# Exploring *Leishmania* secretory proteins to design B and T cell multi-epitope subunit vaccine using immunoinformatics approach

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**Supplementary table 1:** Predicted CTL epitopes for *Leishmania donovani* secretory proteins

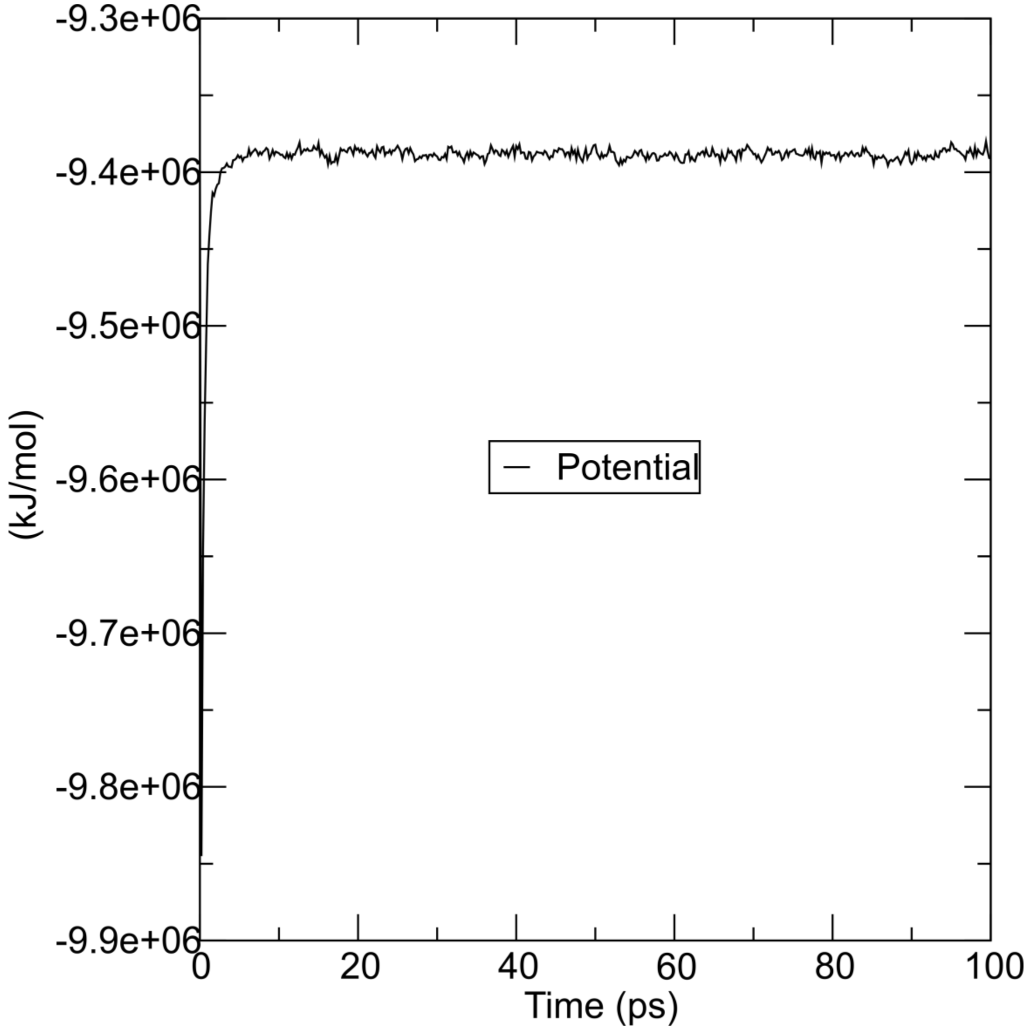
| **S. No.** | **Sequence id** | **Epitopes** | **Score** |
|---|---|---|---|
| **1** | **LdBPK_190160** | TTGIARGAY | 2.1103 |
| | | SSEVPTGSY | 2.8708 |
| | | ASEDDIAAY | 2.7231 |
| | | LSTDDGATY | 2.0833 |
| | | STCTMDAAY | 2.9323 |
| | | QLTLSSLFY | 2.1468 |
| | | **LSSLFYLPY** | **3.3553** |
| | | **NSSTDLLDY** | **3.0863** |
| | | LLDYKAAQY | 2.5937 |
| | | GSAGKSFNY | 2.0306 |
| **2** | **LdBPK_211410** | CTHASMALV | 0.7588 |
| | | **YTEAQQLHT** | **1.4547** |
| | | ATNWAQLAV | 0.9146 |
| | | **WMDLHSNRL** | **1.0307** |
| | | MTFLNTLLL | 0.9509 |
| | | TVDEAVMSV | 0.829 |
| | | AVDGSDATF | 0.8317 |
| **3** | **LdBPK_310120** | SAHVGSSVY | 1.0079 |
| | | FMHPRMKTY | 1.239 |
| | | **QVDWLVALY** | **3.1899** |
| | | GQDGKVQGY | 1.0879 |
| | | AAAVKSVEY | 1.442 |
| | | DTEGKVRCY | 1.7273 |
| | | LLNLNGMLY | 2.1102 |
| | | VTTIKGGVY | 2.4195 |
| | | YVFQTSTPY | 1.2417 |
| | | TVGTRIRLY | 1.0238 |
| | | **FTDSISLSF** | **3.2792** |
| | | IIEPEAVQY | 1.3645 |
| **4** | **LdBPK_220130** | PAEDSNAIY | 1.8882 |
| | | **KSETVSIQY** | **3.0954** |
| | | DSATNQTYF | 1.0139 |
| | | GSTGYDPAY | 1.2708 |
| | | YINADHQRY | 1.736 |
| **5** | **LdBPK_310860** | SLQYANVTY | 1.4446 |
| | | **SADFQHVPY** | **2.478** |
| | | KVDMRDHFF | 1.0015 |
| | | GAAGDAMLY | 1.5074 |
| | | QTDARRSLQ | 0.9877 |

**Supplementary table 2:** Predicted HTL epitopes for *Leishmania donovani* secretory proteins

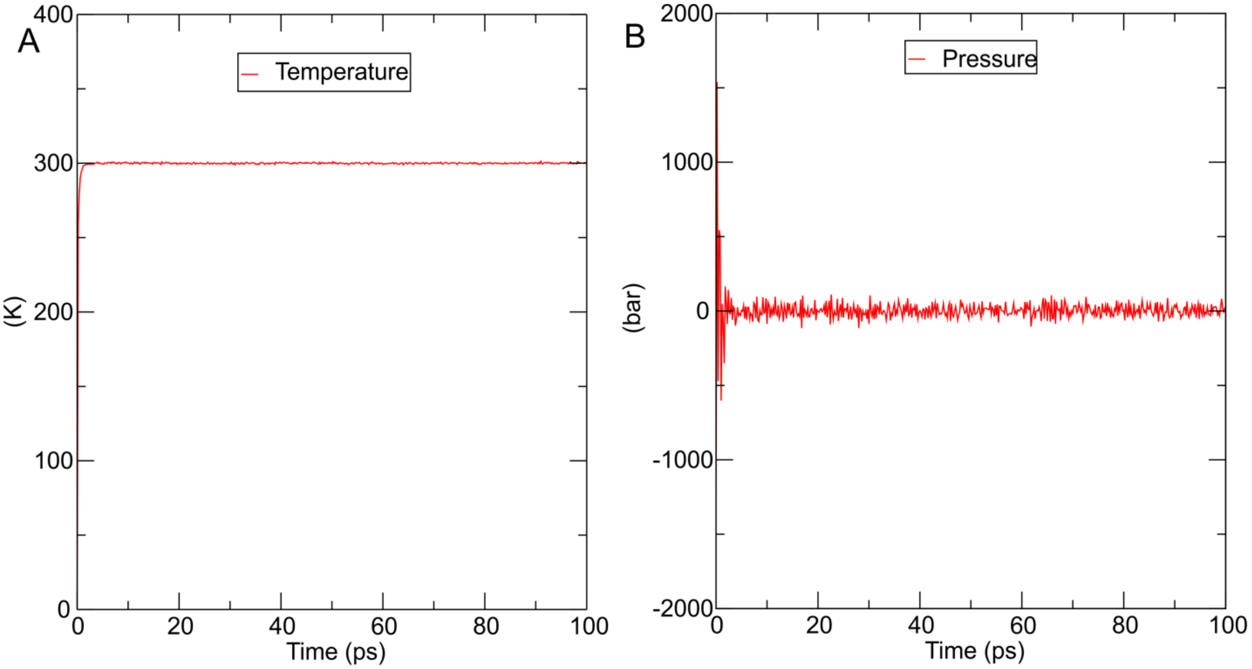
| S. No. | Accession no. | Alleles | Start | End | Sequence | Percentile |
|---|---|---|---|---|---|---|
| **1** | **LdBPK_190160** | H2-IAd | 235 | 249 | VESMQALQAASIVIA | 0.03 |
| | | H2-IAb | 221 | 235 | FTSNVVYLPATATLV | 0.2 |
| | | H2-IEd | 761 | 775 | QVDLASYVRGRRKWM | 4.96 |
| **2** | **LdBPK_211410** | H2-IAd | 1 | 15 | MCTHASMALVAAVAL | 0.03 |
| | | H2-IAb | 451 | 465 | ATFSSWDASASSASN | 1.04 |
| | | H2-IEd | 127 | 141 | LPASWGLLRNLRKVR | 17.41 |
| **3** | **LdBPK_310120** | H2-IAd | 743 | 757 | FNMHFMAAIKYTLIV | 0.54 |
| | | H2-IAb | 398 | 412 | TNAAYALSTPLVINA | 0.48 |
| | | H2-IEd | 691 | 705 | VGTRIRLYRERFHKP | 9.64 |
| **4** | **LdBPK_220130** | H2-IAd | 210 | 224 | LGVVKMIKAMKHSKG | 0.55 |
| | | H2-IAb | 72 | 86 | FPSFHAGSKANVVIA | 3.85 |
| | | H2-IEd | 260 | 274 | EVLHKKLSTSRSRRA | 17.71 |
| **5** | **LdBPK_310860** | H2-IAd | 173 | 187 | VALLAAVDVQAHVNR | 0.19 |
| | | H2-IAb | 247 | 261 | HVPYEVYCAAAAGTN | 1.8 |
| | | H2-IEd | 135 | 149 | FQRSYLAVRRTVRAA | 12.78 |

**Supplementary table 3:** Predicted B cell epitopes for the final vaccine construct protein proteins

| S. No. | Position | Epitope | Score |
|---|---|---|---|
| 1 | 317 | SSWDASASSASNGPGPGLPA | 1 |
| 2 | 500 | YCAAAAGTNGPGPGFQRSYL | 1 |
| 3 | 386 | INAGPGPGVGTRIRLYRERF | 1 |
| 4 | 421 | KAMKHSKGGPGPGFPSFHAG | 1 |
| 5 | 456 | LHKKLSTSRSRRAGPGPGVA | 1 |
| 6 | 219 | YSADFQHVPYGPGPGVESMQ | 1 |
| 7 | 479 | AVDVQAHVNRGPGPGHVPYE | 1 |
| 8 | 262 | PATATLVGPGPGQVDLASYV | 1 |
| 9 | 241 | QAASIVIAGPGPGFTSNVVY | 1 |
| 10 | 360 | AAIKYTLIVGPGPGTNAAYA | 1 |
| 11 | 43 | AAAGAAPAGAAVEAAEEQSE | 0.999 |
| 12 | 339 | GLLRNLRKVRGPGPGFNMHF | 0.999 |
| 13 | 283 | GRRKWMGPGPGMCTHASMAL | 0.998 |



Supplementary figure1: Potential energy of protein ligand (TLR-4 vaccine) complex as a function of energy minimization step during molecular dynamics simulation.



**Supplementary figure 2: Molecular dynamics simulation study of protein ligand (TLR-4 vaccine) complex** (A) Temperature progression curve indicating that temperature of the system reaches a up to 300K and remains stable for rest of the equilibration period (100 ps) (B) Pressure progression curve indicating pressure fluctuation up to 1bar.