SCOP: Structural Classification of Proteins

Structural Classification of Proteins



Protein: Platelet factor 4, PF4 from Cow (Bos taurus)

Lineage:

- 1. Root: scop
- Class: <u>Alpha and beta proteins (a+b)</u> Mainly antiparallel beta sheets (segregated alpha and beta regions)
- Fold: <u>IL8-like</u> beta(3)-alpha
- 4. Superfamily: Interleukin 8-like chemokines form dimers with different dimerisation modes
- 5. Family: Interleukin 8-like chemokines
- 6. Protein: Platelet factor 4, PF4
- 7. Species: Cow (Bos taurus)

PDB Entry Domains:

1. <u>1plf</u> 🚨 📽

complexed with tcn

- 1. <u>chain a</u> 🚨 📽 🖪
- 2. <u>chain b</u> 🚨 📽 🗳
- 2 1 1 1 1 1 10 10 10

Murzin et al. 1995

Il8-like Domain

MMS-Code

- : 54117
- Class :

Number of Members

Average Size : 71

- Alpha and Beta Proteins (a+b)
- : 2

Percentage Identity Matrix

| | 1ikl- | 1huma |
|-------|-------|-------|
| 1ikl- | 100.0 | 21.0 |
| 1huma | 21.0 | 100.0 |

Alignment Based On Similarities In Structural Features in Interleukin Superfamily

1ikl-elrçqçikTyskpfhpkfIkeL1humaapmgsdpptaç-çfsytarklprnfVvdy

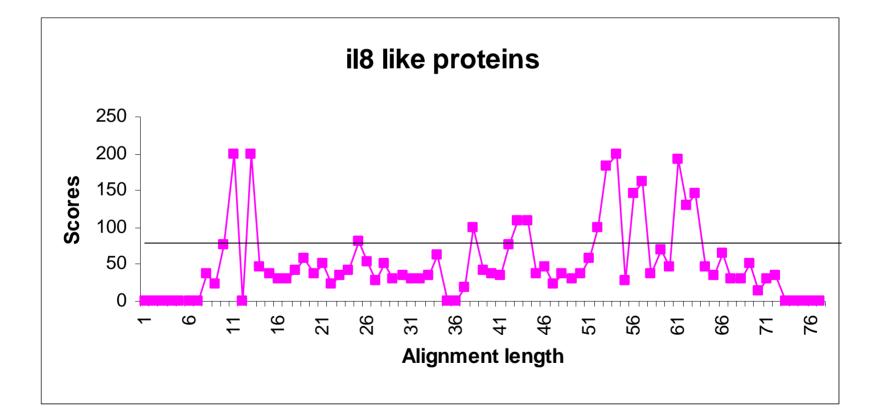
- 1ikl- rviesgphçantelivklsdg
 1huma yeTslçsqpAvVFqTkrs--bb bbbb

Alignment with Homologues in HOMSTRAD database

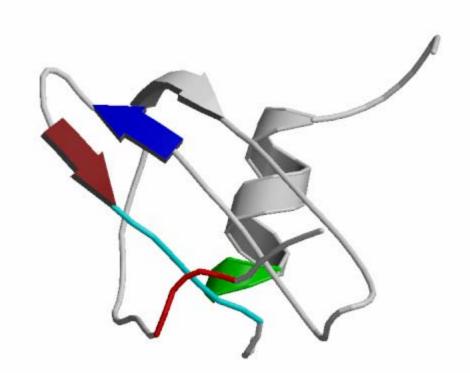
| 1huma 1b3aa 2eot 1plfa 1rhpa 1tvxa 1mi2a 1mi2a 1roda 1il8a 1sdf | 1 23 7 23 1 1 2 1 |))))))))))))))))))))))))))))))))))))))) | py s s-d- gpa asva avva sa a | ttpçÇfa svpttÇçfn lqçvçlkt d <i>lq</i> ç <i>l</i> Çvkt lrçlÇikt telrçqÇlqt sel <u>rçqç</u> lkt kelrç <u>q</u> çikt | jiarplp <u>r</u> ah lanrkiplqr ts-qVrprh ts-qVrprh lq-Gihpkn lq-Gihpkn yskpfhpkf yskpfhPkf | IkeyfyT- Lesyrrit IssLevid IgsLevid Igslevid Igsvnvk Igslsvtg ikelrvid Ikelrvid | 40 ss-lçs <u>q</u> pAvVF sg-kÇs <u>n</u> pAVVF sg-kÇpqkaVif gaglhÇpsp qLif gaglhÇpsp qLif gaghÇngveVif spgphÇaqt <u>EVif</u> sggp <u>h</u> Çaqt <u>EVif</u> sggp <u>h</u> Çanteii sggp <u>h</u> Çant <u>e</u> ii bbbb | Fvtr Sktk Atlk Atlk Atlk Atlk VkLs Vkls ArLk |
|---|--|---|--|---|--|---|--|--|
| 1huma 1b3aa 2eot 1plfa 1rhpa 1tvxa 1mgsa 1mi2a 1roda 1il8a 1sdf | 4654646546464644654444544466464464444444 | | k- <i>n</i> rqvçA 1- <i>a</i> kdiÇA t- <i>g</i> rkiçI n- <i>g</i> rkiçI d- <i>g</i> rkiçI n- <i>g</i> rkaçI <i>g</i> - <i>g</i> qkvÇI d-grelÇI <u>d</u> - <i>g</i> relÇI nn <u><i>n</i></u> rqvçI | 60 dpseswVqey npekkwV <u>rey</u> dpkkkwV <u>qd</u> dqqnplykki dlqaplykki dpdaprI <u>kki</u> dpdaprI <u>kki</u> dpa <u>s</u> piVkki dpsenwVqrv dpklkwI <u>q</u> ey | ZInslems Smkyldqksp Iik <u>r</u> llks Ii <u>k</u> kll <i>es</i> Ivq <u>kk</u> lagd Iie <u>k</u> mln <u>sd</u> k iiqkilnkgk iiekml <u>n</u> sdk vvekflkrae /lekaln | <i>sn</i> an <u>s</u> n | | |

bbbb aaaaaaaaaaa

Alignment Score of il8-like Superfamily

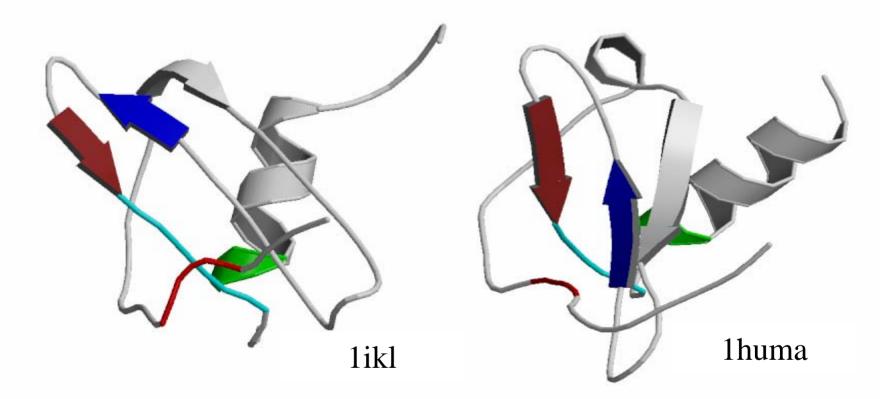


Interacting Motifs of the il8 superfamily



| likl- (| 4) | e l rçqçi kTyskpf h pkfIkeLrviesgp h çant <mark>eIiVkls</mark> dg |
|---------|-----|---|
| 1huma (| 1) | apmgsdpptaç-çfsytarklp <mark>rnf</mark> Vvdyye r sslçs <u>q</u> pAvVF gr krs |
| | | bb bbb |
| likl- (| 47) | relÇL d pk <u>enw</u> Vgrvv <u>e</u> kflk <i>r</i> aens |
| lhuma (| 48) | kqvçAdpseswVqeyvy <u>d</u> leln |
| | | bb aaaaaaaaaa |

Conservation of the motifs in the structures



Bhaduri, A., Ravishankar, R. & Sowdhamini, R., Proteins Structure, Function and Genetics (in press)

Employing structural motifs for sensitive sequence searches

Step 1:

Homologous sequences of individual superfamily members are aligned and amino acid exchanges at individual positions were scored for conservation.

Step 2:

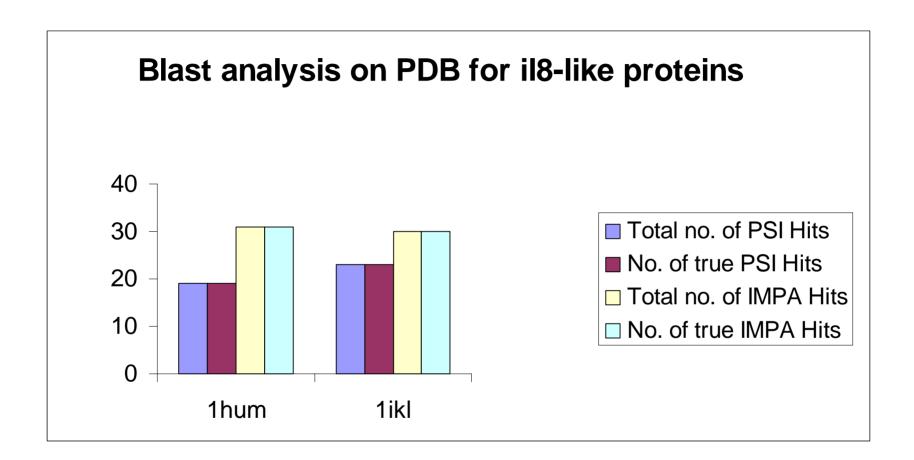
Homologous sequences of individual superfamily members are aligned and amino acid exchanges at individual positions were scored for conservation.

Step 3:

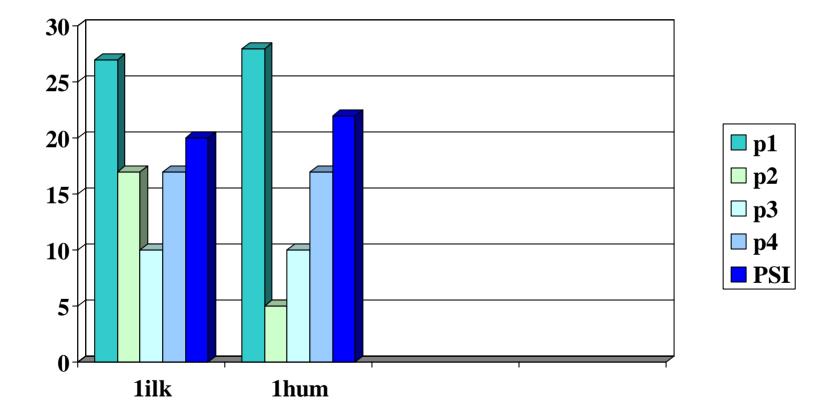
Spatially interacting motifs, when mapped on the superfamily alignment if in equivalent positions are considered for constrained sequence searches

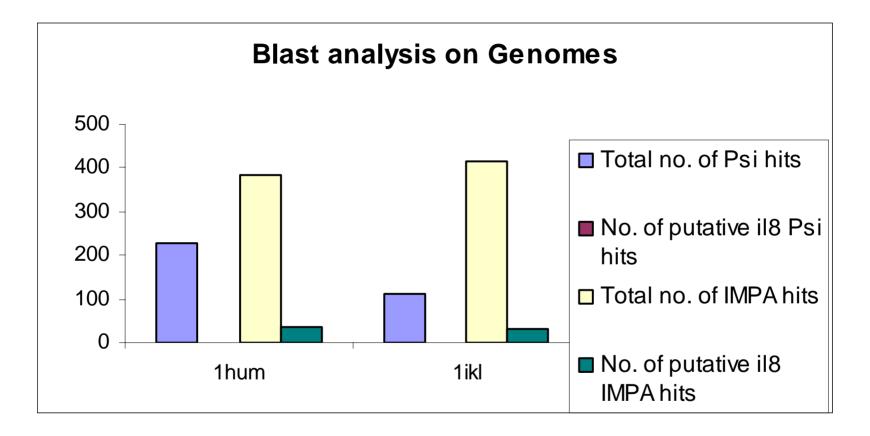
Interacting Motif Pattern Assisted (IMPA) Search: PHI-Blast Parameters

- Patterns obtained from Interactive Motifs
- E –value 1 (Standard value 0.0001)
- Iterations used 1(Standard value 3 or 5)
- Each superfamily Member of CAMPASS was used as a query Sequence

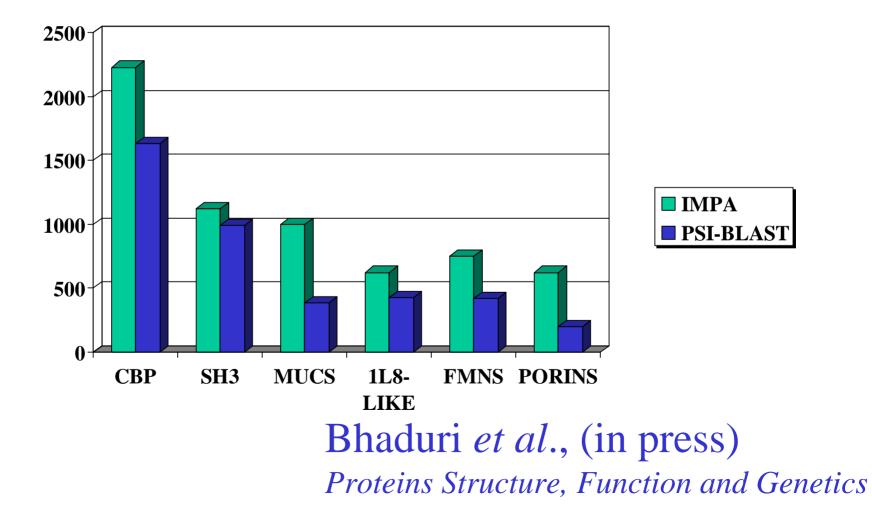


Contribution of individual motifs of the il8-like proteins

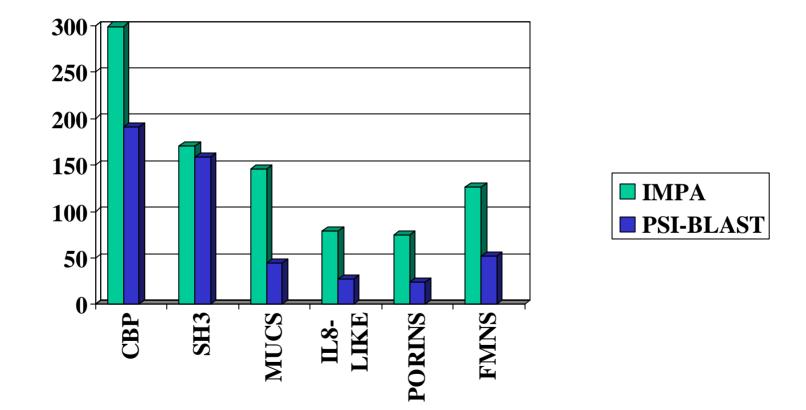




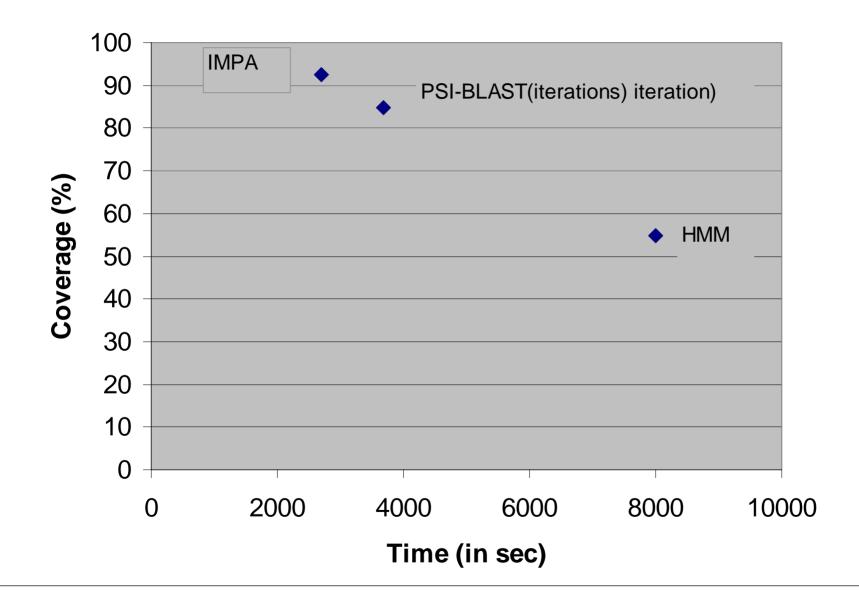
Genome Distribution across 91 Genomes



Distribution of Hypothetical Proteins in the genome : Putative members of the Superfamily



Performance with respect to time



Testing of The Coverage against SCOP

| Superfamily | IMPALA | BLAST | IMPA | TOTAL |
|-------------|--------|-------|------|-------|
| SH3 | 58 | 54 | 56 | 67 |
| Porins | 31 | 24 | 33 | 33 |
| Mucs | 20 | 18 | 18 | 20 |
| FMNs | 17 | 5 | 16 | 18 |
| Il8-like | 34 | 34 | 34 | 35 |
| CBP | 111 | 99 | 105 | 125 |
| | | | | |

Bhaduri *et al.*, (in press) *Proteins Structure, Function and Genetics*