Implementation of flexible search for proteomics metadata



http://dev.jpost.org/px-rdf

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Introduction

The ProteomeXchange (PX) Consortium (http://www.proteomexchange.org) provides a globally coordinated data submission and dissemination platform for mass spectrometry proteomics data in the public domain, involving the main existing proteomics repositories. The members of the Consortium are PRIDE (https://www.ebi.ac.uk/pride), PeptideAtlas/PASSEL (http://www.peptideatlas.org/passel), MassIVE (https://massive.ucsd.edu), and jPOST, which has just joined the Consortium (http://jpost.org). Public datasets from the different members can be accessed into a common interface called ProteomeCentral (http://proteomecentral.proteomexchange.org). A set of technical and biological common metadata about the datasets has been agreed by the PX members. Although the ProteomeCentral web interface (Fig. 1) provides a state-of-the-art search functionality, it is not well-suited to construct more complex searches. In the context of 'Linked Open Data', a concept about connecting data independently of the involved biological data types, we chose the Resource Description Framework (RDF) data model to achieve this intended more advanced search functionality, to improve dataset discoverability.

Methods

We designed a PX-RDF schema (Fig. 3) based on the PX-XML schema (Fig. 2). In addition to well-known ontologies (such as Dublin Core and Friend of a Friend) and domain specific controlled vocabularies for proteomics (such as PSI-MS and UNIMOD) (Fig. 4), we defined a new ontology, PX ontology, which makes up for deficiencies in existing vocabularies (Fig. 5). The PX ontology and a conversion program from PX-XML to PX-RDF are available at https://github.com/PX-RDF/ontology and https://github.com/PX-RDF/RDF, respectively. The converted PX-RDF files were loaded into Virtuoso, which is a database management system for RDF. The Virtuoso server can be searched by SPARQL (SPARQL Protocol and RDF Query

Language), which is a query language for RDF (Fig. 6).

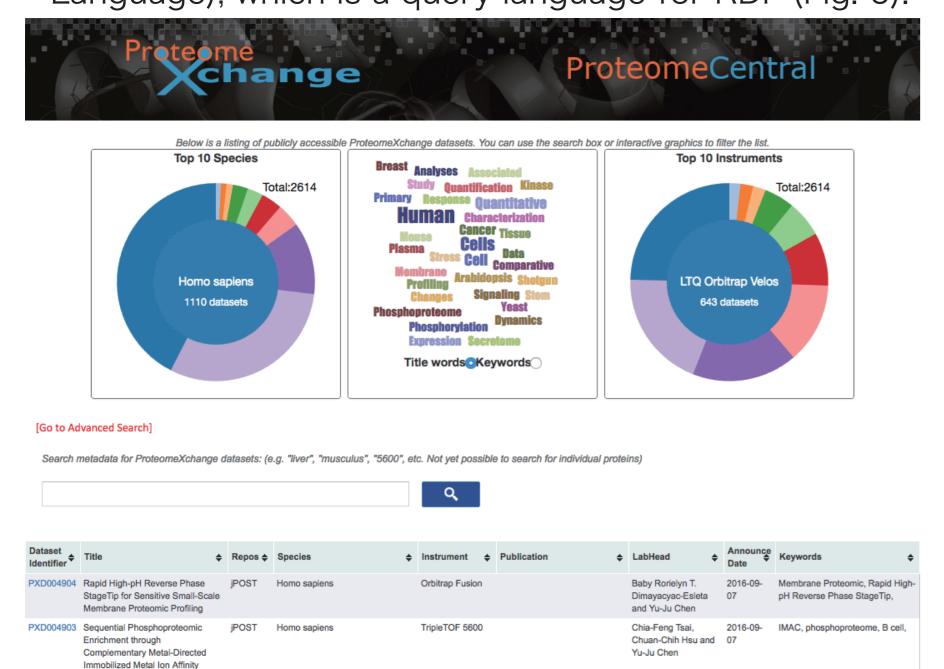


Fig. 1 The front page of ProteomeCentral http://proteomecentral.proteomexchange.org/

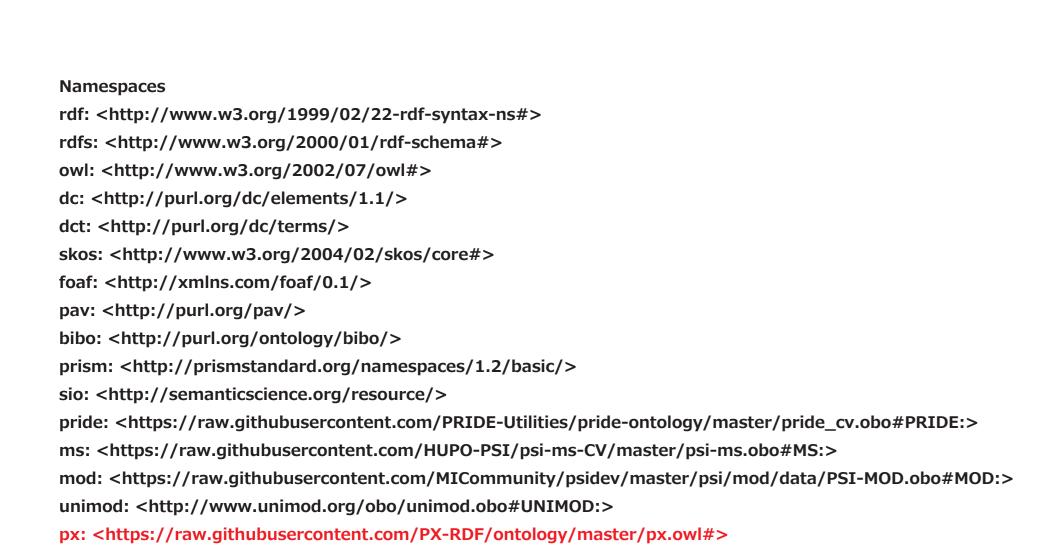


Fig. 4 Used controlled vocabularies and ontologies for PX-RDF

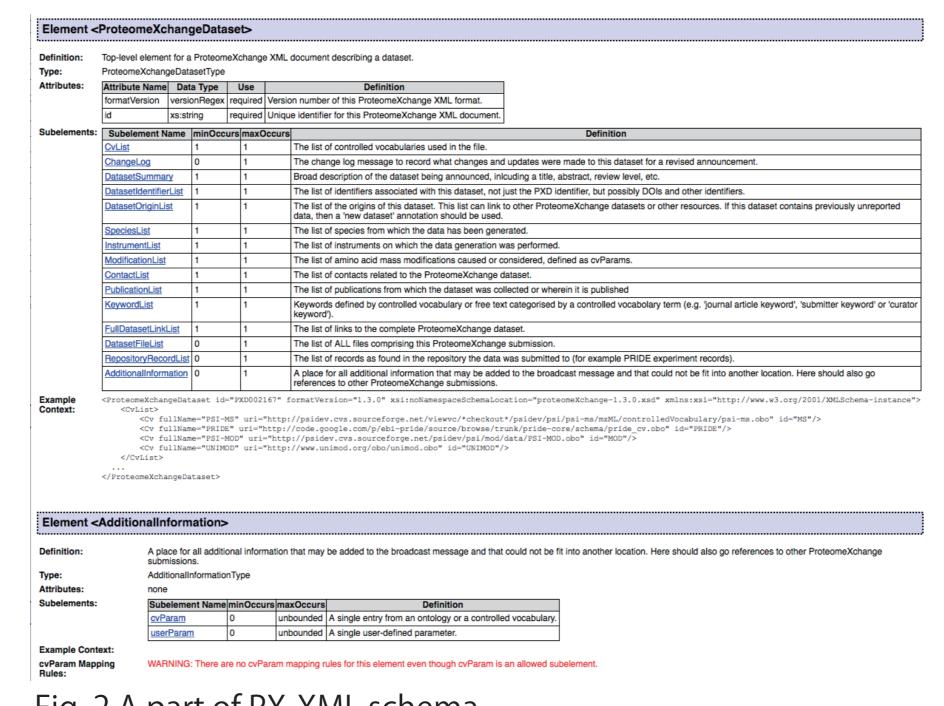


Fig. 2 A part of PX-XML schema http://proteomecentral.proteomexchange.org/schemas/proteomeXchange-1.3.0.html

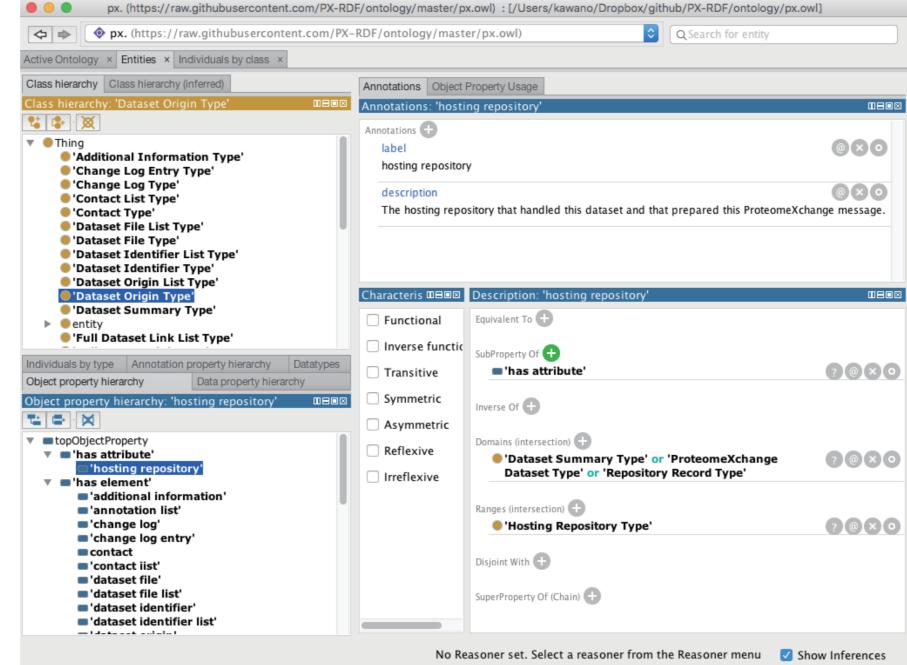


Fig. 5 The PX ontology on the Protege ontology editor

PREFIX px: ">PREFIX px: PREFIX px: https://raw.githubusercontent.com/PX-RDF/ontology/master/px.owl

PREFIX rdfs: http://www.w3.org/2000/01/rdf-schema">

PREFIX dct: http://purl.org/dc/terms/

SELECT?id

?px dct:identifier ?id .

WHERE {

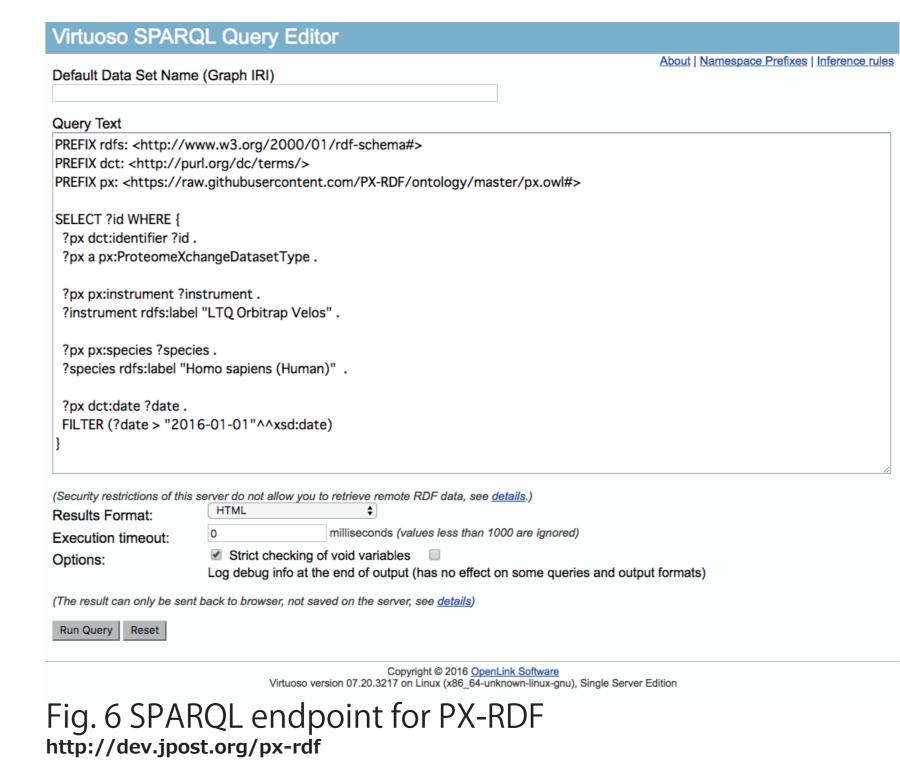


Fig. 3 The PX-RDF schema for PX metadata

https://github.com/PX-RDF/RDF/blob/master/PX-RDF.png

id	<< Full experiment listing PXD000117
"PXD000117"	
"PXD000332"	DataSet Summary
"PXD000261"	 HostingRepository: PRIDE AnnounceDate: 2016-08-25 AnnouncementXML: Submission 2016-08-25 04:54:54.xml
"PXD000275"	DigitalObjectIdentifier: http://dx.doi.org/10.6019/PXD000117 ReviewLevel: Peer-reviewed dataset
"PXD000301"	DatasetOrigin: Original data RepositorySupport: Supported dataset by repository
"PXD000302"	PrimarySubmitter: Laurent Gatto Title: Human exosome proteome
"PXD000437"	 Description: Proteomics study of human urine exosomes. This data describes the proteomic complement of the human exosomal urine fraction from 10 healthy volunteers (5 male, 5 female) aged 23 to 36 years. 50 µg protein from each
"PXD000787"	sample were fragmented on a 4%/12% SDS-polyacrylamide gel. Following staining, each gel track was separated into 28 equal sections, which were processed individually. Peptides were separated by reverse-phase chromatography
"PXD000883"	(Dionex, Sunnyvale, CA) and LC-MS/MS was performed using an Eksigent NanoLC-1D Plus (Eksigent Technologies, Dublin, CA) HPLC system and an LTQ Orbitrap mass spectrometer (ThermoFisher, Waltham, MA). Peptides from each
"PXD000895"	gel segment were analysed twice: (1) with a dynamic exclusion list and (2) a fixed exclusion list for the abundant protein uromodulin which was superimposed on a dynamic exclusion. MS data were processed using SEQUEST Bioworks
"PXD001222"	Browser (version 3.3.1 SP1, ThermoFisher) to generate MS/MS peak lists. Combined peak list files were submitted to the MASCOT search algorithm (version 2.2.1, Matrix Science, London UK) and searched against the IPI-Human
"PXD001485"	database. • SpeciesList: scientific name: Homo sapiens (Human); NCBI TaxID: 9606;
"PXD001501"	 ModificationList: monohydroxylated residue; iodoacetamide derivatized residue Instrument: instrument model: LTQ Orbitrap; LTQ Orbitrap

Fig. 8 Output of the query and one of the listed entry.

Results and Discussion

Statistics at the end of August were:

- Entries: 2,611
- · Triples: 2,064,628
- File size (tar.gz): 9.5 MB

Figs. 7 and 8 show an example of SPARQL query and its output, respectively.

Since we employed the RDF data model, which is globally used e.g. in federated queries, we will not only be able to search for proteomics datasets, but also integrate these searches with datasets from other fields such as genomics, transcriptomics and metabolomics.

Future work

- Implementation of automatic update of PX-RDF using the PX RSS notification feed.
- · Implementation of SPARQL endpoint on ProteomeCentral.

?px a px:ProteomeXchangeDatasetType . ?px px:instrument ?instrument . ?instrument rdfs:label "LTQ Orbitrap Velos" . ?px px:species ?species . ?species rdfs:label "Homo sapiens (Human)" . ?px dct:date ?date . FILTER (?date > "2016-01-01"^^xsd:date) Fig 7 An example of SPAROL query List IDs of datasets which were measured.

Prefixes for simplifying query

Getting ID

Fig. 7 An example of SPARQL query. List IDs of datasets which were measured by "LTQ Orbitrap Velos" instruments, for "Homo sapiens" samples, and published after 2016.

Conclusion

- · We designed an RDF schema of PX metadata, and converted from PX-XML to PX-RDF.
- PX-RDF enables users to perform much more complex and flexible query searches using SPARQL.

Acknowledgment

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