

Supplementary Material



Figure S1. Structural alignment of eight VH10 containing PDB models. CDR2 residues that are depicted in Figure 4 is marked in green. Alignment was performed with Chimera for the V_H segment (residues 1–100).

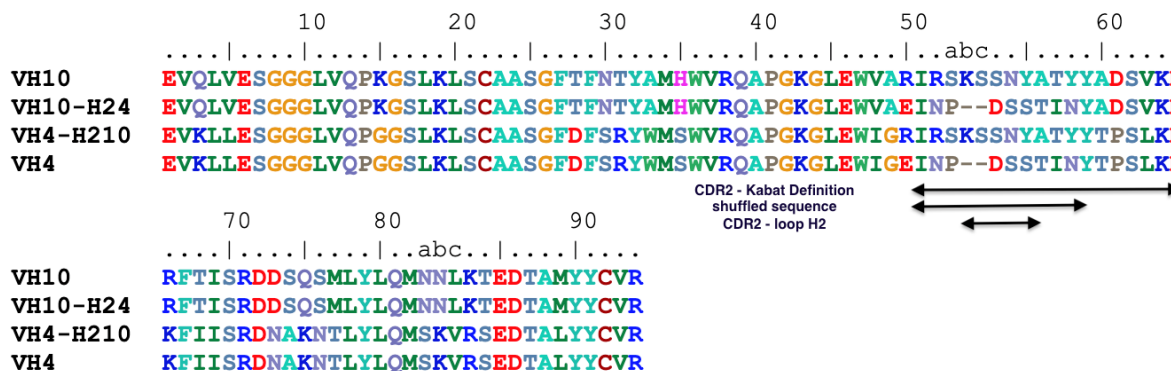
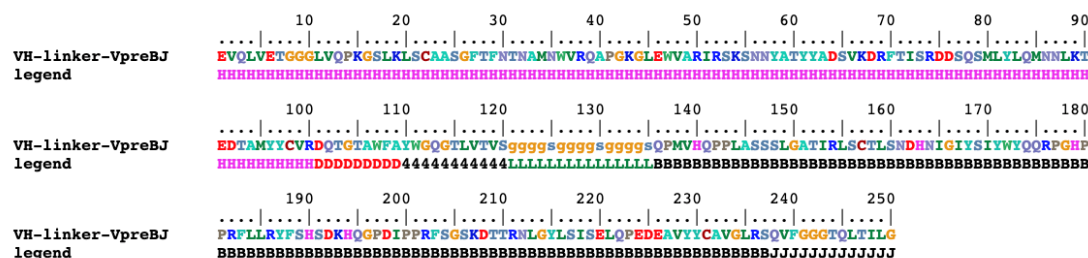


Figure S2. Alignment of recombinant V_h gene segment produced as scpre-BCR. VH10, VH4 and the two CDR2 shuffled variants. VH10-H24 correspond to the VH10 germline containing the CDR2 loop region of VH4 germline. VH4-H210 correspond to the VH4 germline containing the CDR2 loop region of VH10 germline. CDR2 Kabat definition, shuffled region and H2 loop is marked with double headed arrows.



H – Germline heavy chain (V_H10)
D – Synthetic D segment
4 – J_H4 gene segment
L – linker sequence
B- VpreB
J – λ5 J-like FW4

Figure S3. Scheme of scpre-BCR recombinant protein.

Table 1. WdV contacts and H-Bonds in model scpre-BCR-VH10. The number of times a residue makes contacts or bonds among the best 10 models is tabulated. Residues <5.0 Å apart are considered counted as WdV contact residues. H Bonds and distances are calculated with Chimera.

| Residue | Contact | H-Bond | Location |
|---------|---------|--------|----------|
| T31 | 10 | 0 | CDR1 |
| A33 | 10 | 0 | |
| R50 | 10 | 4 | CDR2 |
| R52 | 10 | 5 | |
| S52c | 10 | 6 | |
| S53 | 3 | 0 | |
| E95 | 8 | 0 | CDR3 |
| Q98 | 1 | 0 | |
| R100 | 3 | 0 | |
| R237 | 1 | 0 | VpreB |