**Riding the Wave of Innovation: Immunoinformatics in Fish Disease Control**

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**Supplemental file**

**Table 1:** A summary of tools useful in immunoinformatics vaccine design for fish diseases.

|  |  |  |  |
| --- | --- | --- | --- |
| **Application** | **Method** | **Tools/ server** | **URL** |
| Epitope Prediction | B-cell prediction | ABCpred | https://webs.iiitd.edu.in/raghava/abcpred/ |
| IEDB B-cell epitope tools | http://tools.iedb.org/bcell/ |
| SVMTriP | http://sysbio.unl.edu/SVMTriP/index.php |
| BCPred | http://ailab-projects1.ist.psu.edu:8080/bcpred/predict.html |
| LBtope | http://crdd.osdd.net/raghava/lbtope/ |
| BepiPred 2.0 | https://services.healthtech.dtu.dk/service.php?BepiPred-2.0 |
| DiscoTope-2.0 | https://services.healthtech.dtu.dk/service.php?DiscoTope-2.0 |
| BEpro | http://pepito.proteomics.ics.uci.edu/ |
| ElliPro | http://tools.iedb.org/ellipro/ |
| EPCES | http://sysbio.unl.edu/EPCES/ |
| EPSVR | http://sysbio.unl.edu/EPSVR/ |
| EPMeta | http://sysbio.unl.edu/EPMeta/ |
| Epitopia | http://epitopia.tau.ac.il/ |
| SEPPA | http://www.badd-cao.net/seppa3/index.html |
| T-cell prediction | IEDB database | http://tools.immuneepitope.org/mhcii/ |
| RANKPEP server | http://imed.med.ucm.es/Tools/rankpep.HTML |
| ProPred | http://crdd.osdd.net/raghava/propred/ |
| NetMHCIIpan- 4.0 | https://services.healthtech.dtu.dk/service.php?NetMHCIIpan-4.0 |
| NetMHCIIpan- 3.2 | https://services.healthtech.dtu.dk/service.php?NetMHCIIpan-3.2 |
| NetCTL-1.2 | https://services.healthtech.dtu.dk/service.php?NetCTL-1.2 |
| ProPred1 | http://crdd.osdd.net/raghava/propred1/ |
| NetMHCpan-4.1 | https://services.healthtech.dtu.dk/service.php?NetMHCpan-4.1 |
| MHCpred 2.0 | http://www.ddg-pharmfac.net/mhcpred/MHCPred/ |
| EpiJen | http://www.ddg-pharmfac.net/epijen/EpiJen/EpiJen.htm |
| CTLPred | http://crdd.osdd.net/raghava/ctlpred/index.html |
| Expitope | http://webclu.bio.wzw.tum.de/expitope/ |
| Construction of multi-epitope vaccine | Adjuvant selection | Vaxjo | http://www.violinet.org/vaxjo/ |
| VaccineDA | https://webs.iiitd.edu.in/raghava/vaccineda/ |
| imRNA | https://webs.iiitd.edu.in/raghava/imrna/ |
| VaxinPAD | https://webs.iiitd.edu.in/raghava/vaxinpad/ |
| Linker selection | Linker DB | https://www.ibi.vu.nl/programs/linkerdbwww/ |
| Structural modeling | EasyModeller 4.0 | https://sites.google.com/site/bioinformatikz/homology-modelling/homology-modelling?authuser=0 |
| SWISS-MODEL | https://swissmodel.expasy.org/ |
| Phyre2 | http://www.sbg.bio.ic.ac.uk/~phyre2/ |
| I-TASSER | https://zhanggroup.org/I-TASSER/ |
| RaptorX | http://raptorx.uchicago.edu/ |
| ROBETTA, | http://robetta.bakerlab.org/ |
| Structure validation | PROCHECK | https://www.ebi.ac.uk/thornton-srv/software/PROCHECK/ |
| Verify3D | https://saves.mbi.ucla.edu |
| ERRAT | https://saves.mbi.ucla.edu |
| Prediction of vaccine antigenicity, allergenicity and toxicity | Antigenicity | VaxiJen 2.0 | http://www.ddg-pharmfac.net/vaxijen/VaxiJen/VaxiJen.html |
| ANTIGENpro | http://scratch.proteomics.ics.uci.edu/ |
| Allergenicity | AllerTOP v 2.0 | http://www.ddg-pharmfac.net/AllerTOP/ |
| AlgPred | https://webs.iiitd.edu.in/raghava/algpred/submission.html |
| AllerCatPro | https://allercatpro.bii.a-star.edu.sg/ |
| Toxicity | ToxinPred | http://crdd.osdd.net/raghava/toxinpred/ |
| T3DB | http://www.t3db.ca/biodb/search/target\_bonds/sequence |
| Physicochemical properties | Protparam | https://web.expasy.org/protparam/ |
| Molecular interaction of immunogenic vaccine | Molecular docking | Autodock Vina | https://vina.scripps.edu/ |
|  Autodock 4 | https://autodock.scripps.edu/ |
| ZDOCK | https://zdock.umassmed.edu/ |
| Glide | https://www.schrodinger.com/products/glide |
| GOLD | https://www.ccdc.cam.ac.uk/solutions/csd-discovery/components/gold/ |
| RosettaDock | https://rosie.graylab.jhu.edu/ |
| ClusPro | https://cluspro.org/login.php |
| HADDOCK | https://wenmr.science.uu.nl/haddock2.4/ |
| EpiDOCK | http://www.ddg-pharmfac.net/epidock/EpiDockPage.html |
| Molecular dynamics simulation | GROMACS | https://www.gromacs.org/ |
| CHARMM | https://www.charmm.org/charmm/ |
| AMBER | http://ambermd.org/ |
| NAMD | https://www.ks.uiuc.edu/Research/namd/ |