

Health and Environmental Sciences Institute

740 15th Street, NW Suite 600 Washington, DC 20005 USA 1.202.854.8404 office 1.202.659.3859 fax www.hesiglobal.org



## **COMPARE 2024 Update Documentation**

The COMPARE Team is pleased to present the release of the COMPARE 2024 database, released on 01/25/2024 (www.comparedatabase.org).

A new version was updated on 02/02/2024. This version corrected a duplicate header line in the fasta file. No sequences were added/removed or changed between the two releases.

### 1. COMPARE 2024: General Overview

### 1.1. Database entries

The COMPARE 2024 database consists of **2748 sequence entries**. Overall updates to the 2024 COMPARE database include:

- 151 unique additions to the COMPARE 2023 database.
  - o 35 full-length proteins
  - 116 mass spectrometry (MS) additions
- The removal of 34 entries from COMPARE 2023 (see table below).

Therefore, COMPARE 2024 = 2361 entries (COMPARE 2023) - 34 entries (removal from COMPARE 2023) + 151 new unique entries = 2748 sequence entries.







Figure 1: Constant and consistent growth of sequence entries in COMPARE. In 2020 a historical data review was undertaken, and MS sequences were included in the database.

All decisions result from the COMPARE Peer-Review Panel (PRP)'s review of sequence candidates with record dates ranging between May 15, 2022 – May 15, 2023, and associated literature. As in previous years, the candidate sequences were sourced from <u>NCBI Protein</u>, <u>UniProt</u>, <u>AllergenOnline</u>, and <u>IUIS</u> databases, as well as a targeted literature search, for the same time window.

<b>Retired Sequence</b>	Replacement Sequence	Justification
(Removed from COMPARE 2023)	(new or updated sequence in COMPARE 2024)	
COMPARE167	ALQ56981.1	Duplicate: COMPARE167 is fully contained in ALQ56981.1
COMPARE227	(removed)	Sequence does not contain 10 consecutive amino acids (criteria for inclusion)
COMPARE00433	Q9SPL3.1	Duplicate: COMPARE00433 is fully contained in Q9SPL3.1
COMPARE00438	Q9SPL3.1	Duplicate: COMPARE00438 is fully contained in Q9SPL3.1
COMPARE00442	Q9SPL3.1	Duplicate: COMPARE00442 is fully contained in Q9SPL3.1
COMPARE00443	Q9SPL3.1	Duplicate: COMPARE00443 is fully contained in Q9SPL3.1
COMPARE00445	Q9SPL3.1	Duplicate: COMPARE00445 is fully contained in Q9SPL3.1
COMPARE00446	Q9SPL3.1	Duplicate: COMPARE00446 is fully contained in Q9SPL3.1
COMPARE00447	Q9SPL3.1	Duplicate: COMPARE00447 is fully contained in Q9SPL3.1
COMPARE00448	Q9SPL3.1	Duplicate: COMPARE00448 is fully contained in Q9SPL3.1
COMPARE00449	Q9SPL3.1	Duplicate: COMPARE00449 is fully contained in Q9SPL3.1
COMPARE00455	Q9SPL3.1	Duplicate: COMPARE00455 is fully contained in Q9SPL3.1
COMPARE00458	Q9SPL3.1	Duplicate: COMPARE00458 is fully contained in Q9SPL3.1
COMPARE00460	Q9SPL3.1	Duplicate: COMPARE00460 is fully contained in Q9SPL3.1
COMPARE00461	Q9SPL3.1	Duplicate: COMPARE00461 is fully contained in Q9SPL3.1
COMPARE00462	Q9SPL3.1	Duplicate: COMPARE00462 is fully contained in Q9SPL3.1





COMPARE00464	Q9SPL3.1	Duplicate: COMPARE00464 is fully contained in Q9SPL3.1
COMPARE00436	Q9SPL4.1	Duplicate: COMPARE00436 is fully contained in Q9SPL4.1
COMPARE00437	Q9SPL4.1	Duplicate: COMPARE00437 is fully contained in Q9SPL4.1
COMPARE00439	Q9SPL4.1	Duplicate: COMPARE00439 is fully contained in Q9SPL4.1
COMPARE00451	Q9SPL4.1	Duplicate: COMPARE00451 is fully contained in Q9SPL4.1
COMPARE00452	Q9SPL4.1	Duplicate: COMPARE00452 is fully contained in Q9SPL4.1
COMPARE00454	Q9SPL4.1	Duplicate: COMPARE00454 is fully contained in Q9SPL4.1
COMPARE00456	Q9SPL4.1	Duplicate: COMPARE00456 is fully contained in Q9SPL4.1
COMPARE00327	QDO73345.1	Duplicate: COMPARE00327 is fully contained in QDO73345.1
ABF21078.1	AHM25029.1	Duplicate: ABF21078.1 is fully contained in AHM25029.1
COMPARE105	C0HLQ2	Duplicate: COMPARE105 is fully contained in C0HLQ2
COMPARE106	C0HLQ2	Duplicate: COMPARE106 is fully contained in C0HLQ2
COMPARE00422	XP_042518524.1	Duplicate: COMPARE00422 is fully contained in XP_042518524.1
COMPARE00423	XP_042518524.1	Duplicate: COMPARE00423 is fully contained in XP_042518524.1
COMPARE00424	XP_042518524.1	Duplicate: COMPARE00424 is fully contained in XP_042518524.1
COMPARE00425	XP_042518524.1	Duplicate: COMPARE00425 is fully contained in XP_042518524.1
COMPARE00428	XP_042518524.1	Duplicate: COMPARE00428 is fully contained in XP 042518524.1
BAF47264.1	CBY17558.1	Duplicate: Identical to CBY17558.1

COMPARE 2024 has otherwise followed specifications set in 2019 - e.g., use of "COMPARE #" Accessions when no other public accession number is known for a specific sequence (see paragraph A in "<u>COMPARE 2019 Documentation</u>" file); information sharing via documentation and transparency files, available in the database page under the <u>Documentation tab</u>.





### 1.2. Accession number updates (past entries)

The "Accession" field was updated for 3 allergen entries.

PAST COMPARE	NEW COMPARE	COMPARE Description
Accession	Accession	
MANUAL2	COMPARE247	cysteine protease
MANUAL3	COMPARE248	vitellogenin, partial
COMPARE022	QFG58557.1	7S globulin, vicilin, beta-conglutin

## 1.3. Description updates (past entries)

## The "Description" field was updated for 13 entries.

COMPARE Accession	PAST COMPARE Description	NEW COMPARE Description
2MC9_A	peptidyl-prolyl isomerase	cyclophilin/peptidyl-prolyl isomerase
CAB44442.1	peptidyl-prolyl isomerase	cyclophilin/peptidyl-prolyl isomerase
CAC84116.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
CAI78448.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
AAP35065.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
AEY79726.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
ALM24136.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
AVV30163.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
CAA09884.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
P81531.2	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
XP_025675300.1	cyclophilin	cyclophilin/peptidyl-prolyl isomerase
ANQ43386.1	chitinase	glyceraldehyde-3-phosphate- dehydrogenase
CAA45085.1	alpha-amylase, partial	alpha-amylase inhibitor, partial



### 1.4. Other updates to past entries

Accession	Old IUIS Name	New IUIS Name
ABM53752.1	Tyr p 13	None
Accession(s)	Old Species Name	New Species Name
P80273.2, P33556.1, P80274.1	Vitis sp.	Vitis vinifera
AKV72166.1	Acacia farnesiana	Acacia farnesiana (Vachellia
		farnesiana)
AIV43662.1	Vachellia farnesiana	Acacia farnesiana (Vachellia
		farnesiana)
BAH10157.1	Venerupis philippinarum	Ruditapes philippinarum
		(Venerupis philippinarum)
Accession	Old Sequence	New Sequence
COMPARE086	IEIESFYEGD <mark>O</mark> FSETLTR	IEIESFYEGD <mark>D</mark> FSETLTR

1.5. New! Links to NCBI Protein database have been included on the allergen record page.

		NIH National Library of Medicine
ADK662	280.1	Protein V
Accession External DB Link	ADK66280.1	GenPept - Intracellular fatty acid-binding protein [Penaeus vannamei] GenBank ADK66280.1 Identical Proteins EASTA Coophics
Species	Litopanaeus vannamei (Penaeus vannamei)	Garlas (9
Common Name	white shrimp	LOCUS ADX65288 136 as linear DW 28-301-2018 DEFDNITOW Intractibular fatty acid-binding protein [Penaeus vannamel].
Description	fatty acid-binding protein	VENSION AUXOGUBE DESOURCE ACCESSION 1 DESOURCE ACCESSION 10100007-1
IUIS Name	Lit v 13	KENAGR5 - SDURCE Panasus vannamsi (Pacific white shrimp) ORGANISH Pengeus vannamsi
Length	136	Eukaryota; Petazoa; Ecdysozoa; Arthropoda; Crustacea; Pulticrustacea; Palacostraca; fumalacostraca; Eucarida; Decapoda; Dendrobraccidata: Proacoldea: Proactida: Penavut.
Year Adopted	2023	
Sequence	>ADK66280.1 Lit v 13; fatty acid-binding prot MAKIEGKFKMESSENFDEFMKALGVGLVMRKMGMAATPTVEITKD EIKFKLGEEFEETTADGRVVKSTITLDGNKLVMKQVGDKEKKEKD CKVDDVVCKRVYSRLE	ein [Litopanaeus vannamei (Penaeus vannamei)] GDTYTMKTTTTFKTT SELLREFTDOKMLME





# 1.6. New! A list of biochemical names in COMPARE has been included on the Documentation page.

In 2021, the Peer Review Panel reviewed the description lines of all COMPARE entries to clean-up irrelevant wording from automated text imported from the source databases in order to generate meaningful description lines to the eyes of allergy experts. This list is now included in the Documentation tab <u>here</u>.

# 1.7. Enhanced visibility for Mass Spectrometry (MS) fragments: Visualization of MS fragments mapped to their Parent Accession has been incorporated.

**New!** A visual representation of MS sequences mapped to their known full length parent sequence (even though the full-length parent protein sequence is not an entry in the database itself) has been included as part of our commitment to continuous improvement. An example is shown in Figure 2 below. COMPARE030 maps to parent sequence Q9FSH9.1. The graphic demonstrates where the peptide sequence is located on the parent and which other peptide sequences in COMPARE are associated with that parent sequence. This helps the user identify the portion of the parent sequence that has published IgE binding evidence.







### ABOUT DATABASE PROCESS DEVELC

## Allergen

## COMPARE030

Accession	COMPARE030
External DB Link	
Species	Lupinus albus
Common Name	white lupine
Description	7S globulin, vicilin, gamma-conglutin, partial from Q9FSH9.1
IUIS Name	
Length	21
Year Adopted	2020H_MS
Sequence	>COMPARE030 75 globulin, vicilin, gamma-conglutin, partial from Q9FSH9.1 [Lupinus albus] AGIALGTHQLEENLVVFDLAR
Parent Accession	<u>Q9FSH9.1</u>

#### **Related Sequences**

Peptide sequences mapped to Parent Accession



Figure 2: New visualization in COMPARE2024 for records with known Parent Accessions is now available. Allergen record page for <u>COMPARE030</u>.





REMINDER: bioinformatics companion tool, COMPASS (COMPare Analysis of with Software)

As of June 2019, the COMPARE database is equipped with its companion tool, <u>COMPASS</u> (COMPare Analysis of Sequences with Software), as a built-in feature. COMPASS is a comparative sequence search software, incorporating the <u>open source FASTA software</u> <u>package</u> (FASTA v36). With this tool, COMPARE users can conduct website-based, real-time use of the COMPARE database to identify similarities between a protein sequence of interest and COMPARE's allergens via amino acid sequence alignments (between two or more amino acid sequences). COMPASS offers a visualization option to view results in a color-coded graphic display. To access the tool, go <u>www.comparedatabase.org</u>, click on the "<u>Database</u>" tab and click on the green button "<u>Run COMPASS</u>." For detailed information, instructions on how to use and supporting references, visit the <u>COMPASS</u>' "About" page.

As part of COMPARE 2024's release, COMPASS is also updated to screen against COMPARE 2024 sequences.

### Your Feedback is Appreciated - Contact Us

The HESI COMPARE database program is committed to transparency and open dialog. Individuals or organizations are invited to submit feedback, questions, or inquiries via the "<u>Contact us</u>" portal in the COMPARE database website, or email to <u>comparedatabase@hesiglobal.org</u>. HESI staff will respond if the information is readily available or will relay the inquiries to the Peer Review Panel if a more in-depth response is required.

## Licensing

This work is licensed under a Creative Commons Attribution 4.0 International Public License: This license requires that reusers give credit to the creator. It allows reusers to distribute, remix, adapt, and build upon the material in any medium or format, even for commercial purposes. For the text of the license, see <u>https://creativecommons.org/licenses/by/4.0/</u>.

When using the database or referring to it in a publication, please cite the COMPARE publication:

van Ree et al., 2021. The COMPARE Database: A Public Resource for Allergen Identification, Adapted for Continuous Improvement. *Frontiers in Allergy*. <u>https://doi.org/10.3389/falgy.2021.700533</u>.





### Support COMPARE!

Is COMPARE useful as a resource and do you like its commitment to continuous improvement? If so, support COMPARE! We have other ideas to continue improving this resource and making it as comprehensive and thorough as possible. The COMPARE database is a collaborative HESI program. The annual update of the database is a resource intensive process that involves many more partners and collaborators, rolling on a steady annual cycle schedule. The execution of the program relies on scientific expertise and in-kind and direct financial support from both public sector and private sector scientific organizations to maintain this free, public resource. If you would like to learn more about how you or your organization can contribute, please contact us at <u>comparedatabase@hesiglobal.org</u>.

<u>Your support is tax deductible in the US</u>: HESI is a non-profit, 501(c)(3) organization committed to generating science for a safer, more sustainable world. <u>Financial support to HESI's scientific programs is considered a tax-deductible charitable donation in the United States</u>. Your support to our mission, through funding and participation, makes our scientific collaborations and outreach possible, and helps improve both human and environmental health across the globe.

We look forward to hearing from you!

**About HESI** (<u>www.hesiglobal.org</u>): The Health and Environmental Sciences Institute (HESI) is a non-profit institution whose mission is to collaboratively identify and help resolve global health and environmental challenges through the engagement of scientists from academia, government, industry, NGOs, and other strategic partners. Since 1989, HESI has provided the framework for scientists from public and private sectors to meaningfully collaborate in developing science for a safer, more sustainable world.

