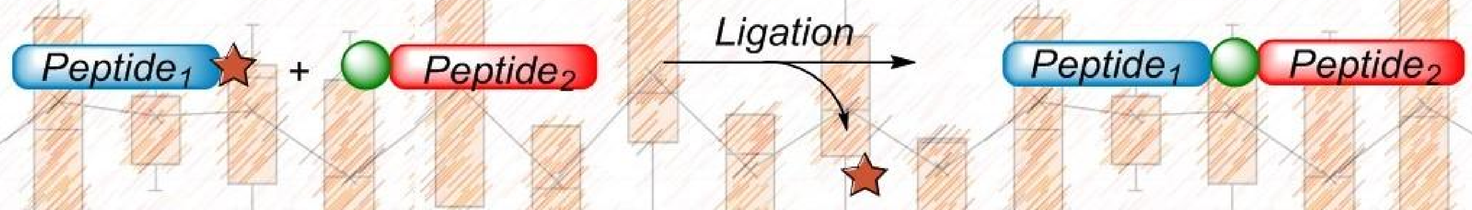
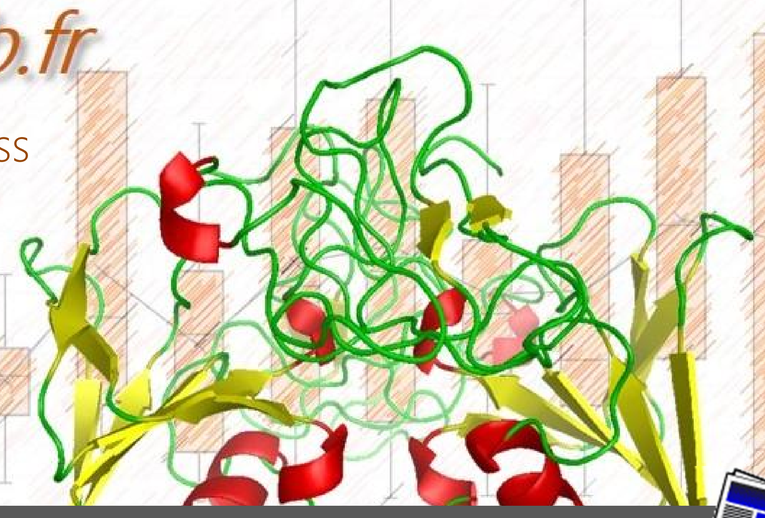
Protein Chemical Synthesis Database > *pcs-db.fr*

V. Agouridas, O. El Mahdi, M. Cargoet and O. Melnyk *Bioorg. Med. Chem.* 2017, in press





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Over the last 20 years, amide-bond forming ligation reactions have established themselves as an essential tool for the total chemical synthesis of challenging peptides and proteins. This spectacular development is echoed in an abundant literature that we wanted to compile in a database : the Protein Chemical Synthesis DataBase (http://pcs-db.fr). The aim of this work is to provide the community a comprehensive tool along with a user-friendly interface (PC or cellphone browsable) to rapidly identify targets pursued by protein chemists but also compare how the various ligation methodologies are used according to the length of targets, the nature of junctions or post-ligation manipulations…

Methodological approach

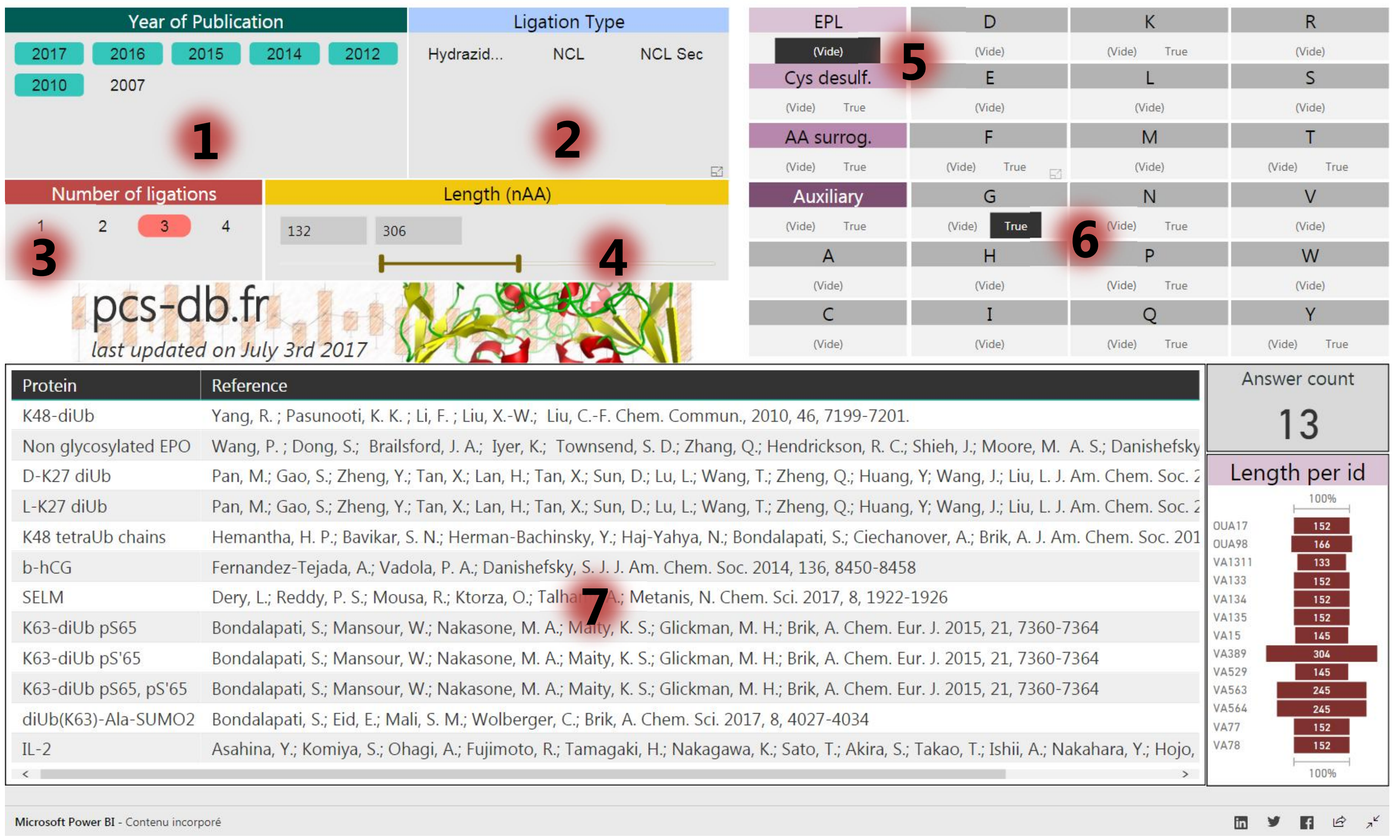
Proteins or analogs of **biological significance** (model peptides, polymers, hybrid material excluded)

Synthetic proteins assembled by **at least one or any combination of the following ligation methodologies**: **NCL and extended methodologies** (by extended methodologies, we mean the methods for which the thioester segment is substituted by a thioester surrogate – *i.e. selenoester, hydrazide, Nbz, O,S, N,S, and N,Se acyl shift systems* - or for which the Cys segment is substituted by a thiol or selenol amino acid residue – *i.e. thiol-based auxiliaries linked to the α-amino group, mercapto or seleno amino acid surrogates* -), **serine/threonine ligation (STL)** or **α-ketoacid-hydroxylamine (KAHA) ligation**, **Additive-Free Selenoester Diselenide Ligation (AFSDL)** and miscellaneous.

Name, **year of publication**, **length** and **origin** collected. Details about the synthetic design, such as the **type of ligation chemistry** used, **nature of the junctions** formed, **use of amino acid surrogates** or **thiol auxiliaries** and/or **use of dechalcogenation reactions** were also compiled.

725 entries from ~500 unique references published over the period 1994 - Jun. 2017 (July 3rd 2017 update)

An example of research on pcs-db.fr (full instructions can be found directly on the website)



1 Years 2017, 2016, 2015, 2014, 2012 and 2010 were selected by Ctrl+ mouse click

2 Ligation types are refreshed accordingly to what has been selected in other fields

3 Proteins assembled by 3 ligations (4 segments) were selected

4 The range of protein lenght was defined with the numeric range slidebar (from 132 aa to 306 aa)

5 Proteins produced by EPL are excluded (*(Vide)* selected). Other fields work the same way.

6 Only proteins assembled with at least one Gly-X junction are considered (*True* selected). Other fields work the same way.

7 Results display area

The pcs-GO module

I The interactive PCS-GO module provides a synoptic view of the type or the number of ligations used to assemble proteins over the years.

II Mouse-clicking an histogram bar instantly modifies the treemap charts below to deliver adjusted statistics (multiple selection is allowed).

III Mouse-clicking a rectangle of the treemap charts filters the data accordingly in all other charts (multiple selection is allowed).

IV View all proteins synthesized thanks to at least a dechalcogenation step