Identification of Putative Neuropeptides that Alter the Behaviour of *Schistosoma mansoni* Cercariae

Conor E. Fogarty et al.

File S1. Comparative sequence analysis of all precursor proteins identified in this study.

Alignment of Cercariae neuropeptide

Method

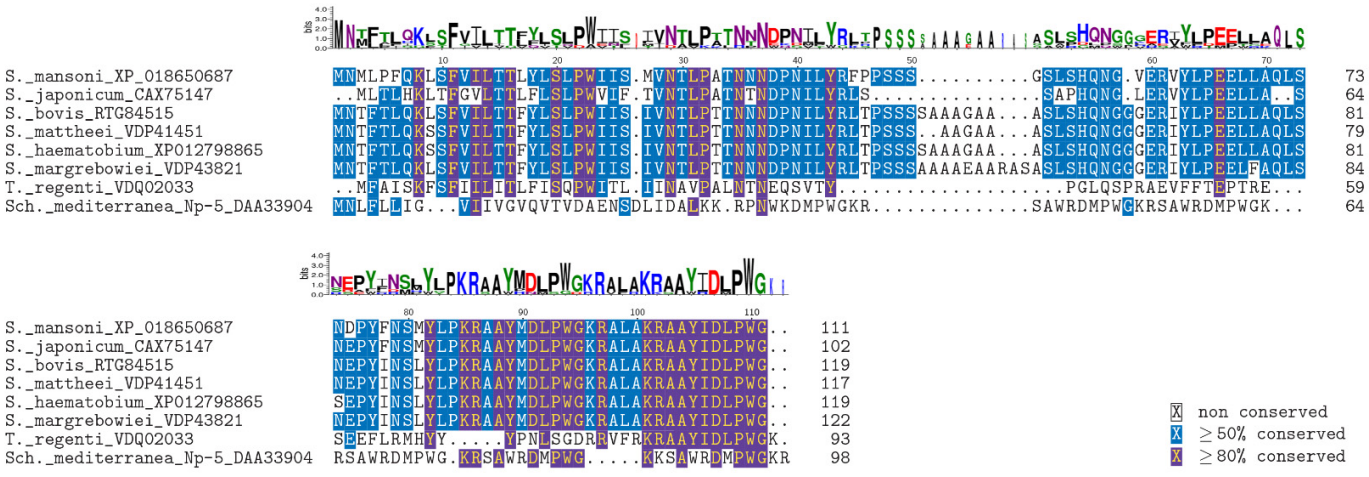
Annotation of putative *S. mansoni* neuropeptides was performed by BLASTp search against non-redundant protein database, NCBI (May, 21st 2020). Homologous proteins match with *S. mansoni* neuropeptides with *E*-value≤0.5 were retrieved from NCBI and used for multiple sequence alignment. Amino acid alignment was generated using MEGA X software (version 10.1.8) (Kumar, Stecher et al. 2018) with parameter set as follows: algorithm, ClustalW; gap opening penalty, 10; gap extension penalty, 0.2. Visualization of alignment was carried out on TeXworks software. Sequence logo was generated by using WebLogo application (Crooks et al., 2004).

Table 1. Species and species abbreviations used in the alignments.

Species	Species abbreviation
Clonorchis sinensis	*C. sinensis*
Dugesia japonica	*D. japonica*
Echinococcus granulosus	*E. granulosus*
Echinococcus multilocularis	*E. multilocularis*
Echinostoma caproni	*E. caproni*
Fasciola gigantica	*F. gigantica*
Fasciola hepatica	*F. hepatica*
Fasciolopsis buski	*F. buski*
Macrostomum lignano	*M. lignano*
Mesocestoides corti	*M. corti*
Opisthorchis felineus	*O. felineus*
Opisthorchis viverrini	*O. viverrini*
Paragonimus westermani	*P. westermani*
Schistosoma bovis	*S. bovis*
Schistosoma curassoni	*S. curassoni*
Schistosoma haematobium	*S. haematobium*
Schistosoma japonicum	*S. japonicum*
Schistosoma mansoni	*S. mansoni*
Schistosoma margrebowiei	*S. margrebowiei*
Schistosoma mattheei	*S. mattheei*
Schmidtea mediterranea	*Sch. mediterranea*
Trichobilharzia regenti	*T. regenti*

Npp-1

Npp-5



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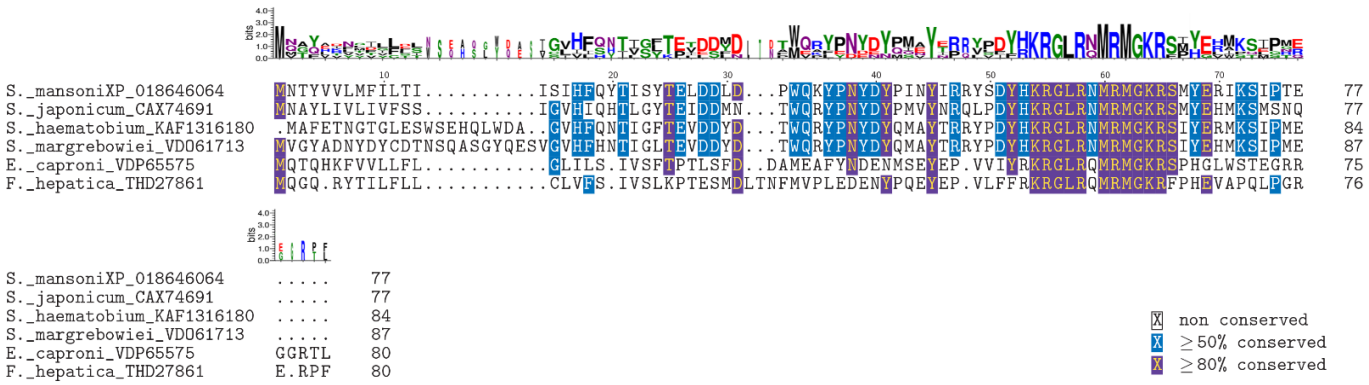

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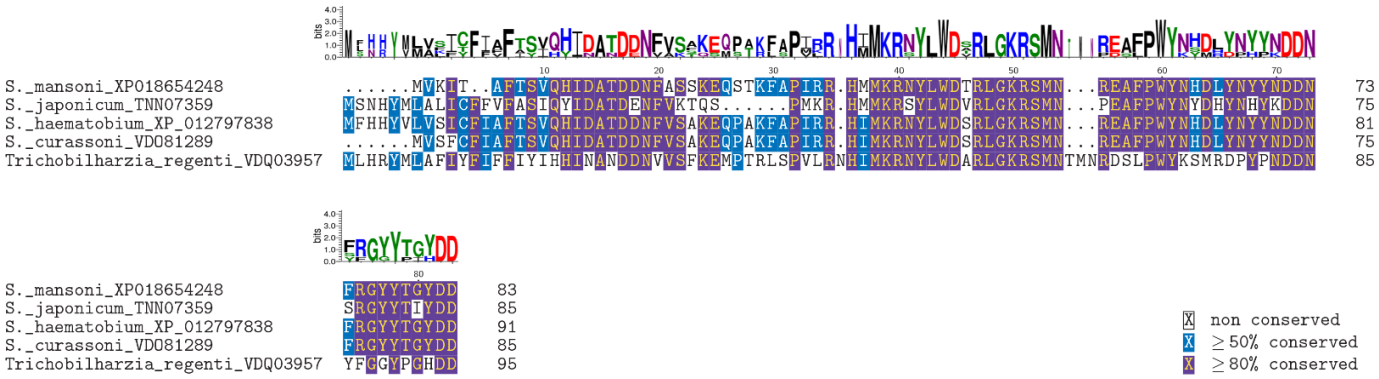
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S._haematobium_XP_012797838 MFHHYVLVSICFIAFTSVQHIDATDDNFVSAKEQPAKFAPIRR.HIMKRNYLWDSRLGKRSMN...REAFPWYNHDLYNYYNDDN 81
S._curassoni_VDO81289 ......MVSFCFIAFTSVQHIDATDDNFVSAKEQPAKFAPIRR.HIMKRNYLWDSRLGKRSMN...REAFPWYNHDLYNYYNDDN 75
Trichobilharzia_regenti_VDQ03957 MLHRYMLAFIYFIFFIYIHHINANDDNVVSFKEMPTRLSPVLRNHIMKRNYLWDARLGKRSMNTMNRDSLPWYKSMRDPYPNDDN 85
FRGYYTGYDD
S._mansoni_XP018654248 FRGYYTGYDD 83
S._japonicum_TNN07359 SRGYYTIYDD 85
S._haematobium_XP_012797838 FRGYYTGYDD 91
S._curassoni_VDO81289 FRGYYTGYDD 85
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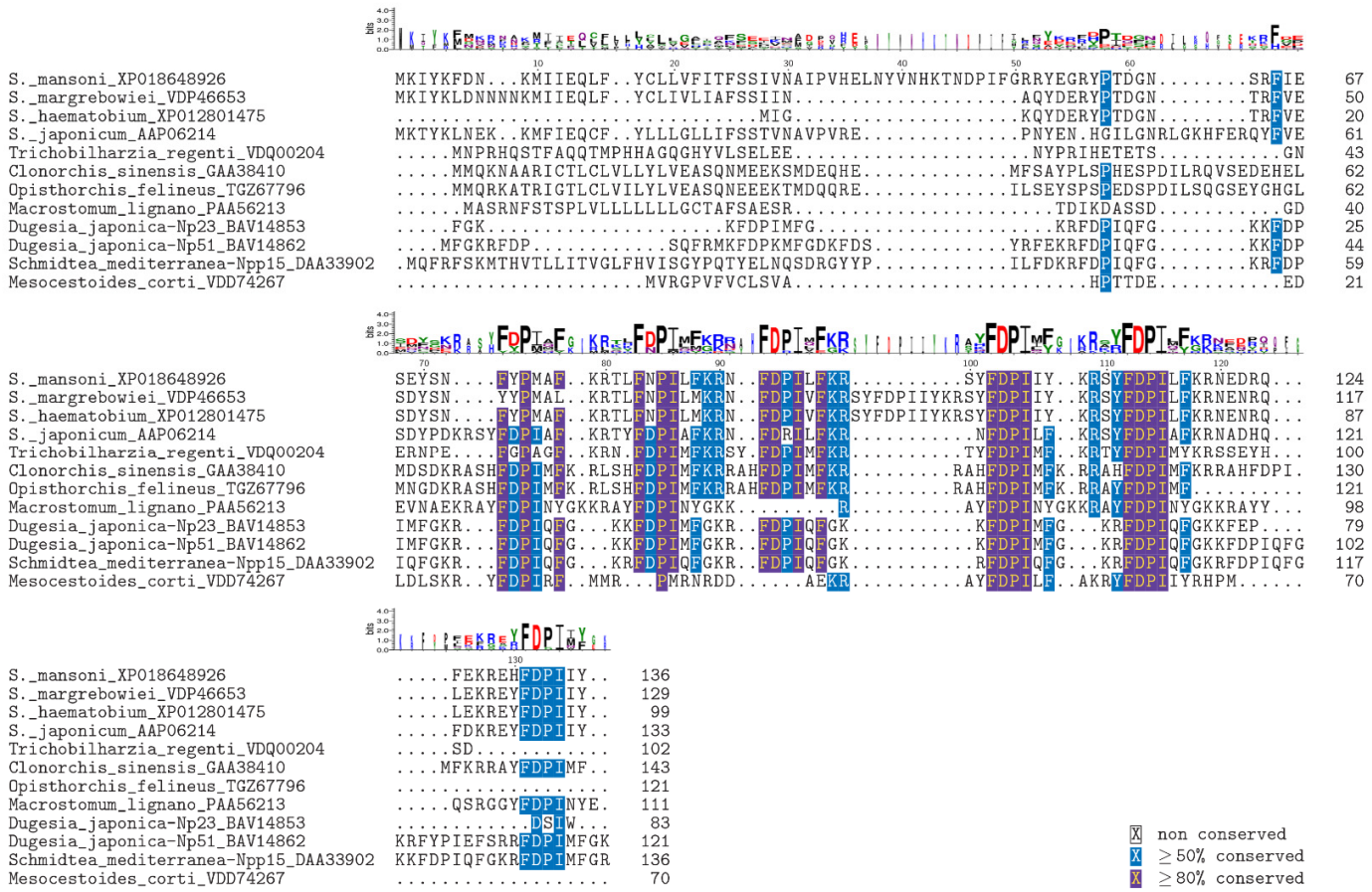
≥50% conserved
≥80% conserved

Npp-26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S._haematobium_XP012801475 .....MIG.....KQYDERYFTDGN........TRFVE 20
S._japonicum_AAP06214 MKTYKLNEK..KMFIEQCF..YLLLGLLIFSSTVNAVPVRE.....PNYEN.HGILGNRLGKHFERQYFVE 61
Trichobilharzia_regenti_VDQ00204 .....MNPRHQSTFAQQTMPHHAGQGHYVLSELEE.....NYPRIHETETS.....GN 43
Clonorchis_sinensis_GAA38410 .....MMQKNAARICTLCLVLLYLVEASQNMEEKSMDEQHE.....MFSAYPLSFHESPDILRQVSEDEHEL 62
Opisthorchis_felineus_TGZ67796 .....MMQRKATRIGTLCLVILYLVEASQNEEEKTMDQQRE.....ILSEYSPSFEDSPDILSQGSEYGHGL 62
Macrostomum_lignano_PAA56213 ......MASRNFSTSPLVLLLLLLGCTAFSAESR.....TDIKDASSD.....GD 40
Dugesia_japonica-Np23_BAV14853 .....FGK.....KFDPIMFG.....KRFDFIQFG.....KKFDP 25
Dugesia_japonica-Np51_BAV14862 ....MFGKRFDP.....SQFRMKFDPKMFGDKFDS.....YRFEKRFDFIQFG.....KKFDP 44
Schmidtea_mediterranea-Npp15_DAA33902 .MQFRFSKMTHVTLLITVGLFHVISGYPQTYELNQSDRGYYP.....ILFDKRFDFIQFG.....KRFDP 59
Mesocestoides_corti_VDD74267 .....MVRGPVFVCLSVA.....HFTTDE.....ED 21
S._mansoni_XP018648926 SEYSN....FYPMAF..KRTLFNPILFKFN..FDPILFKR.....SYFDPIIY..KFSYFDPILFKRNEDRQ... 124
S._margrebowiei_VDP46653 SDYSN....YYPMAL..KRTLFNPILMKRN..FDPIVFKRSYFDPIIYKRSYFDPIIY..KRSYFDPILFKRNENRQ... 117
S._haematobium_XP012801475 SDYSN....FYPMAF..KRTLFNPILMKRN..FDPIVFKRSYFDPIIYKRSYFDPIIY..KRSYFDPILFKRNENRQ... 87
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Trichobilharzia_regenti_VDQ00204 ERNPE....FGFAGF..KRN.FDPIMFKRSY.FDPIMFKR.....TYFDPIMF..KRTYFDPIMYKRSSEYH... 100
Clonorchis_sinensis_GAA38410 MDSDKRASHFDPIMFK.RLSHFDPIMFKRRAHFDPIMFKR.....RAHFDPIMFK.RRAHFDPIMFKRRAHFDPI. 130
Opisthorchis_felineus_TGZ67796 MNGDKRASHFDPIMFK.RLSHFDPIMFKRRAHFDPIMFKR.....RAHFDPIMFK.RRAYFDPIMF..... 121
Macrostomum_lignano_PAA56213 EVNAEKRAYFDPINYGKKRAYFDPINYGKK.....R.....AYFDPINYGKKRAYFDPINYGKKRAYY... 98
Dugesia_japonica-Np23_BAV14853 IMFGKR...FDPIQFG...KKFDPIMFGKR..FDPIQFGK.....KFDPIMFG...KRFDPIQFGKKFEP.... 79
Dugesia_japonica-Np51_BAV14862 IMFGKR...FDPIQFG...KKFDPIMFGKR..FDPIQFGK.....KFDPIMFG...KRFDPIQFGKKFDPIQFG 102
Schmidtea_mediterranea-Npp15_DAA33902 IQFGKR...FDPIQFG...KRFDPIQFGKR..FDPIQFGK.....RFDPIQFG...KRFDPIQFGKRFDPIQFG 117
Mesocestoides_corti_VDD74267 LDLSKR..YFDPIRF..MMR...PMRNRDD.....AEKR.....AYFDPILF..AKRYFDPIIYRHPM..... 70
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S._margrebowiei_VDP46653 .....LEKREYFDPIIY.. 129
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Clonorchis_sinensis_GAA38410 ....MFKRRAYFDPIMF.. 143
Opisthorchis_felineus_TGZ67796 121
Macrostomum_lignano_PAA56213 .....QSRGGYFDPINYE. 111
Dugesia_japonica-Np23_BAV14853 .....PSIW... 83
Dugesia_japonica-Np51_BAV14862 KRFYPIEFSRRFDPIMFGK 121
Schmidtea_mediterranea-Npp15_DAA33902 KKFDPIQFGKRFDPIMFGR 136
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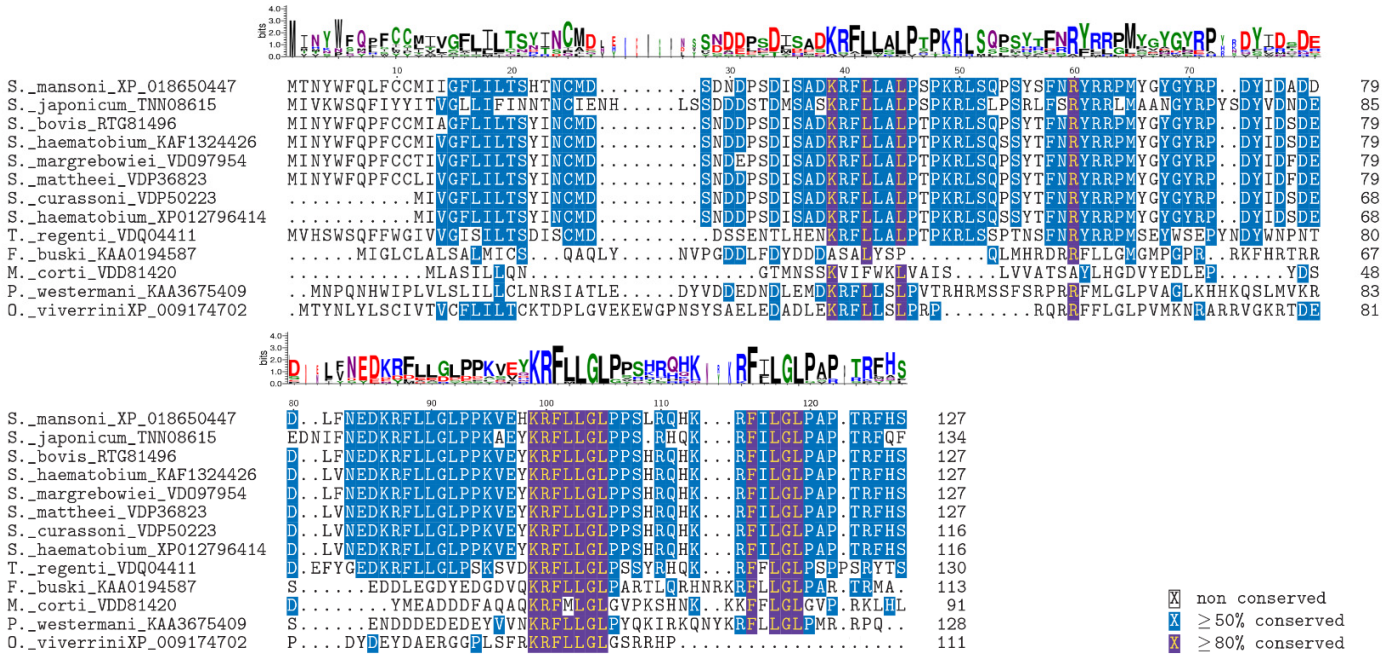
non conserved
≥50% conserved
≥80% conserved

Npp-30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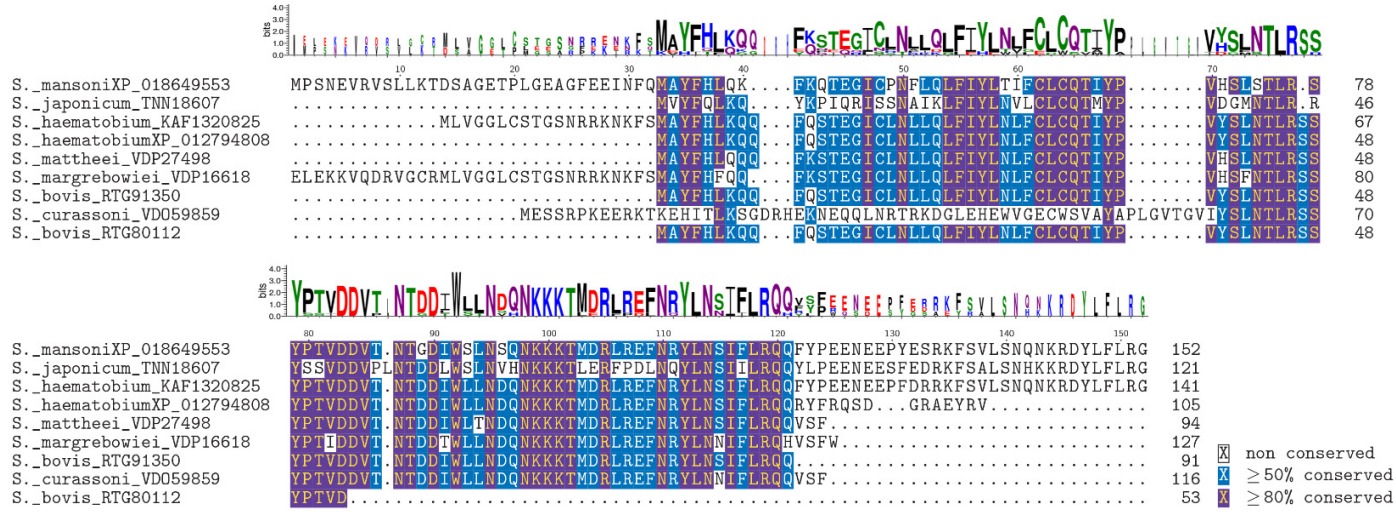
X non conserved
X ≥50% conserved
X ≥80% conserved

Npp-31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S._margrebowiei_VDP16618
S._bovis_RTG91350
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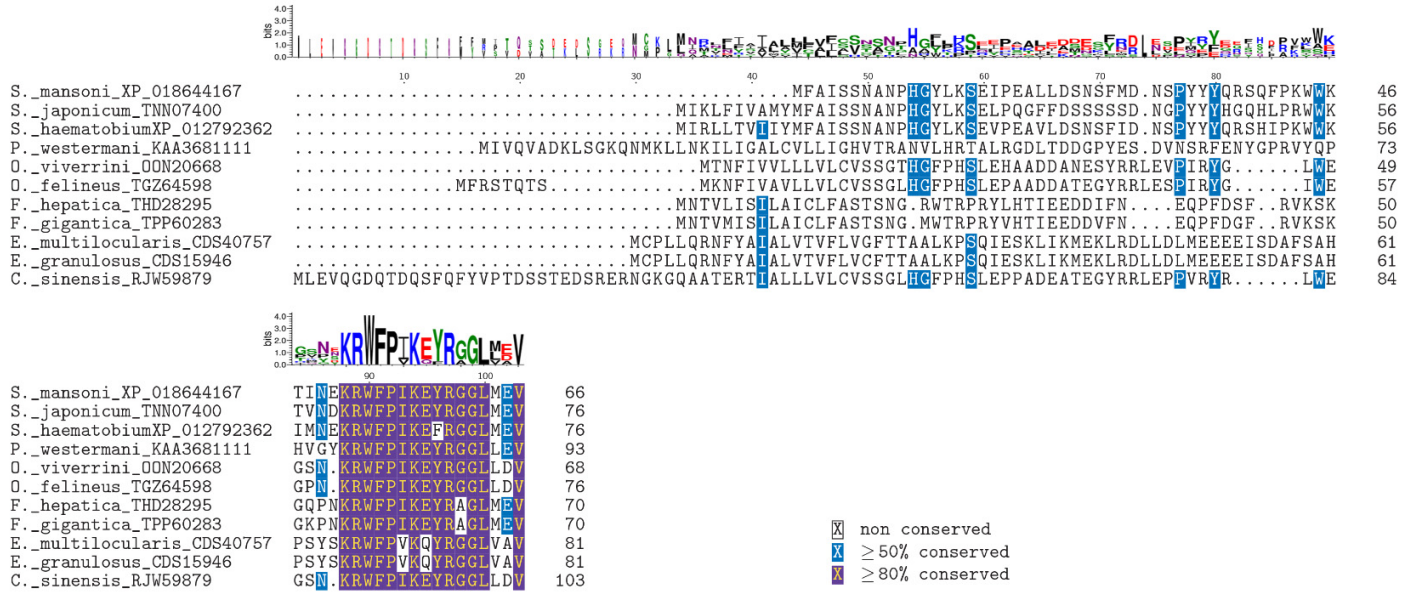
X non conserved
X ≥50% conserved
X ≥80% conserved

Npp-32



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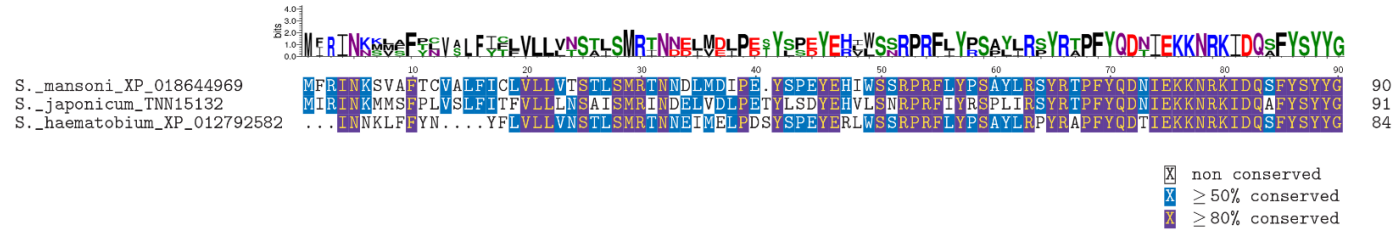

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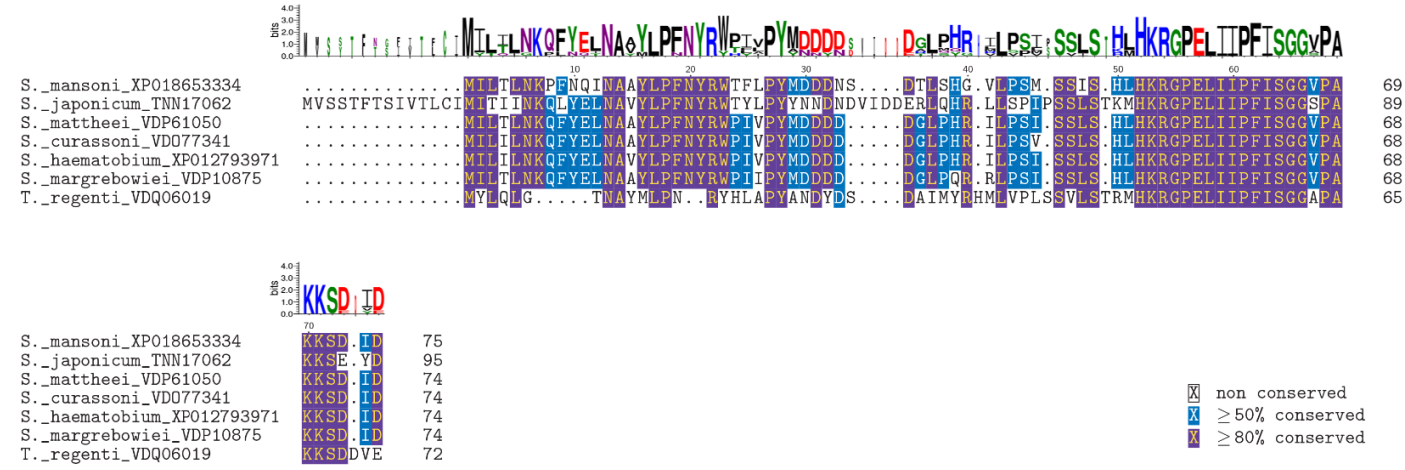
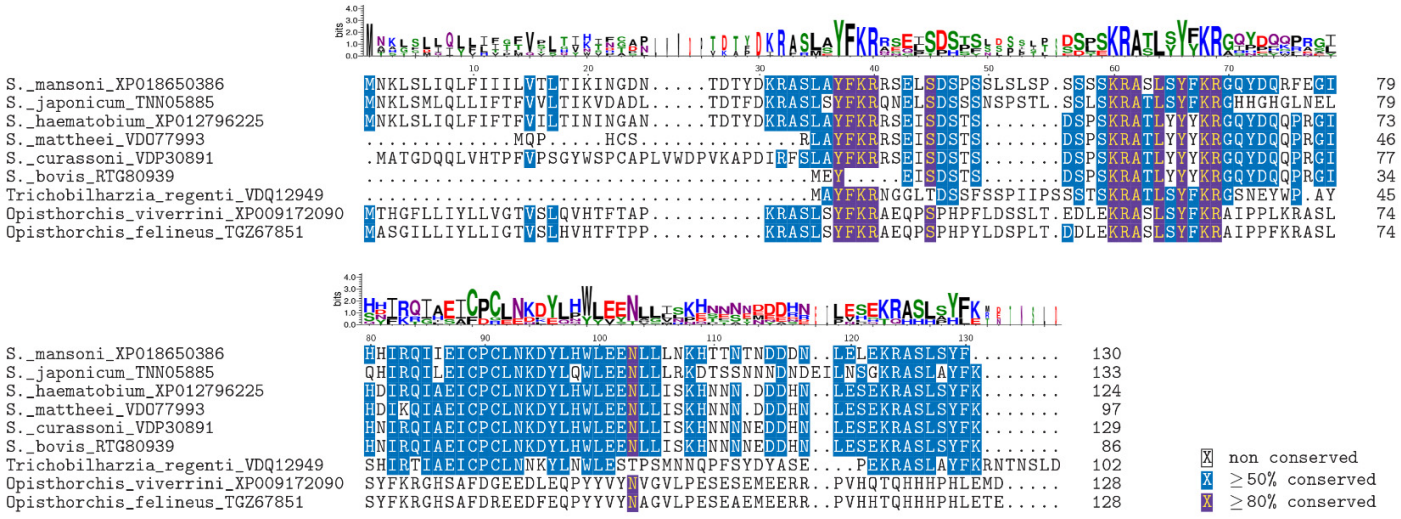


Npp-35

Npp-36



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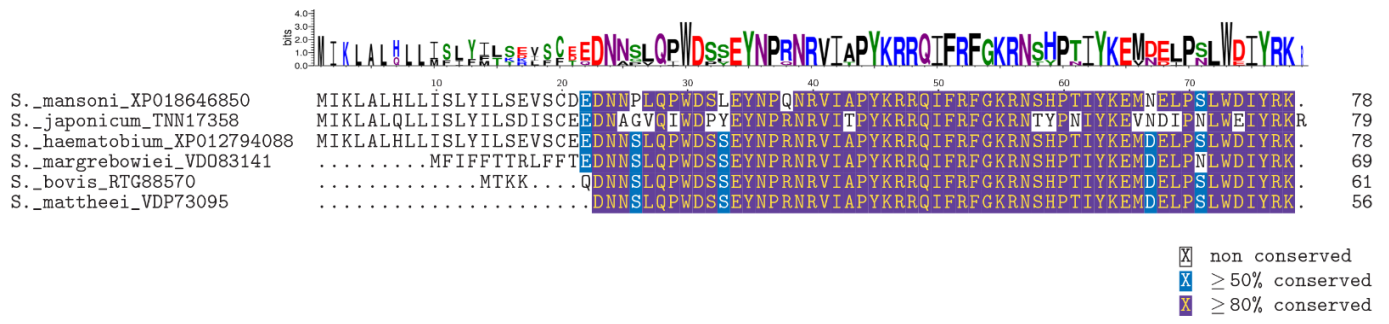
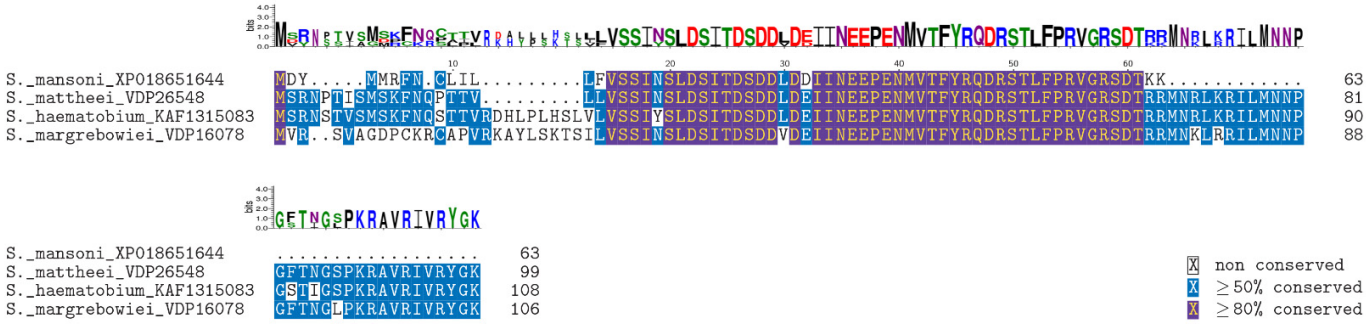


Npp-38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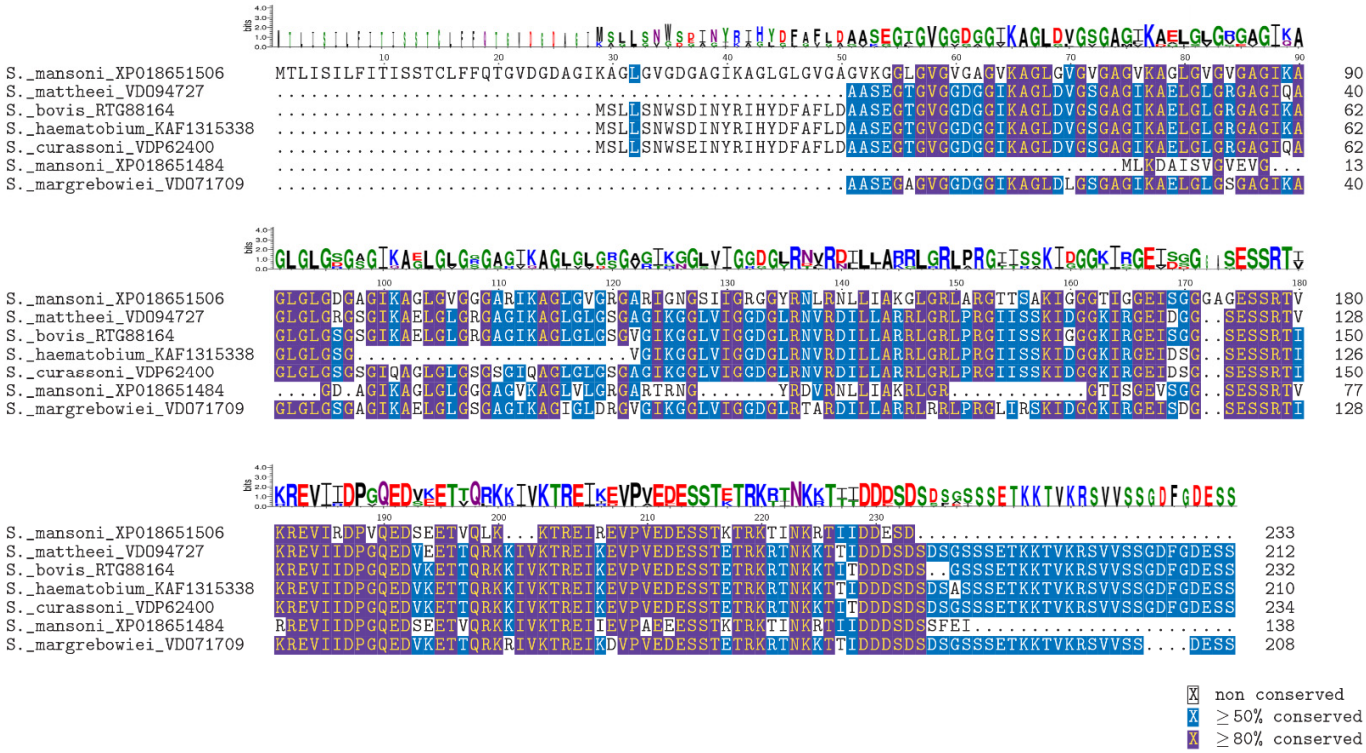
non conserved
≥50% conserved
≥80% conserved

Npp-39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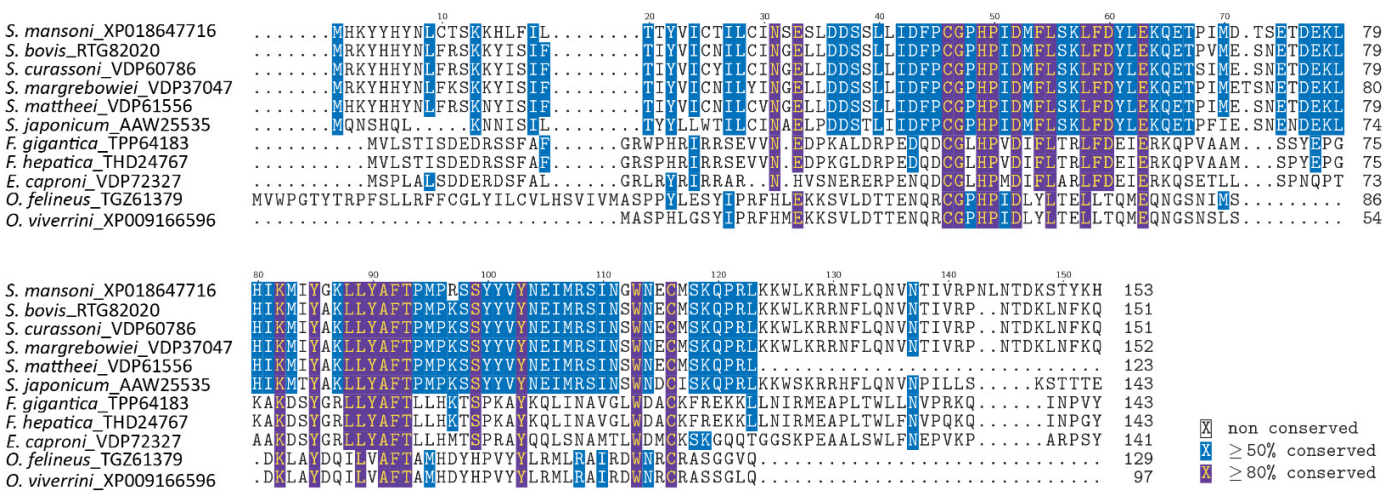
non conserved
≥50% conserved
≥80% conserved

Npp-40



References:

Kumar, S., et al. (2018). "MEGA X: Molecular Evolutionary Genetics Analysis across Computing Platforms." Mol Biol Evol **35**(6): 1547-1549.

The Molecular Evolutionary Genetics Analysis (Mega) software implements many analytical methods and tools for phylogenomics and phylomedicine. Here, we report a transformation of Mega to enable cross-platform use on Microsoft Windows and Linux operating systems. Mega X does not require virtualization or emulation software and provides a uniform user experience across platforms. Mega X has additionally been upgraded to use multiple computing cores for many molecular evolutionary analyses. Mega X is available in two interfaces (graphical and command line) and can be downloaded from www.megasoftware.net free of charge.

Crooks GE, Hon G, Chandonia JM, Brenner SE WebLogo: A sequence logo generator, Genome Research, 14:1188-1190, (2004)