MILLENNIUM®

Breakthrough science. Breakthrough medicine.℠

Alan Ruttenberg
Senior Scientist, Computational Biology

Experiences Collecting and Representing Information about Antibodies for the Semantic Web

ISWC 2006 HCLS Workshop
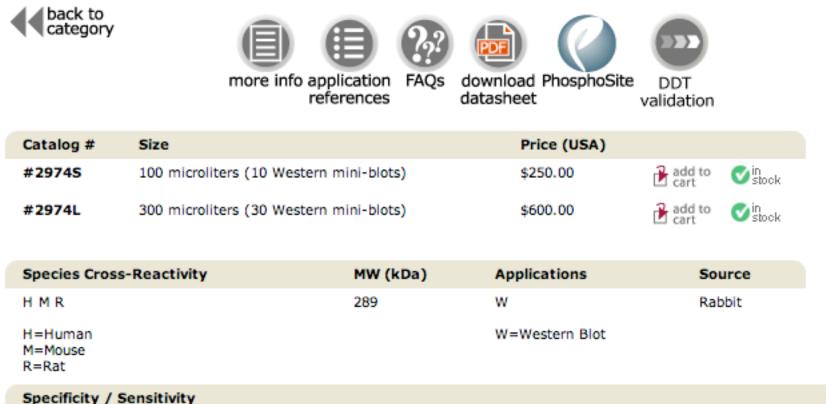**November 6, 2006**

Background/Goals

- Part of a goal articulated by Tim Clark/BioRDF - make available information to help scientists design experiments.

- A typical problem is finding appropriate reagents.

- Antibodies are widely used in molecular biology
  – Checking for presence/quantitation of protein
  – Cell type determination (FACS)
  – Interfering with protein function

- http://www.alzforum.org/ has curated antibodies for Alzheimer Research

- Make these (and others) available on the SW

- Learn/communicate how to do these sorts of projects

Ingredients: Alzforum Record

AntibodyID: 13396

Antigen: MAPKs, ERK, MEK, ASK1, p38

Datasheet: NULL

Datasheet link text:ERK1/2

Clonality: polyclonal

Company Name:ACCURATE CHEMICAL & SCIENTIFIC CORPORATION

Company URL: http://www.accuratechemical.com/

Distributor info: Cat# YSGKA PMA001C/E

Host: rabbit

Specificity: polyclonal rabbit

methodFastOutput: IH, IP, WB

reactivityFastOutput: ~43 and 42 kDa ERK1/2, ~44 kDa doubly phos. ERK1

reactivityExtraOutput: human, rat, mouse, sheep, bovine, drosophila, mussel, xenopus, chicken

Ingredients: Commercial Web Page

Phospho-mTOR (Ser2481) Antibody

back to category

more info | application references | FAQs | download datasheet | PhosphoSite | DDT validation

Catalog #	Size		Price (USA)		
#2974S	100 microliters (10 Western mini-blots)		$250.00	add to cart	in stock
#2974L	300 microliters (30 Western mini-blots)		$600.00	add to cart	in stock

Species Cross-Reactivity	MW (kDa)	Applications	Source
H M R	289	W	Rabbit
H=Human M=Mouse R=Rat		W=Western Blot	

Specificity / Sensitivity

Phospho-mTOR (Ser2481) Antibody detects endogenous levels of mTOR only when phosphorylated at serine 2481.

Scraping

```
((:ID 2517)
 (:TITLE   "Phospho-Estrogen Receptor alpha (Ser104/106) Antibody  #2517")
 (:PAGE "http://www.cellsignal.com/product.asp?productid=2517")
 (:SPECIFICATION "http://www.cellsignal.com/pdf/2517.pdf")
 (:CITATIONS)
 (:SPECIES "Human" "Mouse")
 (:METHODS "Western Blot"  "Immunofluorescence (Immunocytochemistry)")
 (:SPECIFICITY
 . "Phospho-Estrogen Receptor alpha (Ser104/106) Antibody detects overexpressed levels of
    ER alpha only when phosphorylated at Ser104/106. It does not cross-react with the
    phosphorylated ER isoform beta. ; ")
 (:SOURCE
 . "Polyclonal antibodies are produced by immunizing rabbits with a synthetic phospho-
    peptide (KLH-coupled) corresponding to residues surrounding serine 104/106 of human
    ER alpha. Antibodies are purified by protein A and peptide affinity chromatography. ; ")
 (:PTM ("Ser" "104" "106")))
```

So Far

Cell Signal Technologies
Abcam
Santa Cruz Biotechnology
R&D Systems
Panomics

Challenges

- Most antibodies are identified by name only

- Often the names are ambiguous, idiosyncratic

- Many antibodies are constructs - what should the property relating genes be.

- Intellectual property

- There is a lack of standardized vocabulary, for, e.g. epitopes, "species",

Names Strategy

- Synonym database - Entrez Gene, OMIM, Enzyme
- Simple transformations
  - Lowercase, only letters and numbers
- General rewrite rules (beta->b, Anti-p->p, etc)
- Company specific synonyms, e.g. Panomics ER->ESR1 - curated by noticing and investigating failures
- Company specific rewrites. A/B -> try matching A or matching B (not safe in general) - curated
- "Helper" synonym databases to make suggestions on failure - InfoBiogen cancer gene synonyms, Ingenuity,COPE response element names.

Tools

- LSW = Lisp Semantic Web
- Armed Bear Common Lisp
- Jena
- OWLAPI
- Pellet OWL DL Reasoner

```
(define-ontology alzantibodies (:base "http://www.w3.org/2001/sw/hcls/ontologies/reagent.owl"
        :includes '(reagent))
 (let ((individuals nil) (count 0))
  (block limit
   (foreach-antibody-entry
    (lambda(entry)
          (flet ((field (field)
                   (let ((value (cdr (assoc field entry))))
                    (if (and (char= (char value 0) #\")
                             (char= (char value (1- (length value))) #\"))
                        (setq value (subseq value 1 (- (length value) 2))))
                    (if (or (equal value "NULL") (equal value " "))
                        nil
                        (progn
                         (#"replaceAll" (#"replaceAll" value "&" "&amp;") "\"" "%22")))))))
           (let* ((name (make-uri-base-relative (format nil "antibody-~a" (field :antibodyid)) "alz:"))
                  (individual
                   (individual name
                    (annotation !alz:hasAntibodyId (field :antibodyid))
                    (and (field :epitope)
                         (annotation !hasEpitopeDescription (field :epitope)))
                    (and (field :specificity)
                         (annotation !hasSpecificityDescription (field :specificity)))
                    (annotation !hasHostDescription
                      (format nil "~a~a" (field :hostfastoutput)
                      (if (field :hostExtraInfo) (format nil " (~a)" (field :hostExtraInfo)) "")))
                    (annotation !hasReactivityDescription
                      (format nil "~a~a"
                        (field :reactivityfastoutput)
                        (if (field :reactivityextrainfo)
                            (format nil " (~a)" (field :reactivityextrainfo)) "")))
                    (annotation !hasCompanyDescription (field :companyname))
                    (annotation !alz:hasAntigenClass (field :antigenId))
                    (type !Antibody))))
             (push individual individuals))))))
   individuals))
```

Links

- http://www.alzforum.org/res/com/ant/default.asp
- http://esw.w3.org/topic/HCLSIG_BioRDF_Subgroup/Tasks/Reagents
- http://svn.mumble.net:8080/svn/lsw/trunk/

Acknowledgements

- AlzForum: June Kinoshita, Elizabeth Wu, Colin Knep, Tim Clark

Breakthrough science. Breakthrough medicine.[SM]