Gene expression

Homology-driven assembly of NOn-redundant protEin Sequence Sets (NOmESS) for mass spectrometry

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Supplementary Material

This supplement contains:

-Fig. S1-S4

Fig. S1

Graphical User interface of NOmESS -

BLASTp ² Cd-hit ³ Input set ⁴ Scaffold set ⁵	UsersitemuiNOmESS UsersitemuiProgramsit UsersitemuiNOmESSit UsersitemuiNOmESSit	d-hit-windows Browse Browse Browse Browse	 ¹ Folder storing the output ² Folder containing blastp.exe and makeblastdb.exe ³ Folder containing cd-hit.exe ⁴ Fasta file containing amino acid sequences of the organism of interest ⁵ Fasta file containing amino acid sequences of the scaffold set (homolog organism) 	st
		Indication, whether pre-processing should be applied Characters that will be cut out of the sequences of the input set prior to the assembly Sequence length threshold of the input set	ID prefixes Pre-processing identity thresholds (cd-ht) Homology thresholds (BLASTp) Pre-processing (step 1) Image: Comparison of the state	
		Sequence identity thresholds for cd-hit clustering of the scaffold set and the generated sequence sets after each step	Reset all ID prefixes Pre-processing identity thresholds (cd-hit) Homology thresholds (BLASTp) Scaffold set 0.95 Step 1: Pre-processing 1.0 Step 2: Assembly 0.95 Step 3: Concatenation 0.95 Reset Reset	
		Thresholds to filter BLAST hits for every step Sequence identity of overlapping sequences in the assembly step	ID prefixes Pre-processing Identity thresholds (cd-hit) Homology thresholds (BLASTp) Step 2: Assembly Step 3: Concatenation Step 4: Representative selection Percentage identity 0.6 Percentage identity 0.6	.6 0e-10 00 00

Fig. S1 Graphical User interface of NOmESS. The graphical user interface consists of a main window containing the required parameters, whereas the optional parameters can be found in a pop-up window with 4 tabs. The optional parameter values of the screenshots above are NOmESS' default values. Parameter descriptions are highlighted in blue.

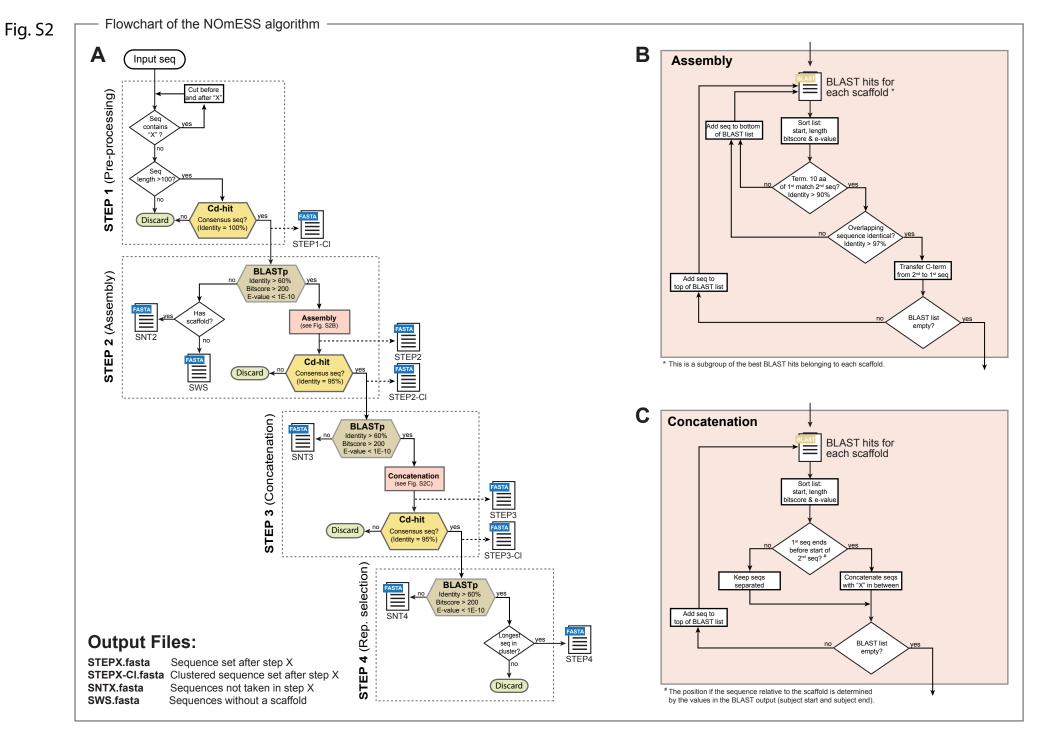


Fig. S2 Flowchart of the NOmESS algorithm. (A) Iterative BLAST searches and cd-hit clustering are used to align sequences to the scaffold, retrieve their relative position and find the representative of each sequence after each step. (B-C) Detailed view of the assembly and the concatenation module (step 2 and step 3 respectively). Abbreviations: seq: sequence, rep.: representative, Term.: terminal, aa: amino acid

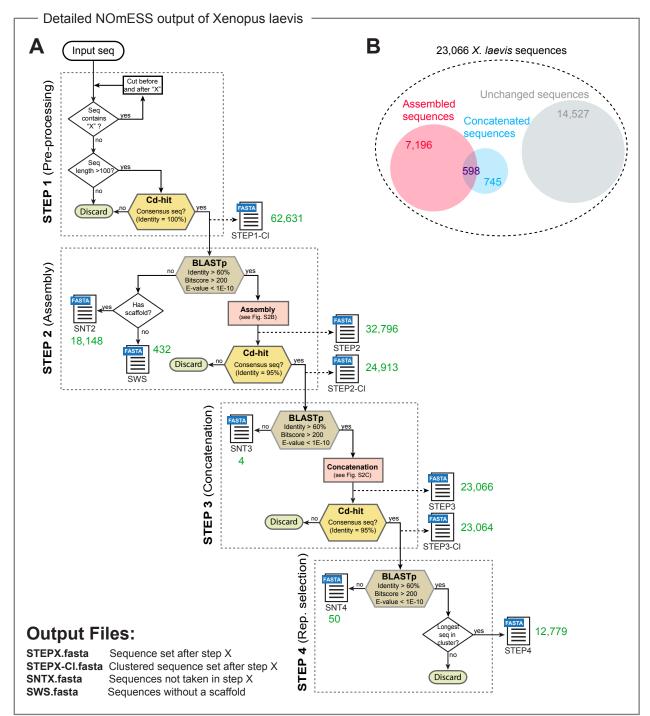


Fig. S3 NOmESS assembly of X. laevis sequences along a X. tropicalis scaffold. (A) Sequences retrieved from various repositories (e.g. TIGR gene indices, Xenbase, contigs from Gurdon, Unigene or XGI, see http://www.biochem.mpg.de/cox) were assembled using amino acid sequences from *X. tropicalis* as a scaffold. The Flowchart indicates the number of sequences generated during each step of the NOmESS procedure (see green numbers next to the output files). (B) Venn diagram showing the number of *X. laevis* sequences that were assembled and/or concatenated. Divergence of *X. laevis* and *X. tropicalis* has been estimated to have occurred about 63.7 million years ago (Evans et. al., 2007).

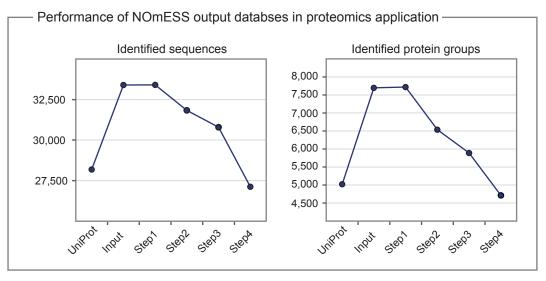


Fig. S4 Comparison of proteomic analyses of a X. laevis egg extracts using NOmESS or UniProt databases. A small mass spectrometry data set acquired from a fractionated egg extract (see Räschle, et al., 2015) was analysed with MaxQuant using the latest available UniProt database or various outputs of the NOmESS pipeline (see Fig. S3). The number of identified peptides (left panel) or "protein groups" (right panel) are plotted for each analysis.