Plateforme IMGT®
Bases de données anticorps
http://www.imgt.org

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IMGT

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Module Anticorps monoclonaux
Parcours Immunotechnologies et Biothérapies
UPMC, Paris, 12 novembre 2012

IMGT®: the adaptive immune response

http://www.imgt.org

Vertebrates

Immunoglobulin (IG)

T lymphocyte

B lymphocyte

peptide

T cell receptor (TR)

Major histocompatibity (MH)

Trimolecular complex
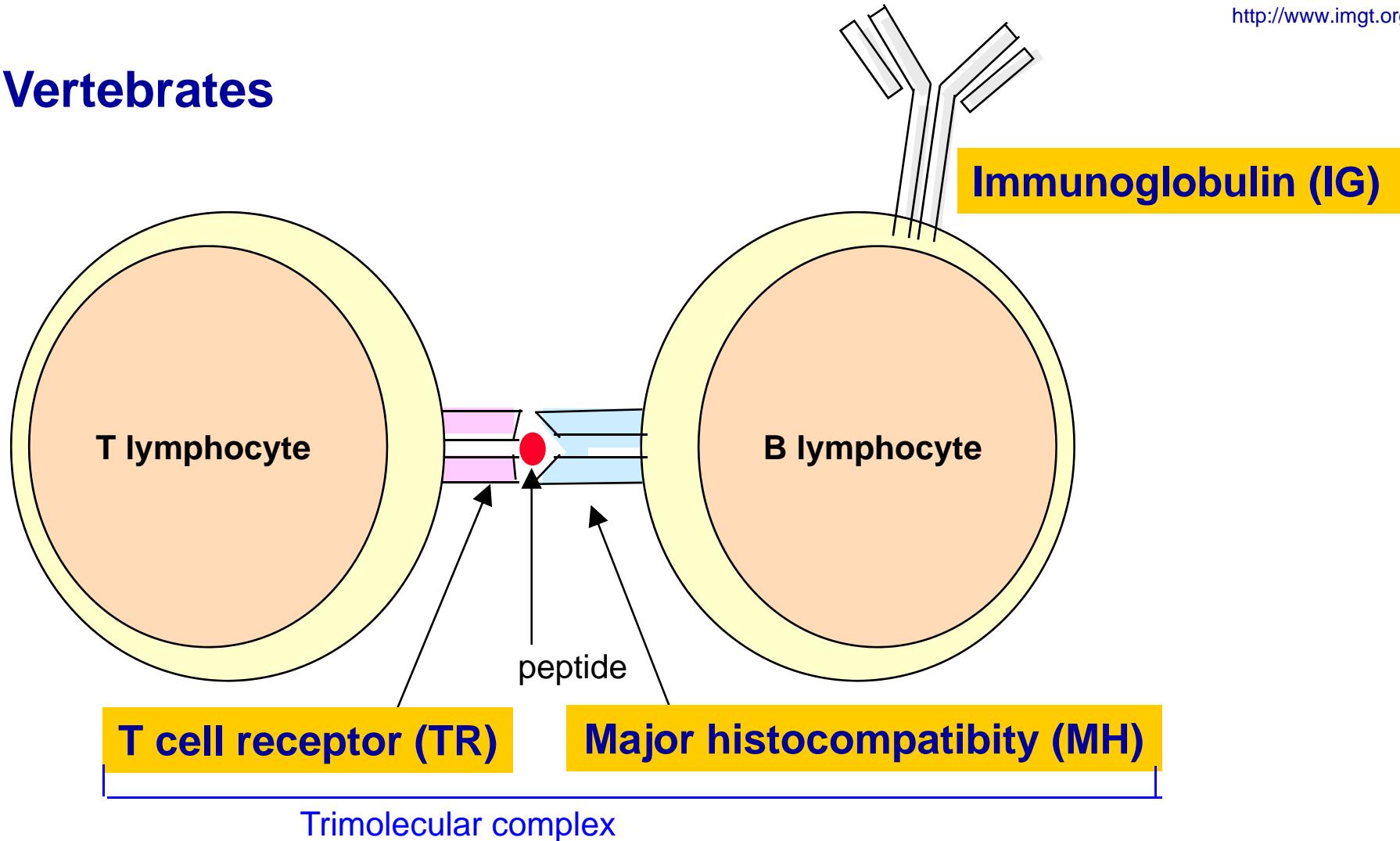
Immunoglobulin (IG) synthesis

150 FUNCTIONAL IG GENES
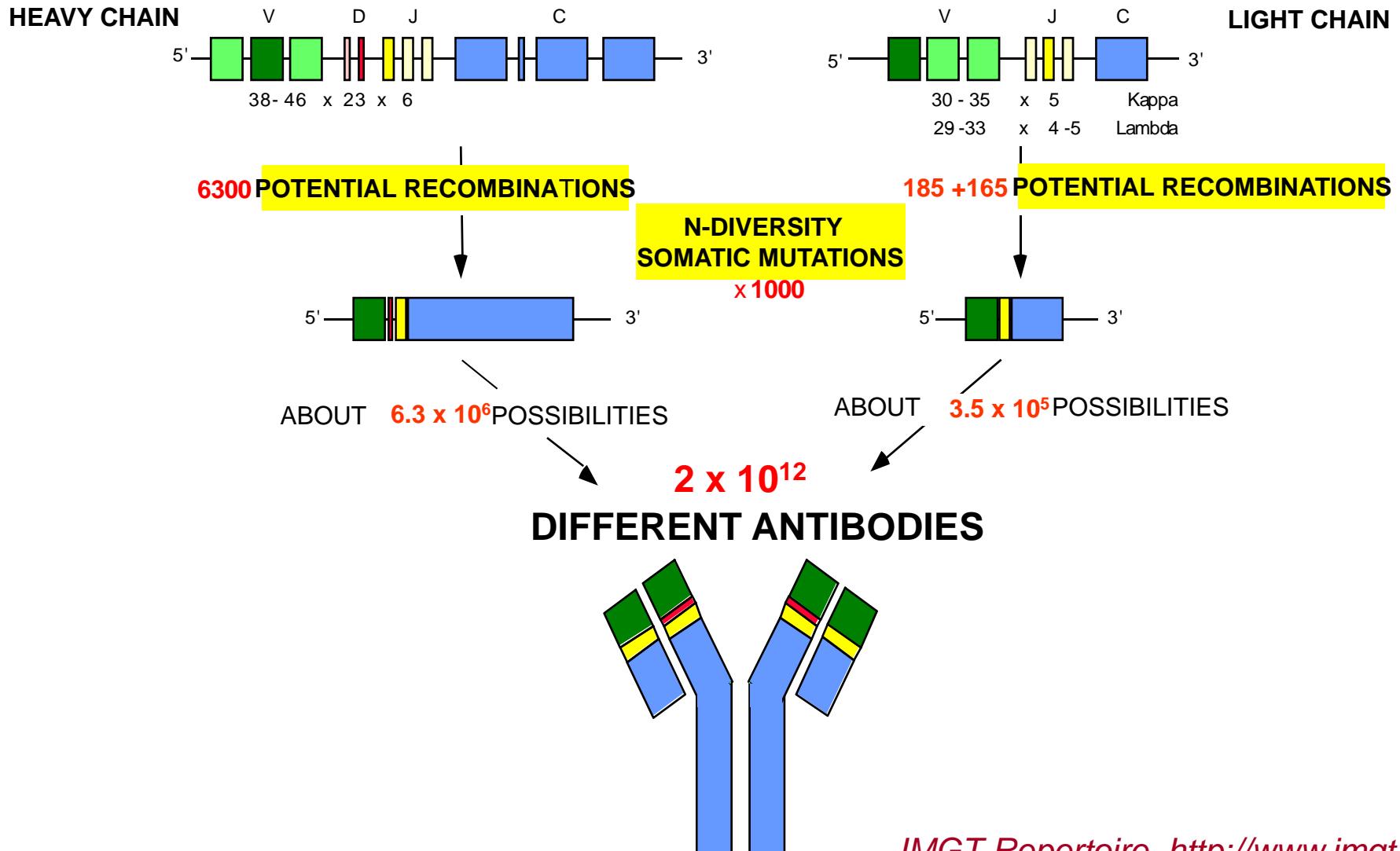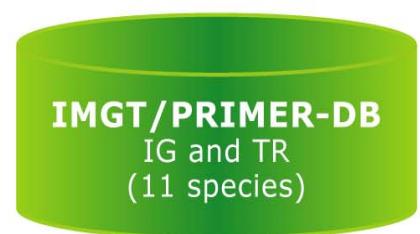
HEAVY CHAIN

5' — V — D — J — C — 3'

38 - 46 x 23 x 6

LIGHT CHAIN

5' — V — J — C — 3'

30 - 35 x 5 Kappa
29 -33 x 4 -5 Lambda

6300 POTENTIAL RECOMBINATIONS

185 +165 POTENTIAL RECOMBINATIONS

N-DIVERSITY SOMATIC MUTATIONS x **1000**

5' — — 3'

5' — — 3'

ABOUT **6.3 x 10^6** POSSIBILITIES

ABOUT **3.5 x 10^5** POSSIBILITIES

2 x 10^12
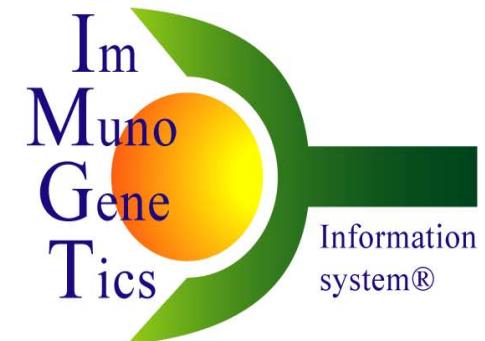
DIFFERENT ANTIBODIES

IMGT standards based on IMGT-ONTOLOGY

IMGT-ONTOLOGY

http://www.imgt.org

IMGT-ONTOLOGY seven axioms:

To share, reuse and represent knowledge in Immunogenetics and Life Sciences

IDENTIFICATION

OBTENTION

CLASSIFICATION

ORIENTATION

DESCRIPTION

LOCALIZATION

NUMEROTATION
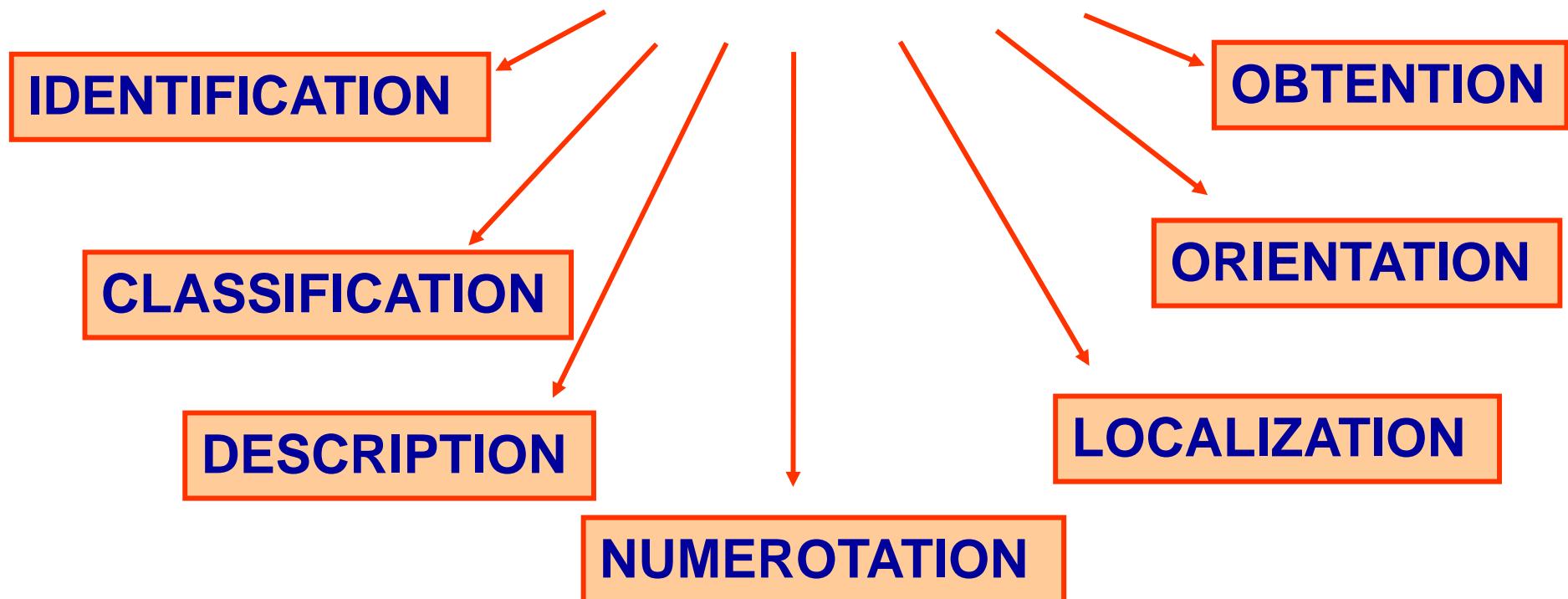
Giudicelli and Lefranc, Bioinformatics (1999)

CLASSIFICATION axiom
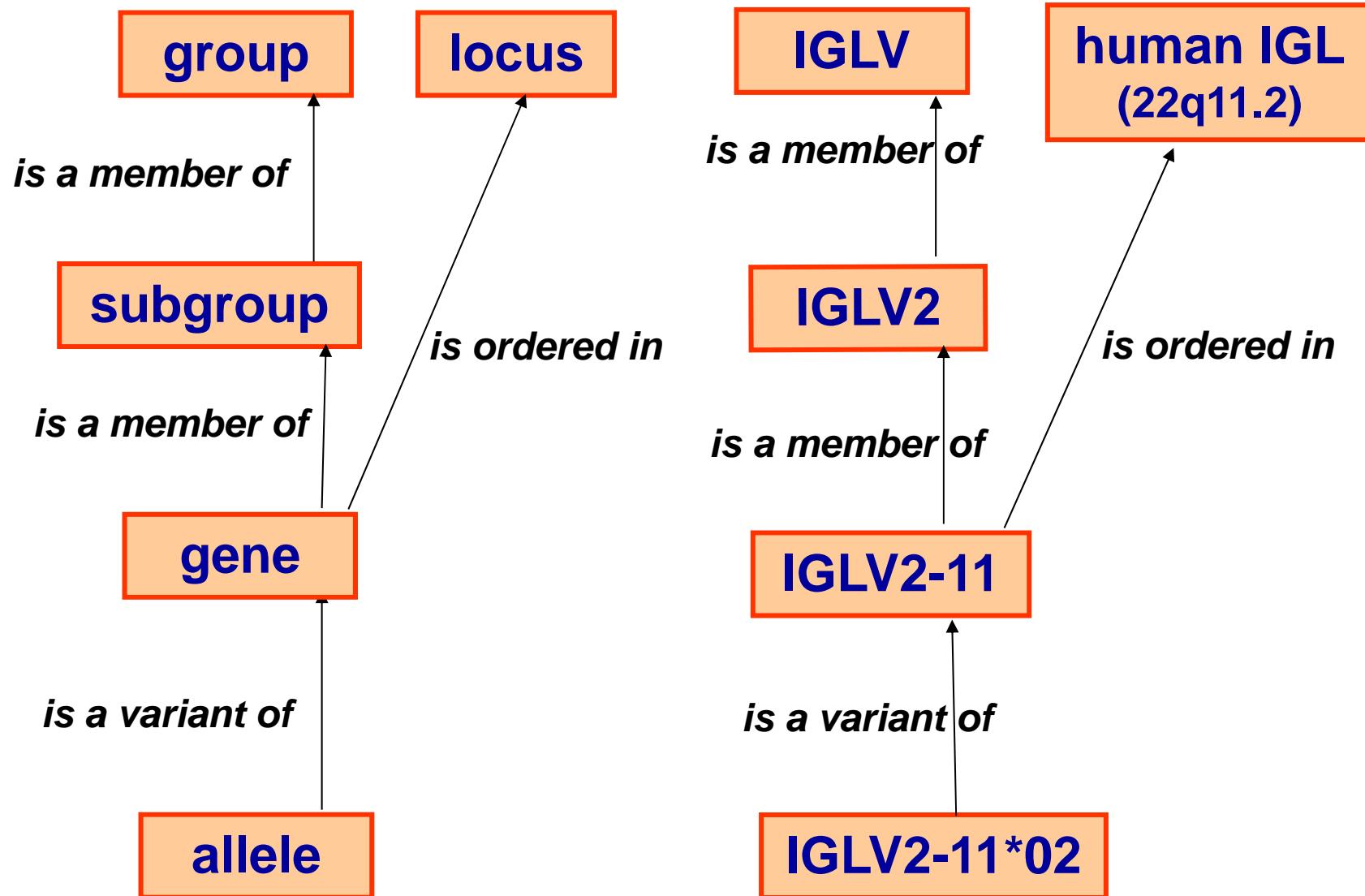
http://www.imgt.org

group

locus

subgroup

is a member of

gene

is a member of

is ordered in

allele

is a variant of

IGLV

human IGL
(22q11.2)

is a member of

IGLV2

IGLV2-11

is a member of

is ordered in

IGLV2-11*02

is a variant of

Concepts of CLASSIFICATION

1. The IMGT-ONTOLOGY main concepts of classification
   - include 'group', 'subgroup', 'gene', 'allele'.
   - have allowed to set up the nomenclature of the immunoglobulin (IG) and T cell receptor (TR) genes (V, D, J, C genes).

2. IMGT gene names have been approved by the HUGO Nomenclature Committee (HGNC) in 1999.

3. New alleles are validated by the WHO-IUIS/IMGT nomenclature committee and entered in IMGT/GENE-DB.

4. IMGT/GENE-DB is the international reference database for IG and TR genes (direct links from NCBI Entrez Gene) and alleles.

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DESCRIPTION axiom

PROTOTYPE for a V-GENE
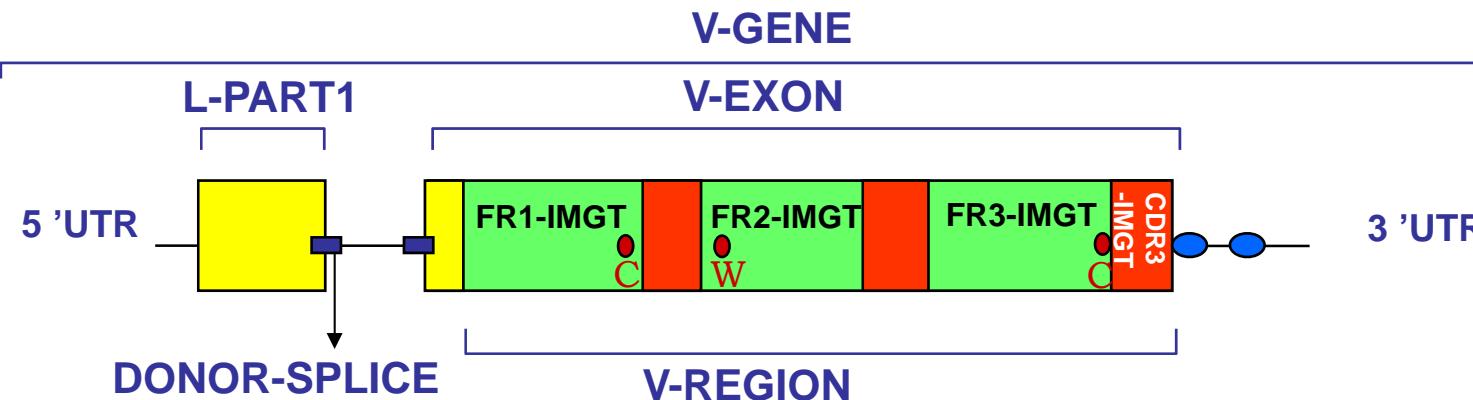
Label 1	Label 2	Relations entre Labels
V-GENE	V-EXON	
FR3-IMGT	CDR3-IMGT	
L-PART1	DONOR-SPLICE	
V-REGION	FR1-IMGT	
V-REGION	CDR3-IMGT	

IMGT/LIGM-DB

http://www.imgt.org

IMGT/LIGM-DB Consultation module v3 - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

```
FH    Key                    Location/Qualifiers
FH
FT    L-V-D-J-C-SEQUENCE     <1..375>
FT                           /partial
FT                           /db_xref="taxon:9606"
FT                           /cell_type="B-cell hybridoma 2F7"
FT                           /IMGT_note="automatically annotated with IMGT tools"
FT                           /organism="Homo sapiens"
FT    V-D-J-REGION           1..375
FT                           /translation="QVHLVESGGAVFHPGRSLRLSRAASGFTFSSYGMHWVRQAP
FT                           AKGLEWVAVIWYDGSNKYYADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYYC
FT                           AKHVTIAAAGRRGAGMDVWGQGTTVTVSS"
FT    V-REGION               1..296
FT                           /allele="IGHV3-33*01, putative"
FT                           /gene="IGHV3-33"
FT                           /CDR_length="[8.8.18]"
FT                           /putative_limit="3' side"
FT                           /translation="QVHLVESGGAVFHPGRSLRLSRAASGFTFSSYGMHWVRQAP
FT                           AKGLEWVAVIWYDGSNKYYADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYYC
FT                           AK"
FT    FR1-IMGT               1..75
FT                           /AA_IMGT="1 to 26, AA 10 is missing"
FT                           /translation="QVHLVESGGAVFHPGRSLRLSRAAS"
FT    CDR1-IMGT              76..99
FT                           /AA_IMGT="27 to 34"
FT                           /translation="GFTFSSYG"
FT    FR2-IMGT               100..150
FT                           /AA_IMGT="39 to 55"
FT                           /translation="MHWVRQAPAKGLEWVAV"
FT    CONSERVED-TRP          106..108
FT    CDR2-IMGT              151..174
FT                           /AA_IMGT="56 to 63"
FT                           /translation="IWYDGSNK"
FT    FR3-IMGT               175..288
FT                           /AA_IMGT="66 to 104, AA 73 is missing"
FT                           /translation="YYADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYYC"
```

Done

D E S C R I P T I O N

167 356 sequences from 323 species

IMGT-ONTOLOGY:
286 IMGT labels for sequences
**285 IMGT labels for 3D structures**

Concepts of DESCRIPTION

http://www.imgt.org

1. The IMGT-ONTOLOGY concepts of description:
- comprise the standardized IMGT labels and their relations.
- have allowed to describe the IG (or antibody) and TR sequences and structures, whatever the receptor type, the chain type or the species.

2. IMGT labels are used in all IMGT® databases and tools for the description of:
- nucleotide and amino acid sequences (IMGT/LIGM-DB…)
- 2D and 3D structures (IMGT/3Dstructure-DB…).

3. Sequence Ontology (SO) includes IMGT labels.

4. IMGT® databases can be queried using labels (a big 'plus' compared to generalist databases).

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NUMEROTATION axiom

IMGT Collier de Perles

Based on the **IMGT unique numbering**
(first one in **1997**)

CDR-IMGT lengths
[8.10.12]
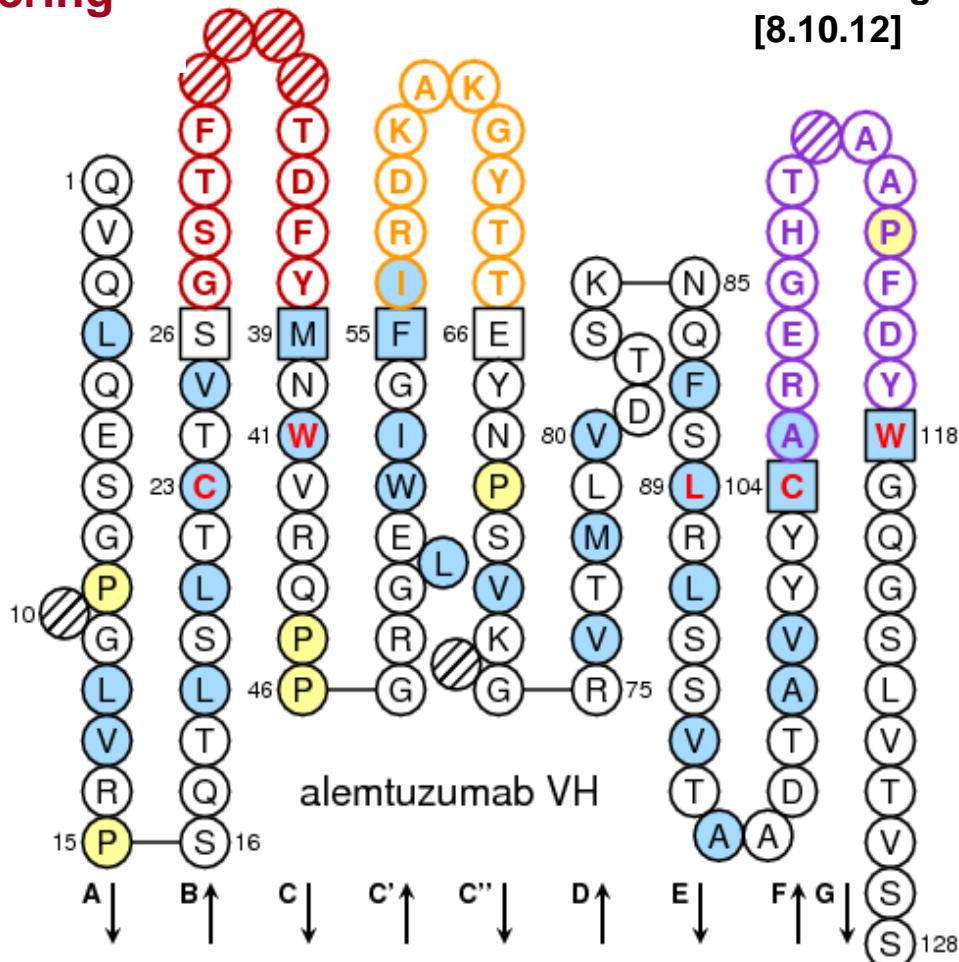
alemtuzumab VH

NUMEROTATION axiom

## IMGT Collier de Perles

Based on the **IMGT unique numbering**
(first one in **1997**)

- conserved AA (and codons)
are always at the **same positions**:

    23   1st-CYS
    41   CONSERVED-TRP
    89   hydrophobic
  104   2nd-CYS
  118   J-PHE, J-TRP

- delimitation of the **FR-IMGT**
and **CDR-IMGT** is standardized

- **CDR-IMGT lengths** are crucial
information
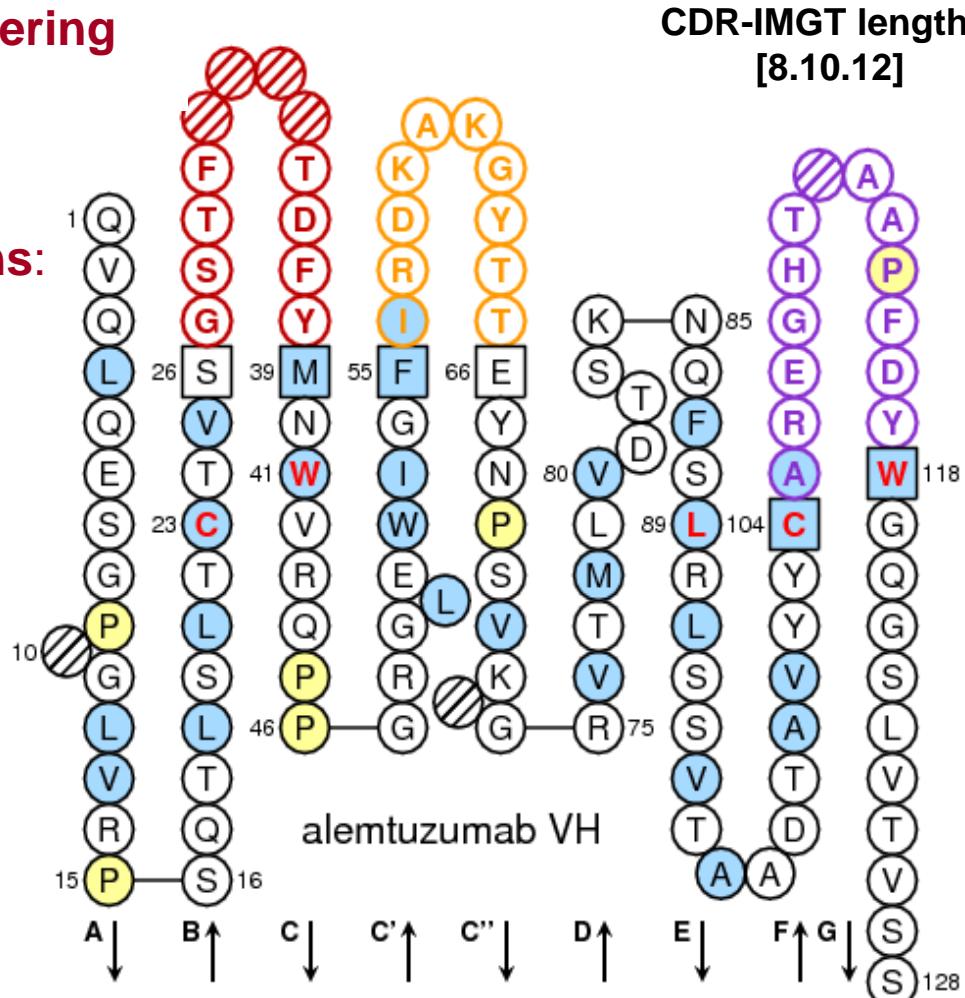
**CDR-IMGT lengths
[8.10.12]**

alemtuzumab VH

Lefranc et al. Dev. Comp. Immunol. 27, 55-77 (2003)

Concepts of NUMEROTATION

http://www.imgt.org

1. The IMGT-ONTOLOGY concepts of numerotation include:
- IMGT unique numbering
- IMGT Collier de Perles.

2. The concepts bridge the gap between sequences and 3D structures, at the amino acid (and codon) level, for:
- the variable domains (V-DOMAIN and V-LIKE-DOMAIN)
- the constant domains (C-DOMAIN and C-LIKE-DOMAIN).

4. The concepts are used for:
- mutations, polymorphisms
- CDR-IMGT lengths
- contact analysis, paratope definition.

5. WHO-INN programme requires the CDR-IMGT lengths for antibody.

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- contact analysis, paratope definition.

5. WHO-INN programme requires the CDR-IMGT lengths for antibody.

V-DOMAIN: VH and V-KAPPA

VH   V-KAPPA

V-D-J junction   V-J junction

Side view of the V-DOMAIN

VH   V-KAPPA

View from above the CDR-IMGT
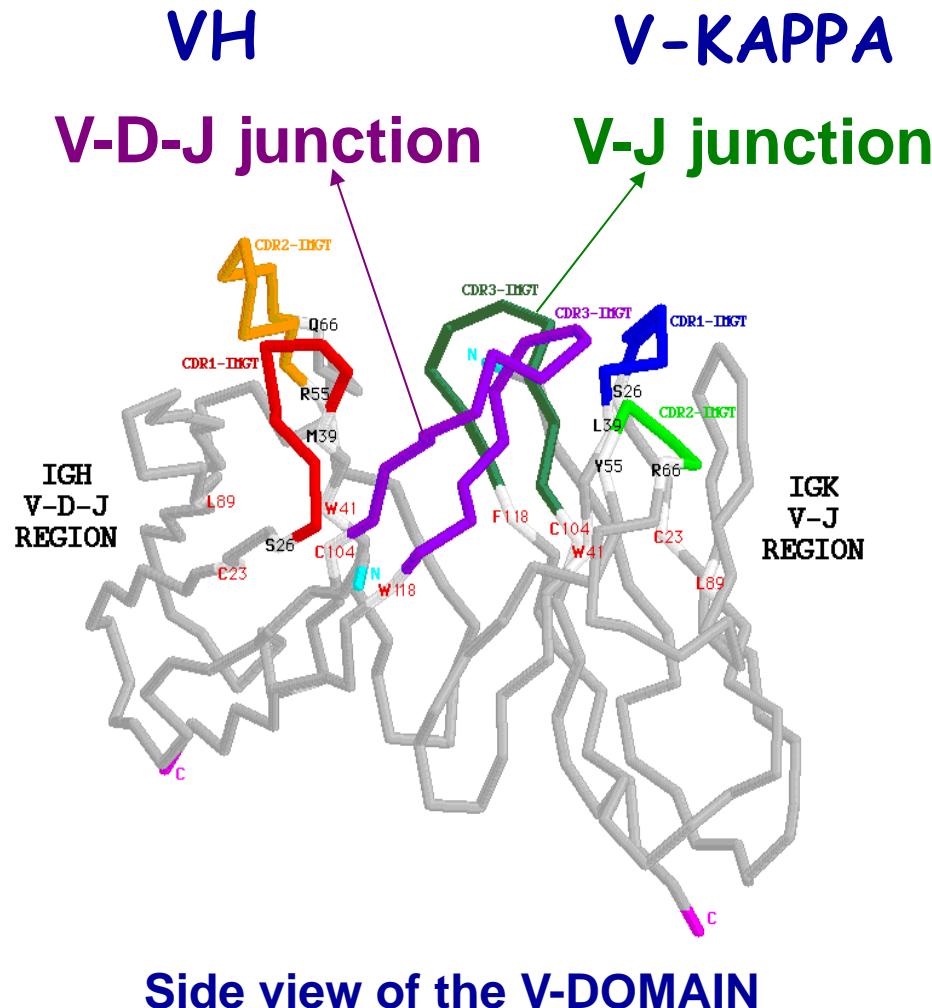
CDR: complementarity determining region
CDR3-IMGT (105-117)
V-D-J junction (104-118), V-J junction (104-118)

IMGT® http://www.imgt.org
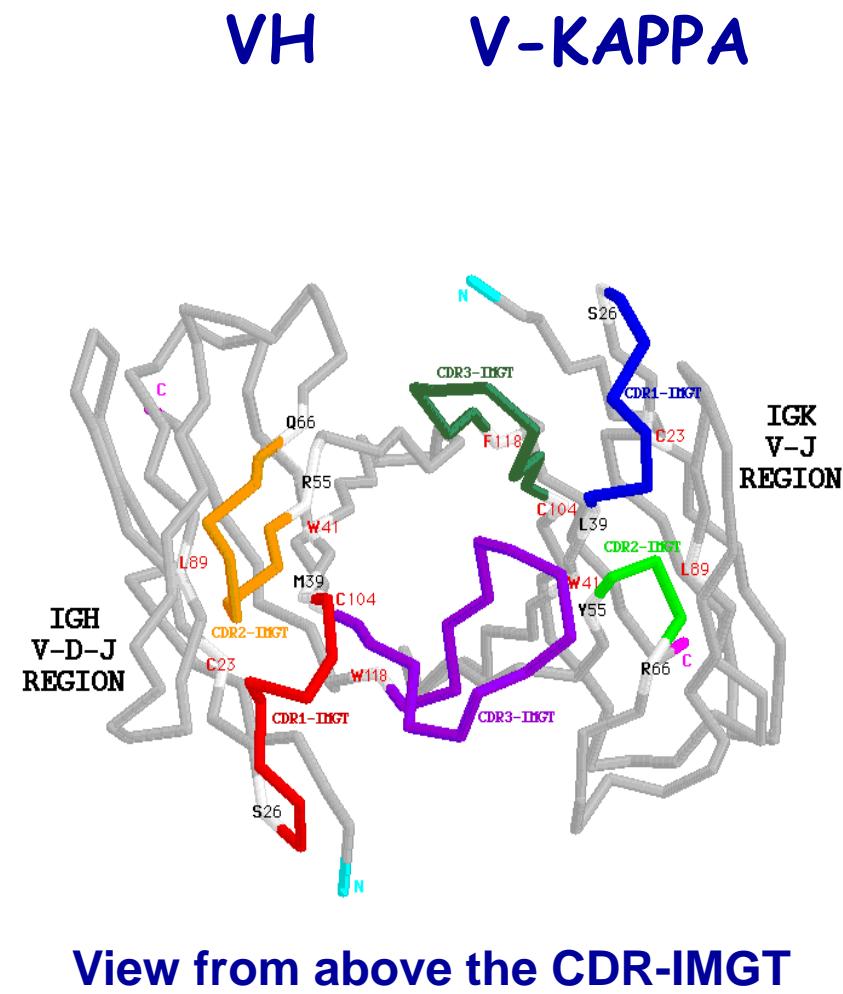
Immunoglobulin V-D-J generation of sequence diversity
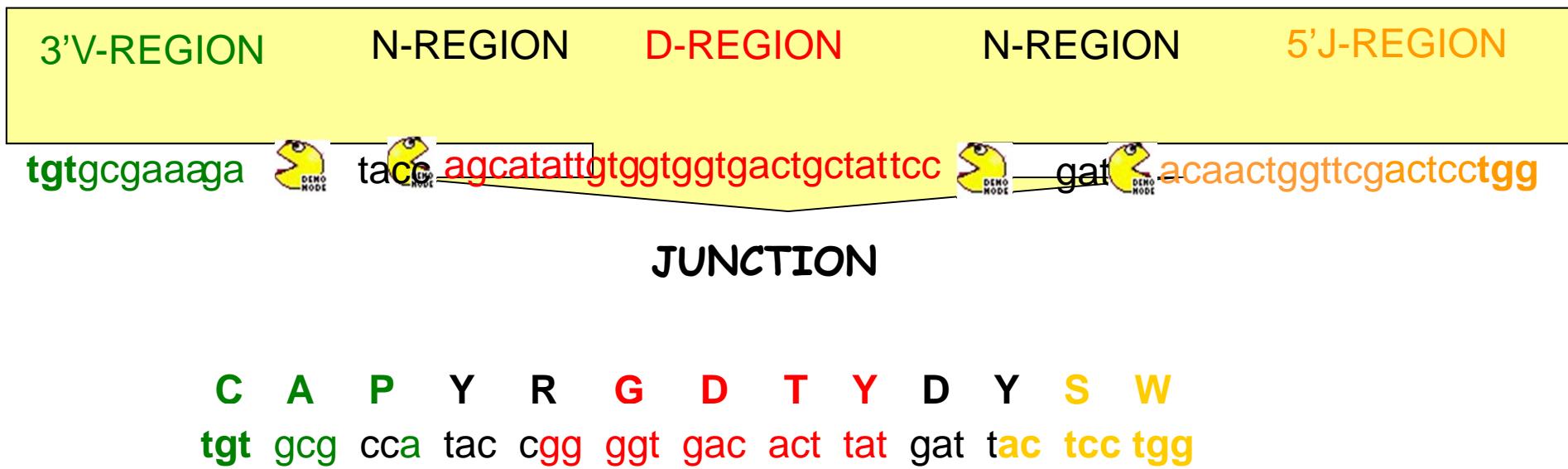
3'V-REGION	N-REGION	D-REGION	N-REGION	5'J-REGION

tgtgcgaaaga   tacc agcatattgtggtggtgactgctattcc   gat acaactggttcgactcctgg

JUNCTION

C A P Y R G D T Y D Y S W

tgt gcg cca tac cgg ggt gac act tat gat tac tcc tgg

IMGT/JunctionAnalysis: analysis of the IG and TR junctions

http://www.imgt.org

IMGT/JunctionAnalysis: analysis of the IG and TR junctions

The 11 IMGT physicochemical AA classes

'Volume' classes		'Hydropathy' classes								
	in Å³	Hydrophobic			Neutral			Hydrophilic		
Very large	189-228	F		W		Y				
Large	162-174	I L	M					K R		
Medium	138-154	V					H		E	Q
Small	108-117		C	P	T				D	N
Very small	60-90	A		G	S					
		Aliphatic	Sulfur		Hydroxyl		Basic		Acidic	Amide
					Uncharged		Charged			Uncharged
		Nonpolar				Polar				

Pommié et al. J. Mol Recognit. 17, 17-32 (2004)
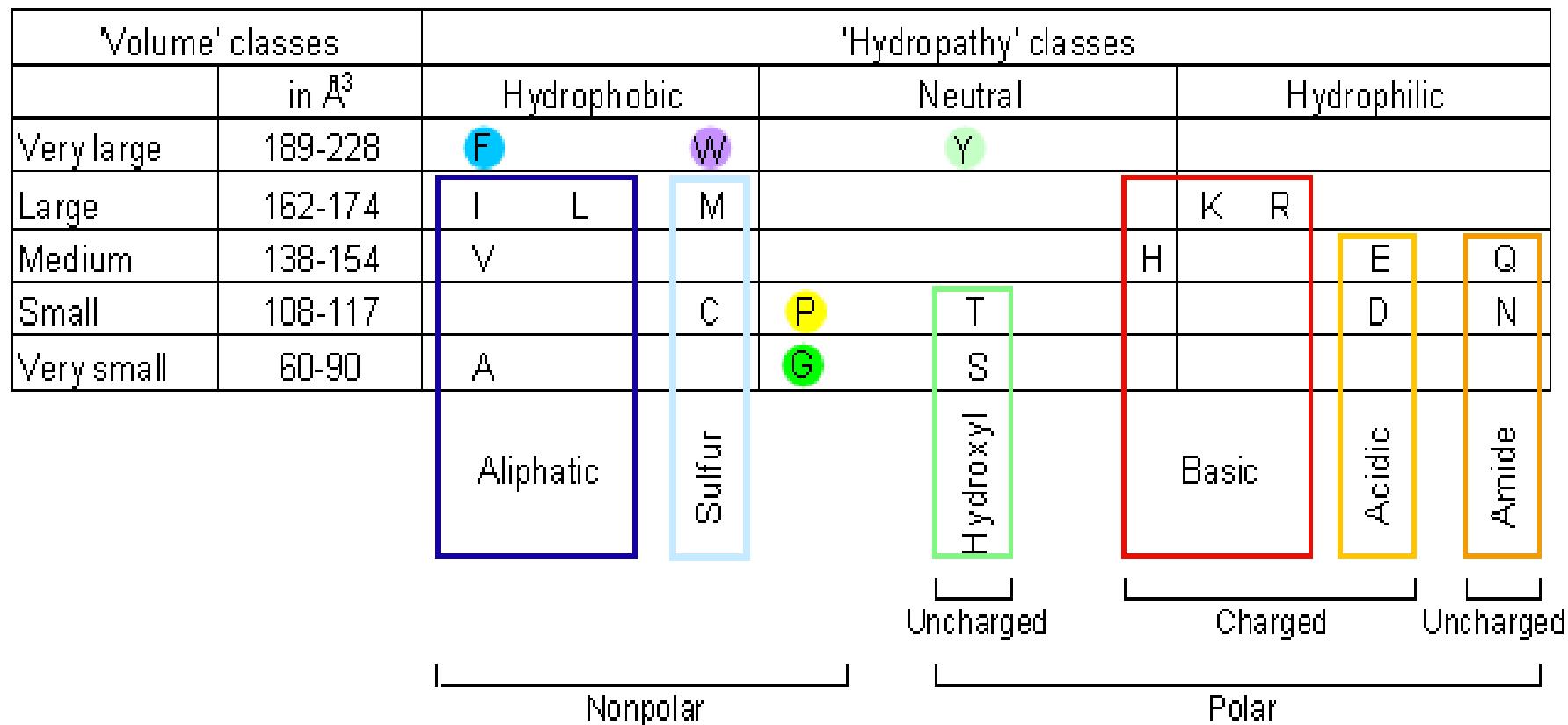
IMGT/JunctionAnalysis

Analysis of the IG and TR junctions

JUNCTION alignments with translation and IMGT AA classes

Click on mutated (underlined) amino acid to see the original one: [ ]

		104	105	106	107	108	109	110	111	111.1	111.2	111.3	112.3	112.2	112.1	112	113	114	115	116	117	118
		C	S	P	G	G	S	A	Y						Y	H	E	H	F	Q	Q	W
#1	AY393054	tgt	agt	ccc	ggg	ggt	agt	gct	tat	...	...	...	...	...	tac	cac	gaa	cac	ttc	cag	cag	tgg
		C	V	K	P	T	D	D	D	G				H	R	A	E	Y	F	Q	Y	W
#2	AY393055	tgt	gtg	aaa	ccc	acg	gat	gat	gat	ggc	...	...	...	cac	cgg	gct	gaa	tac	ttc	cag	tac	tgg
		C	S	P	G	G	S	A	Y						Y	H	E	D	F	Q	Q	W
#3	AY393058	tgt	agt	ccc	ggg	ggt	agc	gct	tat	...	...	...	...	...	tac	cac	gaa	gac	ttc	cag	cag	tgg
		C	S	P	G	G	S	A	Y						Y	H	E	H	F	Q	Q	W
#4	AY393072	tgt	agt	ccc	ggg	ggt	agt	gct	tat	...	...	...	...	...	tac	cac	gaa	cac	ttc	cag	cag	tgg
		C	A	R	Q	N	P	P	E	Y	S	G	A	Y	H	D	G	W	F	D	P	W
#5	AY393088	tgt	gcg	aga	caa	aac	ccc	ccc	gag	tat	agt	ggc	gca	tat	cat	gat	ggg	tgg	ttc	gac	ccc	tgg
		C	A	R	E	M	L	Y	G	S	G	G	Y	Y	P	P	D	A	F	E	L	W
#6	AY393089	tgt	gcg	aga	gag	atg	ctc	tat	ggt	tcg	ggg	ggt	tat	tac	ccc	cct	gat	gca	ttc	gag	ctc	tgg
		C	A	R	Q	N	P	P	E	Y	S	G	A	Y	H	D	G	W	F	D	P	W
#7	AY393091	tgt	gcg	aga	cag	aat	ccc	ccc	gag	tat	agt	ggc	gca	tat	cat	gat	ggg	tgg	ttc	gac	ccc	tgg
		C	A	R	E	M	L	Y	G	S	G	G	Y	Y	P	P	D	A	F	E	V	W
#8	AY393092	tgt	gcg	aga	gag	atg	ctc	tat	ggt	tcg	ggg	ggt	tat	tac	ccc	cct	gat	gca	ttc	gag	gtc	tgg
		C	A	R	Q	N	P	P	E	Y	S	G	A	Y	H	D	G	W	F	D	P	W
#9	AY393094	tgt	gcg	aga	cag	aac	ccc	ccc	gag	tat	agt	ggc	gca	tat	cat	gat	ggg	tgg	ttc	gac	ccc	tgg

Yousfi Monod et al. Bioinformatics 20, i379-385 (2004)
Pommié et al. J. Mol Recognit. 17, 17-32 (2004)

IMGT/V-QUEST   http://www.imgt.org

IMGT/V-QUEST   http://www.imgt.org

IMGT/V-QUEST online: analysis by batches of up to
50 sequences in a single run

IMGT/HighV-QUEST:
batches of 150.000 sequences (output: text for Excel)

IMGT/V-QUEST 'Detailed view': Result summary

http://www.imgt.org

IMGT/V-QUEST provides **22 different output results** (analysis of IG nucleotide sequences and of their translation)

IMGT/V-QUEST 'Detailed view':
Result summary table

Number of analysed sequences: 7

CLASSIFICATION

Sequences compared with the human IG set from the IMGT reference directory

DESCRIPTION

NUMEROTATION

Summary table:

Sequence ID	V-GENE and allele	Functionality	V-REGION score	V-REGION identity % (nt)	J-GENE and allele	D-GENE and allele	D-REGION reading frame	CDR-IMGT lengths	AA JUNCTION	JUNCTION frame
seq1	IGHV1-69*06	Productive	1050	95,63% (219/229 nt)	IGHJ3*02	IGHD3-16*02	2	[8.8.21]	CARGGDYDYIWGSYRASDAFDIW	in-frame
seq2	IGHV1-69*06	Productive	1300	94,79% (273/288 nt)	IGHJ4*01	IGHD6-13*01	1	[8.8.21]	CARERVGAYTSSWYGDYVSFDYW	in-frame
seq3	IGHV4-34*01	Productive	1411	99,30% (283/285 nt)	IGHJ6*02	IGHD2-2*02	3	[8.7.20]	CWIVVVPAAIVPNYYYYGMDVW	in-frame
seq4	IGHV4-34*01	Productive	1294	95,09% (271/285 nt)	IGHJ6*02	IGHD3-10*01	2	[8.7.20]	CARDFSPSPPGHYDARNDMDVW	in-frame
seq5	IGHV4-34*01	Productive	1285	94,74% (270/285 nt)	IGHJ6*03	IGHD3-22*01	2	[8.7.21]	CARWYYFDTSGYYPRNFYYMDVW	in-frame
seq6	IGHV4-34*01	Productive	1258	93,68% (267/285 nt)	IGHJ6*02	IGHD2-2*02	3	[8.7.25]	CARGHKTAIREPPTIGPIYYSYDMDVW	in-frame
seq7	IGHV4-34*01	Productive	1420	100,00% (285/285 nt)	IGHJ5*02	IGHD2-2*01	3	[8.7.25]	CARGDWRIVVVPAAVDTAMAANWFDPW	in-frame

Results of IMGT/JunctionAnalysis for : IGH junctions

Alignment with the closest alleles:

The analysed sequences are aligned with the closest allele (with number of aligned sequences in parentheses):

IGHV1-69*06 (2) IGHV4-34*01 (5)

Terminé

zotero

http://www.imgt.org

Antibody humanization and engineering

Alemtuzumab (CAMPATH®)

2 mutations:
S31>T, S28>F
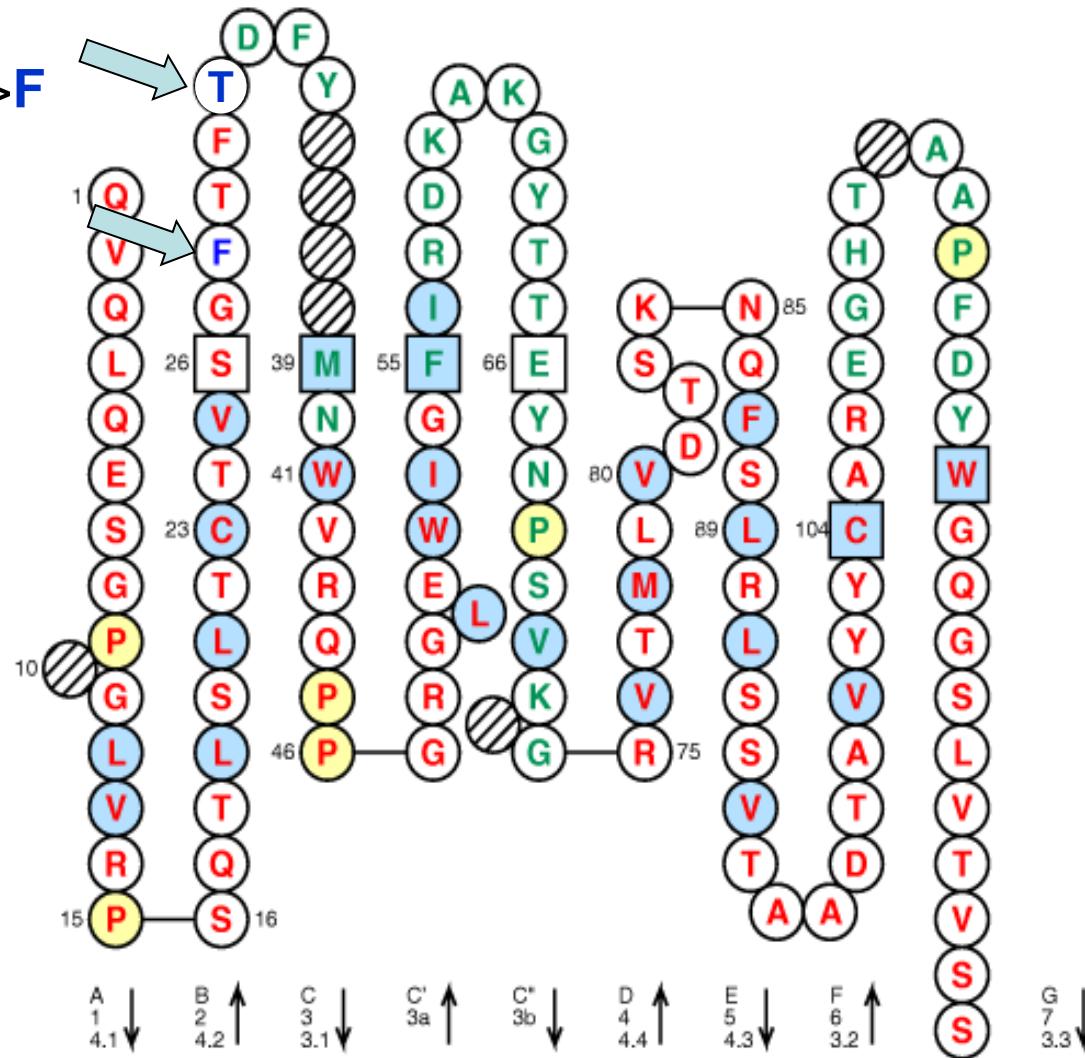
VH domain
[8.10.12]

■ human

■ rat

Towards «Potential immunogenicity evaluation»

http://www.imgt.org

- Comparison with the closest human germline genes and alleles
- Number of different AA in FR-IMGT

		V-REGION identity percent	FR-IMGT AA differences
VH	alemtuzumab	73 %	14 /91
	bevacizumab	72.40 %	23
	trastuzumab	81.63 %	9
V-KAPPA	alemtuzumab	86.32 %	2 /89
	bevacizumab	87.40 %	7
	trastuzumab	86.32 %	6

Magdelaine-Beuzelin C. et al. Crit. Rev. Oncol. Hemat. 64, 210-225 (2007)

IMGT/DomainGapAlign

Sequence name: alemtuzumab_H

ℹ Move your mouse over the amino acids in bold for the characterization of AA class changes

Closest reference gene and allele(s) from the IMGT domain directory

V gene and allele	Species	Domain	Smith-Waterman Score	Identity percentage	Overlap
IGHV4-59*01	Homo sapiens	1	494	73.0	100

J gene and allele	Species	Domain	Smith-Waterman Score	Identity percentage	Overlap
IGHJ4*01	Homo sapiens	1	94	92.9	14
IGHJ4*02	Homo sapiens	1	94	92.9	14
IGHJ4*03	Homo sapiens	1	94	92.9	14

Alignment with the closest genes and alleles from the IMGT domain directory

```
                    FR1-IMGT              CDR1-IMGT        FR2-IMGT         CDR2-IMGT                    FR3-IMGT                          CDR3-IMGT    FR4-IMGT
                     (1-26)                (27-38)         (39-55)          (56-65)                      (66-104)                          (105-117)    (118-128)

                A              B             BC          C       C'       C'C'       C"        D         E          F                       FG           G
              (1-15)        (16-26)       (27-38)     (39-46) (47-55)   (56-65)   (66-74)   (75-84)   (85-96)   (97-104)                 (105-117)    (118-128)
              --------->     --------->     -------->   ------->  ------->  -------->  -------->  ------->  -------->  ------->                 ------->      --------->
              1      10 15 16           23 26 27       38 3941  46 47    55 56      65 66    74 75   80 84 85   89    96 97    104 105 11112 117 118           128
              |........|....| |......|..| |........| |.|....| |......| |.......| |........| |....|...| |..|......| |.....| |.....||....| |.........|
alemtuzumab_H QVQLQESGP.GLVRP SQTLSLTCTVS GFTF....TDFY MNWVRQPP GRGLEWIGF IRDKAKGYTT EYNPSVK.G RVTMLVDTSK NQFSLRLSSVTA ADTAVYYC AREGHTAAPFDYW GQGSLVTVSS.
IGHV4-59*01   QVQLQESGP.GLVKP SETLSLTCTVS GGSI....SSYY WSWIRQPP GKGLEWIGY IYYS...GST NYNPSLK.S RVTISVDTSK NQFSLKLSSVTA ADTAVYYC AR           FDYW GQGTLVTVSS.
(Homo sapiens)                R   Q          FTF    TDF  MN V      R        F  RDK      YT   E    V  G    ML         R                         S
              |------------------------------------------------V-REGION------------------------------------------------------|  |—N—| |—J-REGION—|
```

Region(s) and domain(s) identified in your sequence (corresponding to the closest genes and alleles)

```
QVQLQESGPGLVRPSQTLSLTCTVSGFTFTDFYMNWVRQPPGRGLEWIGF
IRDKAKGYTTEYNPSVKGRVTMLVDTSKNQFSLRLSSVTAADTAVYYCAR
EGHTAAPFDYWGQGSLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLV
KDYFPEPVTVSWNSGALTSGVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQ
TYICNVNHKPSNTKVDKKVEAPELLGGPSVFLFPPKPKDTLMISRTPEVT
CVVVDVSHEDPEVKFNWYVDGVEVHNAKTKPREEQYNSTYRVVSVLTVLH
QDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSRDELTK
NQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTPPVLDSDGSFFLYSKL
TVDKSRWQQGNVFSCSVMHEALHNHYTQKSLSLSPGK
```

Without gaps — Sequence in FASTA format — 💾 Download

With gaps — Sequence in FASTA format — 💾 Download

🖼 IMGT Collier de Perles

IMGT/DomainGapAlign

Towards «Potential immunogenicity evaluation»

http://www.imgt.org

V-REGION identity percent

CDR-IMGT lengths

FR-IMGT lengths

Closest human germline
IGHV4-59*01

Sequence name	V-REGION identity percentage	CDR-IMGT lengths	Number of different AA in CDR1- and CDR2-IMGT	FR-IMGT lengths	Number of different AA in FR-IMGT
alemtuzumab_H	73.0%	[8,10,12]	11	[25,17,38,11] = 91 AA	14

11 different AA in CDR1- and CDR2-IMGT

14 different AA in FR-IMGT 14/91

Ehrenmann et al. Nucl. Acids Res. 38, D301-307 (2010)
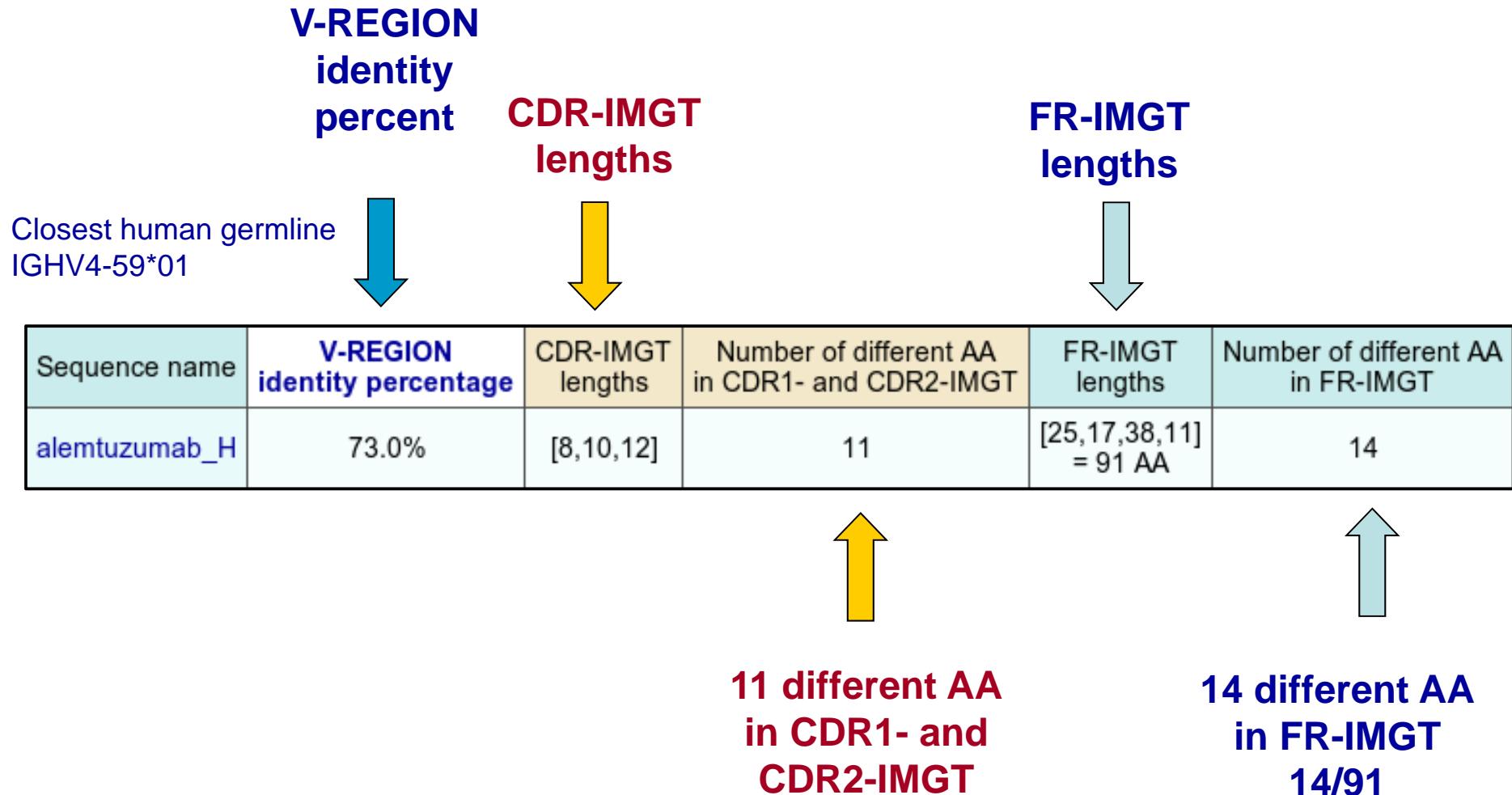
IMGT/DomainGapAlign

Towards «Potential immunogenicity evaluation»

Characteristics of the AA class changes:

CDR-IMGT	Number of different AA	Different AA with class changes
CDR1-IMGT (27-38)	6	G28>F (- - -) very dissimilar S29>T (+ - +) similar I30>F (+ - -) dissimilar S35>T (+ - +) similar S36>D (- - -) very dissimilar Y37>F (- + -) dissimilar
CDR2-IMGT (56-65)	5	Y57>R (- - -) very dissimilar Y58>D (- - -) very dissimilar S59>K (- - -) very dissimilar G63>Y (+ - -) dissimilar S64>T (+ - +) similar

FR-IMGT	Number of different AA	Different AA with class changes
FR1-IMGT (1-26)	2	K14>R (+ + +) very similar E17>Q (+ + -) similar
FR2-IMGT (39-55)	5	W39>M (+ - -) dissimilar S40>N (- - -) very dissimilar I42>V (+ - +) similar K48>R (+ + +) very similar Y55>F (- + -) dissimilar
FR3-IMGT (66-104)	6	N66>E (+ - -) dissimilar L71>V (+ - -) similar S74>G (+ + -) similar I78>M (+ + -) similar S79>L (- - -) very dissimilar K90>R (+ + +) very similar
FR4-IMGT (118-129)	1	T122>S (+ - +) similar

(Hydropathy Volume Physicochemical)
+ : conserved classes
- : different classes

- **very similar (+ + +)**
- **similar (+ - +), (+ + -)**
- **dissimilar (+ - -), (- + -), (- - +)**
- **very dissimilar (- - -)**

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IMGT/DomainGapAlign:

Towards «Potential immunogenicity evaluation»

http://www.imgt.org

IMGT Collier de Perles
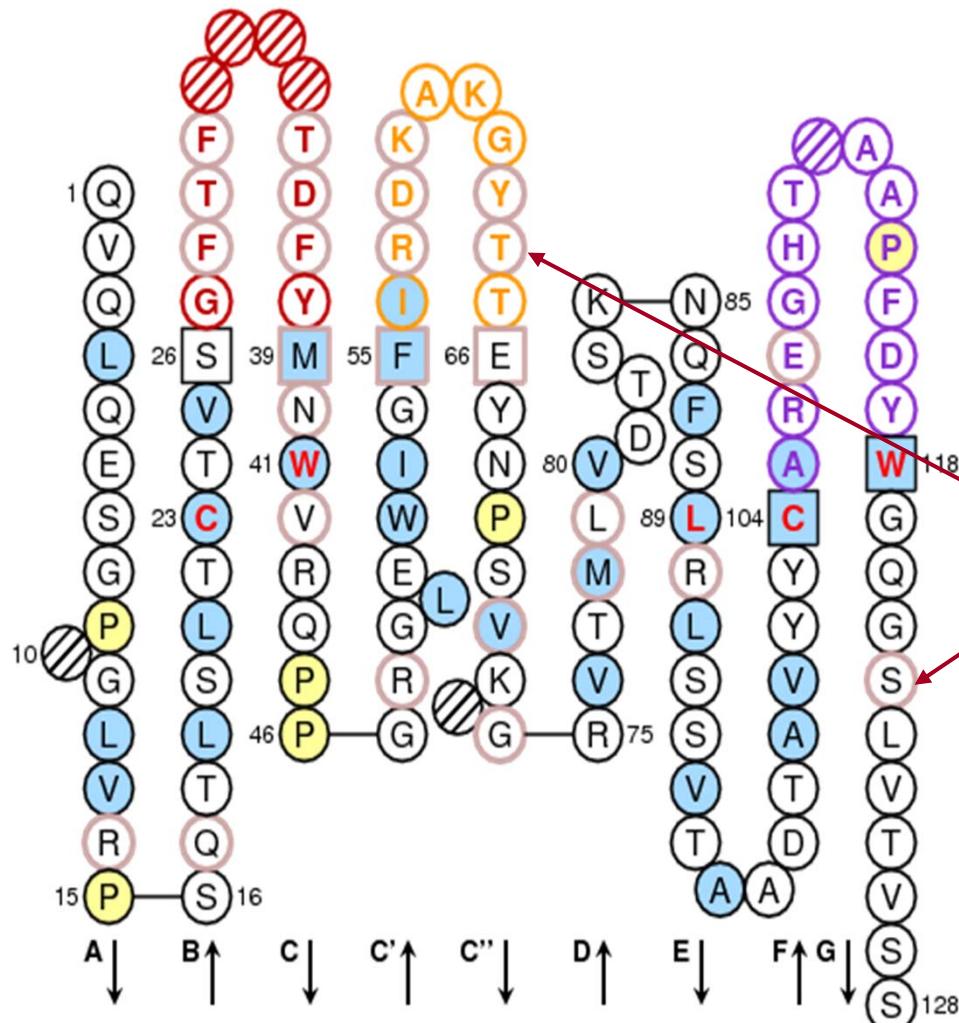
AA that are different compared to the closest germline V and J genes and alleles

(e.g. for alemtuzumab: 11 AA in CDR1- and CDR2-IMGT and 14 AA in the FR-IMGT, compared to *Homo sapiens* IGHV4-59*01)

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IMGT/3Dstructure-DB

IMGT Collier de Perles : *Homo sapiens* (Human) IGHV V-DOMAIN from b12 (1hzh_H)

CDR-IMGT lengths [8.8.20]

Hydrogen bonds

V-DOMAIN

http://www.imgt.org

Lefranc et al. Nucl. Acids Res. 37, D1006-1012 (2009)
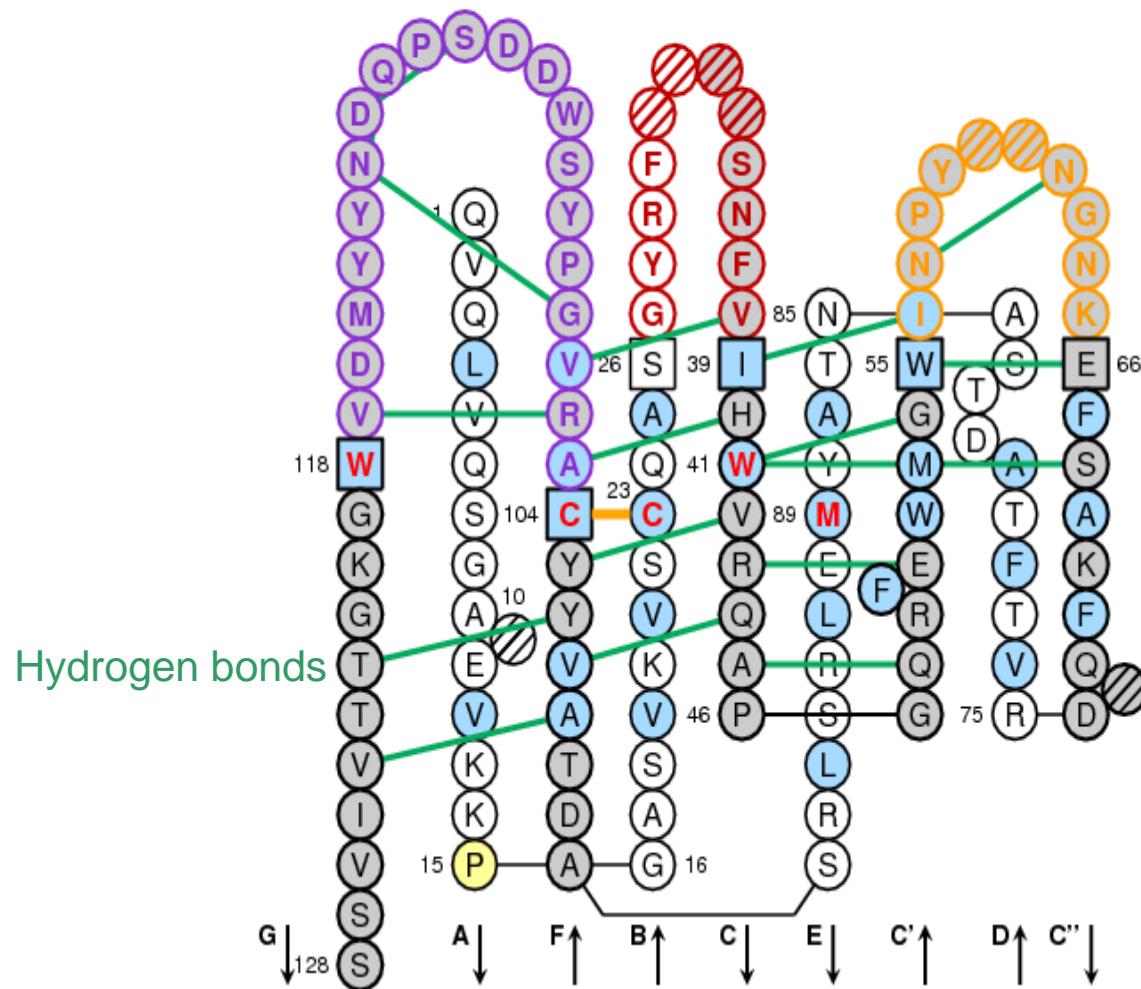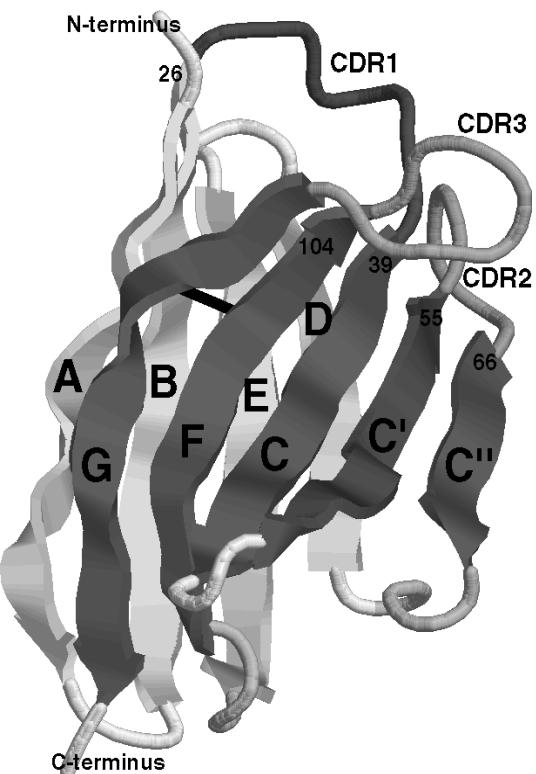
Contacts VH-(Ligand), V-KAPPA-(Ligand)

IMGT molecule name	IMGT description	Chain ID	IMGT chain description	Domain number	IMGT domain description
CAMPATH-1H, alemtuzumab, MABCAMPATH®	FAB-GAMMA-1_KAPPA	1ce1_H	VH-CH1	[D1]	VH
				[D2]	CH1
		1ce1_L	L-KAPPA	[D1]	V-KAPPA
				[D2]	C-KAPPA
CD52 (synthetic peptide)	Peptide	1ce1_P	Peptide		

	Unit 1 Domain	Unit 1 Chain	Unit 2 Domain	Unit 2 Chain	Residue contacts	Number of residues Total	Number of residues From 1	Number of residues From 2	Atom contact types Total	Atom contact types Polar	Atom contact types Hydrogen
DomPair	VH	1ce1_H	CH1	1ce1_H	19	17	8	9	125	9	1
DomPair			V-KAPPA	1ce1_L	63	45	24	21	532	61	6
DomPair			(Ligand)	1ce1_P	25	19	12	7	216	40	9
DomPair	CH1	1ce1_H	VH	1ce1_H	19	17	9	8	125	9	1
DomPair			C-KAPPA	1ce1_L	68	58	28	30	498	40	6
DomPair	V-KAPPA	1ce1_L	VH	1ce1_H	63	45	21	24	532	61	6
DomPair			C-KAPPA	1ce1_L	18	18	8	10	137	19	2
DomPair			(Ligand)	1ce1_P	16	14	7	7	171	37	5
DomPair	C-KAPPA	1ce1_L	CH1	1ce1_H	68	58	30	28	498	40	6
DomPair			V-KAPPA	1ce1_L	18	18	10	8	137	19	2

Contacts V-KAPPA-(Ligand)

Summary:

Residue contacts	Number of residues			Atom contact types		
	Total	From 1	From 2	Total	Polar	Hydrogen
16	14	7	7	171	37	5

List of the Residue@Position pair contacts:

Click 'R@P' for IMGT Residue@Position cards

	Order					Order				Atom contacts		
	IMGT Num	Residue	Domain	Chain		IMGT Num	Residue	Domain	Chain	Total	Polar	Hydrogen
R@P	38	TYR	Y	V-KAPPA	1ce1_L	R@P	3	SER	S		1ce1_P	1	0	0
R@P	38	TYR	Y	V-KAPPA	1ce1_L	R@P	5	PRO	P		1ce1_P	21	0	0
R@P	56	ASN	N	V-KAPPA	1ce1_L	R@P	3	SER	S		1ce1_P	3	2	0
R@P	107	HIS	H	V-KAPPA	1ce1_L	R@P	4	SER	S		1ce1_P	20	4	1
R@P	107	HIS	H	V-KAPPA	1ce1_L	R@P	5	PRO	P		1ce1_P	12	2	0
R@P	107	HIS	H	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	14	3	1
R@P	108	ILE	I	V-KAPPA	1ce1_L	R@P	5	PRO	P		1ce1_P	12	1	0
R@P	108	ILE	I	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	12	3	0
R@P	109	SER	S	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	11	2	0
R@P	114	ARG	R	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	18	3	1
R@P	114	ARG	R	V-KAPPA	1ce1_L	R@P	7	ALA	A		1ce1_P	4	2	0
R@P	114	ARG	R	V-KAPPA	1ce1_L	R@P	8	ASP	D		1ce1_P	6	2	0
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	2	THR	T		1ce1_P	1	1	0
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	4	SER	S		1ce1_P	9	4	1
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	6	SER	S		1ce1_P	20	6	1
R@P	116	ARG	R	V-KAPPA	1ce1_L	R@P	7	ALA	A		1ce1_P	7	2	0

http://www.imgt.org
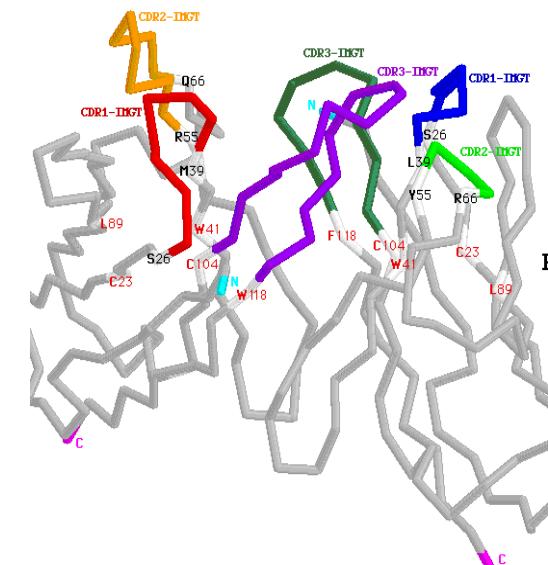
Kaas Q. et al.
Nucl. Acids Res. (2004)

Contacts VH-(Ligand)

R@P	IMGT Num	Residue	Domain		Chain	R@P	IMGT Num	Residue	Domain	Chain	Total	Polar	Hydrogen
R@P	38	TYR	Y	VH	1ce1_H	R@P	2	THR	T	1ce1_P	4	0	0
R@P	38	TYR	Y	VH	1ce1_H	R@P	7	ALA	A	1ce1_P	13	1	0
R@P	38	TYR	Y	VH	1ce1_H	R@P	8	ASP	D	1ce1_P	14	2	2
R@P	55	PHE	F	VH	1ce1_H	R@P	6	SER	S	1ce1_P	5	0	0
R@P	55	PHE	F	VH	1ce1_H	R@P	7	ALA	A	1ce1_P	16	0	0
R@P	55	PHE	F	VH	1ce1_H	R@P	8	ASP	D	1ce1_P	1	0	0
R@P	57	ARG	R	VH	1ce1_H	R@P	7	ALA	A	1ce1_P	9	3	2
R@P	57	ARG	R	VH	1ce1_H	R@P	8	ASP	D	1ce1_P	20	6	1
R@P	61	LYS	K	VH	1ce1_H	R@P	8	ASP	D	1ce1_P	11	2	1
R@P	66	GLU	E	VH	1ce1_H	R@P	7	ALA	A	1ce1_P	1	0	0
R@P	107	GLU	E	VH	1ce1_H	R@P	2	THR	T	1ce1_P	13	2	1
R@P	107	GLU	E	VH	1ce1_H	R@P	4	SER	S	1ce1_P	5	2	0
R@P	107	GLU	E	VH	1ce1_H	R@P	7	ALA	A	1ce1_P	5	0	0
R@P	108	GLY	G	VH	1ce1_H	R@P	1	GLY	G	1ce1_P	2	1	0
R@P	108	GLY	G	VH	1ce1_H	R@P	2	THR	T	1ce1_P	9	2	0
R@P	109	HIS	H	VH	1ce1_H	R@P	1	GLY	G	1ce1_P	24	4	0
R@P	109	HIS	H	VH	1ce1_H	R@P	2	THR	T	1ce1_P	21	5	0
R@P	109	HIS	H	VH	1ce1_H	R@P	3	SER	S	1ce1_P	9	2	1
R@P	110	THR	T	VH	1ce1_H	R@P	1	GLY	G	1ce1_P	1	1	0
R@P	110	THR	T	VH	1ce1_H	R@P	3	SER	S	1ce1_P	11	4	1
R@P	112	ALA	A	VH	1ce1_H	R@P	3	SER	S	1ce1_P	3	1	0
R@P	113	ALA	A	VH	1ce1_H	R@P	2	THR	T	1ce1_P	3	0	0
R@P	113	ALA	A	VH	1ce1_H	R@P	3	SER	S	1ce1_P	7	2	0
R@P	113	ALA	A	VH	1ce1_H	R@P	4	SER	S	1ce1_P	4	0	0
R@P	114	PRO	P	VH	1ce1_H	R@P	4	SER	S	1ce1_P	5	0	0
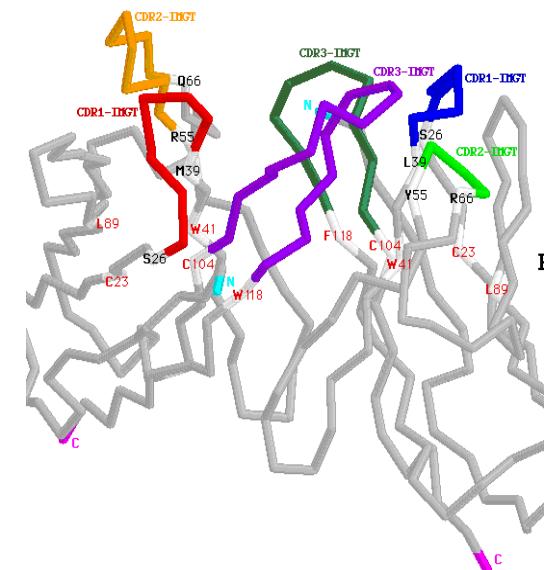
Kaas Q. et al.
Nucl. Acids Res. (2004)

IMGT/2Dstructure-DB

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IMGT/3Dstructure-DB Results

www.imgt.org/3Dstructure-DB/cgi/3Dquery.cgi

Overview

Your query: Entry type INN

Number of results: 161

Entry code [ ] Search

Query page

Click on IMGT entry ID (2nd column) for entry card

International Nonproprietary Name (INN)

	IMGT entry ID	IMGT molecule name	IMGT entry type	IMGT receptor description	Species	Proposed list	Recommended list	CAS number
1	7164	daclizumab	INN	IG-GAMMA-1_KAPPA	Humanized	L78 (1997)	R40 (1998)	152923-56-3
2	7602	infliximab, cA2, REMICADE®	INN	FV-HEAVY_KAPPA	Chimeric	L77 (1997)	R39 (1998)	170277-31-3
3	7609	rituximab, IDEC-C2B8, RITUXAN®, MABTHERA®	INN	IG-GAMMA-1_KAPPA	Chimeric	L77 (1997)	R39 (1998)	174722-31-7
4	7637	trastuzumab, 4D5-humanized variant 8, Herceptin, HERCEPTIN®	INN	IG-GAMMA-1_KAPPA	Humanized	L78 (1997)	R40 (1998)	180288-69-1
5	7783	etanercept, TNFR-immunoadhesin, ENBREL®	INN	FUSION-TNFRSF1B-FC-GAMMA-1	Homo sapiens	L81 (1999)	R43 (2000)	185243-69-0
6	7860	adalimumab, D2E7, LU200134, HUMIRA®	INN	FV-HEAVY_KAPPA	Homo sapiens	L82 (1999)	R44 (2000)	331731-18-1
7	7906	cetuximab, IMC-225, Fab C225 [IgG1κ], ERBITUX®	INN	IG-GAMMA-1_KAPPA	Chimeric	L82 (1999)	R44 (2000)	205923-56-4
8	8005	alemtuzumab, CAMPATH-1H, LDP-03, MABCAMPATH®	INN	IG-GAMMA-1_KAPPA	Humanized	L83 (2000)	R45 (2001)	216503-57-0
9	8017	bevacizumab, 12-IgG1, F(ab)-12 IgG1, Fab-12 IgG1, rhuMAb-VEGF, AVASTIN®	INN	IG-GAMMA-1_KAPPA	Humanized	L83 (2000)	R45 (2001)	216974-75-3
10	8039	omalizumab, IGE25, olizumab, rhuMAb-E25	INN	IG-GAMMA-1_KAPPA	Humanized	L84 (2000)	R46 (2001)	242138-07-4
11	8122	efalizumab, hu1124	INN	IG-GAMMA-1_KAPPA	Humanized	L85 (2001)	R47 (2002)	214745-43-4
12	8313	ranibizumab, Fab-12 variant Y0317, RhuFab, LUCENTIS®	INN	FAB-GAMMA-1_KAPPA	Humanized	L90 (2004)	R52 (2004)	347396-82-1
13	8380	pertuzumab, rhuMAB 2C4 OMNITARG™, PERJETA™	INN	FAB-GAMMA-1_KAPPA	Humanized	L89 (2003)	R51 (2004)	380610-27-5
14	8394	tocilizumab, RO4877533	INN	IG-GAMMA-1_KAPPA	Humanized	L90 (2004)	R52 (2004)	375823-41-9
15	8598	naptumomab estafenatox, ABR-217620, ANYARA, TTS CD3	INN	FAB-GAMMA-1-SAG_KAPPA	Mus musculus	L96 (2006)	R58 (2007)	676258-98-3
16	8651	tadocizumab, C4G1, YM-337	INN	FAB-GAMMA-1_KAPPA	Humanized	L94 (2005)	R56 (2006)	339086-80-5
17	8658	efungumab, HSP90mab, anti- Candida albicans heat shock protein 90 homolog , MYCOGRAB	INN	SCFV-HEAVY-KAPPA	Homo sapiens	L95 (2006)	R57 (2007)	762260-74-2
18	8659	abagovomab, ACA125 MEN-2234	INN	IG-GAMMA-1_KAPPA	Mus musculus	L95 (2006)	R57 (2007)	792921-10-9
19	8669	atacicept, TACI-Fc, TACI-Ig	INN	FUSION-TNFRSF13B-FC-GAMMA-1	Homo sapiens	L95 (2006)	R57 (2007)	845264-92-8
20	8693	motavizumab, MEDI-524	INN	IG-GAMMA-1_KAPPA	Humanized	L95 (2006)	R57 (2007)	677010-34-3
21	8734	bavituximab, Tarvacin ch3G4	INN	IG-GAMMA-1_KAPPA	Chimeric	L95 (2006)	R57 (2007)	648904-28-3
22	8739	aflibercept, VEGF Trap, VEGF TrapR1/R2, VEGF-trapR1, VEGF-TRAPR1R2, ZALTRAP®	INN	FUSION-FLT1-KDR-FC-GAMMA-1	Homo sapiens	L95 (2006)	R57 (2007)	862111-32-8
23	8750	rilonacept, ARCALYST™	INN	FUSION-IL1RAP-IL1R1-FC-GAMMA-1	Homo sapiens	L95 (2006)	R57 (2007)	501081-76-1
24	8753	lexatumumab, HGS-ETR2	INN	IG-GAMMA-1_LAMBDA	Homo sapiens	L95 (2006)	R57 (2007)	845816-02-6
25	8818	ibalizumab, Hu5A8, TNX-355	INN	IG-GAMMA-4_KAPPA	Humanized	L97 (2007)	R59 (2008)	680188-33-4
26	8832	tenatumomab, ST2146	INN	IG-GAMMA-2B_KAPPA	Mus musculus	L98 (2007)	R60 (2008)	592557-43-2 592557-41-0
27	8836	canakinumab, ACZ885	INN	IG-GAMMA-1_KAPPA	Homo sapiens	L97 (2007)	R59 (2008)	402710-27-4 402710-25-2
28	8862	etaracizumab, hLM60, MEDI-522	INN	IG-GAMMA-1_KAPPA	Humanized	L99 (2008)	R61 (2009)	892553-42-3
29	8864	otelixizumab, ChAglyCD TRX4	INN	IG-GAMMA-1_LAMBDA	Chimeric Humanized	L98 (2007)	R60 (2008)	881191-44-2
30	8869	teplizumab, hOKT3-gamma-1 (Ala-Ala), humanized OKT3, MGA031	INN	IG-GAMMA-1_KAPPA	Humanized	L97 (2007)	R59 (2008)	876387-05-2
31	8887	lucatumumab, CHIR-12,12, HCD122	INN	IG-GAMMA-1_KAPPA	Homo sapiens	L98 (2007)	R60 (2008)	903512-50-5
32	8888	panobacumab, Aerumab 11KBPA101, KBPA-101	INN	(J-CHAIN) IG-MU_KAPPA	Mus musculus Homo sapiens	L100 (2008)	R62 (2009)	885053-97-4

IMGT/2Dstructure-DB

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IMGT/2Dstructure-DB card for INN: **7637**

Entry code [ ] Search

Query page

IMGT molecule name		IMGT receptor type	IMGT receptor description	Specificity	Species	Chain ID
INN name	trastuzumab	IG	IG-GAMMA-1_KAPPA	ERBB2 (epidermal growth factor receptor 2, receptor tyrosine-protein kinase erbB-2, EGFR2, HER2, HER-2, p185c-erbB2, NEU, CD340)	*Humanized* (humanized)	[7637_H 7637_L]
Common name	4D5-humanized variant 8, Herceptin					
Commercial name	HERCEPTIN®					

Proposed INN list L78 (1997)   Recommended INN list R40 (1998)

IMGT Notes
Trastuzumab has been engineered with two amino acid changes IGHG1 CH3 D12>E, L14>M to convert the G1m1 allotype
to the isoallotype nG1m1, the resulting gamma1 chain being Gm17, nG1m1, in an attempt to reduce the risk of anti-G1m1 antibodies interfering with therapy:
Carter P. et al. Proc. Natl Acad. Sci. USA, 89, 4285-4289 (1992) PMID: 1350088.
* Trastuzumab constant genes and alleles, and allotypes, based on sequence analysis are:
IGHG1*01, CH3 D12>E, L14>M [allotypes G1m17 (CH1 K120),nG1m1 (CH3 E12, M14)]
IGKC*01 (100%) [allotype Km3 (A45.1, V101)].
* The G1m allotypes have been confirmed serologically:Jefferis R. and Lefranc M.-P., mAbs, 1:4, 332-338 (2009).
* Sequence source: Harris R. et al., Journal of Chromatography B, 752 (2001).

Chain details | Contact analysis | 3D visualization Jmol or QuickPDB | Renumbered IMGT file | INN definitions | References and links | Printable card

Chain details

Differences with the closest IMGT allele sequence are in orange.

Chain details of trastuzumab, 4D5-humanized variant 8, Herceptin, IG, IG-GAMMA-1_KAPPA *Humanized* (humanized) [7637_H,7637_L]

Chain ID	INN 7637_H
Chain length	450
IMGT chain description	H-GAMMA-1 = VH (1-120) [D1] + CH1 (121-218) [D2] + HINGE-REGION (220-233) + CH2 (234-343) [D3] + CH3 (344-448) [D4]

Chain sequence	`[                                        VH (1-120) [D1]`
	 `EVQLVESGGGLVQPGGSLRLSCAASGFNIKDTYIHWVRQAPGKGLEWVARIYPTNGYTRYADSVKGRFTISADTSKNTAYLQMNSLRAED`
	 `           ](N-D)[    J-REGION   ][                          CH1 (121-218) [D2]`
	 `TAVYYCSRWGGDGFYAMDYWGQGTLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVLQSS`
	 `                        ] HINGE-REGION ([`
	 `GLYSLSSVVTVPSSSLGTQTYICNVNHKPSNTKVDKKVEPKSCDKTHTCPPCPAPELLGGPSVFLFPPKPKDTLMISRTPEVTCVVVDVS`
	 `         CH2 (234-343) [D4]                                                           ][`
	 `HEDPEVKFNWYVDGVEVHNAKTKPREEQYNSTYRVVSVLTVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSREE`
	 `               CH3 (344-448) [D5]                                         ]`
	 `MTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTPPVLDSDGSFFLYSKLTVDKSRWQQGNVFSCSVMHEALHNHYTQKSLSLSPGK`

Sequence in FASTA format   Sequence in IMGT format

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IMGT/2Dstructure-DB

Chain details of trastuzumab, 4D5V8, IG, IG-GAMMA-1_KAPPA Humanized [7637_H,7637_L]

Chain ID	INN 7637_H
Chain length	450
IMGT chain description	H-GAMMA-1 = VH(1-120) + CH1(121-218) + HINGE-REGION(219-233) + CH2(234-343) + CH3(344-450)

DESCRIPTION

Chain sequence

```
                                                V-REGION
[
EVQLVESGGGLVQPGGSLRLSCAASGFNIKDTYIHWVRQAPGKGLEWVARIYPTNGYTRYADSVKGRFTISADTSKNTAYLQMNSLRAED
       ]N-AND[    J-REGION    ][                                            CH1
TAVYYCSRWGGDGFYAMDYWGQGTLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVLQSS
                       ][HINGE-REGION ][
GLYSLSSVVTVPSSSLGTQTYICNVNHKPSNTKVDKKVEPKSCDTPPPCPRCPAPELLGGPSVFLFPPKPKDTLMISRTPEVTCVVVDVS
           CH2                                                                      ][
HEDPEVKFNWYVDGVEVHNAKTKPREEQYNSTYRVVSVLTVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSRDE
                  CH3                                                                  ]
LTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTPPVLDSDGSFFLYSKLTVDKSRWQQGNVFSCSVMHEALHNHYTQKSLSLSPGK
```

Sequence in FASTA format   *Sequence in IMGT format*

V-DOMAIN

IMGT domain description	VH	
IMGT gene and allele name	IGHV3-66*01 (81.60%)(Human) , IGHV3-66*02 (81.60%)(Human) , IGHV3-66*04 (81.60%)(Human) *Alignment details*	
IMGT gene and allele name	IGHJ6*01 (76.50%)(Human) , IGHJ6*02 (76.50%)(Human) *Alignment details*	
2D representation	*IMGT Collier de Perles* or *IMGT Collier de Perles on 2 layers*	
Contact analysis	*Not available*	
CDR-IMGT lengths	[8.8.13]	
Sheet composition	*Not available*	

CLASSIFICATION

NUMEROTATION

```
                   [   CDR1   ]                      [   CDR2   ]
EVQLVESGG.GLVQPGGSLRLSCAASGFNI....KDTYIHWVRQAPGKGLEWVARIYPT..NGYTRYADSVK.GRFTISADTSKNTAYLQ
                  [   CDR3   ]
MNSLRAEDTAVYYCSRWGGDGFYAMDYWGQGTLVTVSS
```

IMGT/DomainGapAlign results

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IMGT/mAb-DB - Mozilla Firefox

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IMGT/mAb-DB Query page

Version: 1.3.3 (11/09/2012) Database release: 201237-2 (11/09/2012)

murine
mAb-DB

Today is Thursday, Nov 08 2012
Database contains 430 entries
272 -mab
18 -cept

> Citing IMGT/mAb-DB:
> Poiron, C. et al., JOBIM 2010, Paper 13 (2010). Abstract [PDF]

💡 If the display of drop-down list is not optimal with Internet Explorer, use Firefox, Opera or Chrome.

Search by:

IMGT/mAb-DB
ID   [-]

[Search] [Clear]

INN   [-]   [   ]   INN proposed
                                           list   [-] ○ and before ○ and after

INN number   [-]

                                           INN
                                           recommended
                                           list   [-] ○ and before ○ and after

Common name [-]

                                           Proprietary
                                           name   [-]

[Search] [Clear]

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IMGT/mAb-DB

Fichier   Édition   Affichage   Historique   Marque-pages   Outils   ?

IMGT/mAb-DB

www.imgt.org/mAb-DB/query

Kidney transplant rejection dictionnaire medical ang

Species [-]

IMGT receptor type   ◉ any ○ IG ○ FPIA ○ CPCA ○ RPI ○ none

IG class and subclass (for complete IG)
```
-
any
none
IgA - nd
IgE - nd
```

IG format (for IG fragments or constructs)
```
-
any
none
scFv (any)
Fab (any)
```

FPIA chain identification
```
-
any
none
ACVR2A (activin receptor type 2a, activin receptor type IIA ) - IGHG1 Fc
ACVRL1 (activin A receptor type I-like 1, activin receptorlike kinase 1, ALK1, ALK-1, serine/threonine-protein kinase rece
```

CPCA chain identification
```
-
any
none
ALB (albumin 25-609) - IFNA2 (interferon alpha 2, IFN-Alpha, IFNA, 24-188)
ALPL (alkaline phosphatase, TNSALP, tissue non-specific alkaline phosphatase, 18-502) - IGHG1 Fc
```

RPI chain identification
```
-
any
none
CD4- Pseudomonas aeruginosa exotoxin A
CR1 (complement receptor type 1, C3b/C4b receptor, C3BR, Knops blood group, KN, CD35)
```

Radiolabelled with [-]

Conjugated with [-]

Origin clone species [-]

Entries in IMGT/2Dstructure-D [-]

Origin clone name [-]

Entries in IMGT/3Dstructure-D [-]

Search   Clear

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IMGT/mAb-DB

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WELCOME !
to IMGT/mAb-DB

ImMunoGeneTics Information system®

http://www.imgt.org

Your query: IMGT/mAb-DB INN = trastuzumab

Number of results: 1

IMGT/ mAb-DB id	INN (International Nonproprietary Name)	INN Num.	INN Prop. list	INN Rec. list	Common name	Proprietary name	IMGT/mAb-DB section	IMGT/ 2D	IMGT/ 3D	Isotype and format	Specificity (target) [origin]	Company	Clinical indication	Development status	Regulatory agency status and year	Application
97	trastuzumab	7637	78 (1997)	40 (1998)	4D5V8, Herceptin	HERCEPTIN®	Humanized	7637	1n8z	IgG1κ	ERBB2 (Epidermal Growth Factor Receptor 2; HER-2; p185c-erbB2; NEU; EGFR2) [*Homo sapiens*]	F. Hoffmann-La Roche Ltd. (Basel Switzerland) (EU) / Genentech Inc. (S. San Francisco CA USA) (US)	Breast cancers (as adjuvant)	Phase III		Therapeutic
													Metastatic breast cancers overexpressing ERBB2	Phase M	AMM Market authorization (Roche) August 2000, FDA approval October 1998	
													Non-small-cell lung cancers	Phase II		

IMGT/mAb-DB Documentation
Monoclonal antibodies with clinical indications

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Why are IMGT Colliers de Perles so useful?

http://www.imgt.org

- Provide a standardized analysis of domains (V, C and G) for IG, TR, MHC and for all other IgSF and MhcSF.
  - IMGT/Collier-de-Perles
  - IMGT/DomainGapAlign

- Provide a standardized analysis of contacts (antibody/antigen, peptide/MHC, TR/pMHC…)
  - IMGT/3Dstructure-DB

- Bridge the gap between sequences and 3D structures and vice versa
  - IMGT/2Dstructure-DB cards (INN)

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http://www.imgt.org
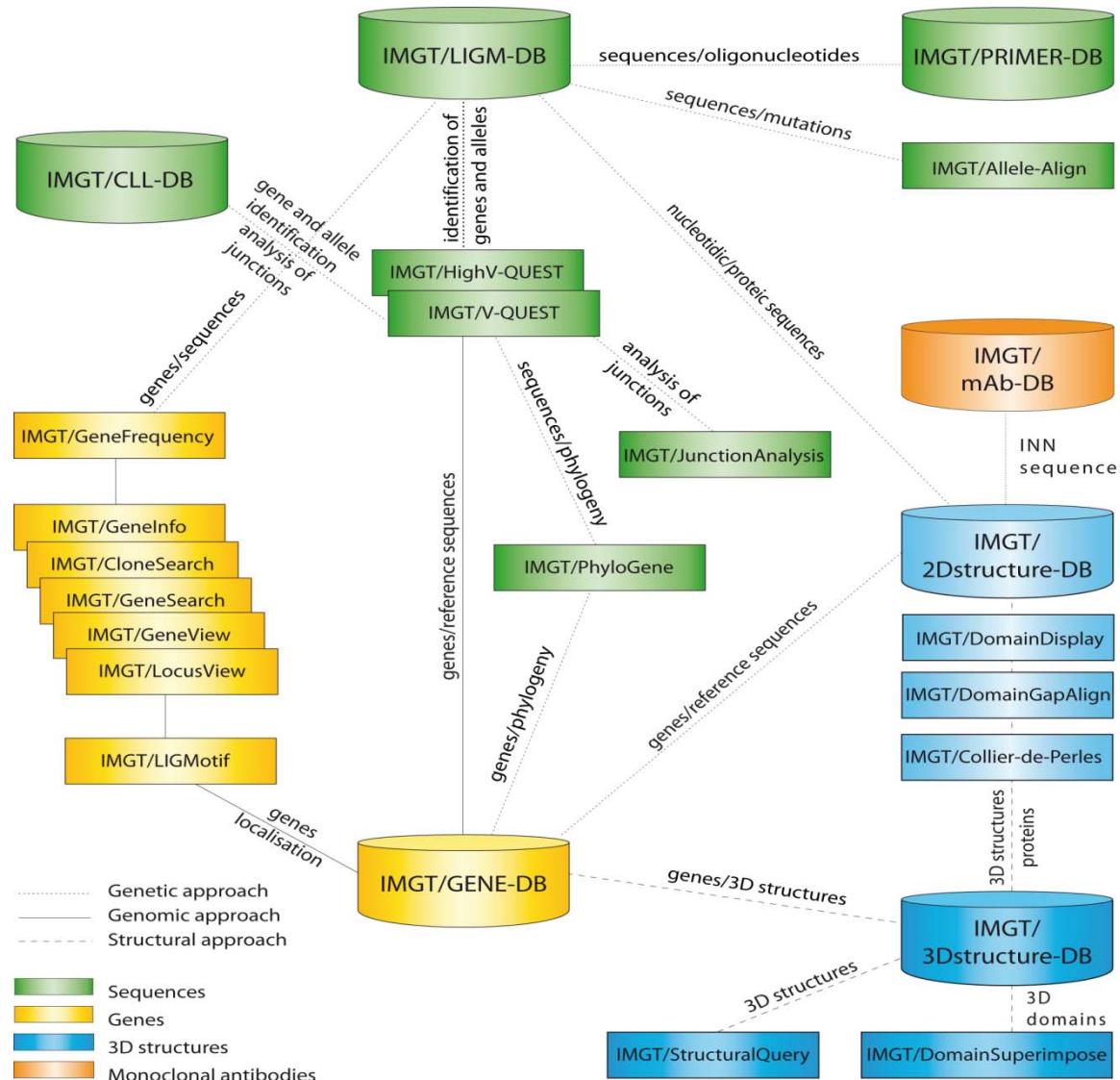
- 7 databases
- 17 online tools
- 15.000 web pages

- Sequences
- Genes
- Structures

- Immunoglobulins (IG) (or antibodies)
- T cell receptors (TR)
- Major Histocompatibility (MH)
- IgSF and MhSF

Acknowledgements

http://www.imgt.org

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the IMGT® team at Montpellier, France

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