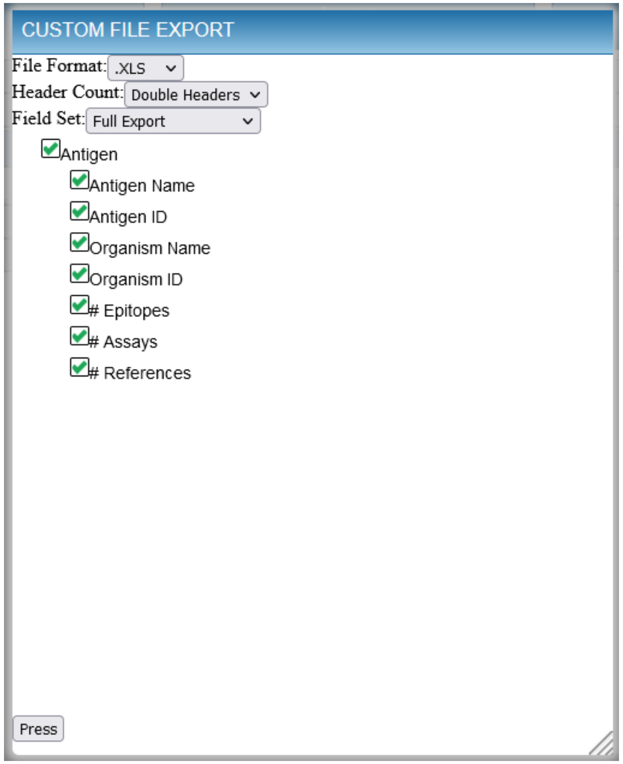
File Format: .XLS

Header Count: Double Headers

Field Set: Full Export

- ☑ Epitope
  - ☑ Epitope ID
  - ☑ Epitope IRI
  - ☑ Object Type
  - ☑ Description
  - ☑ Epitope Modified Residue(s)
  - ☑ Epitope Modification(s)
  - ☑ Starting Position
  - ☑ Ending Position
  - ☑ Non-peptidic epitope ChEBI ID
  - ☑ Non-peptidic epitope IRI
  - ☑ Epitope Synonyms
  - ☑ Antigen Name
  - ☑ Antigen Accession
  - ☑ Antigen IRI
  - ☑ Parent Protein
  - ☑ Parent Protein Accession
  - ☑ Parent Protein IRI
  - ☑ Organism Name
  - ☑ Organism IRI
  - ☑ Parent Organism
  - ☑ Parent Organism ID
  - ☑ Parent Organism IRI
  - ☑ Epitope Comments
- ☑ Related Object
  - ☑ Epitope Relationship
  - ☑ Object Type

Antigen


CUSTOM FILE EXPORT

File Format: .XLS

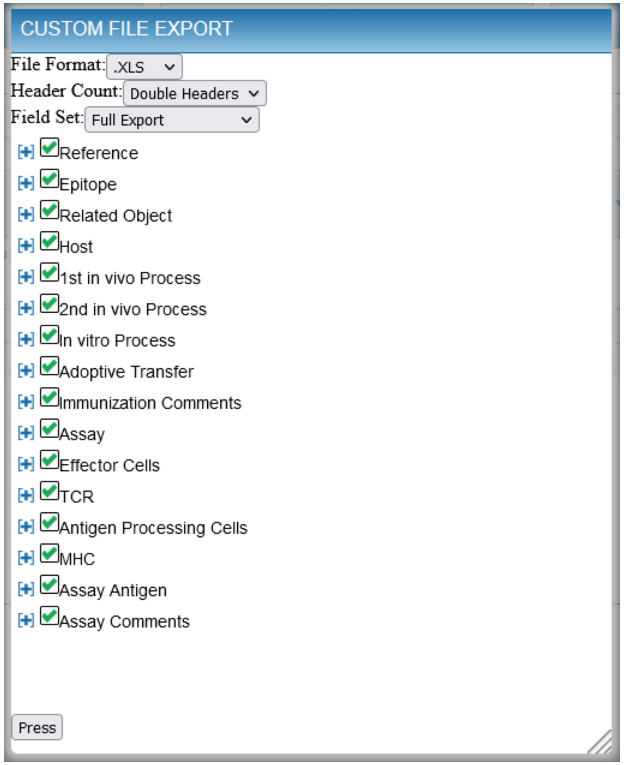
Header Count: Double Headers

Field Set: Full Export

- ☑ Antigen
  - ☑ Antigen Name
  - ☑ Antigen ID
  - ☑ Organism Name
  - ☑ Organism ID
  - ☑ # Epitopes
  - ☑ # Assays
  - ☑ # References

Field Selection Examples

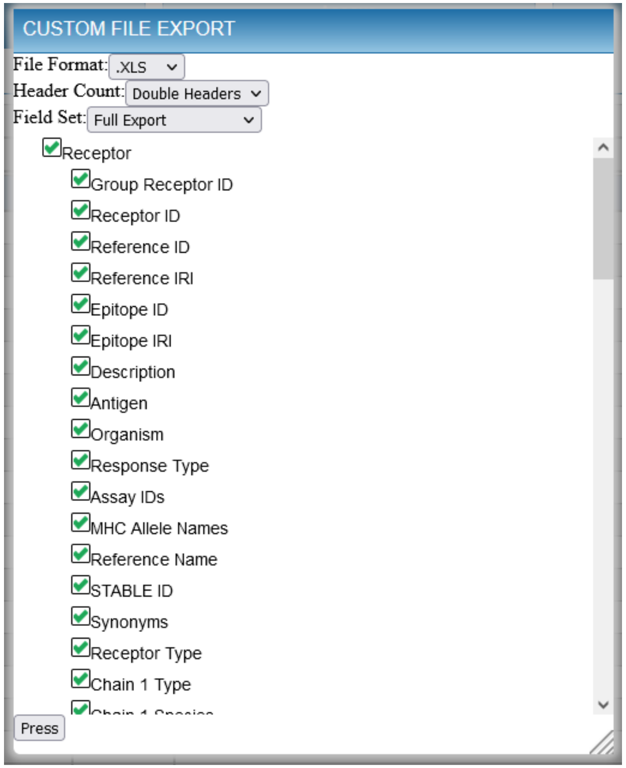
Assay


CUSTOM FILE EXPORT

File Format: .XLS
Header Count: Double Headers
Field Set: Full Export

- [+] ☑ Reference
- [+] ☑ Epitope
- [+] ☑ Related Object
- [+] ☑ Host
- [+] ☑ 1st in vivo Process
- [+] ☑ 2nd in vivo Process
- [+] ☑ In vitro Process
- [+] ☑ Adoptive Transfer
- [+] ☑ Immunization Comments
- [+] ☑ Assay
- [+] ☑ Effector Cells
- [+] ☑ TCR
- [+] ☑ Antigen Processing Cells
- [+] ☑ MHC
- [+] ☑ Assay Antigen
- [+] ☑ Assay Comments

Receptor

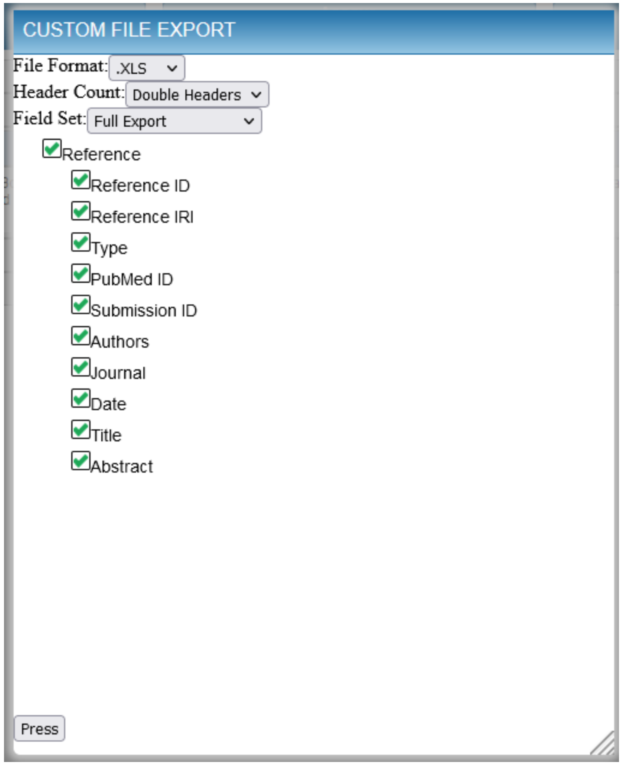

CUSTOM FILE EXPORT

File Format: .XLS
Header Count: Double Headers
Field Set: Full Export

- ☑ Receptor
  - ☑ Group Receptor ID
  - ☑ Receptor ID
  - ☑ Reference ID
  - ☑ Reference IRI
  - ☑ Epitope ID
  - ☑ Epitope IRI
  - ☑ Description
  - ☑ Antigen
  - ☑ Organism
  - ☑ Response Type
  - ☑ Assay IDs
  - ☑ MHC Allele Names
  - ☑ Reference Name
  - ☑ STABLE ID
  - ☑ Synonyms
  - ☑ Receptor Type
  - ☑ Chain 1 Type

Field Selection Examples

Reference



File Format: .XLS

Header Count: Double Headers

Field Set: Full Export

- ☑ Reference
  - ☑ Reference ID
  - ☑ Reference IRI
  - ☑ Type
  - ☑ PubMed ID
  - ☑ Submission ID
  - ☑ Authors
  - ☑ Journal
  - ☑ Date
  - ☑ Title
  - ☑ Abstract

Additional Improvements

- Inclusion of query parameters in the Excel export via a new sheet
- Inclusion of field descriptions in the Excel export via a new sheet
- Re-evaluation of available fields and field names
- Addition of the option to export the fields as shown in the tabs on the website