

MESSAGE FROM THE ESTHER Database
Published occasionally by the ESTHER Team

Since our Newsletter Number 5 of September 2015, it happened the following:

MEETINGS

Thanks to Jorge Estevez, Miguel Angel Sogorb, Eugenio Vilanova and their colleagues, the 12th Meeting on Cholinesterases and Sixth International Conference on Paraoxonases (Elche, Spain, 27 Sept - 2 Oct 2015), nicknamed 12ChE-6PON, and later on “El-ChE”, was a success and a tremendous opportunity to exchange on all aspects of our beloved enzymes ([12th ChE](#)). A ceremony for delivery of the first B.P. Doctor Young Investigator Awards ([XVth ISCM](#)) was held during the meeting. There were 26 applicants, and the committee was able to award five of them ([Satish N. Dighe](#), [Drew R. DeBay](#), [Maja Katalinic](#), [Rahul Sharma](#), [Nir Waiskopf](#)) ([Photo 1](#), [Photo 2](#)). Each awardee received a metal engraved plaque on walnut, a certificate of the honor and a check covering their travel expenses. The organization committee voted unanimously to continue the award at other cholinesterase and cholinergic meetings in the future, so that the tradition and legacy will live on ([link](#)). The proceedings of the meeting will be published soon in a special issue of *Chemico-Biological Interactions*.

The “XVth International Symposium on Cholinergic Mechanisms” (XVth ISCM) in Marseille, France, is now scheduled for October 16-20th, 2016. Please have a look at the web site (<http://iscm.sciencesconf.org/>) and send a note to iscm@afmb.univ-mrs.fr to express your anticipated interest and that of your colleagues and students for this event and be added to the mailing list. Also, should you have close contacts with potential sponsors, please let them know of the package and out-of package sponsoring opportunities posted on the site).

Symposium “A molecular perspective on the cholinergic synapse: A symposium in honor of Israel Silman's 80th birthday” took place at The David Lopatie Conference Centre Weizmann Institute of Science, December 9-11, 2015 ([Poster](#)). A “Symposium in Honor of Palmer Taylor - Scientist, Scholar, Mentor, and Dean, From Toxins to Therapeutics” took place at The UC San Diego Skaggs School of Pharmacy and Pharmaceutical Sciences, January 14-15, 2016 ([Poster](#)). Both events were successful. We all express our warmest congratulations to Sili and Palmer.

NEW TOOLS

We are pleased to announce that

- Tables of substrates and inhibitors have been updated, and compounds linked to the family of their main target enzyme.
- Compounds are now referenced with InChI, InChI Key, Canonical SMILES and links to PubChem and Chembl

STRUCTURES

In February, the number of tridimensional structures in ESTHER reached 1580 entries!

During the latest 6 months (September 2015 - February 2016), 60 new crystal structures of 29 alpha/beta hydrolase proteins from 17 subfamilies were released by the RCSB PDB; for 16 of these proteins they were the first structures to be solved. [Tolzer et al.](#) showed that MekB ([9psed-q0mrg5](#)) from *Pseudomonas veronii* and CgHle ([corgl-CGL0839](#)) from *Corynebacterium glutamicum* are esterases that hydrolyze preferentially acetic acid esters. MekB and CgHle cannot bind homoserine and acetyl-CoA. Accordingly a novel esterase subfamily was extracted from the Homoserine_transacetylase family.

See the table of the families: <http://bioweb.ensam.inra.fr/ESTHER/general?what=overallTable>

MUTATIONS

Multiple mutations on the second acetylcholinesterase gene associated with dimethoate resistance in the Melon Aphid, *Aphis gossypii* (Hemiptera: Aphididae) are published by [Lokeshwari et al.](#) Multiple mutations in the acetylcholinesterase 3 gene associated with organophosphate resistance in *Rhipicephalus (Boophilus) microplus* ticks from Punjab, India are published by [Jyoti et al.](#)

MISCELLANEOUS

A new organophosphate hydrolase with alpha/beta hydrolase fold: crystal structure of diene lactone hydrolase-like promiscuous phosphotriesterase P91 from metagenomic libraries is available ([4ZI5](#)) and published by [Colin et al.](#)

On behalf of the ESTHER Team
Arnaud