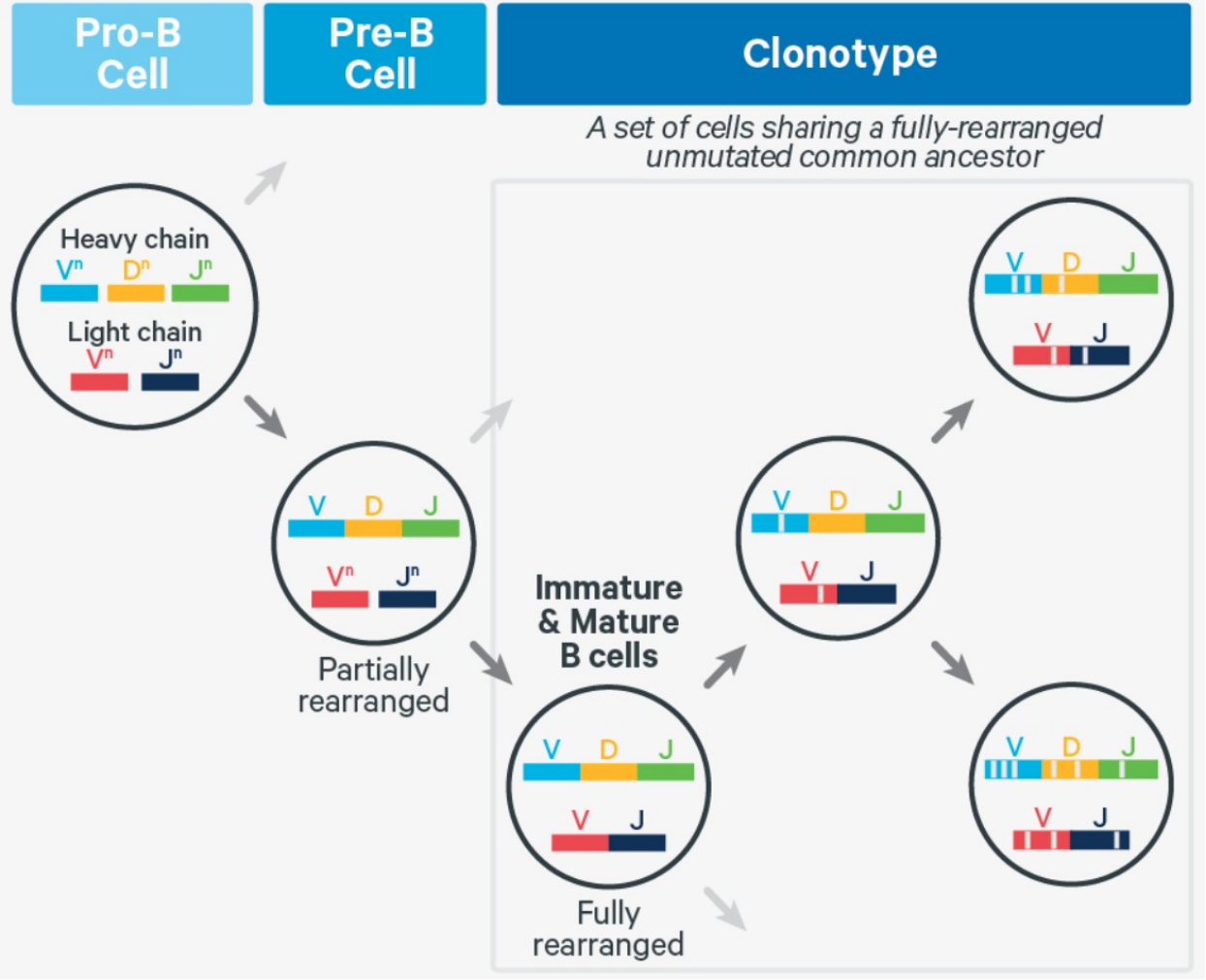
Фонд интеллект

Машинное обучение в иммунологии и медицине

Особенности секвенирования TCR, BCR. Анализ Т- и В-клеточных репертуаров.

Созревание В-клеток



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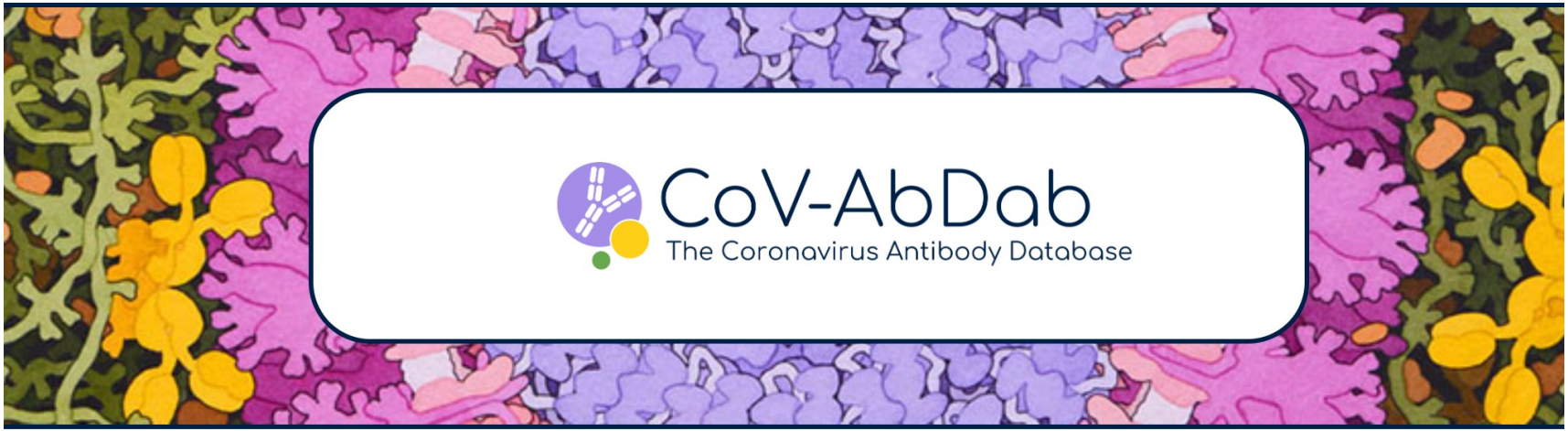

IMGT Repertoire (IG and TR)

The global ImMunoGeneTics Web Resource for immunoglobulins (IG),
T cell receptors (TR), major histocompatibility (MH) and related proteins of the immune system (RPI).
Editor: Marie-Paule Lefranc (LIGM, Université de Montpellier, CNRS, Montpellier, France).

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IMGT Repertoire (MH)
IMGT Repertoire (RPI)

IMGT Repertoire comprises LIGM expertized data on immunoglobulins (IG), T cell receptors (TR), major histocompatibility (MH) and related proteins of the immune sys

1. Locus and genes

1. Chromosomal localizations
2. Locus representations
3. Locus descriptions
4. Gene positions
5. Gene exon/intron organization
6. Gene exon/intron splicing sites
7. Gene tables
8. Potential germline repertoires
9. Lists of human IG and TR genes, groups, loci and orphons
10. Lists of Mouse *(Mus musculus)* IG and TR genes, groups and loci
11. Clans
12. Correspondence between chain types and C genes : IG and TR (all vertebrate species)
13. Correspondence between nomenclatures
14. Correspondence between species

2. Proteins and alleles

1. Protein displays
2. Alignments of alleles
3. Tables of alleles
4. Allotypes
5. Isotypes
6. Particularities in protein designations
7. IMGT reference directory in FASTA format

2. Alignments of alleles

- IGHV:
  - Mammalia: human (*Homo sapiens*), Mouse (*Mus musculus*), Crab-eating macaque (*Macaca fascicularis*), Arabian camel (*Camelus dromedarius*), llama (*Lama glama*), Alpaca (*Vicugna pacos*), sheep (*Ovis aries*), pig (*Sus scrofa*), Norway rat (*Rattus norvegicus*), rabbit (*Oryctolagus cuniculus*), platypus (*Ornithorhynchus anatinus*), bovine (*Bos taurus*), dog (*Canis lupus familiaris*), horse (*Equus caballus*), Rhesus monkey (*Macaca mulatta*), Western lowland gorilla (*Gorilla gorilla gorilla*) NEW!, Ring-tailed lemur (*Lemur catta*) NEW!
  - Sauropsida: spectacled caiman (*Caiman crocodilus*), chicken (*Gallus gallus*)
  - Amphibia: African clawed frog (*Xenopus laevis*),
  - Teleostei: Atlantic cod (*Gadus morhua*), Atlantic salmon (*Salmo salar*), Bastard halibut (*Paralichtys olivaceus*), Blackfin icefish (*Chaenocephalus aceratus*), channel catfish (*Ictalurus punctatus*), charr (*Salvelinus alpinus*), emerald rockcod (*Trematomus bernacchii*), goldfish (*Carassius auratus*), ladyfish (*Elops saurus*), rainbow trout (*Oncorhynchus mykiss*), spotted wolffish (*Anarhichas minor*), torafugu (*Takifugu rubripes*), turbot (*Scophthalmus maximus*), black rockcod (*Notothenia coriiceps*), Zebrafish (*Danio rerio*)
  - Chondrichthyes: bull shark (*Carcharhinus leucas*), sandbar shark (*Carcharhinus plumbeus*), nurse shark (*Ginglymostoma cirratum*), horn shark (*Heterodontus francisci*), Spotted ratfish (*Hydrolagus colliei*), Spotted wobbegong shark (*Orectolobus maculatus*), clearnose skate (*Raja eglanteria*), Little skate (*Leucoraja erinacea*)
  - Other: African lungfish (*Protopterus aethiopicus*)
- IGHD:
  - Mammalia: human (*Homo sapiens*), house mouse (*Mus musculus*), Crab-eating macaque (*Macaca fascicularis*), Alpaca (*Vicugna pacos*), Sheep (*Ovis aries*), pig (*Sus scrofa*), Norway rat (*Rattus norvegicus*), rabbit (*Oryctolagus cuniculus*), platypus (*Ornithorhynchus anatinus*), bovine (*Bos taurus*), dog (*Canis lupus familiaris*), horse (*Equus caballus*), Rhesus monkey (*Macaca mulatta*) Western lowland gorilla (*Gorilla gorilla gorilla*) NEW!, Ring-tailed lemur (*Lemur catta*) NEW!
  - Sauropsida: chicken (*Gallus gallus*)
  - Teleostei: channel catfish (*Ictalurus punctatus*), rainbow trout (*Oncorhynchus mykiss*), Zebrafish (*Danio rerio*), Atlantic salmon (*Salmo salar*)
  - Chondrichthyes: bull shark (*Carcharhinus leucas*), sandbar shark (*Carcharhinus plumbeus*), nurse shark (*Ginglymostoma cirratum*), horn shark (*Heterodontus francisci*), Spotted ratfish (*Hydrolagus colliei*), Spotted wobbegong shark (*Orectolobus maculatus*), clearnose skate (*Raja eglanteria*), Little skate (*Leucoraja erinacea*)
- IGHJ:

Alignment of alleles: human (*Homo sapiens*) IGHV

- IGHV1-2
- IGHV1-3
- IGHV1-8
- IGHV1-18
- IGHV1-24
- IGHV1-38-4
- IGHV1-45
- IGHV1-46
- IGHV1-58
- IGHV1-68 and IGHV1-68D
- IGHV1-69 and IGHV1-69D
- IGHV1-69-2
- IGHV2-5
- IGHV2-26
- IGHV2-70 and IGHV2-70D
- IGHV3-7
- IGHV3-9
- IGHV3-11
- IGHV3-13
- IGHV3-15
- IGHV3-16
- IGHV3-19
- IGHV3-20
- IGHV3-21
- IGHV3-22
- IGHV3-23 and IGHV3-23D


```
                                                 1   2   3   4   5   6   7   8   9   10  11  12  13  14  15  16  17  18  19  20
                                                 E   V   Q   L   V   E   S   G   G       G   L   V   Q   P   G   G   S   L   R
X92217     IGHV3-13*01 F V-REGION gDNA          gag gtg cag ctg gtg gag tct ggg gga ... ggc ttg gta cag cct ggg ggg tcc ctg aga

AB019440   IGHV3-13*01 F V-REGION gDNA          --- --- --- --- --- --- --- --- --- ... --- --- --- --- --- --- --- --- --- ---

U29479     IGHV3-13*01 F V-REGION gDNA          --- --- --- --- --- --- --- --- --- ... --- --- --- --- --- --- --- --- --- ---

Z12348     IGHV3-13*01 F V-REGION gDNA          --- --- --- --- --- --- --- --- --- ... --- --- --- --- --- --- --- --- --- ---

                                                         H                                                               A
M99653     IGHV3-13*02 F V-REGION gDNA          --- --- --t --- --- --- --- --- --- ... --- --- --- --- --- --- --- g-- --- ---

U29582     IGHV3-13*03 F V-REGION gDNA          --- --- --- --- --- --- --- --- --- ... --- --- --- --- --- --- --- --- --- ---

HM855616   IGHV3-13*04 F V-REGION gDNA          --- --- --- --- --- --- --- --- --- ... --- --- --- --- --- --- --- --- --- ---

KC713939   IGHV3-13*05 F V-REGION gDNA          --- --- --- --- --- --- --- --- --- ... --- --- --- --- --- --- --- --- --- ---

IMGT000035 IGHV3-13*05 F V-REGION gDNA          --- --- --- --- --- --- --- --- --- ... --- --- --- --- --- --- --- --- --- ---
```

IMGT Repertoire (IG and TR)

Protein displays: human (*Homo sapiens*) IGHV

Species	Gene	Allele	AccNum	Domain label	Functionality	FR1-IMGT (1-26) A (1-15)	B (16-26)	CDR1-IMGT (27-38) BC (27-38)	C (39-46)	C' (47-55)	CDR2-IMGT (56-65) C'C" (56-65)	C" (66-74)	FR3-IMGT (66-104) D (75-84)	E (85-96)	F (97-104)	CDR3-IMGT (105-117) FG
						1 10 15	16 23 26	27 38	39 41 46	47 55	56 65	66 74	75 84	85 89 96	97 104	105
Homsap	IGHV1-2	IGHV1-2*01	X07448	VH	F	QVQLVQSGA.EVKKP	GASVKVSCKAS	GYTF....TGYY	MHWVRQAP	GQGLEWMGR	INPN..SGGT	NYAQKFQ.G	RVTSTRDTSI	STAYMELSRLRS	DDTVVYYC	AR
Homsap	IGHV1-3	IGHV1-3*01	X62109	VH	F	QVQLVQSGA.EVKKP	GASVKVSCKAS	GYTF....TSYA	MHWVRQAP	GQRLEWMGW	INAG..NGNT	KYSQKFQ.G	RVTITRDTSA	STAYMELSSLRS	EDTAVYYC	AR
Homsap	IGHV1-8	IGHV1-8*01	M99637	VH	F	QVQLVQSGA.EVKKP	GASVKVSCKAS	GYTF....TSYD	INWVRQAT	GQGLEWMGW	MNPN..SGNT	GYAQKFQ.G	RVTMTRNTSI	STAYMELSSLRS	EDTAVYYC	AR
Homsap	IGHV1-18	IGHV1-18*01	M99641	VH	F	QVQLVQSGA.EVKKP	GASVKVSCKAS	GYTF....TSYG	ISWVRQAP	GQGLEWMGW	ISAY..NGNT	NYAQKLQ.G	RVTMTTDTST	STAYMELRSLRS	DDTAVYYC	AR
Homsap	IGHV1-24	IGHV1-24*01	M99642	VH	F	QVQLVQSGA.EVKKP	GASVKVSCKVS	GYTL....TELS	MHWVRQAP	GKGLEWMGG	FDPE..DGET	IYAQKFQ.G	RVTMTEDTST	DTAYMELSSLRS	EDTAVYYC	AT
Homsap	IGHV3-33-2	IGHV3-33-2*01	AB019439	VH	P	EVQLVESGE.DPRQP	GGSLRLSCADS	GLTF....SSY*	MSSVSQAP	GKGLE*VVD	IQCD..GSQI	CYAQSVK.S	KFTISKENAK	NSLYLQMNSLRA	EGTAVCYC	M*G
Homsap	IGHV3-35	IGHV3-35*01	M99666	VH	ORF	EVQLVESGG.GLVQP	GGSLRLSCAAS	GFTF....SNSD	MNWVHQAP	GKGLEWVSG	VSWN..GSRT	HYADSVK.G	RFIISRDNSR	NTLYLQTNSLRA	EDTAVYYC	VR
Homsap	IGHV3-38	IGHV3-38*01	M99669	VH	ORF	EVQLVESGG.GLVQP	RGSLRLSCAAS	GFTV....SSNE	MSWIRQAP	GKGLEWVSS	ISG....GST	YYADSRK.G	RFTISRDNSK	NTLYLQMNNLRA	EGTAAYYC	ARY
Homsap	IGHV3-38-3	IGHV3-38-3*01	KF698732	VH	ORF	EVQLVESRG.VLVQP	GGSLRLSCAAS	GFTV....SSNE	MSWVRQAP	GKGLEWVSS	ISG....GST	YYADSRK.G	RFTISRDNSK	NTLHLQMNSLRA	EDTAVYYC	KK
Homsap	IGHV3-43	IGHV3-43*01	M99672	VH	F	EVQLVESGG.VVVQP	GGSLRLSCAAS	GFTF....DDYT	MHWVRQAP	GKGLEWVSL	ISWD..GGST	YYADSVK.G	RFTISRDNSK	NSLYLQMNSLRT	EDTALYYC	AKD

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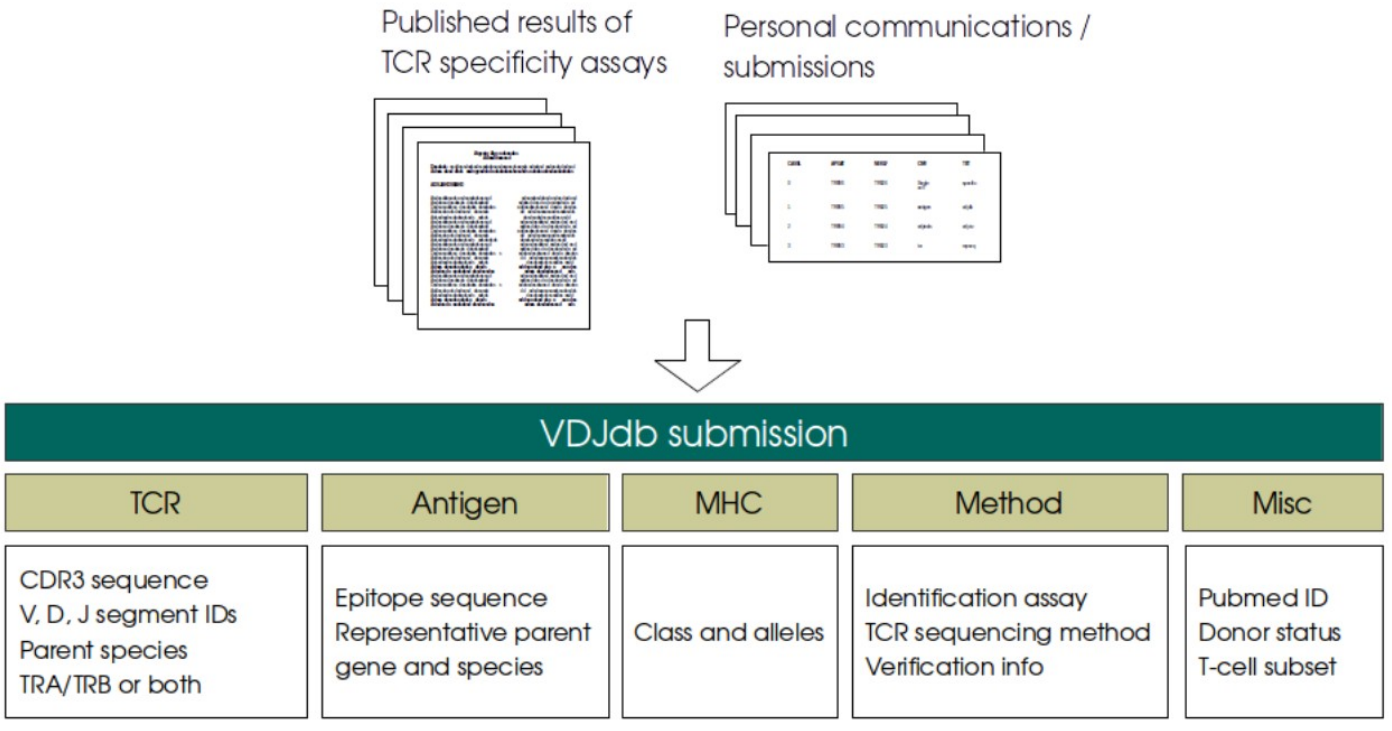
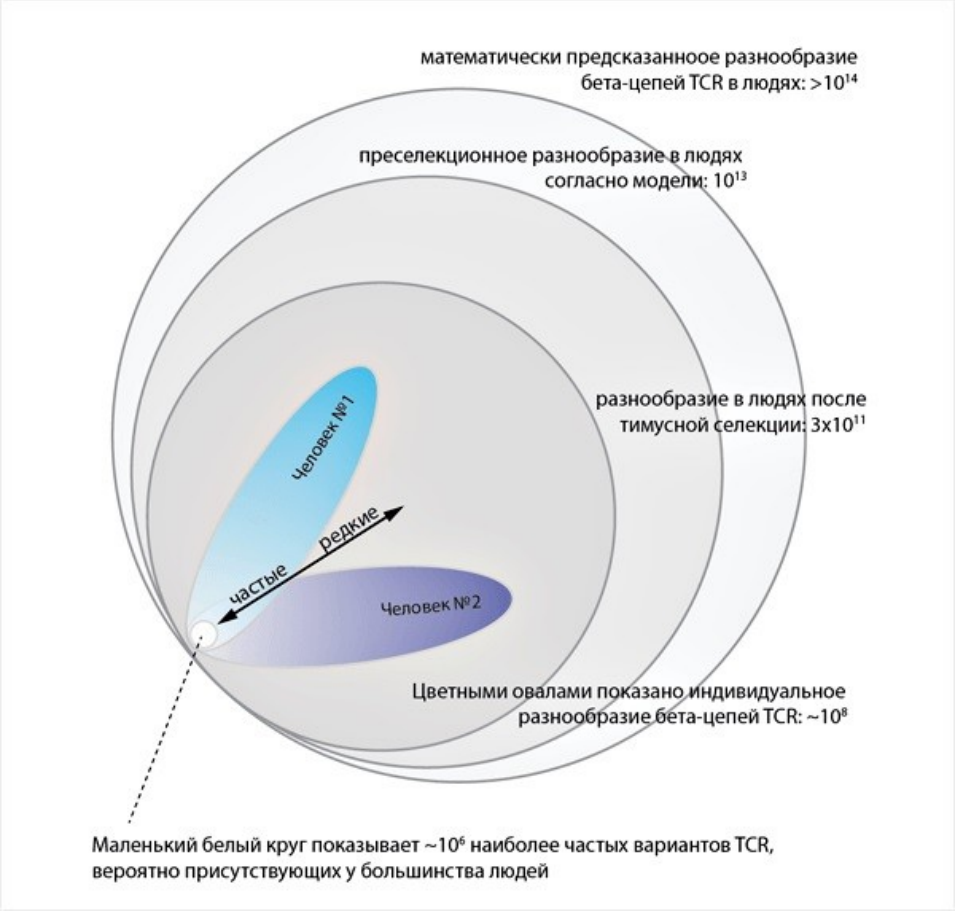


Разнообразие TCR



AmpliSeq for Illumina Immune Repertoire Plus, TCR beta Panel

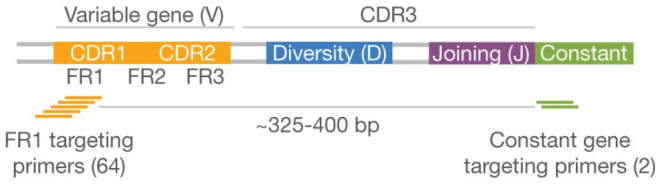


Table 1: AmpliSeq for Illumina Immune Repertoire Plus, TCR beta Panel at a glance

Parameter	Specification
No. of genes	Variable
Targets	TCR beta chain, including CDR1, CDR2, and CDR3
Amplicon size	~ 325 bp
No. of amplicons	Variable
Input RNA requirement	10-1000 ng
No. of pools per panel	1
Supported sample types	Blood, fresh/frozen tissue, FACS cells
Total assay time[a]	5-6 hours
Hands-on time	< 1.5 hours
RNA-to-data time	2.5 days

a. Time represents library preparation only and does not include library quantification, normalization, or pooling.

Data on file at Illumina, Inc. 2017

Oncomine immune repertoire assays

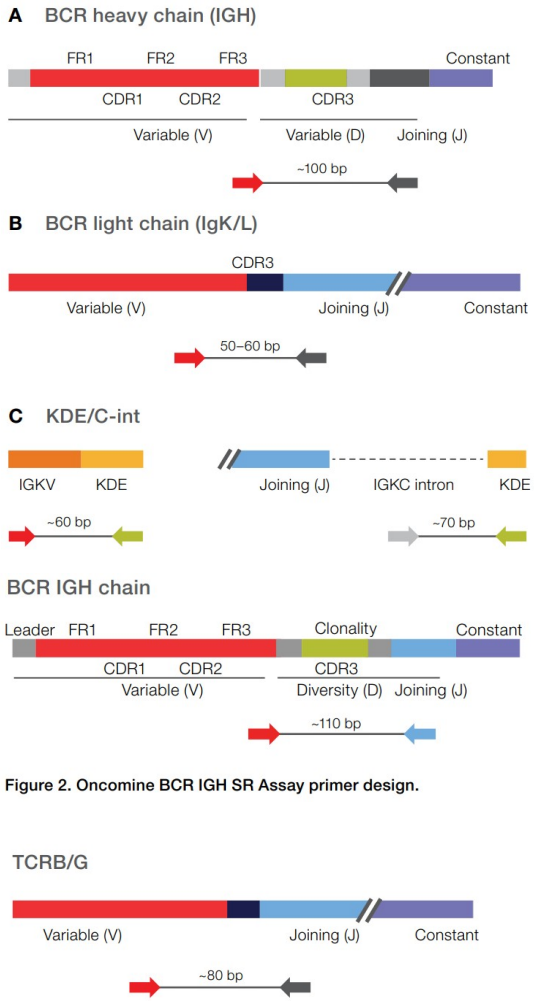


Figure 2. Oncomine BCR IGH SR Assay primer design.

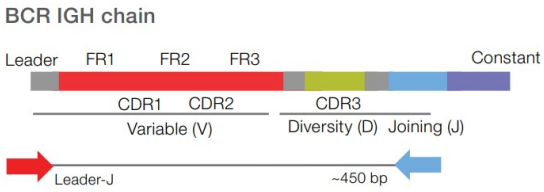
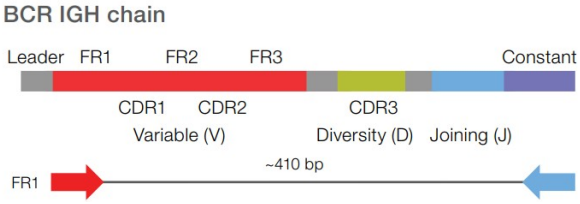


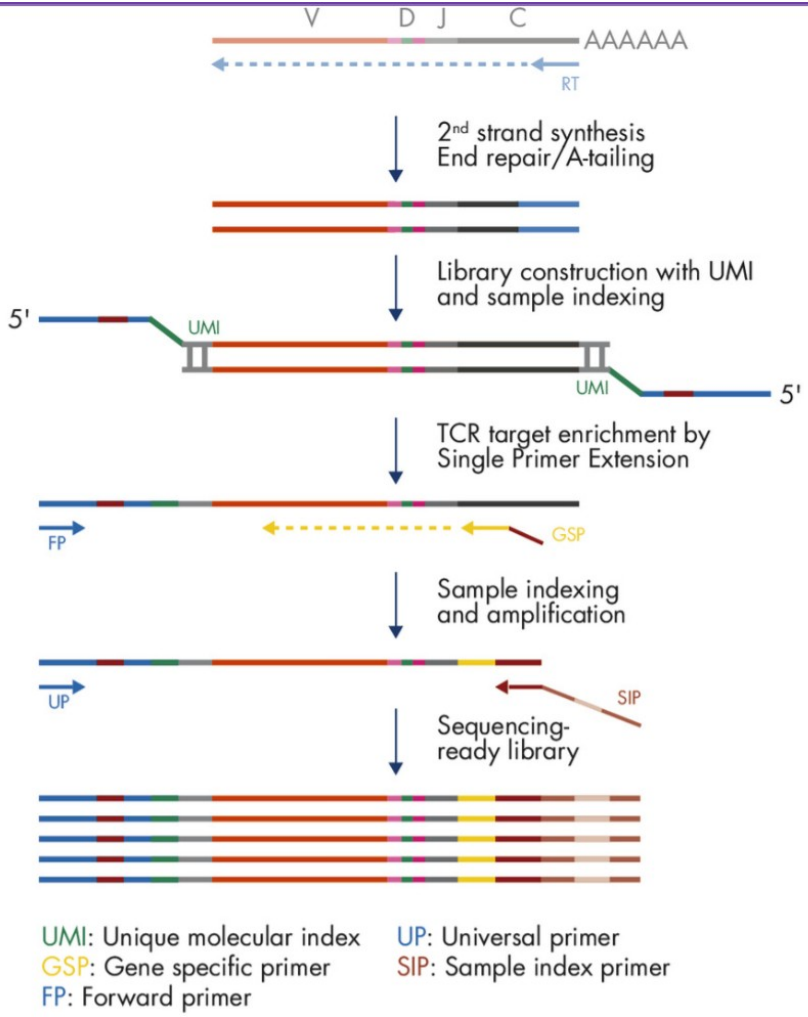
Figure 5. Oncomine IGHV Leader-J Assay primer design.



Research assay summary table

Assay	Target(s)	Nucleic acid input	Sample types	Application(s)	Ion Torrent™ chip compatibility
Oncomine BCR Pan-Clonality Assay	BCR, IGH, IgK, IgL, KDE/ C_{int}, (FR3-J)	gDNA	Whole blood, bone marrow, PBL,* PBMC,* sorted cells, fresh-frozen and FFPE-preserved tissue samples	Clonality, rare clone detection	Ion 530™, Ion 540™, and Ion 550™ Chips**
Oncomine BCR-SR Assay	BCR IGH (FR3-J)	gDNA, RNA			
Oncomine IGH FR3(d)-J Assay	BCR IGH (FR3(d)-J)	gDNA			
Oncomine IGH FR2-J Assay	BCR IGH (FR2-J)	gDNA			
Oncomine TCR Pan-Clonality Assay	TCRB, TCRG (FR3-J)	gDNA			
Oncomine IGHV Leader-J Assay	BCR IGH (Leader-J)	gDNA	Whole blood, bone marrow, PBL, PBMC, sorted cells	SHM	Ion 530 Chip
Oncomine IGH-LR Assay	BCR IGHV (FR1-C)	Non-FFPE RNA	Whole blood, bone marrow, PBL, PBMC, fresh-frozen specimens		
Oncomine IGH FR1-J Assay	BCR IGH (FR1-J)	Non-FFPE RNA			

QIAseq Immune Repertoire RNA Library Kits



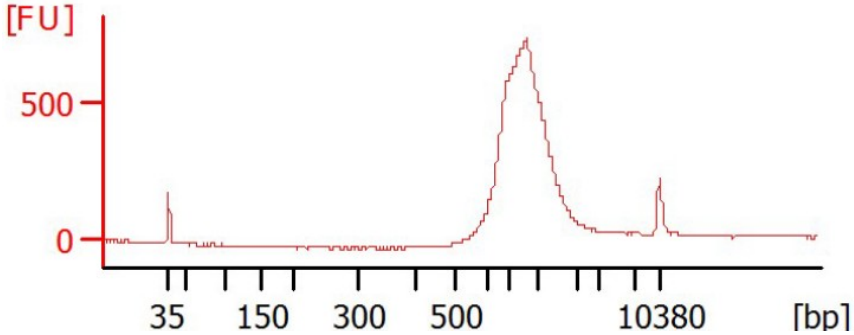


Figure 10. Bioanalyzer image of QIAseq Immune Repertoire RNA Library Kit library for Illumina instruments. A library was prepared using the QIAseq Immune Repertoire RNA Library Kit and assessed using an Agilent 2100 Bioanalyzer. The size of the majority of the library fragments are between 600–2000 bp.

5. **Custom Sequencing Primer for Read 1 preparation and loading**: Use 597 µl HT1 (Hybridization Buffer) to dilute 3 µl QIAseq A Read 1 Custom Primer I (provided) to obtain a final concentration of 0.5 µM. Load 600 µl of the diluted QIAseq A Read 1 Primer I to position 18 of the MiSeq reagent cartridge (Figure 8). For more details, please refer to the Illumina protocol: miseq_using_custom_primers_15041638_b.pdf for the MiSeq.

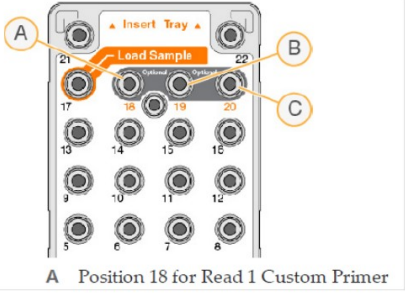


Figure 8. MiSeq Reagent Cartridge. A: Position 18 for Read 1 Custom Primer. B and C are not relevant.

QIAseq Immune Repertoire RNA Library Kit что прочитывается

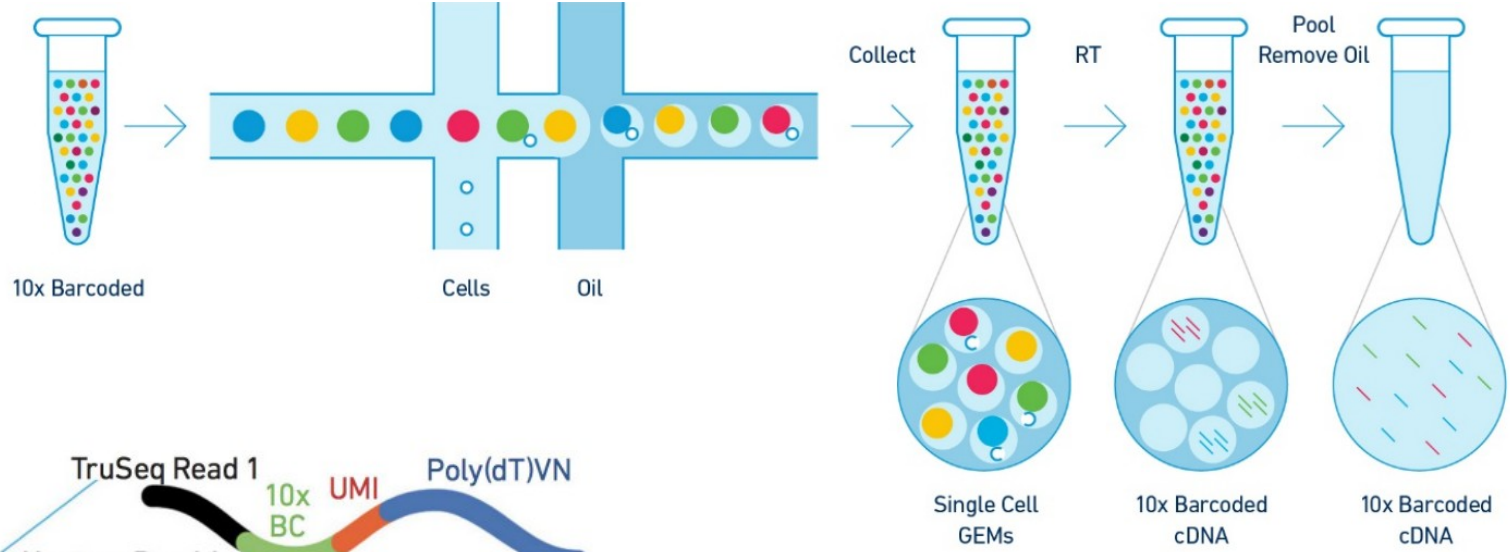
- Index 1 and Index 2 are 8 bp cycles each
- 251 bp paired-end sequencing is recommended for complete variable region sequencing.
- 261/41 bp asymmetrical paired-end sequencing is recommended for CDR3 region sequencing

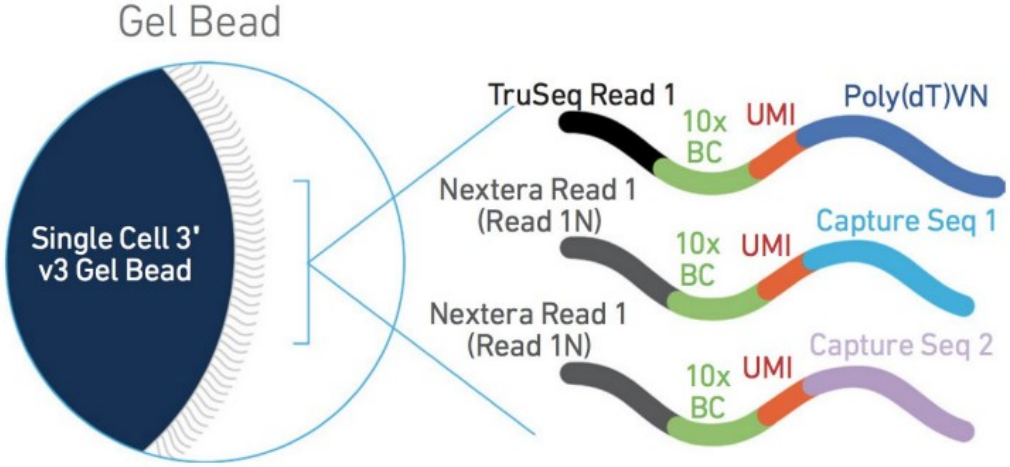
```
                                                   FR1-IMGT          CDR1-IMGT      FR2-IMGT     CDR2-IMGT                FR3-IMGT                CDR3-IMGT
                                                    (1-26)            (27-38)       (39-55)      (56-65)                  (66-104)                (105-117)
                                                A          B          BC        C       C'       C'C"      C"       D          E        F       FG
Species  Gene   Allele   AccNum  Domain label  Functionality      (1-15)     (16-26)   (27-38)   (39-46)  (47-55)  (56-65)  (66-74)  (75-84)  (85-96)  (97-104)
                                                              ----------> ---------> ---------> -------> -------> --------> -------> -------> -------> -------->
                                                              1        10  15 16    23 26 27        38 39 41  46 47     55 56      65 66     74 75      84 85  89    96 97   104 105
                                                              |........|....| |......|..| |..........| |.|....| |.......| |........| |.......| |........| |...|......| |......| |.....
Homsap   TRBV1  TRBV1*01  L36092  V-BETA  P                  DTGITQTPKYLVTAM GSKRTMKREHL GH........DS MYWYRQKA KKSLEFMFY YNC....KEF IENKTVP.N HFTPECP.DS SRLYLHVVALQQ EDSAAYLC TSSQ
Homsap   TRBV2  TRBV2*01  L36092  V-BETA  F                  EPEVTQTPSHQVTQM GQEVILRCVPI SNH.......LY FYWYRQIL GQKVEFLVS FYN....NEI SEKSEIFDD QFSVERP.DG SNFTLKIRSTKL EDSAMYFC ASSE
```

Species	Gene	Allele	AccNum	Domain label	Functionality	Sequence
Homsap	TRBJ1-1	TRBJ1-1*01	K02545	J-REGION	F	NTEAFFGQGTRLTVV
Homsap	TRBJ1-2	TRBJ1-2*01	K02545	J-REGION	F	NYGYTFGSGTRLTVV

```
                                                   A       AB      B         BC       C      CD      D         DE         E      EF   F              FG              G
                                                (1-15)           (16-26)   (27-38)  (39-45)        (77-84)            (85-96)     (97-104)       (105-117)   (118-128)
                                                              ----------> ---------> ---------> -------> ---------> ---------> -------> ---------> ---------> ---------
                                                              1        10  15 16      2326 27      38 39 41 45       77     84             85  89     96  97   104 105                 117 118
                                                              87654321|........|....|123|......|..| |........| |.|...|1234567|......|12345677654321|...|......|12|......| |......123456654321.....| |.......
Homsap   TRBC1  TRBC1*01  M12887  C-BETA-1  F                 EDLNKVFPPEVAVFEPSEAEISH..TQKATLVCLAT GFFP..DHVE LSWWVNGKEVHS..GVSTDPQPLKEQPAL.NDSRYCLSSRLRVSATFWQ.NPRNHFRC QVQFYGLSENDEWTQDRAKPVTQIV SAEAWGRA
```

Single-cell технология от 10x

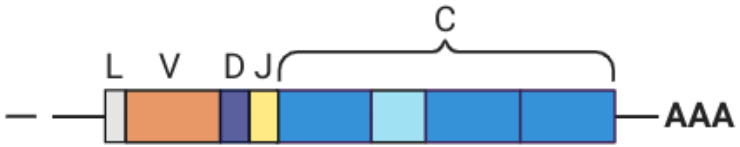




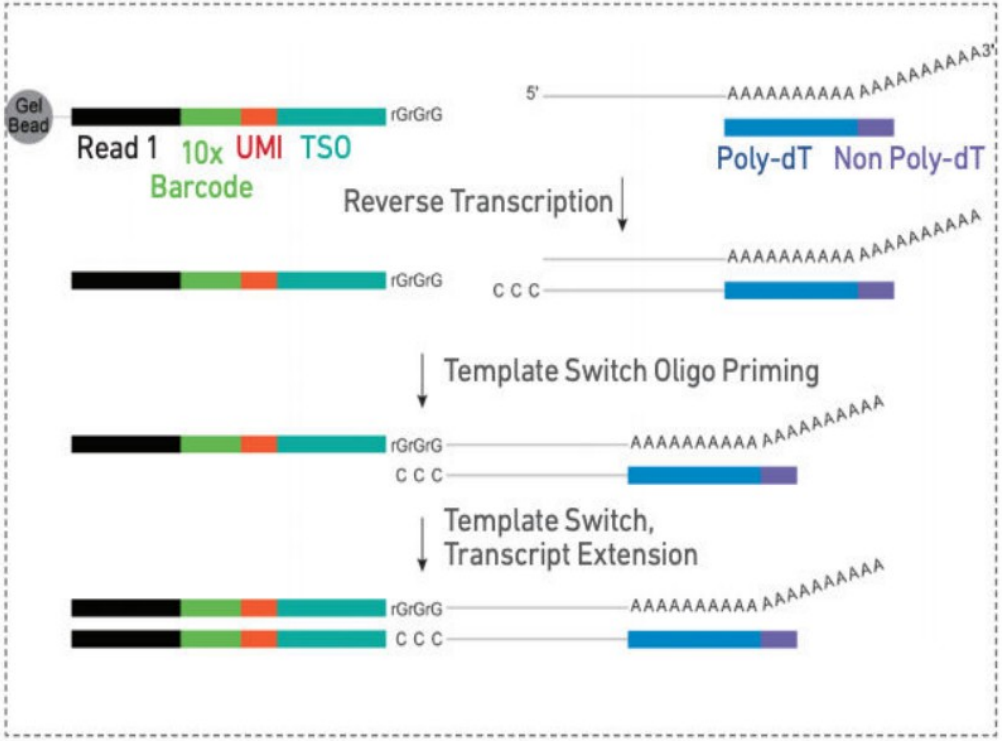
V2: ├─5'- CTACACGACGCTCTTCCGATCT[16-bp cell barcode][10-bp UMI]$(T)_{30}$VN -3'

V3: ├─5'- CTACACGACGCTCTTCCGATCT[16-bp cell barcode][12-bp UMI]$(T)_{30}$VN -3'

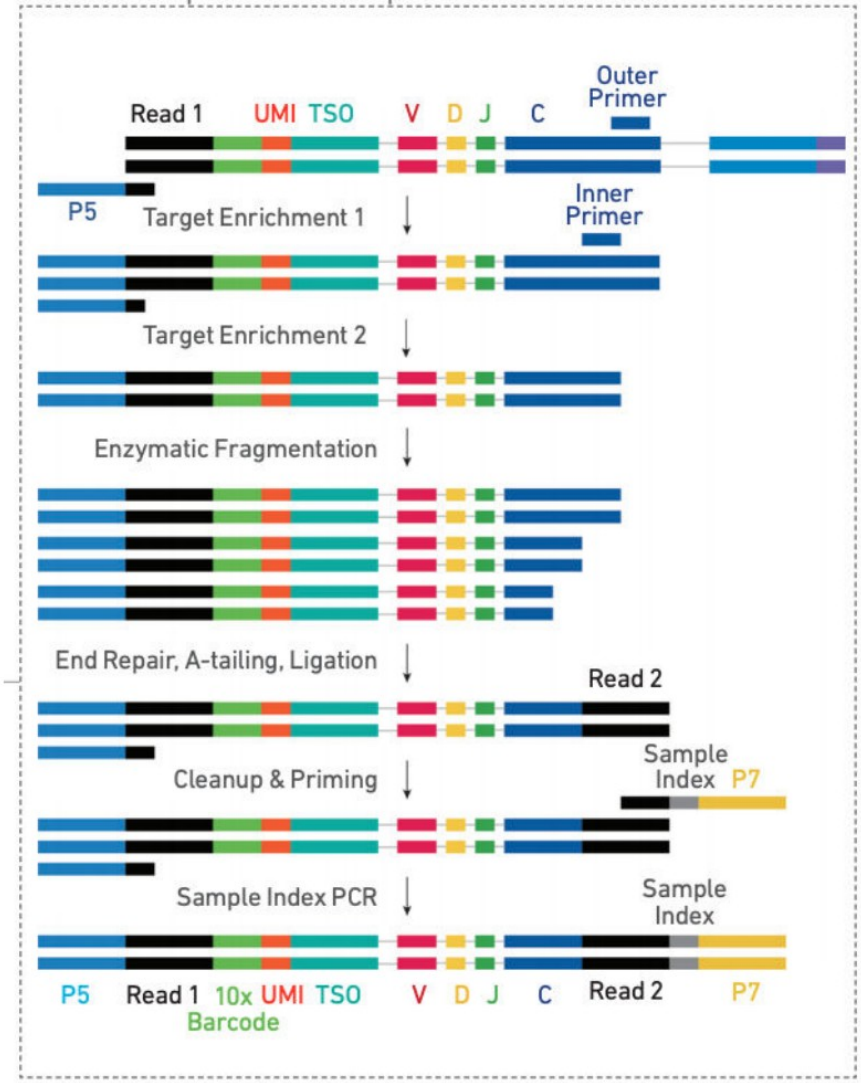
Single-cell V(D)J



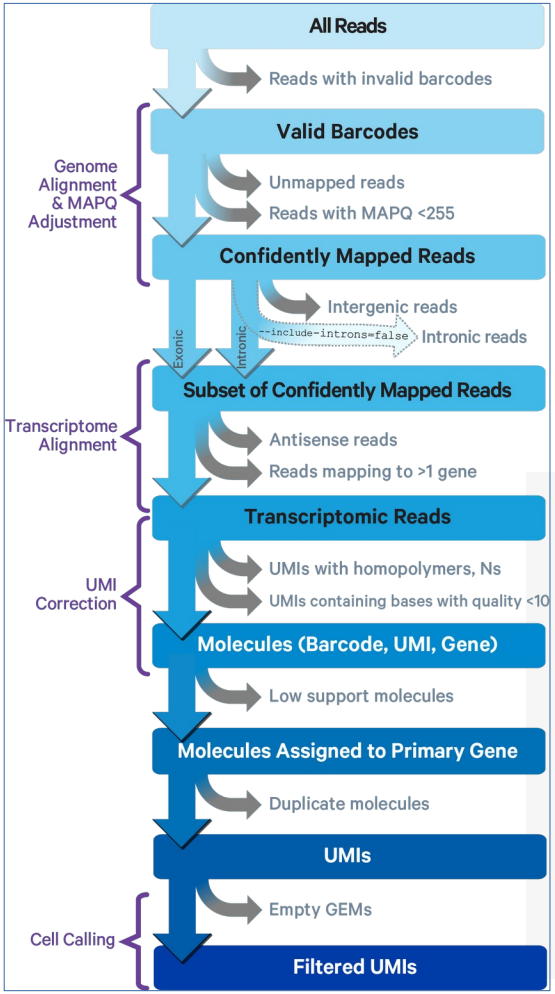
Inside individual GEMs

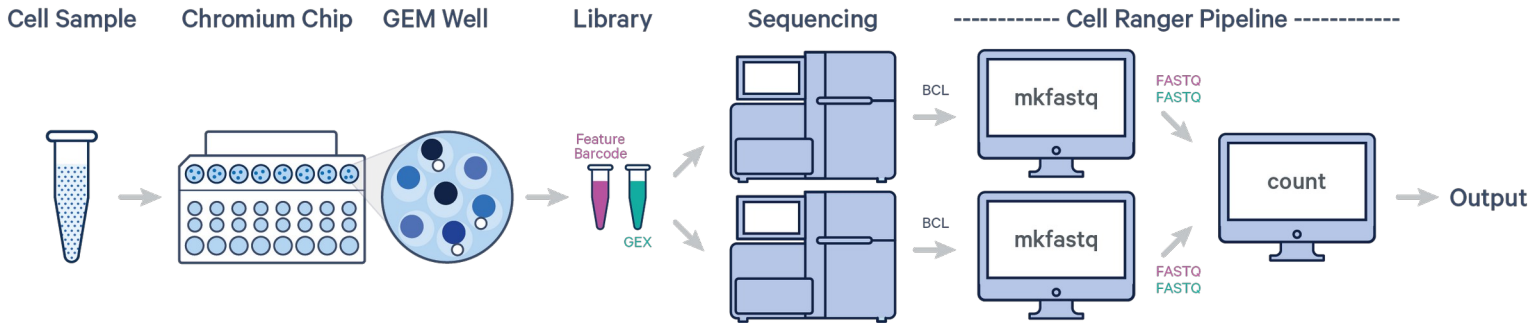


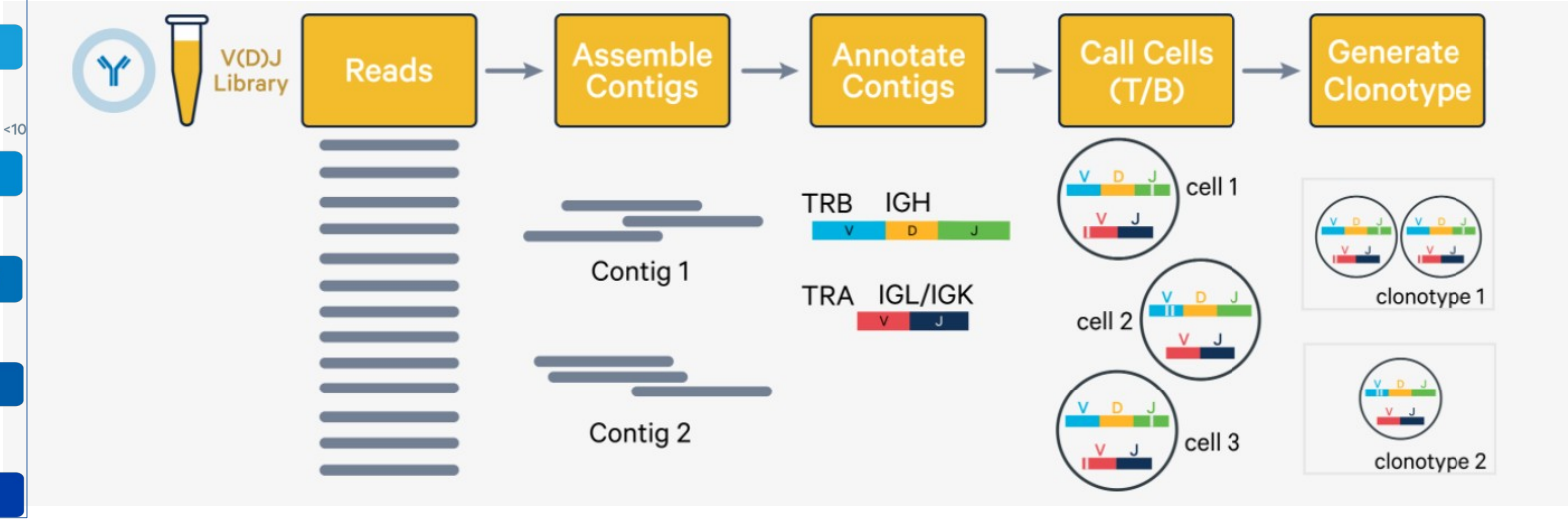
Pooled amplified cDNA processed in bulk



Анализ Single-cell







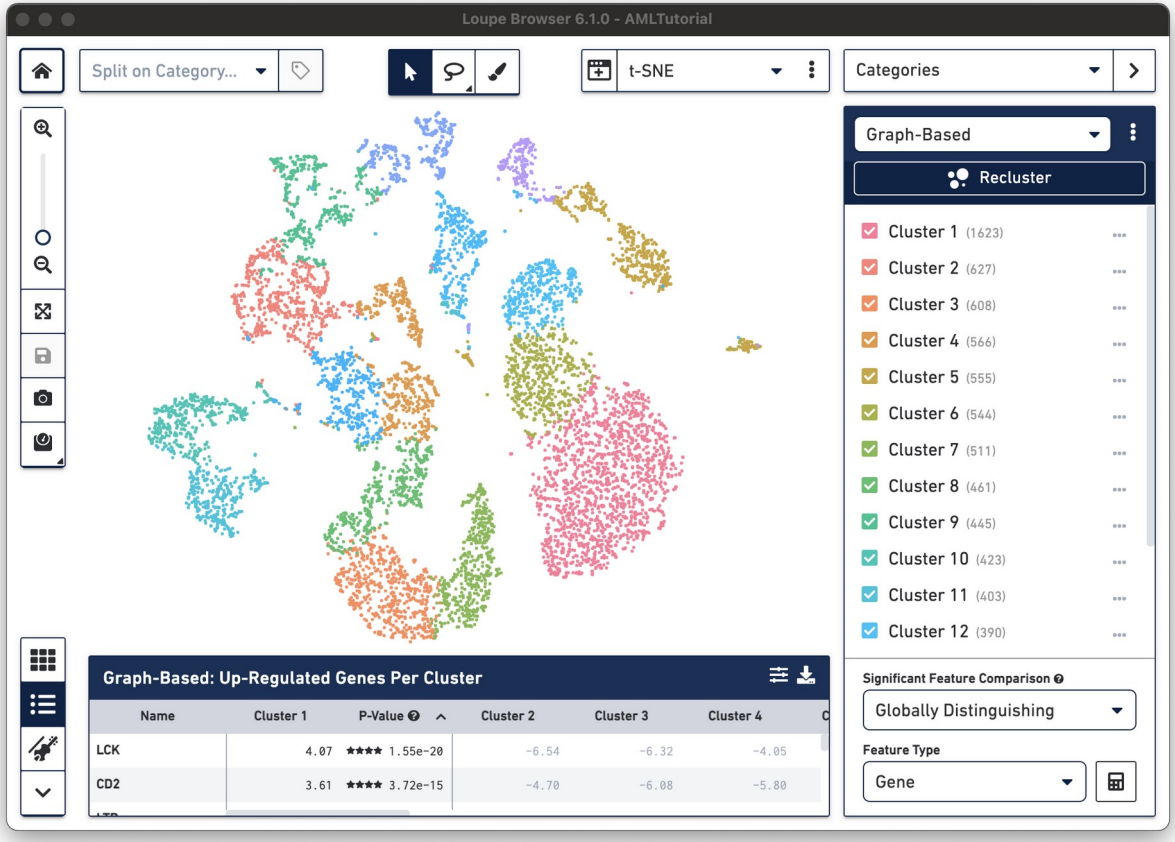
Анализ Single-cell

barcode	is_cell	contig_id	high_confidence	length	chain	v_gene	d_gene	j_gene	c_gene
AAACCTGAGGAGTTTA-1	true	AAACCTGAGGAGTTTA-1_contig_1	true	513	TRB	TRBV31		TRBJ2-1	TRBC2
AAACCTGAGGAGTTTA-1	true	AAACCTGAGGAGTTTA-1_contig_2	true	524	TRA	TRAV6D-4		TRAJ17	TRAC
AAACCTGCAGATGAGC-1	true	AAACCTGCAGATGAGC-1_contig_1	true	505	TRA	TRAV7-5		TRAJ12	TRAC
AAACCTGCAGATGAGC-1	true	AAACCTGCAGATGAGC-1_contig_2	true	599	TRB	TRBV13-3		TRBJ1-4	TRBC1
AAACCTGCAGGACGTA-1	true	AAACCTGCAGGACGTA-1_contig_1	true	523	TRA	TRAV13-4-DV7		TRAJ33	TRAC
AAACCTGCAGGACGTA-1	true	AAACCTGCAGGACGTA-1_contig_2	true	688	TRB	TRBV19	TRBD1	TRBJ1-3	TRBC1
AAACCTGGTAAACCTC-1	true	AAACCTGGTAAACCTC-1_contig_1	true	530	TRA	TRAV6N-7		TRAJ42	TRAC
AAACCTGGTAAACCTC-1	true	AAACCTGGTAAACCTC-1_contig_2	true	590	TRB	TRBV13-3		TRBJ1-3	TRBC1
AAACCTGGTACACCGC-1	true	AAACCTGGTACACCGC-1_contig_1	true	596	TRB	TRBV3		TRBJ1-1	TRBC1
AAACCTGGTACACCGC-1	true	AAACCTGGTACACCGC-1_contig_2	true	649	TRA	TRAV17		TRAJ42	TRAC
AAACCTGTCACCAGGC-1	true	AAACCTGTCACCAGGC-1_contig_1	true	552	TRB	TRBV16		TRBJ1-3	TRBC1
AAACCTGTCACCAGGC-1	true	AAACCTGTCACCAGGC-1_contig_2	true	541	TRA	TRAV8D-1		TRAJ27	TRAC
AAACCTGTCCGAGCCA-1	true	AAACCTGTCCGAGCCA-1_contig_1	true	518	TRB	TRBV26		TRBJ2-2	TRBC2
AAACCTGTCCGAGCCA-1	true	AAACCTGTCCGAGCCA-1_contig_2	true	540	TRA	TRAV8-1		TRAJ30	TRAC

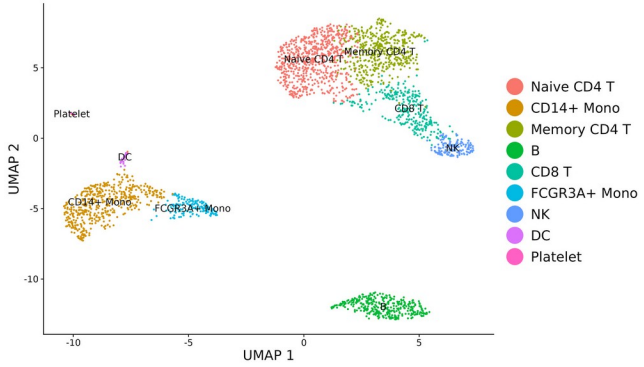
fwr4	fwr4_nt	reads	umis	raw_clonotype_id	raw_consensus_id	exact_subclonotype_id
GPGTRLTVL	GGACCAGGGACACGACTCACCGTCCTAG	13015	23	clonotype54	clonotype54_consensus_1	1
GIGTRVLVRP	GGAATCGGAACCAGGGTGCTGGTCAGGCCAG	3498	11	clonotype54	clonotype54_consensus_2	1
GSGTRLLVSP	GGAAGTGGGACTCGATTGCTGGTAAGCCCTG	10814	23	clonotype221	clonotype221_consensus_2	2
GHGTKLSVL	GGTCATGGAACCAAGCTGTCTGTCCTGG	13070	30	clonotype221	clonotype221_consensus_1	2
GSGTKLIIKP	GGCTCTGGGACCAAGCTAATTATAAAGCCAG	9185	18	clonotype72	clonotype72_consensus_2	1
GEGSRLIVV	GGAGAAGGAAGCCGGCTCATTGTTGTAG	3818	10	clonotype72	clonotype72_consensus_1	1
GKGTKLSVKS	GGGAAAGGCACTAAACTCTCTGTTAAATCAA	7007	17	clonotype7	clonotype7_consensus_2	1
GEGSRLIVV	GGAGAAGGAAGCCGGCTCATTGTTGTAG	10008	24	clonotype7	clonotype7_consensus_1	1
GKGTRLTVV	GGTAAAGGAACCAGACTCACAGTTGTAG	3477	11	clonotype14	clonotype14_consensus_1	3
GKGTKLSVKS	GGGAAAGGCACTAAACTCTCTGTTAAATCAA	5128	11	clonotype14	clonotype14_consensus_3	3
GEGSRLIVV	GGAGAAGGAAGCCGGCTCATTGTTGTAG	31883	71	clonotype774	clonotype774_consensus_1	1
GDGTVLTVKP	GGGGATGGGACCGTGCTCACAGTGAAGCCAA	7618	18	clonotype774	clonotype774_consensus_2	1
GEGSKLTVL	GGTGAAGGCTCAAAGCTGACAGTGCTGG	6449	11	clonotype685	clonotype685_consensus_1	1
GKGTHLHVLP	GGAAAAGGGACACATCTTCATGTTCTCCCTA	2390	4	clonotype685	clonotype685_consensus_2	1
GDGTVLTVKP	GGGGATGGGACCGTGCTCACAGTGAAGCCAA	9301	26	clonotype189	clonotype189_consensus_2	1
GEGSKLTVL	GGTGAAGGCTCAAAGCTGACAGTGCTGG	7335	18	clonotype189	clonotype189_consensus_1	1

Визуализация Single-cell

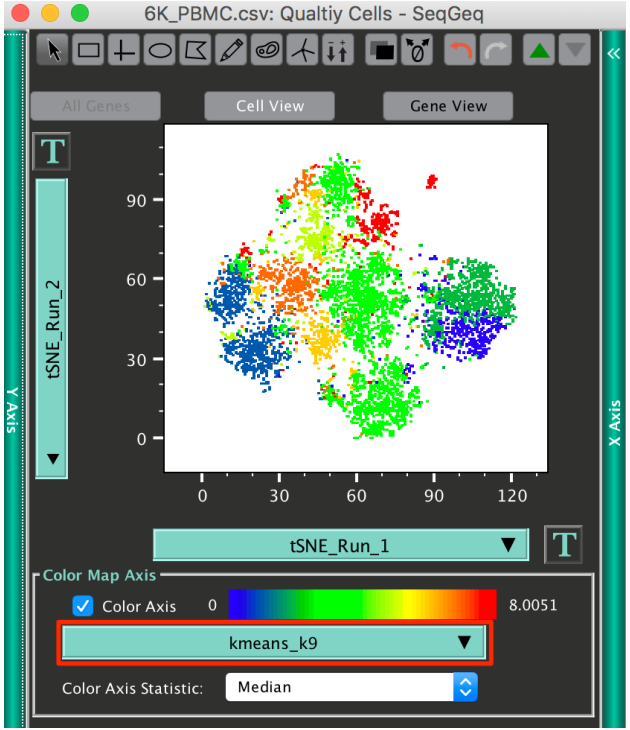
Loupe Browser



Seurat



SeqGeq



5’-RACE (MiLaboratories)

Универсальный адаптер

UMI-Баркод

рибоG

5' -AGATGUGTAUAAGAGACAGNNNNUNNNNUNNNNUCTT(rG)$_4$ -3'

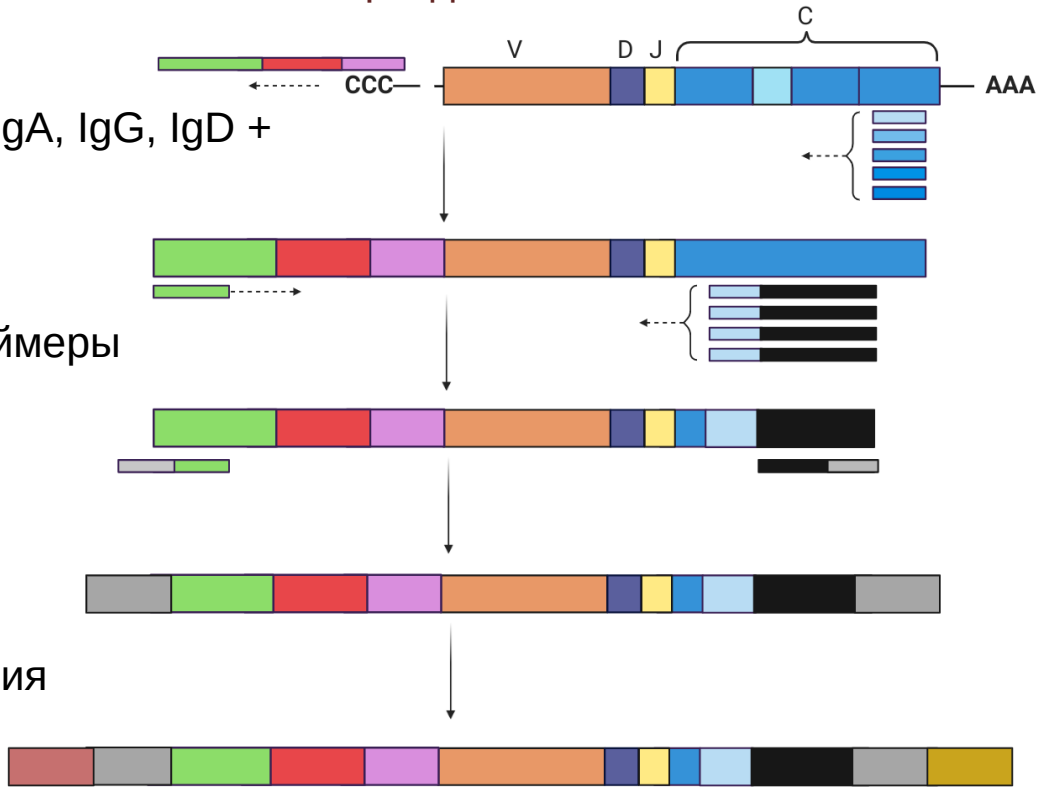
Урацил для разрушения остатков баркода

Праймеры на константный регион IgM, IgE, IgA, IgG, IgD + template switch

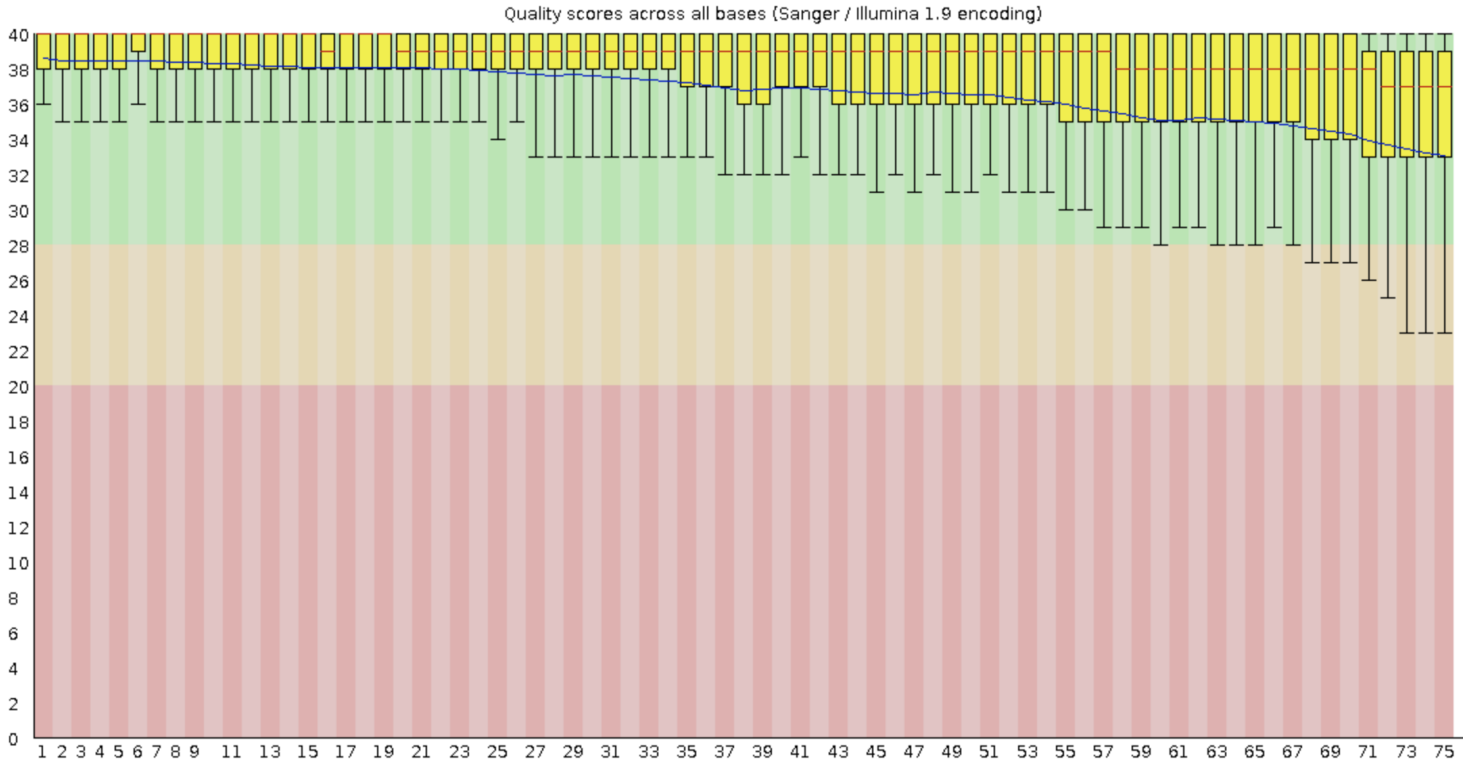
Универсальный праймер + вложенные праймеры

Добавление баркодов

Лигирование адапторов для секвенирования



Молекулярное баркодирование



Инструменты анализа TCR/BCR

Repertoire sequence analysis tools.

Tools	Purpose
IgBLAST IMGT/HighV-QUEST MiXCR TRUST	Bulk Sequence reconstruction
TRAPeS TraCeR VDJPuzzle BASIC BraCeR	Single cell Sequence reconstruction
VDJtools Immcantation Vidjil ASAP ARGalaxy bcRep Immunarch Sumrep	General repertoire analysis
DiVE RDI RECOLD	Specialized in diversity analysis
OLGA IgoR SONIA vampire	Generative model of VDJ recombination

Antibody docking methods.

Tools	Docking mode
ClusPro	Have Ab specific mode
SnugDock/ Rosseta	Have Ab specific mode
FRODOCK2.0	Have Ab specific mode
PatchDock/ FireDock	Have Ab specific mode
HADDOCK2.2	Not Ab specific mode
ZDOCK	Not Ab specific mode
SwarmDock	Not Ab specific mode
LightDock	Not Ab specific mode
pyDockWeb/ pyDock	Not Ab specific mode
HDOCK	Not Ab specific mode
HexServer	Not Ab specific mode
ATTRACT	Not Ab specific mode
GRAMM-X	Not Ab specific mode

BCR or TCR 3D modeling tools.

Tools	BCR	TCR
Repertoire Builder	Yes	Yes
PigsPro	Yes	No
Rosetta Antibody	Yes	No
ABodyBuilder	Yes	No
LYRA	Yes	Yes
TCRpMHCmodels	No	Yes

https://pubmed.ncbi.nlm.nih.gov/32802272/

IgBLAST

NIH U.S. National Library of Medicine | NCBI National Center for Biotechnology Information | Sign in to NCBI

IGBLAST

A tool for immunoglobulin (IG) and T cell receptor (TR) V domain sequences

Documentation: Introduction Reference FAQs Stand-alone IgBLAST Ig Germline Genes Other Resources

Analyze immunoglobulin (Ig) sequences | Analyze T cell receptor (TR) sequences

Reset page Save search parameters Retrieve recent results

Enter Query Sequence

Enter sequence(s) Clear

Or, upload local sequence file

Germline gene databases

Organism for query sequence

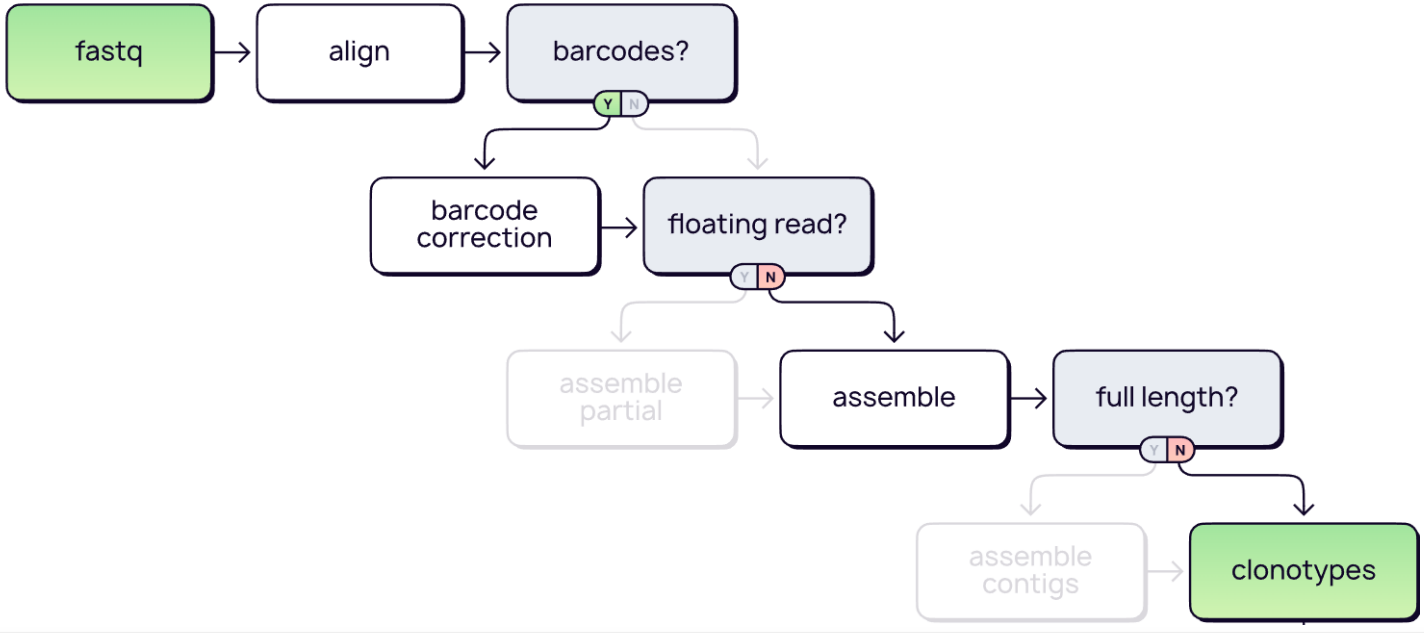
Germline V gene Database IMGT human V genes (F+ORF+in-frame P)

- IMGT human V genes (F+ORF+in-frame P)
- NCBI human V genes
- IMGT human V genes (F+ORF)
- IMGT human V genes (In-frame P)
- IMGT human V genes (F+ORF+in-frame P) including orphons
- IMGT human V genes (F+ORF) including orphons
- IMGT human V genes (In-frame P) including orphons
- NCBI human V genes (old)
- Custom

Germline D gene Database IMGT human D genes (F+ORF)

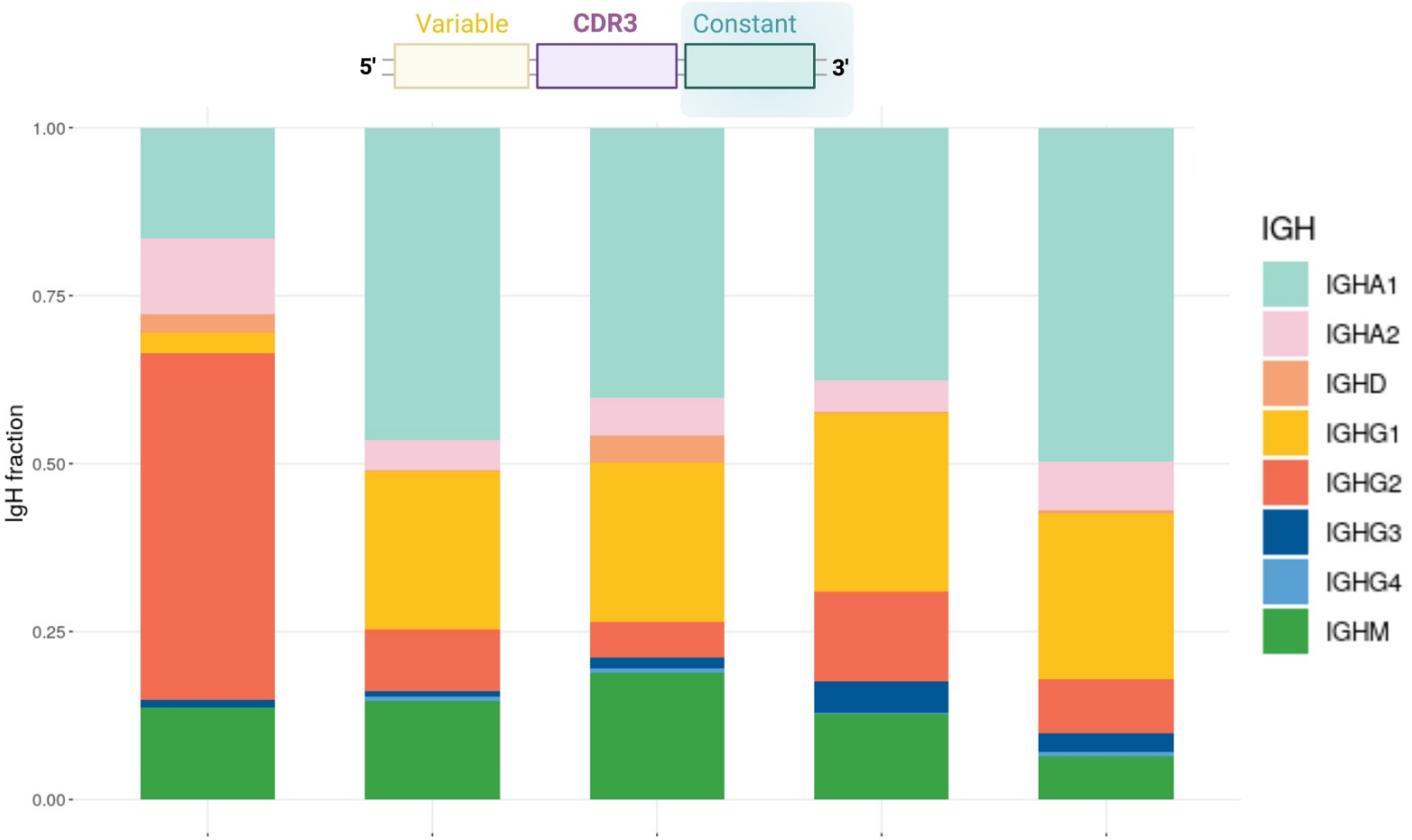
Germline J gene Database IMGT human J genes (F+ORF)

Получение данных

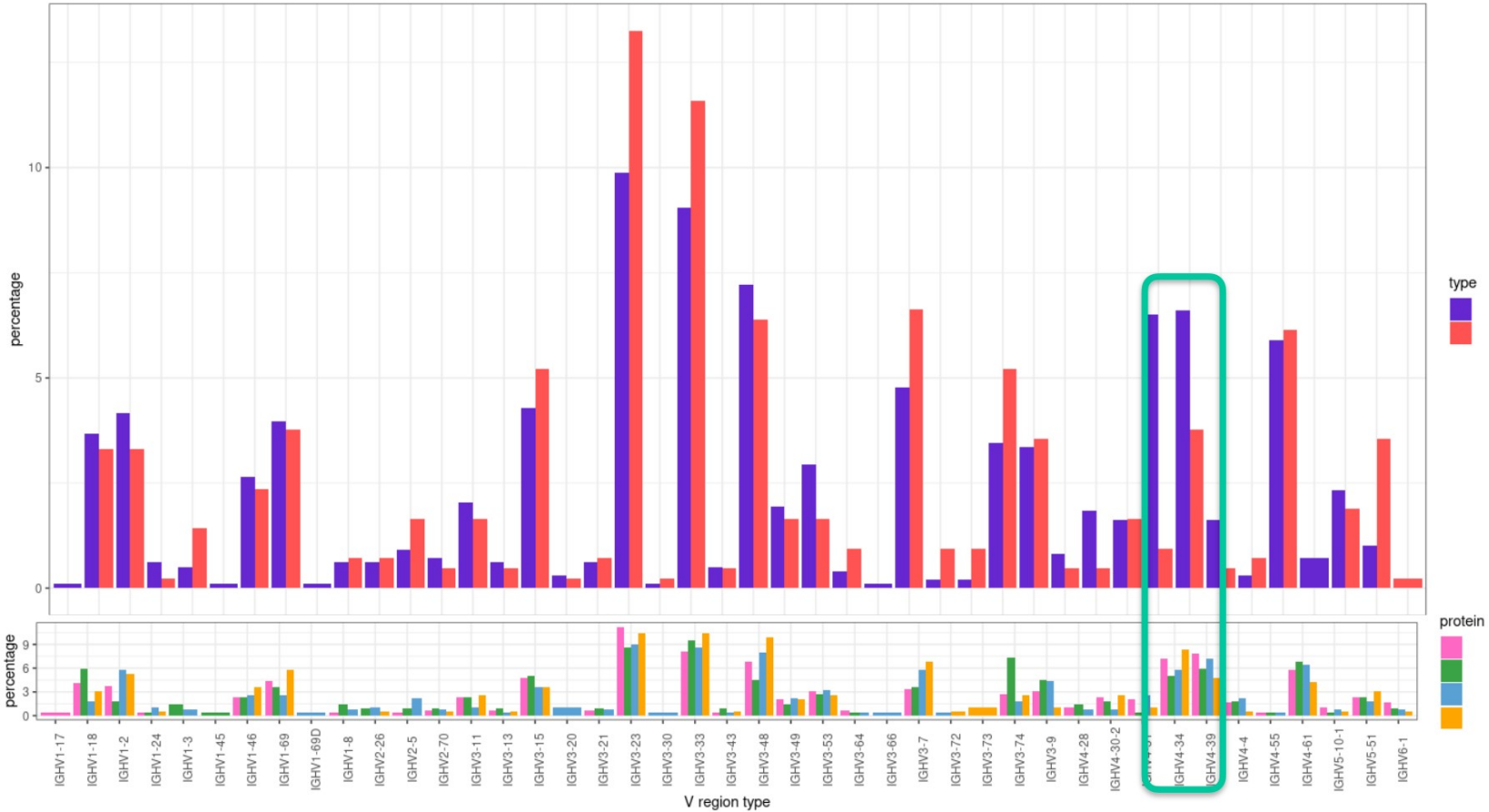


	cloneCount	cloneFraction	targetSequences	allVHitsWithScore	allDHitsWithScore	allJHitsWithScore	allCHitsWithScore	aaSeqImputedCDR3
0	282.0	0.194617	TTTCTGCTGGGTGCGACAGGCCCCTGGACTCGGACTCGAGTGGAT,...	IGHV1-69*00(90.3),IGHV1-69D*00(89.3)	IGHD7-27*00(35),IGHD3-16*00(30)	IGHJ5*00(54),IGHJ4*00(53)	IGHG1*00(155.3),IGHG3*00(141.4)	CARDLNRPIALGDVHW
1	126.0	0.086957	CCGAAACTGGGTCCGCCAGCCCCCAGGAAAGGGGCTGGAGTGGATT...	IGHV4-34*00(197.6)	IGHD6-19*00(60)	IGHJ4*00(54.2)	IGHG3*00(21.7)	CATDSSSGWYW
2	116.0	0.080055	AACCCACACAGACCCTCACGCTGACCTGCACCTTCTCTGGGTTCTC...	IGHV2-5*00(144.1)	IGHD7-27*00(50),IGHD5-24*00(45)	IGHJ4*00(67.5)	IGHM*00(89.7)	CVYNYWGSSLDYW
3	95.0	0.065562	TGGTACAGCCTGGGGGGTCCCTGAGACTCTCCTGTGCAGCCTCTGG...	IGHV3-23*00(156.2)	IGHD2-21*00(54)	IGHJ4*00(69.7)	IGHG1*00(112.9),IGHG3*00(104.1)	CAKDRDRVVVSANLDYW
4	70.0	0.048309	CGTGGTACAGCCTGGGGGGTCCCTGAGACTCTCCTGTGCAGCCTCT...	IGHV3-43*00(242.8)	IGHD4-23*00(50),IGHD4-17*00(45)	IGHJ6*00(53.7)	IGHG1*00(28)	CAKDSNYGGYYYGMDVW

Анализ константного региона

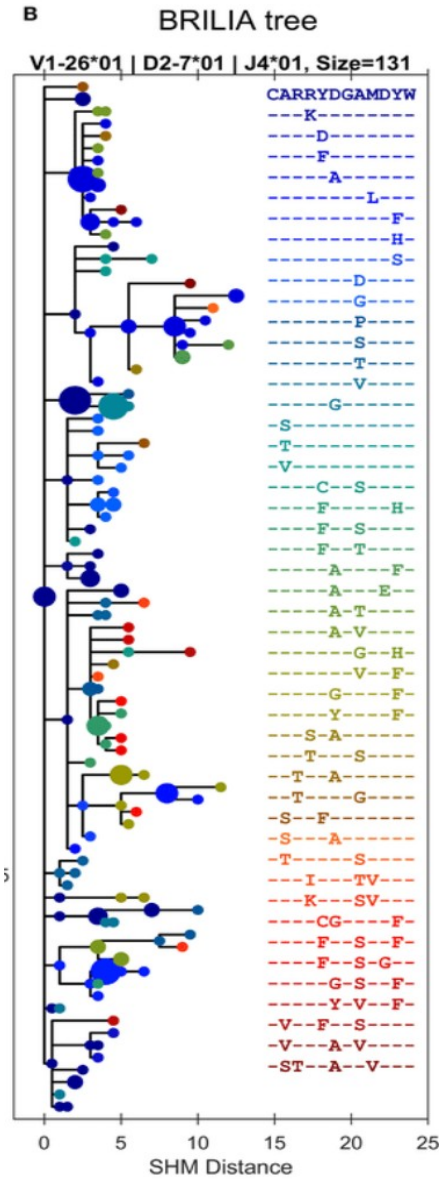


V-segment usage



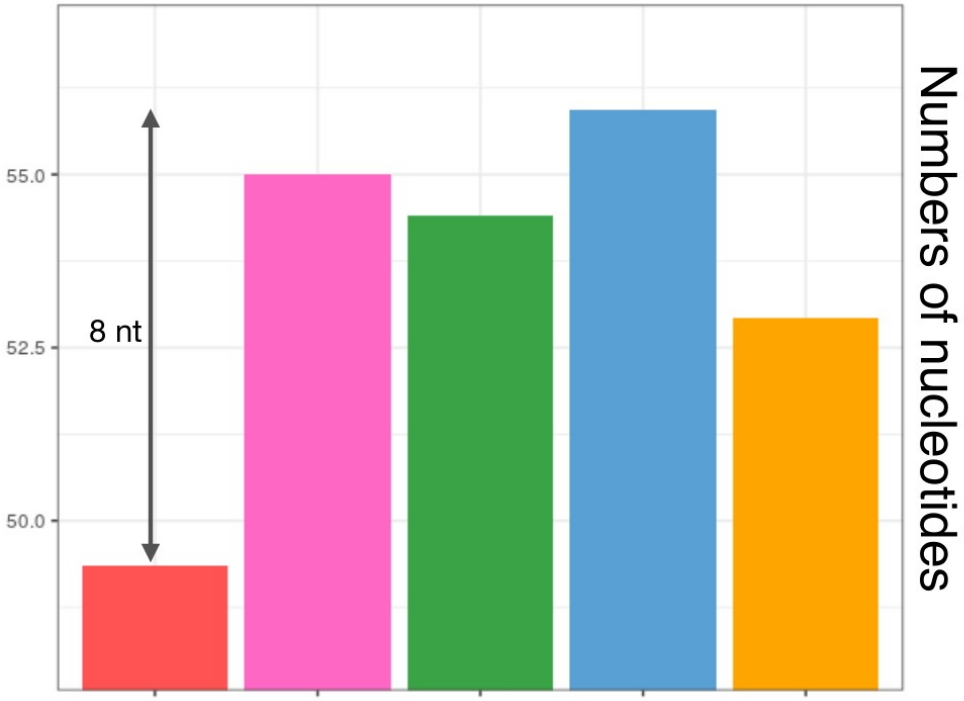
Деревья гипермутаций

https://www.researchgate.net/publication/312479270_BRILIA_Integrated_Tool_for_High-Throughput_Annotation_and_Lineage_tree_Assembly_of_B-Cell_Repertoires

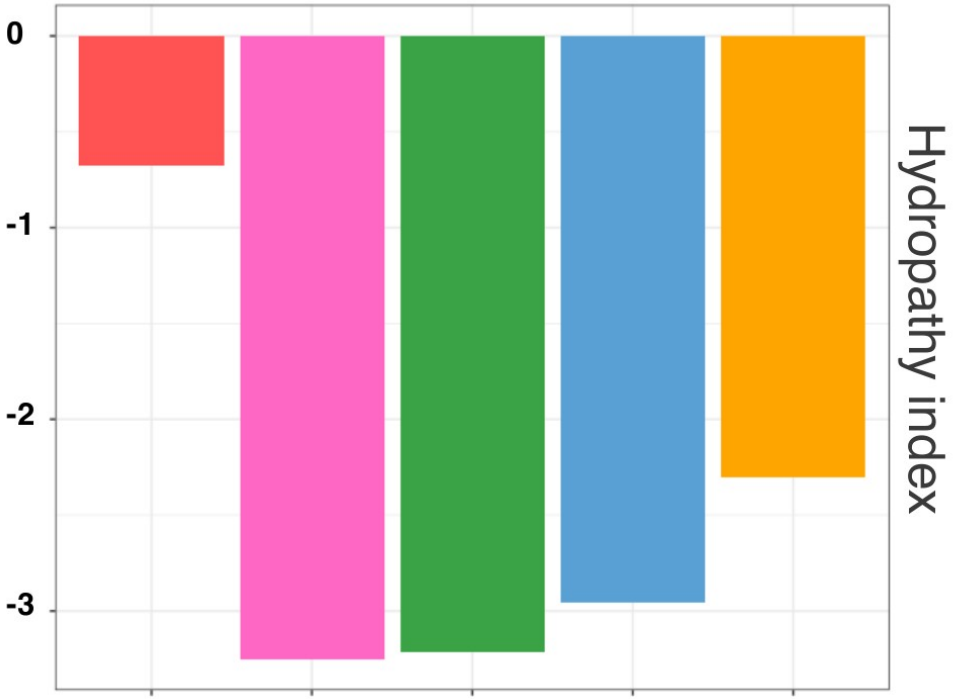


Детальный анализ CDR3

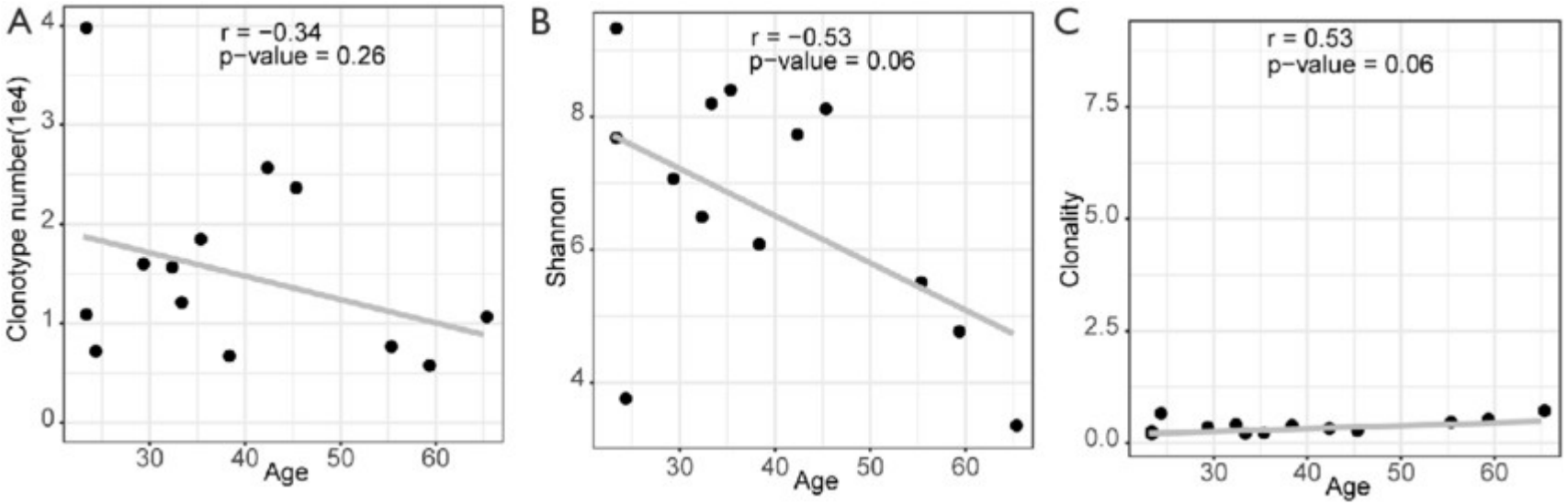
Mean ntCDR3 length



CDR3 hydropathy (5 central residues)



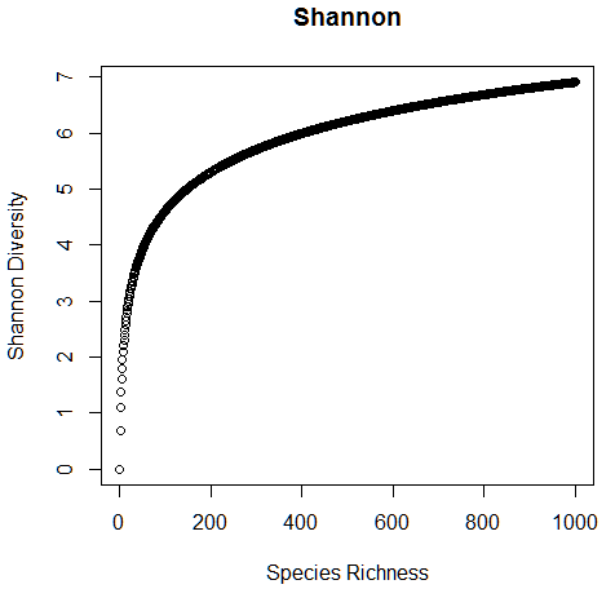
Оценка разнообразия репертуара



$$H' = -\sum_{i=1}^{R} p_i \ln p_i$$

H’ - индекс разнообразия Шеннона;
R - количество клонов;
Pi - доля конкретной последовательности в популяции.

Оценка разнообразия репертуара

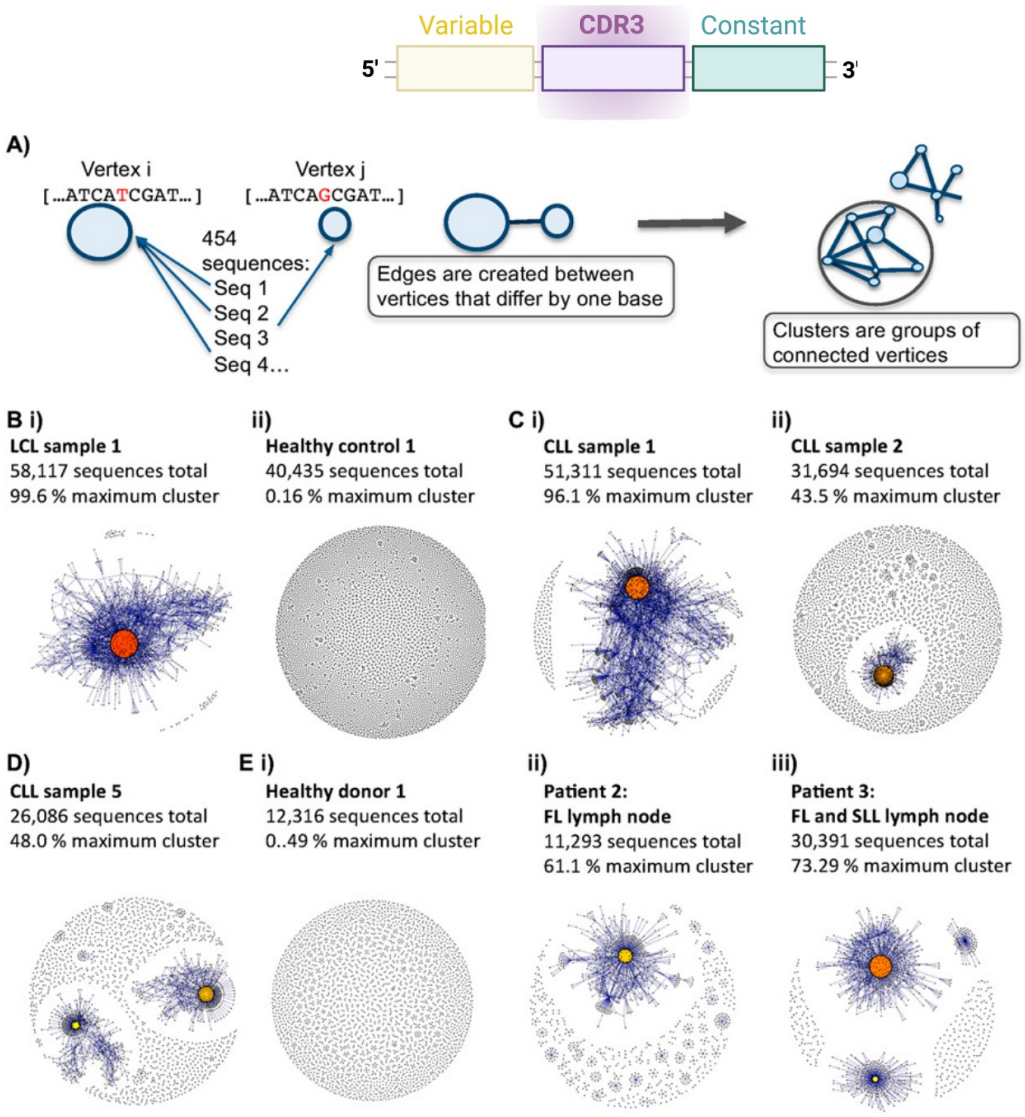


$$-\frac{1}{\log(D)}\sum f_i \log(f_i)$$

D - число клонотипов в образце

Кластеризация CDR3

chronic lymphocytic leukemia (CLL)
follicular lymphoma (FL)
small lymphocytic lymphoma (SLL)
human lymphoblastoid cell lines (LCLs)

Network properties derived from deep sequencing of human B-cell receptor repertoires delineate B-cell populations

https://www.semanticscholar.org/paper/Network-properties-derived-from-deep-sequencing-of-Bashford-Rogers-Palser/4256d7e915f4def83018fc55cb9f3fd7264b3a02