

Index

A

- Adaptable lymphocyte hypothesis, 104–106
Adjuvants
and immunomodulators, computational
vaccinology
Alum, 13
G-protein couple receptors (GPCRs), 13
pharmacophore, 14
T cells (Tregs), 14
vaccination enhancement, 13
innate immunity, 139–140
Allele Query Tool, 22, 23
Allele search tools
Allele Query Tool, 37–38
flat file format, 38
Sequence Retrieval System (SRS) tool,
38–39
AntiBP server, antibacterial peptides, 73–75
AntigenDB database, 9
Antigen-presenting cells (APCs), 146
Artificial immune systems (AIS), tunable
detectors
degeneration framework
algorithm framework, 118–119
patterns of response, 118
population pattern algorithm, parameter
settings, 119–120
degeneration instantiation
algorithm, settings and response shape,
121–123
application and data, 121
k-nearest neighbour, 123–125
pattern classification algorithm
PoRTuDe, 124–126
population patterns
algorithm, 114
antigens stimulation, 115
 α parameter effects, 117
proliferation threshold effects, 116

- tunable activation threshold (TAT)
adaptable lymphocyte hypothesis,
104–106
behaviours, 106–107
dynamics, 105, 106

Artificial neural networks, 7

B

- Basic Formal Ontology (BFO), 51–52
Bayesian multilevel analysis (BMLA),
158, 170–171
Bioinformatic platform
asthma, 172–175, 183
Bayesian data analysis, 179
Bayesian multilevel data analysis,
170–171
network primer, 168
network properties, 169
primer, 166–168
domain exploration, 161–162
genetic association studies (GAS), 157
knowledge and data fusion
Bayesian logic module, 182
factual sources, 179
hybrid knowledge base, 180–181
Markov-Blanket Membership (MBM)
probability, 172, 176–178
Markov Blanket Sets (MBS), 172, 176
multifactorial diseases
candidate gene studies, 159
database of genotypes and phenotypes
(dbGaP), 161
genome wide association studies
(GWAS), 159–160
SNP association studies, DSS
GAS design, 171
issues, 165–166
methods, 163–165

- Bioinformatic platform (*cont.*)
 relevance of, 173–175
 selection process, 163, 165
 standard statistical methods, 172, 176
- Bioinformatics, databases, xiii
- Biological systems, immunology, xii
- Boolean models, xiii
- C**
- Calnexin, 145
- Candidate gene association studies, 159
- Cellular adaptive immunology
 CD1 presentation, 148–149
 major histocompatibility complex (MHC) molecule
 class II MHC expression, 146–148
 class I MHC molecules, 142–146
- ClinMalDB-US database, 8
- Common gateway interface (CGI), 36
- Computational vaccinology
 adjuvants and immunomodulators
 discovery
 Alum, 13
 G-protein couple receptors (GPCRs), 13
 pharmacophore, 14
 T cells (Tregs), 14
 vaccination enhancement, 13
 ageing, 15
 Alzheimer’s disease, 16
 black death, 15
 disease pattern, 16
 epitope prediction
 B cells, 6–8
 T cells, 4–5
 infectious disease, 2, 15
 life-style vaccines, 3
 mortality rate, 1, 2
 Parkinson’s disease, 16
 reverse vaccinology
 NERVE program, 10–11
 open reading frames (ORFs), 10
 subunit vaccines, 10
 surface proteins, 11
 subcellular location prediction, 9–10
 success features, 3
 vaccines delivery, vectors
 CpG optimisation, 13
 DyNAVac, optimisation, 12
 plasmids, DNA vaccine, 12
 virulence factors (VF), identification, 8–9
- Conserved epitopes
 conserved fragments
 HIV-1 gp41, 99
- HIV-1 gp120 and solvent accessibility, 100
 RANKPEP T cell epitope predictions, 98
- materials and methods
 multiple protein-sequence alignments (MSAs), 96
 protein variability server (PVS), 96–97
 vaccine development, 95
 variability-masked sequence, 98, 99
- Copy number variations (CNVs), 157, 161, 166
- Cytokines
 CTKPred, 72–73
 CytoPred, 73
- D**
- Data analysis, Bayesian immunogenomics
 Bayesian methods, 172
 MBM posteriors, 177
 multilevel data analysis, 170–171
 network primer, 168
 network properties, 169
 primer, 166–168
 standard statistical methods, 172
- Database of genotypes and phenotypes (dbGaP), 161
- Decision support system (DSS), SNP design, 162–166
- Dendritic cells (DCs), 147
- Discotope, 7
- Distributed annotation system (DAS), HLA I.
See also TEPIDAS
 architecture, 58–59
 protocol, 58
 registry, 59
- Dizygotic (DZ) twins, 129
- DyNAVac, vaccine optimisation, 12
- E**
- Elusive molecular self, defining, 153–154
- cellular adaptive immunity
 autophagic pathways, 147–148
 CD1 presentation, 148–149
 cell-surface antigen presentation, 142
 class II MHC expression, 146–148
 class I MHC molecules, 142–146
 cross presentation, 147
 dendritic cells (DCs), 147
 glycosylation, 141–142
 immunology dogma, 145
 intracellular peptide fragments, 142
 invariant chain (Ii), 146
 peptidases, 145–146

- proteasome, 144
ubiquitin, 144
- conjoined/Siamese twins, 130
dizygotic (DZ) twins, 129
epitope-paratope network, 133
human symbiosis
host-microbe interactions, 152
microbiome, 151, 152
tolerance, 151
- humoral adaptive immunity
B cell epitopes, 149, 150
sliding-window method, 150
- innate immunity
adjuvants, 139–140
drug-like adjuvants, 140
NOD-like receptors (NLRs), 139
PAMP and PRRs, 138–140
- monozygotic twins, 129–130
network theory, 133
non-self, 131–133
- Polly Matzinger's danger model, 131
- reductionist approaches
autoimmunity, 137
epigenetic inheritance, 135–136
epigenetics, 135
human genomes, 134
post-translational modifications, 136–137
ubiquitination, 136
- self-positive model, 132
- Epitope prediction
B cells
artificial neural networks, 7
complementary determining (CDR)
loops, 6
continuous and discontinuous epitopes, 5–6
paratope-epitope interaction, 6
surface protein, 7
- MHC-peptide-TR binding
comparison of, 87
DQ3.2b, 85
DR and DQ alleles, 85
Dsg3 glycoprotein proteome, 85, 86
HIV-1 p24gag and gp160gag, 85
- T cells, 4–5
- European Searchable Tumour Cell-Line Database (ESTDAB), 30
- F**
- File transfer protocol (FTP), 36, 42
Fish Pathogen Database, 8
- G**
- Gardasil, 3
Genetic association studies (GAS), 157.
See also Bioinformatic platform
Genome wide association studies (GWAS), 159–161
- Global Polio Eradication Program, 1
- H**
- HensBC algorithm, 11
Hidden markov models (HMMs), 5
HLA database. *See* IMGT/HLA database
Human immunodeficiency virus type 1 (HIV-1) infection, 85
Human leukocyte antigen class I (HLA I), 60, 61, 64
- Human platelet antigens (HPA), 27–29
- Human symbiosis, elusive molecular self
host-microbe interactions, 152
microbiome, 151, 152
tolerance, 151
- Humoral adaptive immunity
B cell epitopes, 149, 150
sliding-window method, 150
- I**
- IMGT/HLA database
accessing methods, 36–37
allelic sequences, 33
class I and II alleles, 34, 35
clustal alignment tool, 39
DRB1 consensus sequence, 40
existing database, 34–36
history of, 33–34
tools
alignment formats, 40–42
allele search tools, 37–39
developments, 42
generalist databanks, 42–43
new sequences submittion, 42
similar sequences searching, 39–40
- Immune epitope database (IEDB), ontology
development, 48–49
objects, roles and processes, 52–53
relationships, 53–55
- Immunomics, definition, xi, xii
- Immuno Polymorphism Database (IPD)
centralised system, 21
projects
alignment interface, 27
Allele Query Tool, 22, 23

- Immuno Polymorphism Database (IPD)
(cont.)
- european searchable tumour cell line database (ESTDAB), 30
 - human platelet antigens (HPA), 27–29
 - killer-cell immunoglobulin-like receptors (KIR), 24–26
 - major histocompatibility complex (MHC), 22–24
 - sequence alignments, 26–27
- Immunovaccinology, xv
- Innate immunity
- adaptive immunity, 67
 - adjuvants, 139–140
 - drug-like adjuvants, 140
 - innate immune database (IIDB), 68–69
 - innate immunity interactions database (innate DB), 69–70
 - NOD-like receptors (NLRs), 139
 - PAMPs, 68, 138–140
 - PRRDB, 70–72
 - PRRs, 138–140
 - vaccines, 67
 - web-based tools
 - AntiBP, 73–75
 - CTKPred, 72–73
 - CytoPred, 73
- Invariant NKT (iNKT) cells, 149
- K**
- Killer-cell immunoglobulin-like receptors (KIR)
- Allele Entry, 25
 - cell query tool, 25
 - ligand calculator, 26
 - Probe and Primer Search Tool, 26
- L**
- Leukocyte receptor complex (LRC).
See Killer-cell immunoglobulin-like receptors (KIR)
- Life-style vaccines, 3
- M**
- Major histocompatibility complex (MHC)
- class II MHC expression, 146–148
 - class I MHC molecules, 142–146
- Immuno Polymorphism Database (IPD), 22–24
- T cell epitope prediction, 5
- Major histocompatibility complex (MHC)-peptide-TR binding docking protocol
- binding register refinement, 84
 - flanking residues extension, 84
 - loop closure of, 83–84
 - nonamer termini, 82–83
 - procedure, flowchart of, 82
- epitope prediction
- comparison of, 87
 - DQ3.2 β , 85
 - DR and DQ alleles, 85
 - Dsg3 glycoprotein proteome, 85, 86
 - HIV-1 p24gag and gp160gag, 85
- MHC-peptide Interaction Database - TR (MPID-T)
- gap index and gap volume, 80
 - interface area and intermolecular hydrogen bonds, 79
- Ioga complex, analysis
- gap volume, 91
 - H-bonds, 89
 - LIGPLOT schematic diagram, 90
 - space filling representation, 91
- supertype classification, 80–81
- TR/pMHC interaction
- C α trace ribbon representation, 89
 - inter-residue interactions and schematic structure, 88
- Markov-Blanket Membership (MBM) probability, 172, 176–178
- MenB vaccine, 11
- MHC-peptide Interaction Database - TR (MPID-T)
- gap index and gap volume, 80
 - interface area and intermolecular hydrogen bonds, 79
- Monozygotic (MZ) twins, 129–130
- Multifactorial diseases
- candidate gene association studies, 159
 - database of genotypes and phenotypes (dbGaP), 161
 - genome wide association studies (GWAS), 159
- Multiple protein-sequence alignments (MSAs), conserved epitopes, 96

O

- Ontology development, immune epitope database (IEDB)
Basic Formal Ontology (BFO)
relationships, 51
B cell receptors (BCRs), 48
data consistency approaches, 49
high level BFO/OBI structure, 52
immunization assay, 50
objects, roles and processes, 52–53
Ontology for Biomedical Investigations (OBI), 51–52
open biomedical ontologies (OBO), 51
proxy for, 54, 55
SARS coronavirus nucleoprotein, 50, 54, 55
T cell epitope identification experiment, 54
T cell receptors (TCRs), 48
Ontology for Biomedical Investigations (OBI), 51–52
ONTology of Immune Epitopes (ONTIE), 51–52
Open biomedical ontologies (OBO), 51
Open Reading Frames (ORF)-FINDER, 10

P

- PAMPs. *See* Pathogen associated molecular patterns
Pathogen associated molecular patterns (PAMPs), 68, 138, 140
Pattern recognition receptor database (PRRDB), 70–72
Pattern-recognition receptors (PRRs), 68, 70, 138–140
Population patterns, tunable detectors AIS algorithm, 114
antigens stimulation, 115
 α parameter effects, 117
proliferation threshold effects, 116
Protein variability server (PVS), conserved epitopes
Shannon Diversity Index (H) and metrics used, 97
T cell epitope predictions, 98
web interface, 96
PRRs. *See* Pattern-recognition receptors (PRRs)

Q

- QSAR analysis techniques, 5

R

- Reverse vaccinology
NERVE program, 10–11
open reading frames (ORFs), 10
subunit vaccines, 10
surface proteins, 11

S

- Sequence Retrieval System (SRS)
tool, 38–39
Shannon Diversity Index (H), 97
SignalP, 9–10
Single nucleotide polymorphisms (SNPs).
See also Bioinformatic platform decision support system (DSS)
issues, 165–166
methods, 163–165
selection process, 165
GAS design, 171
ratios and posteriors, 183
SPICE graphical client, TEPIDAS
HLA-B*60 features, 64
viewer window, 63
zooming capability, 64
Structural immunoinformatics. *See* Major histocompatibility complex (MHC)-peptide-TR binding
Support vector machines (SVMs), 5

T

- T cell receptor (TR)/pMHC interaction.
See also Major histocompatibility complex (MHC)-peptide-TR binding
 $\text{C}\alpha$ trace ribbon representation, 89
inter-residue interactions and schematic structure, 88
TEPIDAS
annotations, 60
distributed annotation system (DAS)
architecture, 58–59
protocol, 58
registry, 59
query capabilities
features query, 61–62
XML response, 61
SPICE graphical client
HLA-B*60 features, 64
viewer window, 63
zooming capability, 64
Toll-like receptors (TLRs), 138, 139

Tunable activation threshold (TAT), tunable detectors AIS
adaptable lymphocyte hypothesis, 104–106
antigen and T cell detector shapes, 111–113
dynamics, 105, 106
equation
 excitation, 109–110
 excitation index and activation threshold relationship, 107
 α parameter, 108–109
perturbation, 109

U

UniProt code, 64

V

Vaccines, 67
VaxiJen, reverse vaccinology, 10
Virulence Factors Database (VFDB), 8–9

W

Web-based tools, innate immunity

AntiBP
 query result page, 75
 submission form, 74
CTKPred, 72–73
CytoPred
 query result page, 74
 submission form, 73

WHO Nomenclature Committee for Factors, HLA System, 33–36, 38, 43