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Epitopes in ChEBI - A Collaboration with the IEDB

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Broad range of non-peptidic epitopes unearthed by IEDB and represented in ChEBI on hapten – Ni²⁺ (seen here in ChEBI:53001) 'Fig.1: Nick Fig.2: (ChEBI: 59384) branched tetrasaccharide typical of many bacterial cell wall-derived antigens. represents the most common contact sensitiser in the industrialised world. It acts as a hapten (partial antigen), o-L-Rhap-(1---3)-[o-0-Glcp-(1---4)]-o-L-Rhap-(1---3)-β-0-GlcpNAc-(1---2)-o-L-Rhap (CHEI capable of inducing an immune response upon binding to MHC-associated proteins. Automatic Xrefs ChEER Name Ø o-L-Ribap-(1-43)-1 ChEER ID Ø CHEER 59384 ChEER ASCE Name ølpha-L-Ribap-(1 el sulfate (CHEBI:53001 å Automatic Xosh Definition Abranched tot ChEBI Name nickel sulfat Last Modified 12 May 2010 ChEBI ID CHEBI: 53001 Stars 0 *** 74 Definition Ametal suifale of R Image 20 September 2010 Stars 0 Fig.4: Fatty acid-based epitope (ChEBI: 45573) - a butyric (butanoic) acid-derived epitope.

Main

'Fig.3: Amino acid-based epitope (ChEBI: 59565) an alanine derivative.

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| Main Automatic X | wb . | | |
| | ChEBI Name | N(4-(4-nitrophenylphospho)butanoyl)-c-alanine | |
| | C7EB () | CHEER 55665 | |
| 1 | CHEBI ASCI Name | N-(4-(4-nitrophenylphospho)butanoy()-L-alanine | |
| Jun 10 | Definition 0 | The L-enantiomer of NH4 (4-nitrophenylphospho)butanoy@alanine. | |
| 1 | Last Modified | 02 June 2010 | |
| | San 0 | This entry has been manually associated by the ChEBI Team. | |
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'Fig.5: Steroidal epitope (ChEBI: 8884) - an epitope with a 3α-hydroxy steroid skeleton

| curonium (C | HEB18884) | | | Quick search here! Search for *** only 🗹 |
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| Main | Automatic Xrel | 5 | | |
| | | ChEBI Name | rocuronium | |
| , to | | ChEBI ID | CHEDLOOM | |
| | | Definition 9 | A 6e androstane compound having 3e hydrosy., 178-acetory., 28-morpholino- and 168- NailyRynolder | |
| | | Last Modified @ | 10 November 2009 | |
| State / | HH 1. | 52822 O | *** This entity has been markedly ancotated by the ChERI Team. | |
| | · · · | Secondary ChEBI IDs | CHEB: 340257 | |
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| | more structures >> | | | |

Fig.7: 'Organosilicon epitope (ChEBI: 59555) - an organosilicon compound with a piperidine N-oxide core. CHEBI Name 0 date-4-(din CHEBI Name 0 CHEBI S956 CHEBI ASCI Name 0 trans-4-(din Definition 0 Appendime.) Stars 0 2 Image

Fig.8: 'Glycosphingolipid epitope (ChEBI: 466659) an α -D-galactose-derived glycophytoceramide, the most potent agonistic antigen of the T cell receptor of natural killer T cells.

| -O-(o-0-galactopyranosyl)-N-hexacosanylphytosphingosine (CHEBI:466659) | | | | ABICK SEAFCH HEFEL |
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| Main | Automat | c Xhefs | | |
| | | ChEEL Name | 1-O-(a-o-galaclopyranosy()-N-hexacosanylphylosphingor | ine |
| Substructure Search Similarly Search Identity Search | | CHEBI ID 9 | CHEBE 466660 | |
| | | ChEELASCI Name | 1-O-(alpha-O-galaclopytanosyl) N-hexacosanylphylosphingosine | |
| | | Definition 0 | A glycophytoceramide having an o-o-galdopyranceyl residue at the C-1 position and an hexacosancyl g nitrogen. | |
| | | Last Modified 0 | 21 June 2010 | |
| | | Stars 0 | *** This series has been manually associated by the Chillel Team. | |
| | | Secondary ChEBI IDs | CHEBI 40662 | |
| 10 march | | E Image | | |

References:

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ChEBI, IEDB and their relationship.

What ChEBI is: Chemical Entities of Biological Interest (ChEBI) is a curated database of small chemical entities important in biosystems [1]. Its focus is on entities of no more than 1,500 atomic mass units.

ChEBI evolution: Since its inception in 2004, ChEBI has evolved from an illustrated dictionary of terms into a semantically rich knowledge base with an internal hierarchy that organises entities by their molecular structure types and potential rôles. Its 2009 acquisition of the BioFocus drug discovery dataset [2] exponentially increased the number of entities from 20,000 to 500,000. ChEBI continues to develop automatic curation protocols to maintain the high standards characteristic of the smaller dataset, while the number of manually curated entities continues to rise.

The ChEBI-IEDB collaboration: The Immune Epitope and Analysis Resource (IEDB) is a project supported by contract from the National Institute of Allergy and Infectious Diseases (NIAID) with the aim of making epitope-related data on infectious diseases and immune disorders freely available to researchers worldwide [3]. In addition, the IEDB houses cutting-edge analytical tools [4]. In June 2009, ChEBI began working with the IEDB on a project aimed at incorporating into ChEBI, by manual curation, a pilot subset of immunologically important chemical substances that had been identified as immune epitopes.

IEDB epitopes in ChEBI - the curation process: A list of 1,200 entities was provided by the IEDB, each with one or more PMIDs (PubMed (unique) Identifiers) for publications describing contexts in which the immune epitope status of the structure had been assayed. These chemical

Immune epicope status of the structure had been assayed. These chemical units were treated in one of three ways: -(1) Where the entity already existed in ChEBI, the PMID was entered into the ChEBI database and automatically hyperlinked to the PubMed site; (2) Entities automatically downloaded as part of the BioFocus dataset required definitions, ontology specifications, IUPAC names, synonyms and registry numbers for the various databases linked to ChEBI; (3) New ChEBI identification numbers were generated for entities that did not already exist.

In addition to the data items mentioned in (1) and (2) above, structures were drawn or generated using ChEBI's in-house tools. The rôles played by these structures (e.g. immunogen, antigen, epitope and hapten) were also curated.

The status quo: In the year since the ChEBI-IEDB collaboration began, the pilot 1,200 entities have all been fully curated. Of this number, 50% were newly created for this project, and included a number of new rôles related to immunology. 250 new citations were added to ChEBI from this subset of IEDB data, covering epitopes relating to a variety of entities including antibiotics, organic radicals, oligosaccharides, norligans, transition metal complexes, alkaloids and amino acids. The IEDB continues to request that new structures be processed by ChEBI as new categories of immune epitope-related publications are curated. Approximately 100 structures per month are processed by ChEBI for the IEDB.

The significance of the project: The increasing global prevalence of immune-related diseases, and the complexity of the contributing factors [5, 6], underscore an ever-increasing need for cross-talk among the various scientific disciplines, and makes ChEBI involvement in this project particularly relevant. The ChEBI-IEDB teamwork here described illustrates particularly relevant. The CnEBI-1EDB teamwork here described illustrates the mutual advantages to be gained from such joint endeavours: while the incorporation of IEDB items into ChEBI has effected a significant enrichment of the latter's database content and ontology, IEDB has profited from the ChEBI team's expertise in describing non-peptidic epitopes and from the structure tree lay-out and the multiplicity of synonyms used in ChEBI, which facilitate a simplified search process. The IEDB has recently updated its search interface to make the most of its collaboration with ChEBI.

Conclusion: In identifying and curating these non-classical epitopes, we have highlighted the broad array of non-peptidic epitopes in existence. To date, we have identified over 20 categories of such entities, including antibiotics, resins, food additives and nucleic acid derivatives, in addition to the eight categories depicted in figures 1-8 of this poster. In so doing, we have demonstrated how collaboration among curators working on different databases can lead to reciprocal benefits combined with an enhanced service to our users.

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The ChEBI Team

Ac-Asp-W-(2-(11)), Ac-Asp-W-(2-(11)), Ac-Asp-W-(2-(11)), Ac-Asp-W-(2-(11)), nethylberosyljkATIOFEVQEE (CHEEL80221) is a polyneptide (CHEEL5841 nethylberosyljkATIOFEVQEE (CHEEL80221) is a lopopetide (CHEEL80888 neth-PencosylikATIGFEVQEE (CHEEL80221) has role mimotope (CHEEL80281)

ladder-like polycyclic ether characteristic of certain marine toxins. Main Automat ChEBI Name 0 1,6.5,9.8,12:11,1 disealed

Fig.6: 'Organic heterocycle epitope (ChEBI: 59525) - a

vilbutyric acid (CHEB):45573

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CHEBI 45573

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Fig.9: View of ChEBI ontology relating to a mimotope (molecule whose structure mimics that of an epitope).

△ CHEBI:60221 Ac-Asp-M-(2-(tr

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