SEALAの使い方

藤　博幸
産業技術総合研究所
生命情報工学研究センター

SEALAでできること

（１）アラインメントサイトの各種の保存度、変異度の計算とその立体構造上への表示

（２）アラインメントから相同タンパク質の機能差を決定しているサイトを推測し、それを立体構造上に表示

WindowsXP, 7, 8で動作確認

IE, Fire[ox, Google　chromeなどからアクセス可能

SEALAでできること

（1）アラインメントサイトの各種の保存度、変異度の計算とその立体構造上への表示

（2）アラインメントから相同タンパク質の機能差を決定しているサイトを推測し、それを立体構造上に表示

WindowsXP, 7, 8で動作確認

IE, Fire[ox, Google　chromeなどからアクセス可能

SEALAへのアクセス

- PDBjのリンクから

- http://sseala.cbrc.jp/~seala

Firefox

SEALA PAGE

seala.cbrc.jp/~seala/

よく見るページ　Firefox を使いこなそう　SEALA PAGE　Web スライス ギャ...　おすすめサイト　ブックマーク

SEALA

SEquence ALignment Analyzer

```
...FLV-DTGAQHSVLT...
...ALL-DTGADDTVLE...
...ALL-DSGADITIIS...
...CLI-DTGSTVNMTS...
...CFV-DTGASLCIAS...
...TVVFDTGSSNLWVP...
...TVLFDTGSSDFWVP...
```

Extraction of Functional Sites

Sequence Weight　　**Site-Specific Res. Freq**

Firefox

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...CFV-DTGASLCIAS...
...TVVFDTGSSNLWVP...
...TVLFDTGSSDFWVP...

Extraction of Functional Sites

Sequence Weight help

Site-Specific Res, Freq help

Variability/Conservation help

ET & Relatives help

Plug in software, Chime or jV, is required to see the result of calculation on a tertiary structure.

Link

Link to Related Service : PC-31(Profile Comparison between 3D and 1D)

Conservation/Variability

必要な入力ファイル

（１）アラインメントファイル (align_example.txt)

clustalW format

構造データへの表示をする場合は

立体構造に対応する配列を含めておく

配列名は構造データのファイル名に

一致させておく

（２）構造データ (

pdb format (1UJY.pdb)

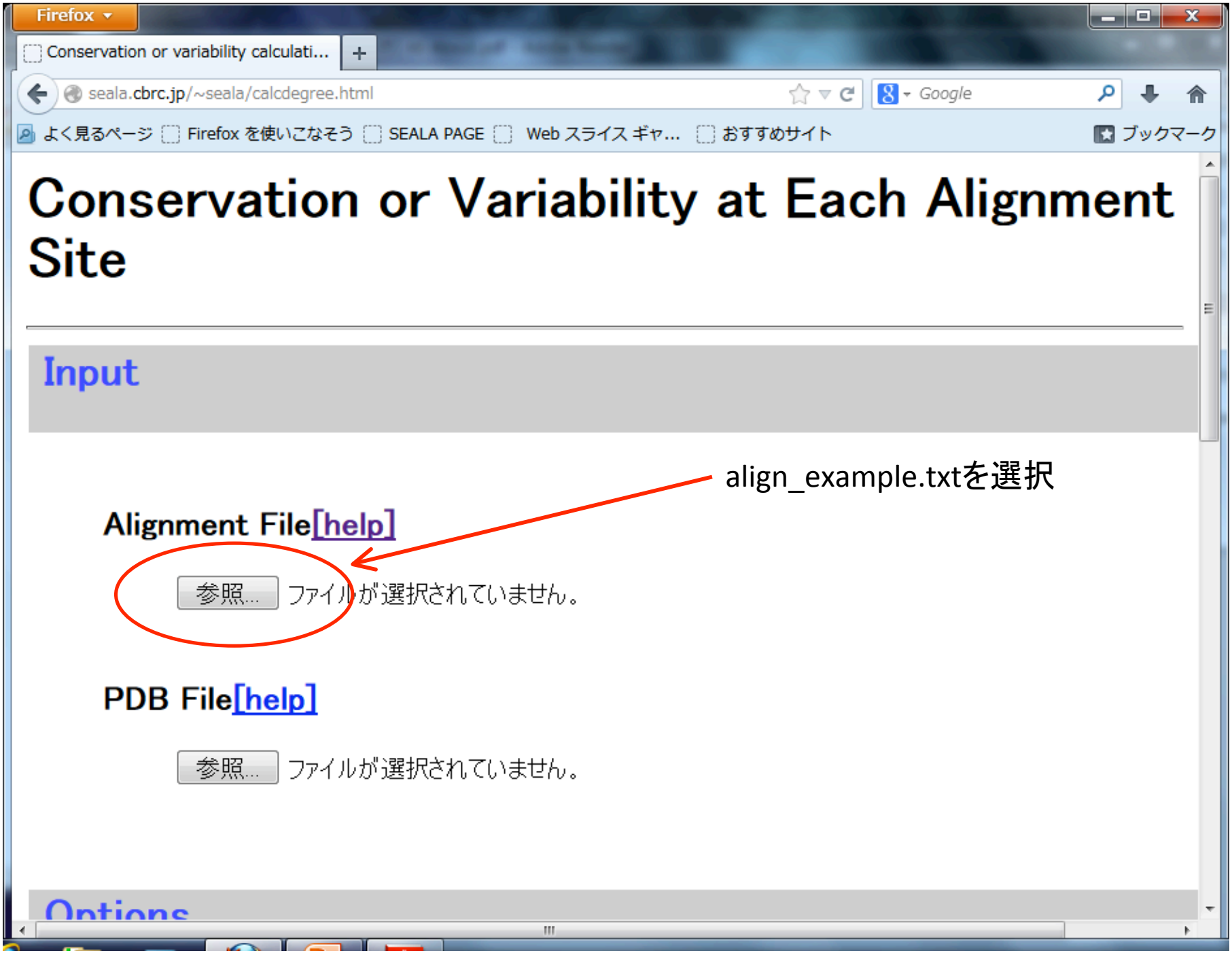
CLUSTAL W (1.81) multiple sequence alignment

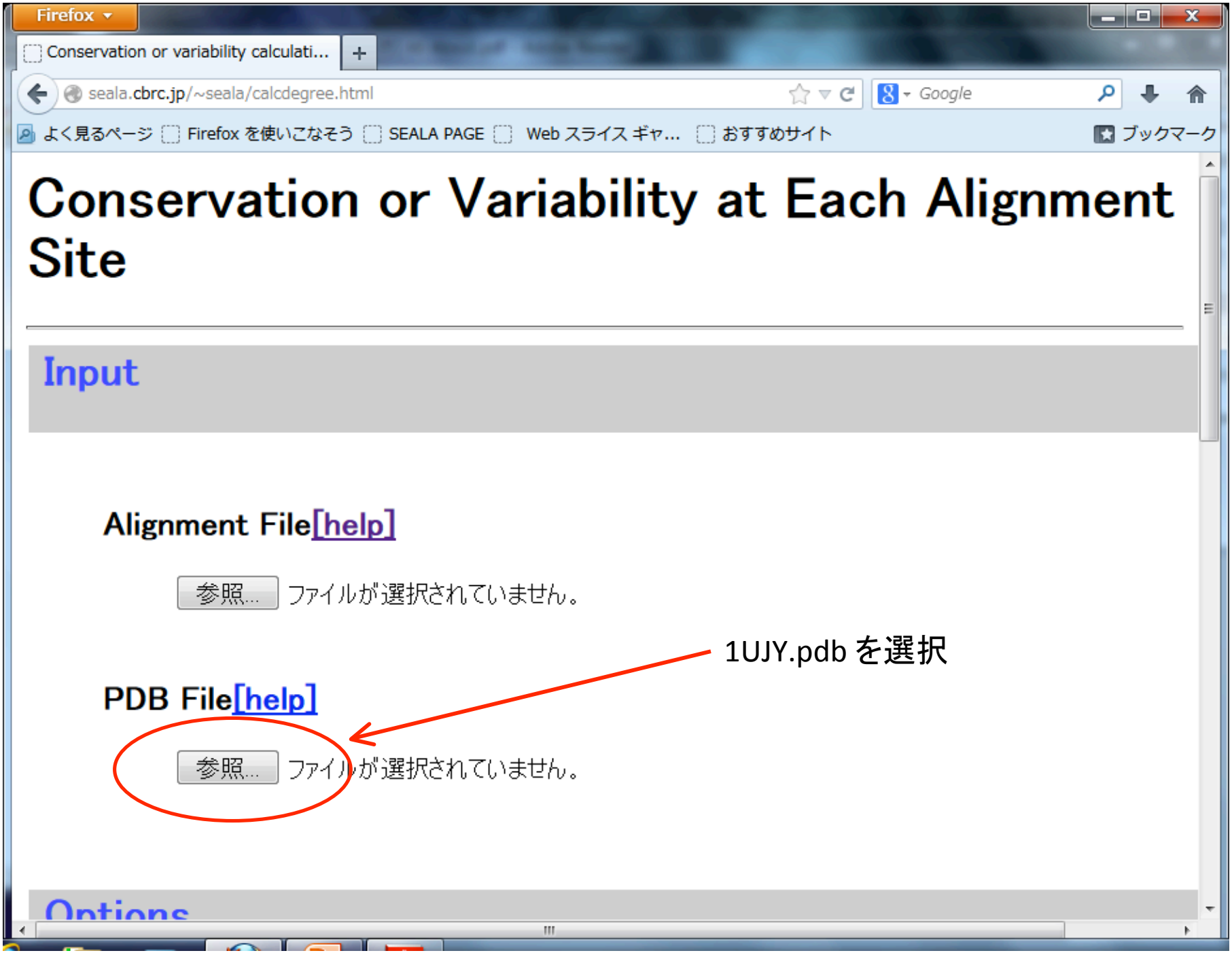
```
YB65_SCHPO/587-642          SYVKALYAYTAQS--DMELSIQEGDIIQVTNRNAG--
1UJY.pdb                    LIVKARFNFKQTN--EDELSVCKGDIIYVTRVEEG--
MYOC_DICDI/1125-1181        QQYIALYEYDAMQ--PDELTFKENDVINLIKKVDA--
MYOB_DICDI/1056-1111        PTAKALYDYDASS--TDELSFKEGDIIFIVQKDNG--
MYSB_ACACA/1093-1147        PQVKALYDYDAQT--GDELTFKEGDTIIVHQKDPA--
VAV_HUMAN/785-840           GTAKARYDFCARD--RSELSLKEGDIIKILNKKGQ--
LASP1_CAEEL/269-325         FAVKAIYDYAAAD--KDEISFLEGDIIVNCEKIDD--
ABP1_SACEX/560-616          PWATAEYDYEAGE--DNELTFAENDKIINIEFVDD--
RV167_YEAST/424-480         ETVTALYDYQAQA--AGDLSFPAGAVIEIVQRTPDV-
PLCG2_HUMAN/772-827         RTVKALYDYKAKR--SDELSFCRGALIHNVSKEPG--
```

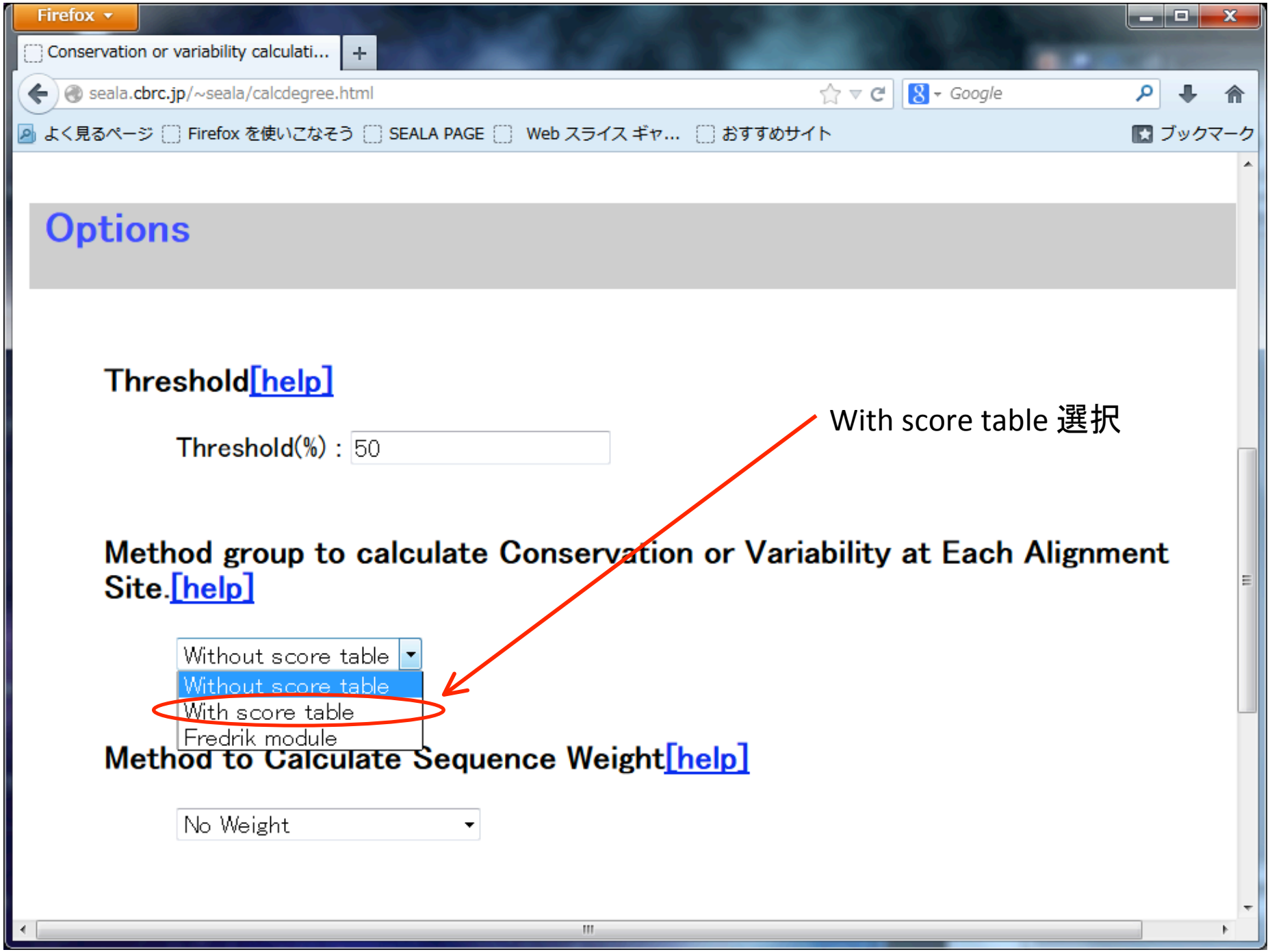
Conservation/Variability

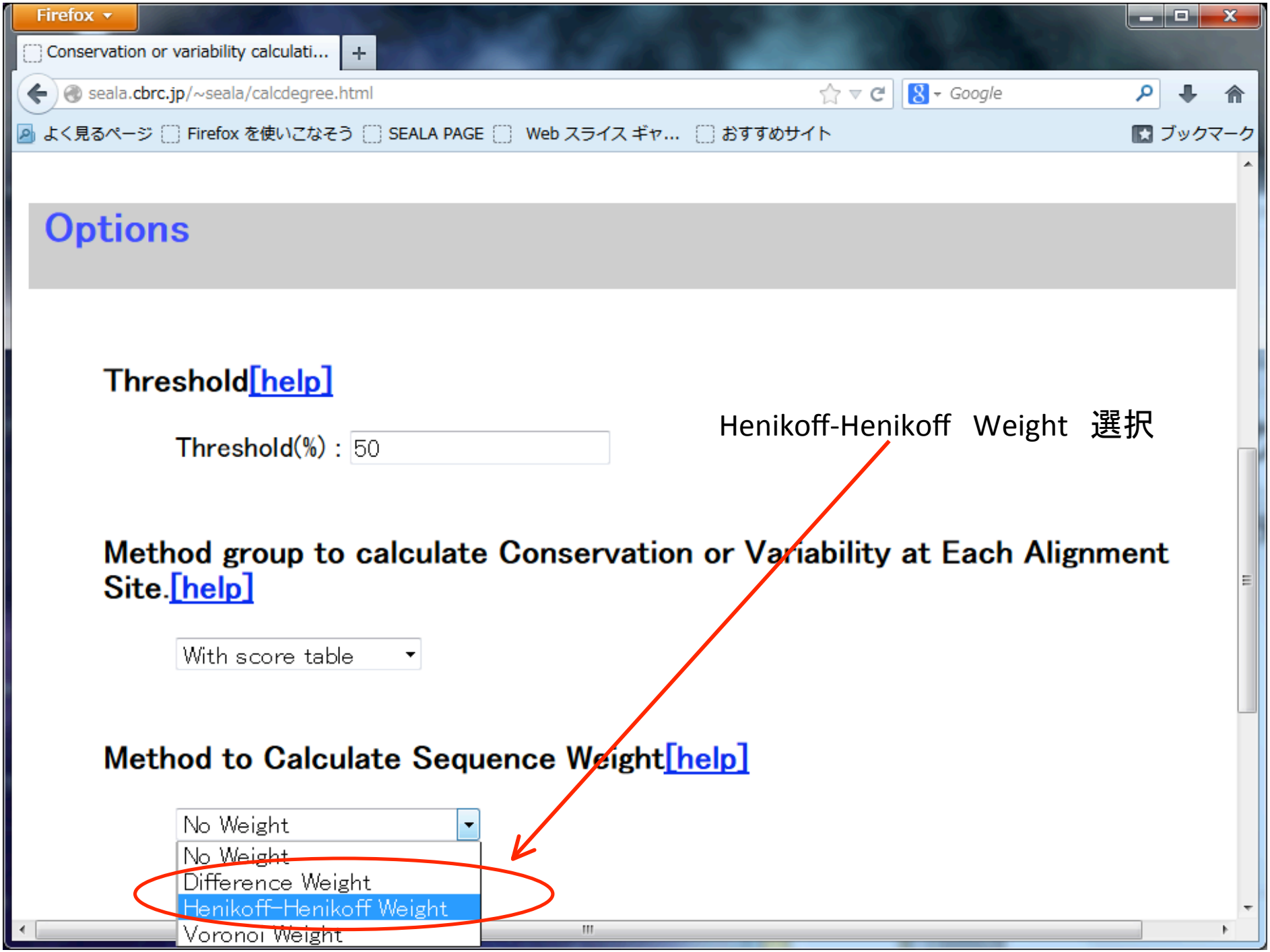
3ページ　選択画面が出てくる

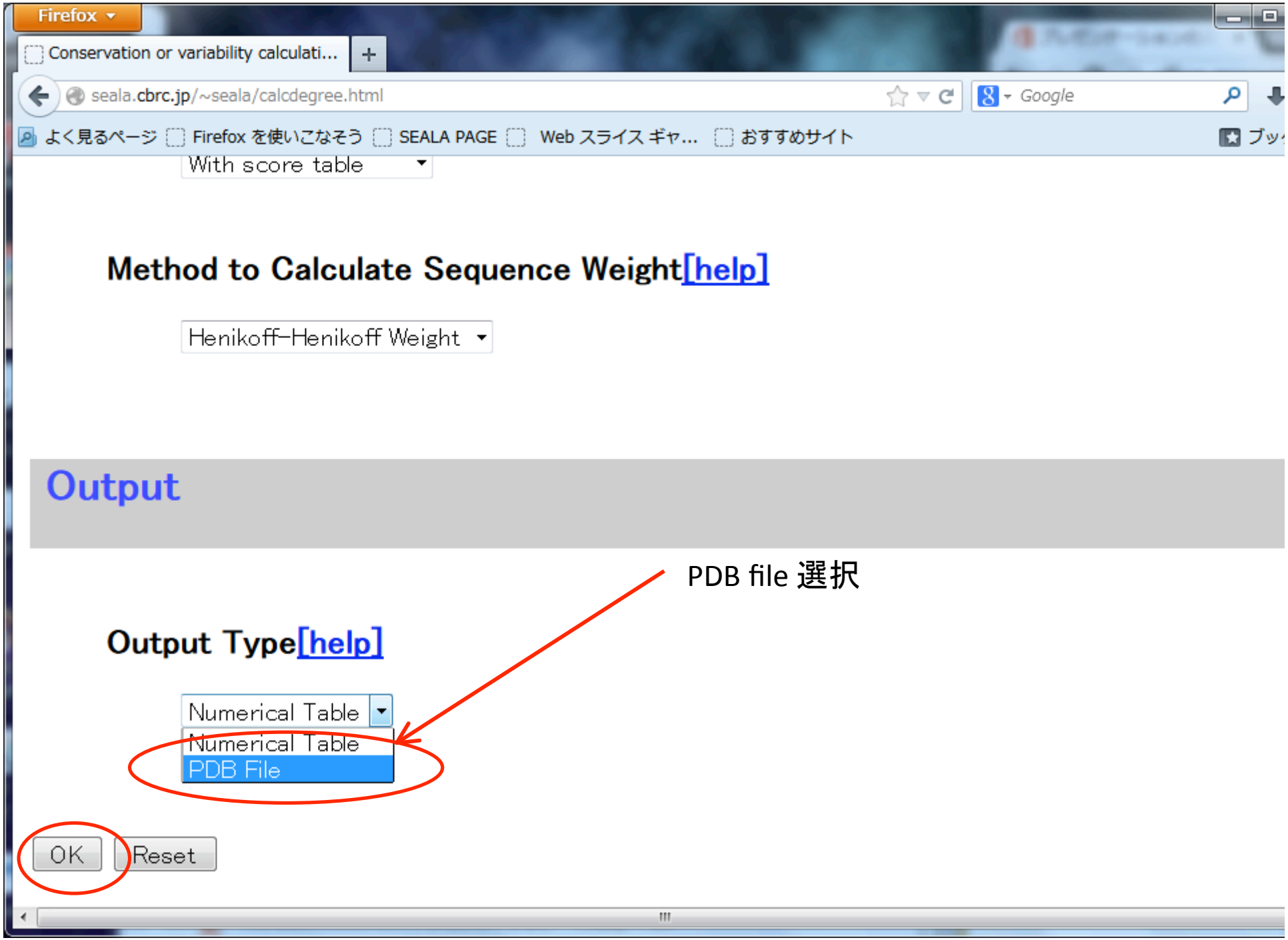
１ページ目


Firefox
Conservation or variability calculati...
seala.cbrc.jp/~seala/calcdegree.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Conservation or Variability at Each Alignment Site
Input
align_example.txtを選択
Alignment File[help]
参照...
ファイルが選択されていません。
PDB File[help]
参照...
ファイルが選択されていません。
Options


Firefox
Conservation or variability calculati...
seala.cbrc.jp/~seala/calcdegree.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Conservation or Variability at Each Alignment Site
Input
Alignment File[help]
参照...
ファイルが選択されていません。
1UJY.pdb を選択
PDB File[help]
参照...
ファイルが選択されていません。
Options


Firefox
Conservation or variability calculati...
seala.cbrc.jp/~seala/calcdegree.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Options
Threshold[help]
Threshold(%) : 50
With score table 選択
Method group to calculate Conservation or Variability at Each Alignment Site.[help]
Without score table
Without score table
With score table
Fredrik module
Method to Calculate Sequence Weight[help]
No Weight


Firefox
Conservation or variability calculati...
seala.cbrc.jp/~seala/calcdegree.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Options
Threshold[help]
Threshold(%) : 50
Henikoff-Henikoff Weight 選択
Method group to calculate Conservation or Variability at Each Alignment Site.[help]
With score table
Method to Calculate Sequence Weight[help]
No Weight
No Weight
Difference Weight
Henikoff-Henikoff Weight
Voronoi Weight


Firefox
Conservation or variability calculati...
seala.cbrc.jp/~seala/calcdegree.html
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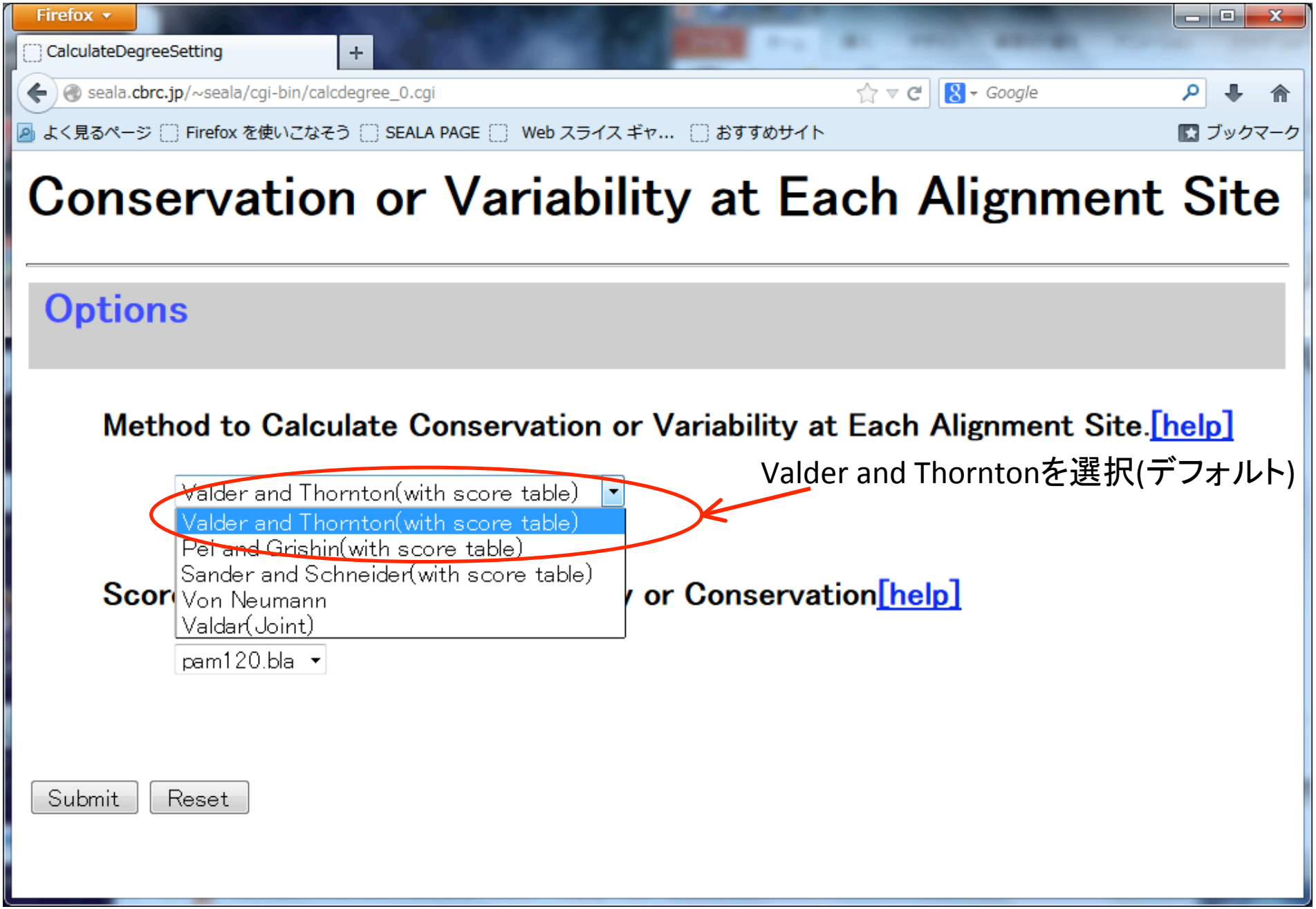
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
With score table
Method to Calculate Sequence Weight[help]
Henikoff-Henikoff Weight
Output
PDB file 選択
Output Type[help]
Numerical Table
Numerical Table
PDB File
OK
Reset

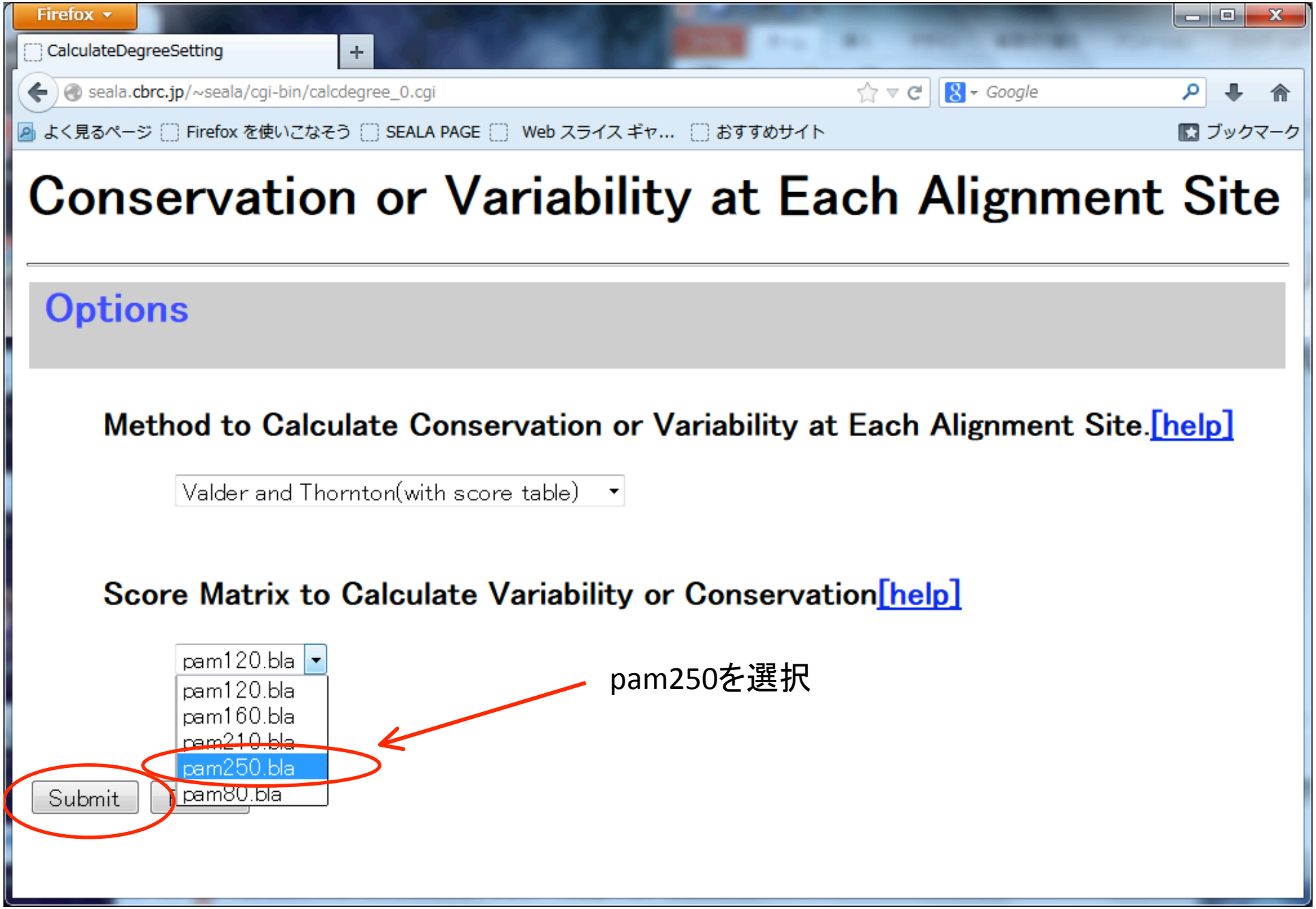
Conservation/Variability

3 ページ　選択画面が出てくる

２ページ目



Valder and Thorntonを選択(デフォルト)


Firefox
CalculateDegreeSetting
seala.cbrc.jp/~seala/cgi-bin/calcdegree_0.cgi
Google
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Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Conservation or Variability at Each Alignment Site
Options
Method to Calculate Conservation or Variability at Each Alignment Site.[help]
Valder and Thornton(with score table)
Score Matrix to Calculate Variability or Conservation[help]
pam120.bla
pam120.bla
pam160.bla
pam210.bla
pam250.bla
pam80.bla
Submit
pam250を選択

Conservation/Variability

3ページ　選択画面が出てくる

3ページ目

Firefox

CalculateDegreeSetting

seala.cbrc.jp/~seala/cgi-bin/calcdegree_1.cgi

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Conservation or Variability at Each Alignment Site

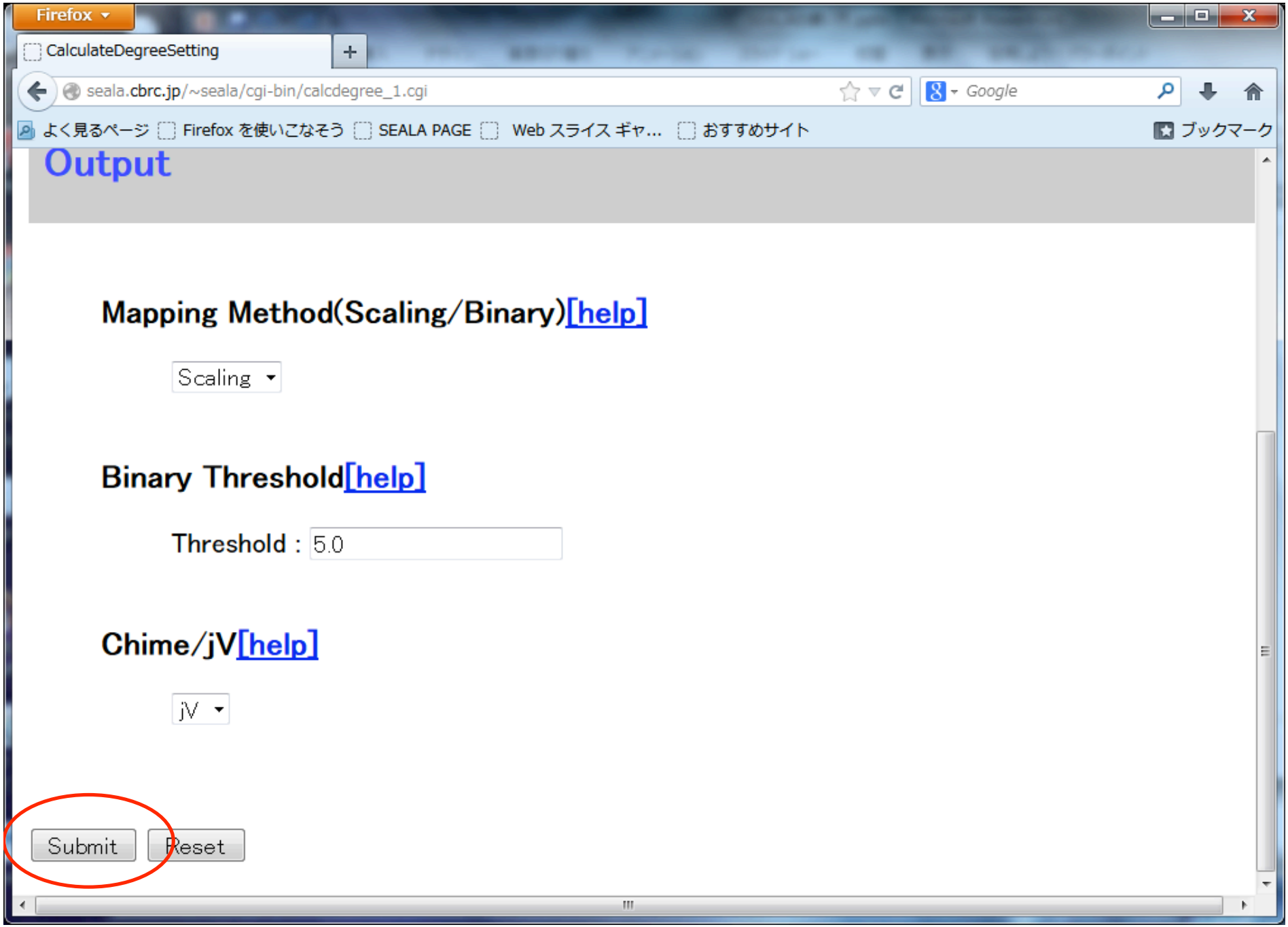
Options

Output

Mapping Method(Scaling/Binary)[help]

Scaling

Binary Threshold[help]


Firefox
CalculateDegreeSetting
seala.cbrc.jp/~seala/cgi-bin/calcdegree_1.cgi
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SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Output
Mapping Method(Scaling/Binary)[help]
Scaling
Binary Threshold[help]
Threshold : 5.0
Chime/jV[help]
jV
Submit
Reset

Firefox

CalculateDegreeResult

seala.cbrc.jp/~seala/cgi-bin/calcdegree_2.cgi

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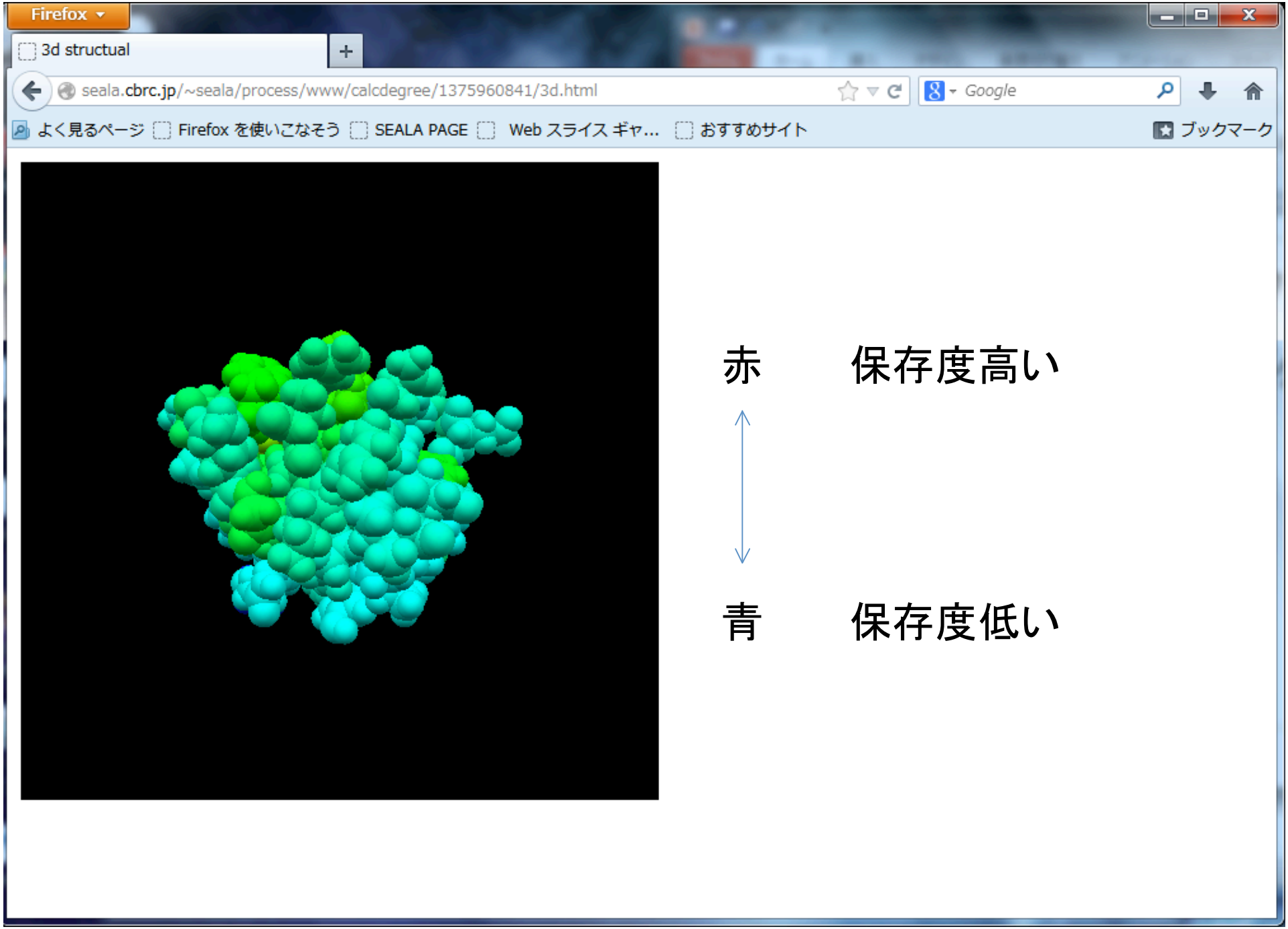
Method by Valder & Thornton(2001)

3D molecular structure選択

3D molecular structure
download pdb file(Please right click, and download the file)
download pdb file whose column for temperature factor is modified with the information about conservation or variability(see help details)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3d structual
seala.cbrc.jp/~seala/process/www/calcdegree/1375960841/3d.html
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赤　保存度高い
青　保存度低い

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CalculateDegreeResult

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Method by Valder & Thornton(2001)

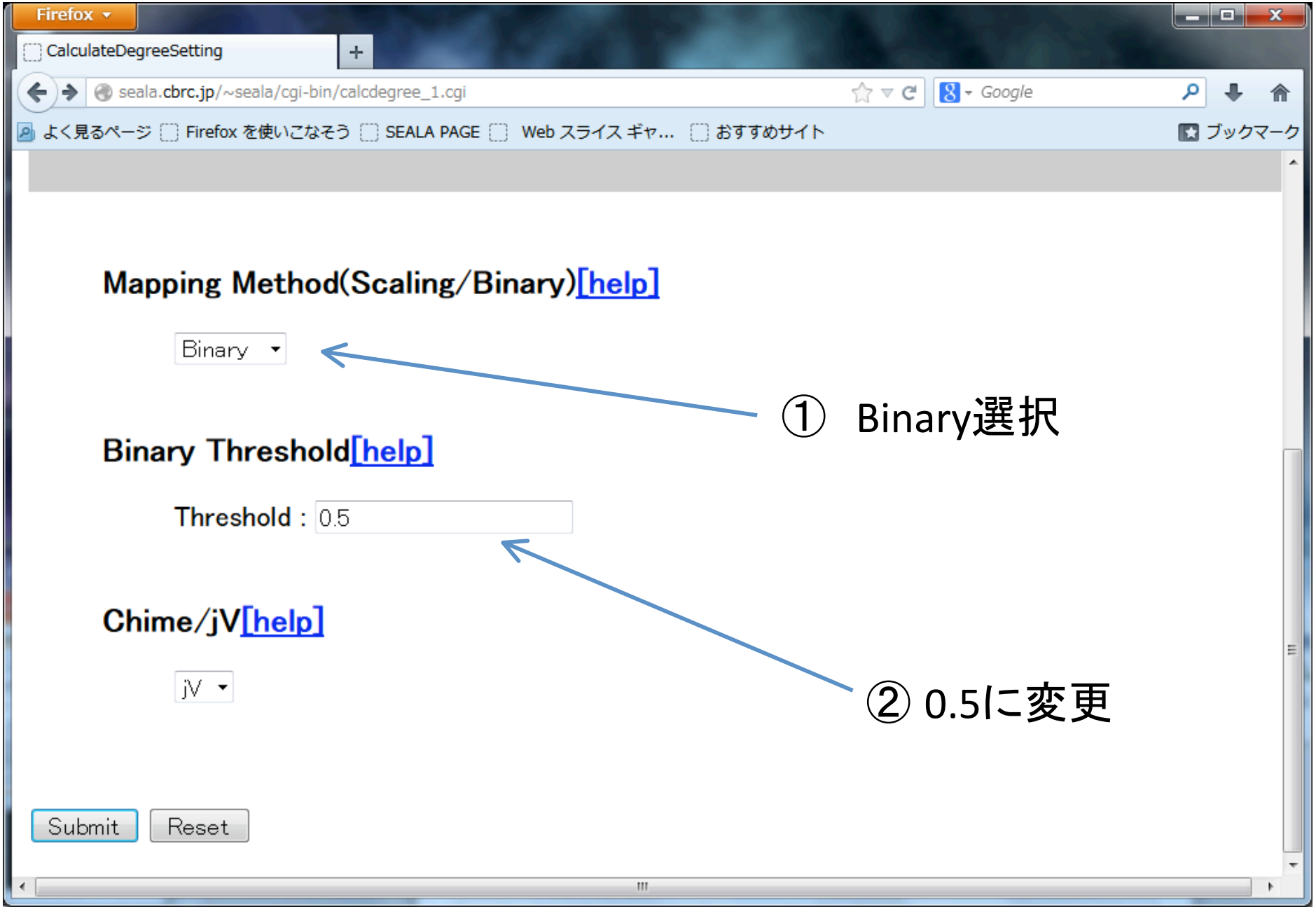
3D molecular structure
download pdb file(Please right click, and download the file)
download pdb file whose column for temperature factor is modified with the information about conservation or variability(see help details)

---

download pdb fileを選択すると
温度因子を保存度で書き換えた
pdb 形式のファイルが得られる。
ローカルなビューアで表示

保存と非保存で二値化したい時

３ページ目の処理を変更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Web スライス ギャ...
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Mapping Method(Scaling/Binary)[help]
Binary
① Binary選択
Binary Threshold[help]
Threshold : 0.5
② 0.5に変更
Chime/jV[help]
jV
Submit
Reset

Firefox

3d structual

seala.cbrc.jp/~seala/process/www/calcdegree/1376800565/3d.html

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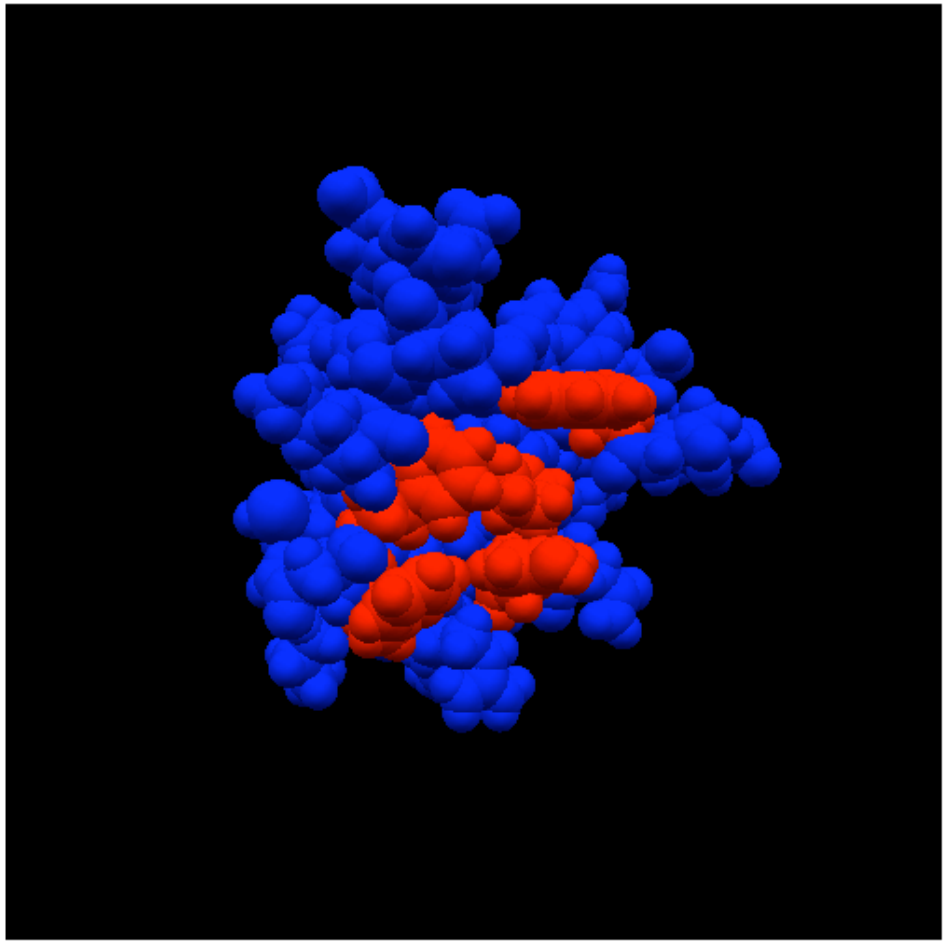

数値として保存度を得る

１ページ目と3ページ目の処理を変更

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Conservation or variability calculati...

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With score table

Method to Calculate Sequence Weight[help]

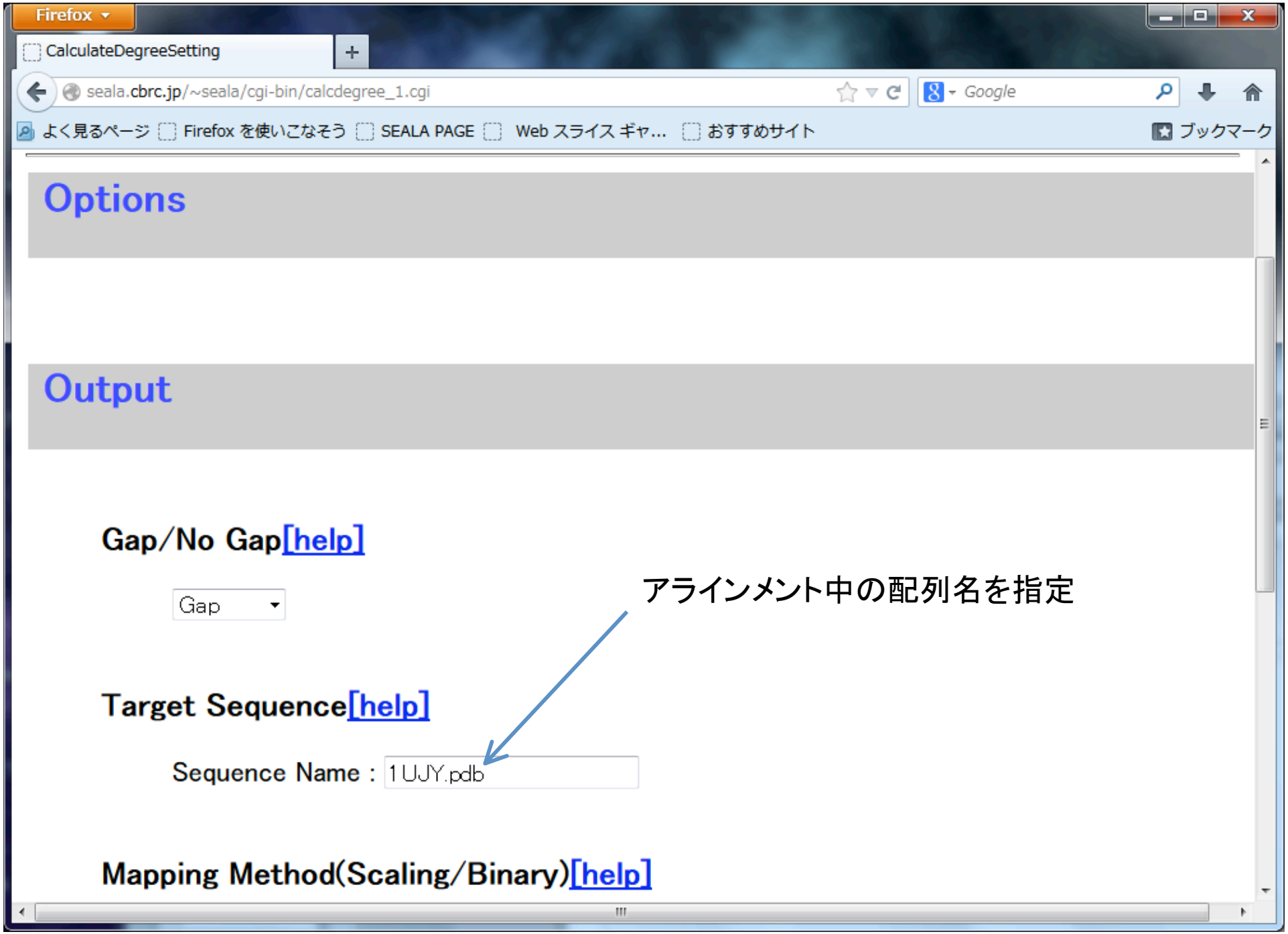
Henikoff-Henikoff Weight

Output

Output Type[help]

Numerical Table

OK Reset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seala.cbrc.jp/~seala/cgi-bin/calcdegree_1.cgi
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Web スライス ギャ...
おすすめサイト
ブックマーク
Options
Output
Gap/No Gap[help]
Gap
Target Sequence[help]
Sequence Name : 1UJY.pdb
Mapping Method(Scaling/Binary)[help]
アラインメント中の配列名を指定

Firefox

CalculateDegreeResult

seala.cbrc.jp/~seala/cgi-bin/calcdegree_2.cgi

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Method by Valder & Thornton(2001) – gap included –

1UJY.pdb

1	L	0.29
2	I	0.29
3	V	0.34
4	K	0.34
5	A	0.38
6	R	0.40
7	F	0.55
8	N	0.40
9	F	0.64
10	K	0.31
11	Q	0.35
12	T	0.32
13	N	0.34
14	–	0.00
15	–	0.00
16	E	0.35
17	D	0.36

Firefox

CalculateDegreeResult

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48	–	0.13
49	–	0.00
50	G	0.00
51	–	0.00
52	–	0.00
53	R	0.27
54	T	0.31
55	G	0.50
56	W	0.37
57	F	0.41
58	P	0.54
59	S	0.33
60	N	0.35
61	Y	0.60
62	V	0.44
63	R	0.35
64	E	0.30
65	I	0.32

3D molecular structure

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download pdb file whose column for temperature factor is modified with the information about conservation or variability(see help details)

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Discussion an...
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Authors' contributions
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A comparative study of conservation and variation scores

Fredrik Johansson[1]* and **Hiroyuki Toh**[2]

* Corresponding author: Fredrik Johansson fredjoha@gmail.com

Author Affiliations

[1] Division of Bioinformatics, Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka 812-8582, Japan

[2] CBRC, AIST Tokyo Waterfront Bio-IT Research Building, 2-42 Aomi, Koto-ku, Tokyo 135-0064, Japan

For all author emails, please log on.

BMC Bioinformatics 2010, **11**:388 doi:10.1186/1471-2105-11-388

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Volume 11

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ページ: 3 of 11 110%

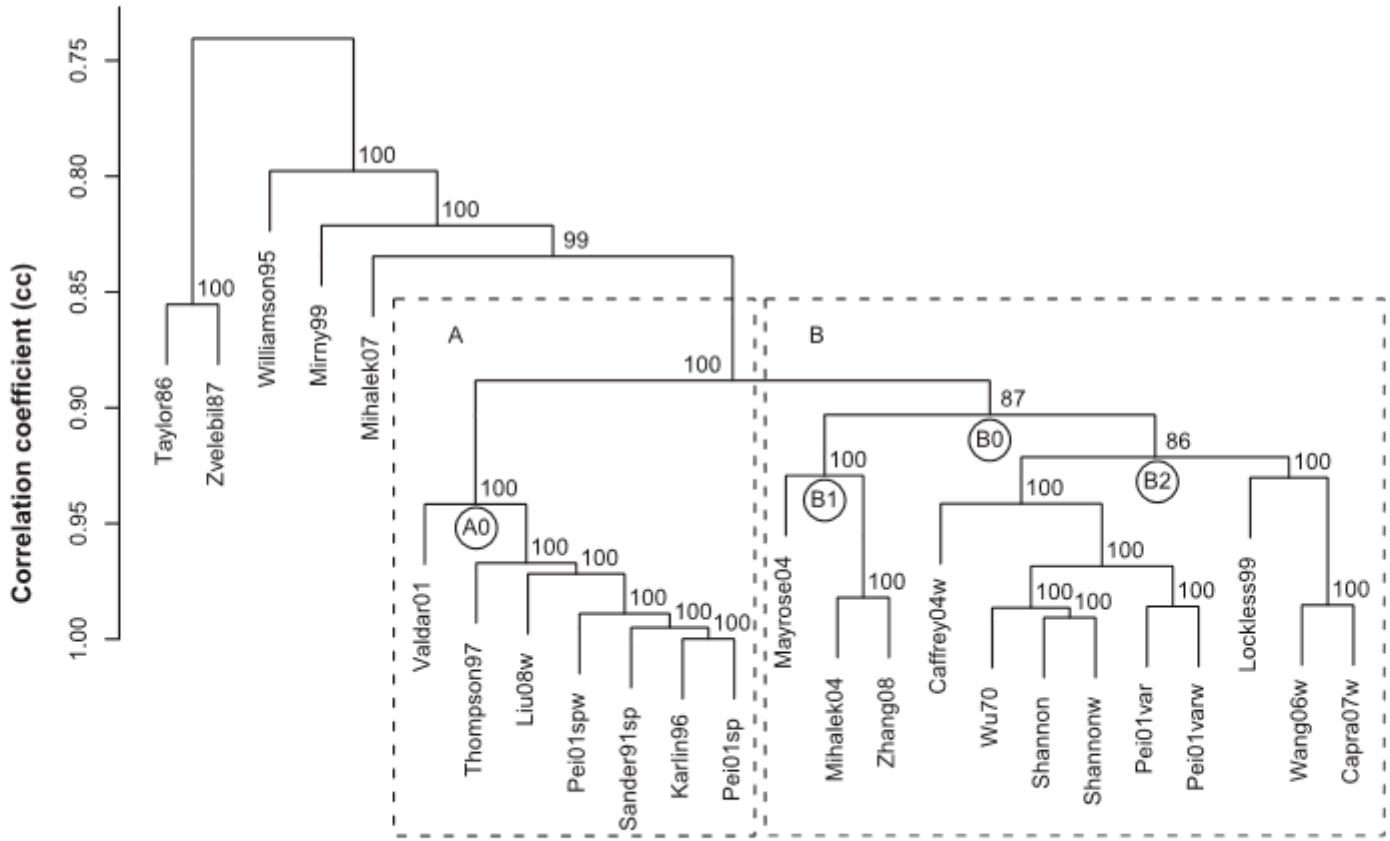

Figure 1 Hierarchical clustering results. Dendrogram obtained from hierarchical clustering of average Spearman correlations on each alignment, using average linking. Each node is labeled by a probability value in percent, given by 1000 iterations of a bootstrap procedure.

dendrogram in Figure 1. However, all scores in this clus- evolutionary rate (hence higher conservation score) for

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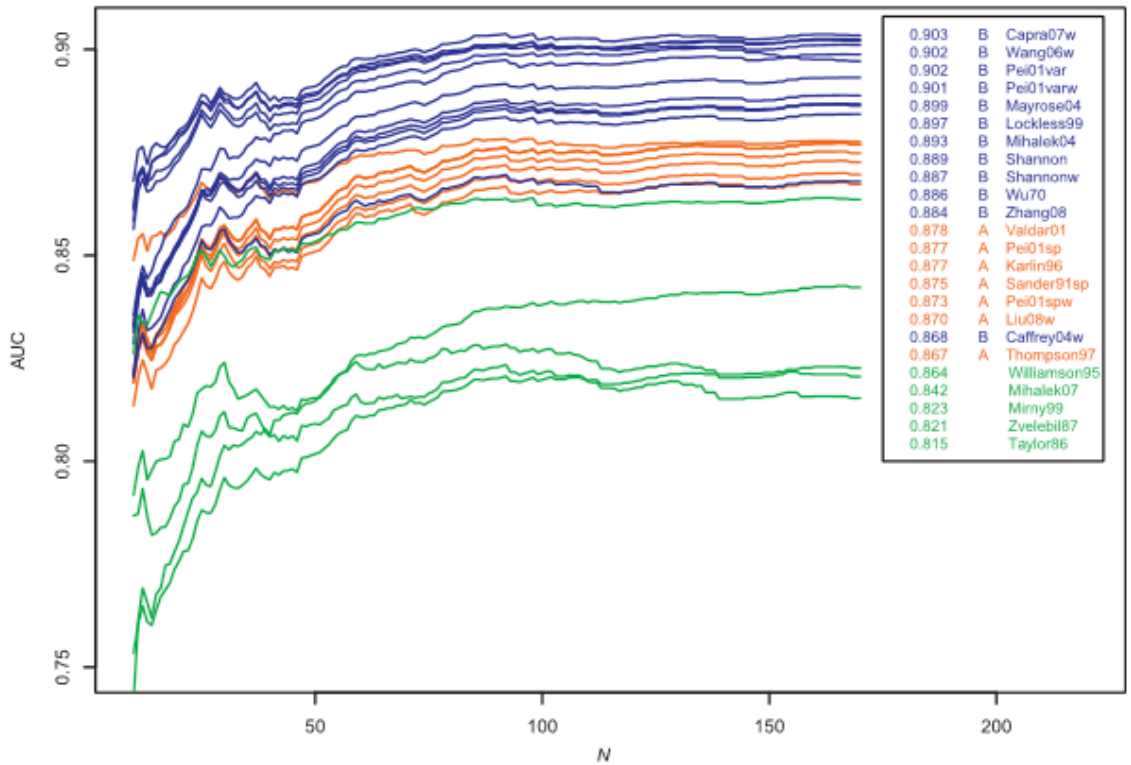

Figure 2 Performance evaluation. Performance evaluation of catalytic site prediction. Lines show the performance measured by the AUC measure for subsets of the original dataset obtained by setting an upper limit on alignment size (ranging from 10 to 168 sequences in an alignment). The legend is sorted on score performance for the original dataset (equal to the right terminal values of the graph), and also shows

検索: Neuman 次を検索(N) 前を検索(P) すべて強調表示(A) 大文字/小文字を区別(C)

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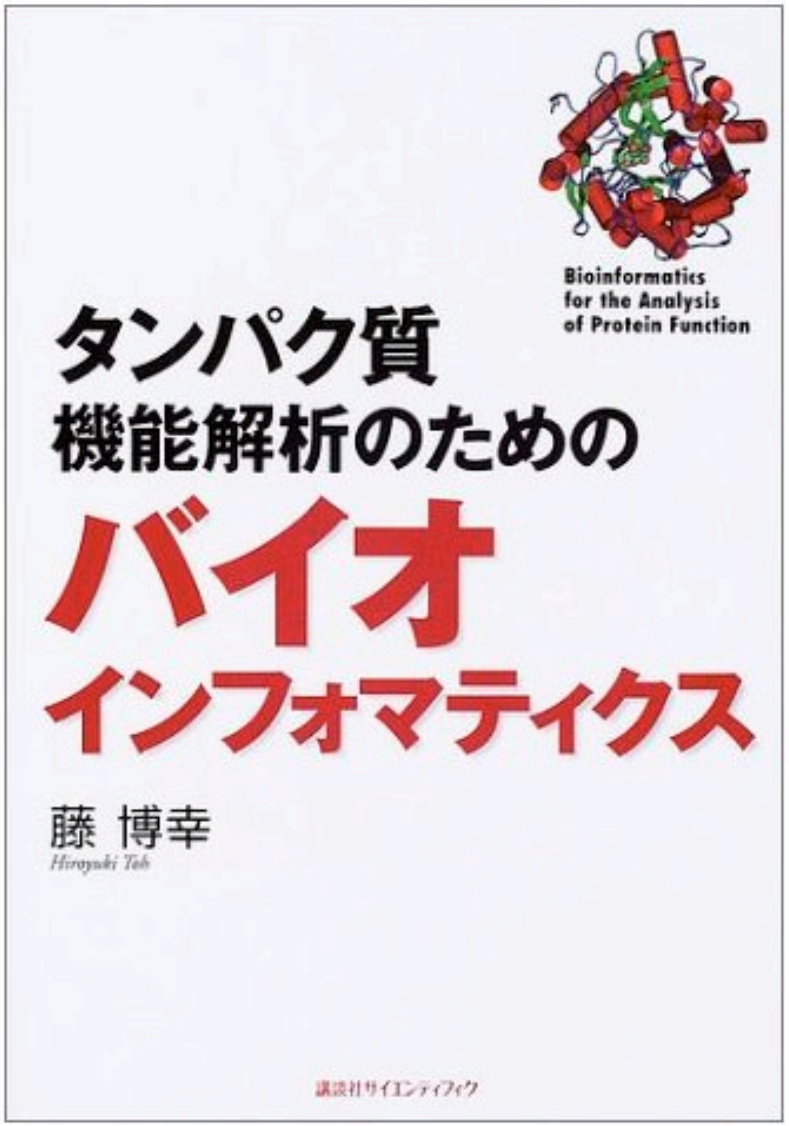
タンパク質機能解析のためのバイオインフォマティクス（KS生命科学専門書）



SEALAでできること

（1）アラインメントサイトの各種の保存度、変異度の計算とその立体構造上への表示

（2）アラインメントから相同タンパク質の機能差を決定しているサイトを推測し、それを立体構造上に表示

WindowsXP, 7, 8で動作確認

IE, Fire[ox, Google　chromeなどからアクセス可能

（1）　進化トレース法

（2）　累積相対エントロピー法

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1 / 17 115%

J. Mol. Biol. (1996) **257**, 342–35

JMB

An Evolutionary Trace Method Defines Binding Surfaces Common to Protein Families

Olivier Lichtarge[1,2], Henry R. Bourne[1] and Fred E. Cohen[1,2*]

[1]*Departments of Cellular and Molecular Pharmacology and Medicine and* [2]*Department of Pharmaceutical Chemistry University of California San Francisco CA 94143-0450, USA*

X-ray or NMR structures of proteins are often derived without the ligands, and even when the structure of a full complex is available, the are of contact that is functionally and energetically significant may be specialized subset of the geometric interface deduced from the spati proximity between ligands. Thus, even after a structure is solved, remains a major theoretical and experimental goal to localize prote functional interfaces and understand the role of their constituent residue The evolutionary trace method is a systematic, transparent and nov predictive technique that identifies active sites and functional interfaces proteins with known structure. It is based on the extraction of functional

215.9 x 279.4 mm

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3 / 17 50%

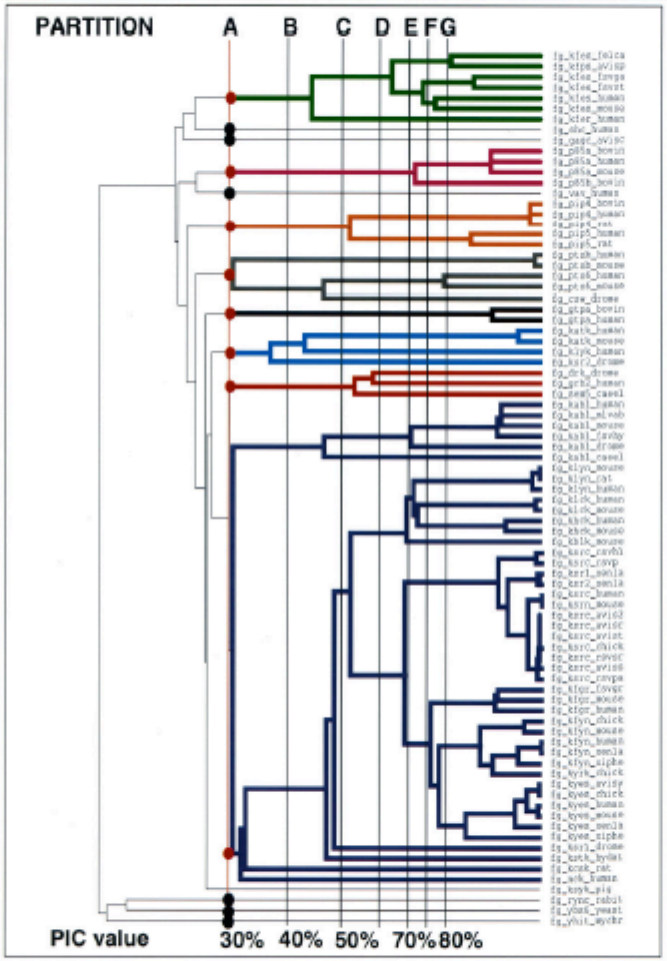

Figure 1. Sequence identity dendrogram of SH2 domains obtained as described in Methods. Vertical lines A to G represent the different partition identity cutoffs (PICs) that are used to define partitions. For each PIC, a partition of the entire family is generated by grouping together sequences that branch off from a node, shown in red, to the right of a PIC line. As PIC increases, from A to G, partitions comprise more groups, each with fewer sequences. Thick colored lines are used in this example to display the different groups in partition A. Six nodes, in black, give rise to singular groups and effectively drop out of the evolutionary trace analysis. ET analysis was performed over this entire tree, see Figure 3, and over the subtree shown in purple, see Figure 4.

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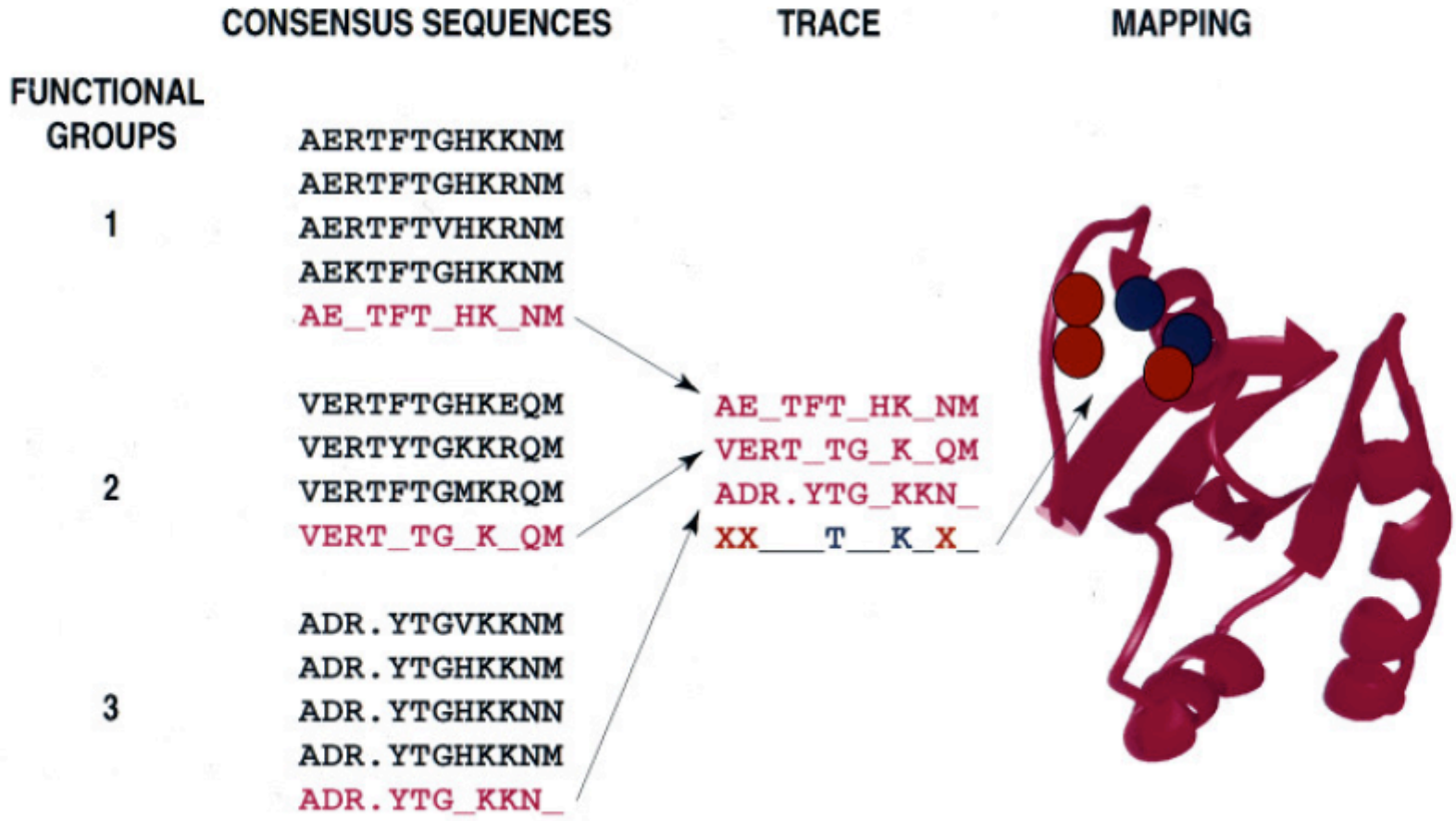
ファイル(F) 編集(E) 表示(V) ウィンドウ(W) ヘルプ(H)
4 / 17 150%



215.9 x 279.4 mm

Figure 2. Derivation of the evolutionary trace. The left panel shows sequences from

1-s2.0-S0022283696901679-main.pdf - Adobe Reader

ファイル(F) 編集(E) 表示(V) ウィンドウ(W) ヘルプ(H)

6 / 17 50%

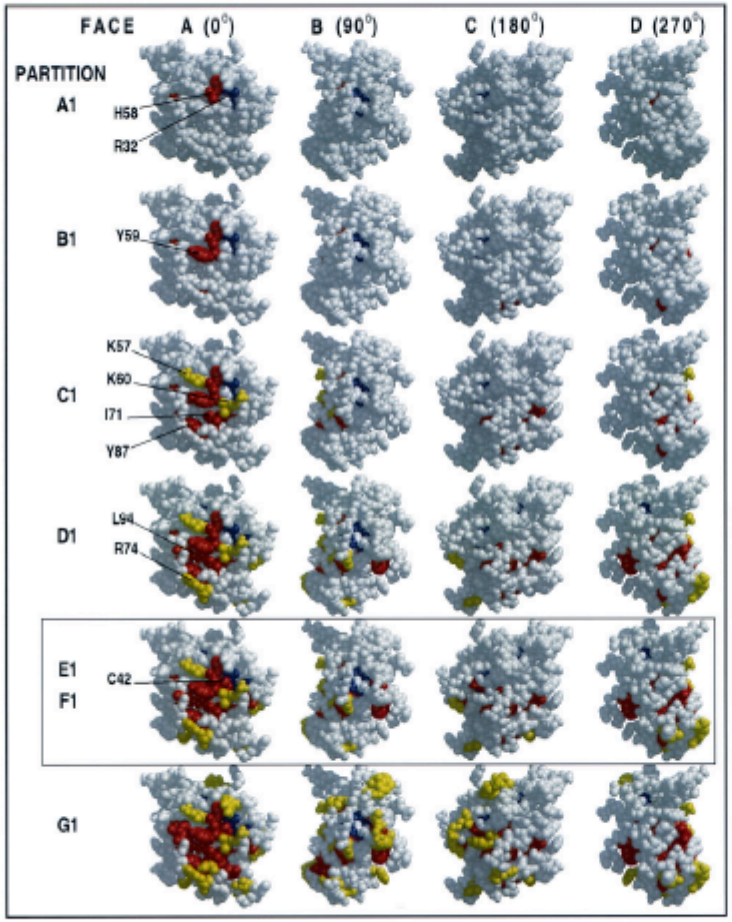


Figure 3. Evolutionary trace of the complete family of SH2 domains mapped onto the 2.7 Å resolution structure of Src SH2 domain (Waksman et al., 1993). Each row displays the protein in sequential 90% rotations about the z-axis, and successive rows show traces that arise from partitions A1 to G1, as defined in Figure 1. The internal positions that are conserved (dark blue) and class-specific (red), and the external class-specific (yellow) and conserved (cyan, though none in this Figure) positions are distributed inhomogeneously and form a single localized cluster on face A. At low PIC, partitions A and B, the trace is specific and points to only three residues, R32, H58 and Y59. To these core residues K57, K60, I71 and Y87 are added contiguously in partition C, L94 and R74 in partition D and C42 in partition E. The other faces remain essentially free of trace signal until partition G1. There, the scattered appearance of trace positions suggests that the useful limit of functional resolution has been reached at that higher PIC value. Partition F1 is not

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```
...CFV-DTGASLCIAS...
...TVVFDTGSSNLWVP...
...TVLFDTGSSDFWVP...
```

Extraction of Functional Sites

Sequence Weight help

Site-Specific Res, Freq help

Variability/Conservation help

ET & Relatives help

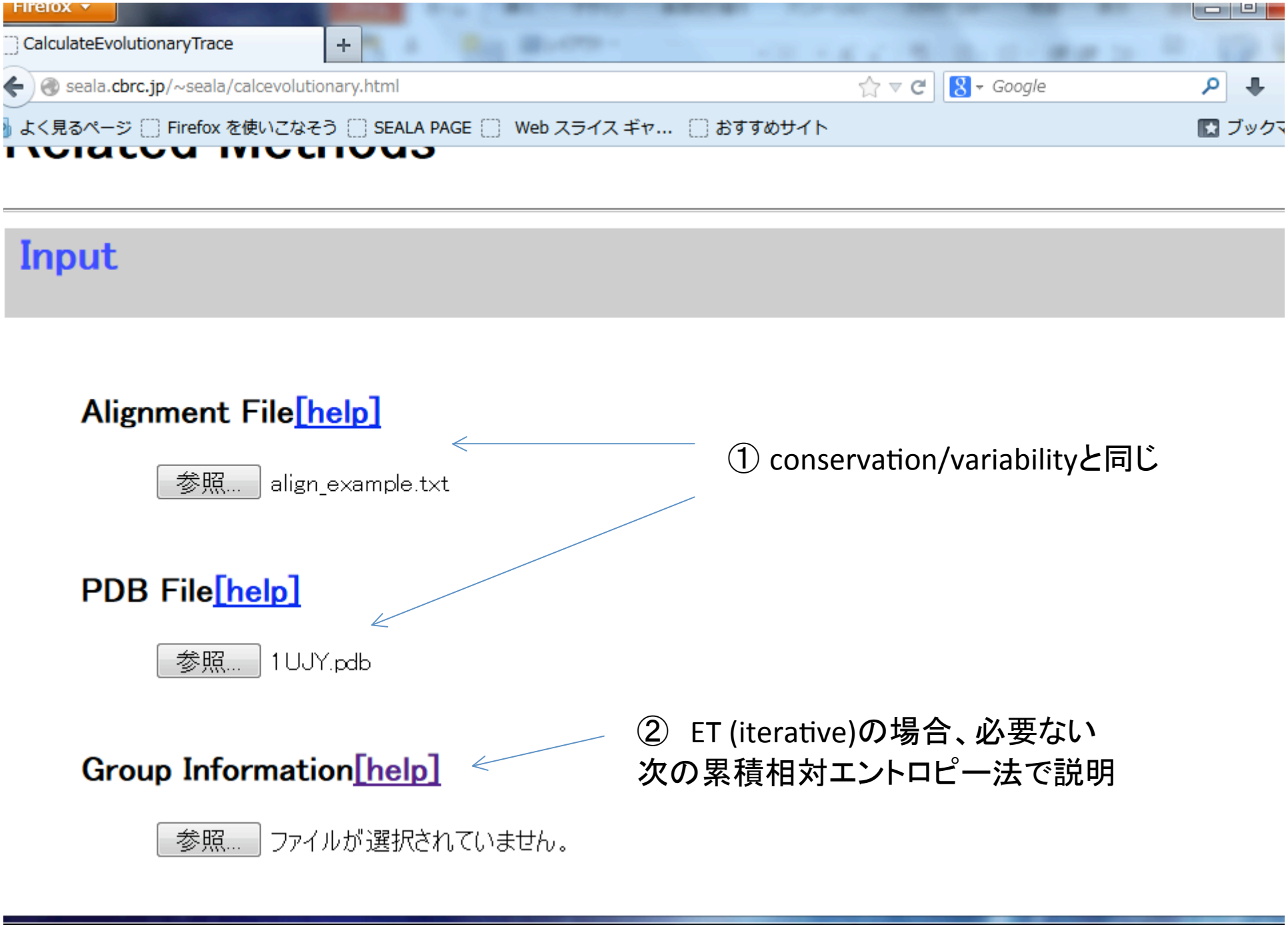
Plug in software, Chime or jV, is required to see the result of calculation on a tertiary structure.

Link

Link to Related Service : PC-31(Profile Comparison between 3D and 1D)

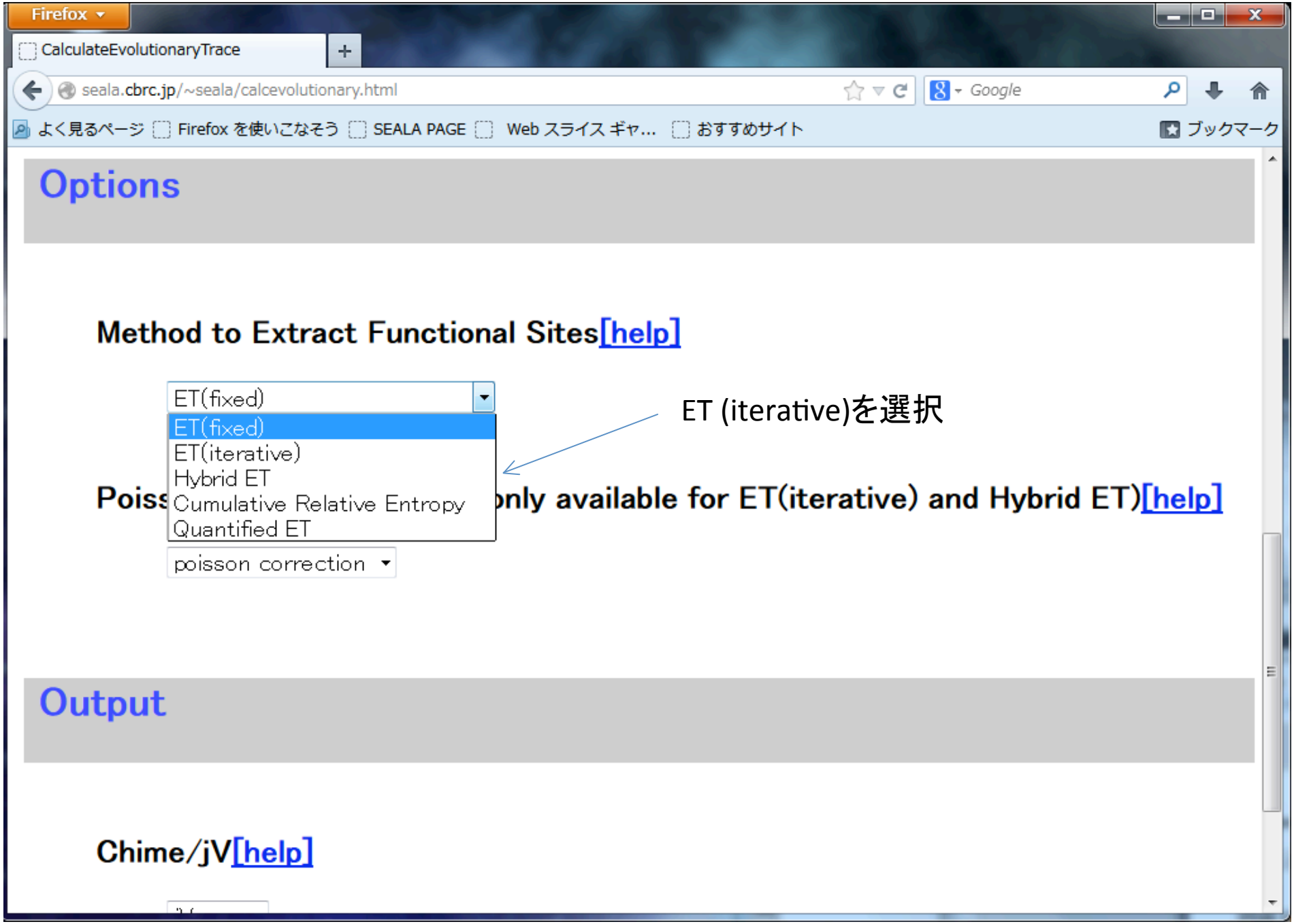
2つの入力画面

入力画面1



① conservation/variabilityと同じ

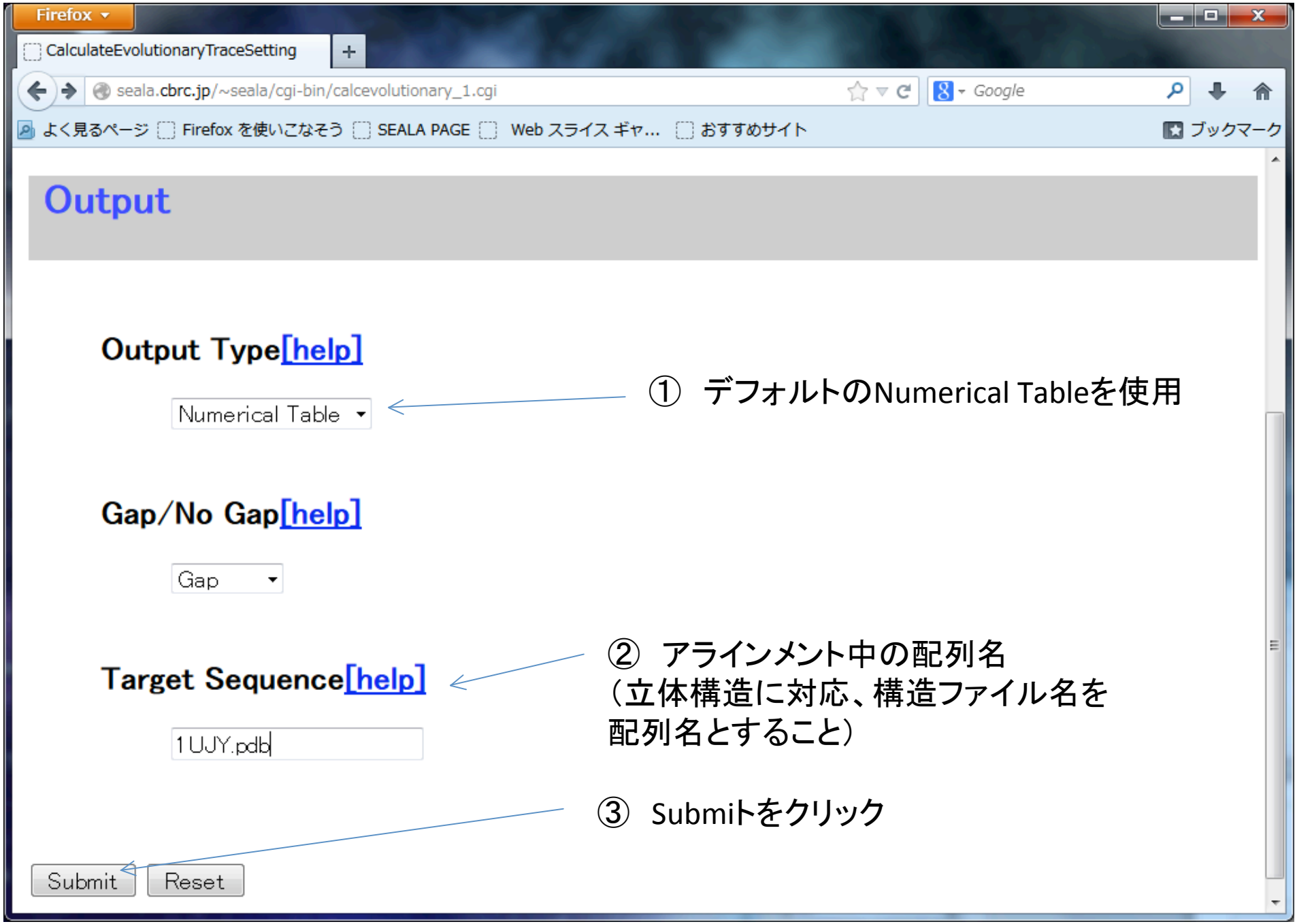
② ET (iterative)の場合、必要ない
次の累積相対エントロピー法で説明

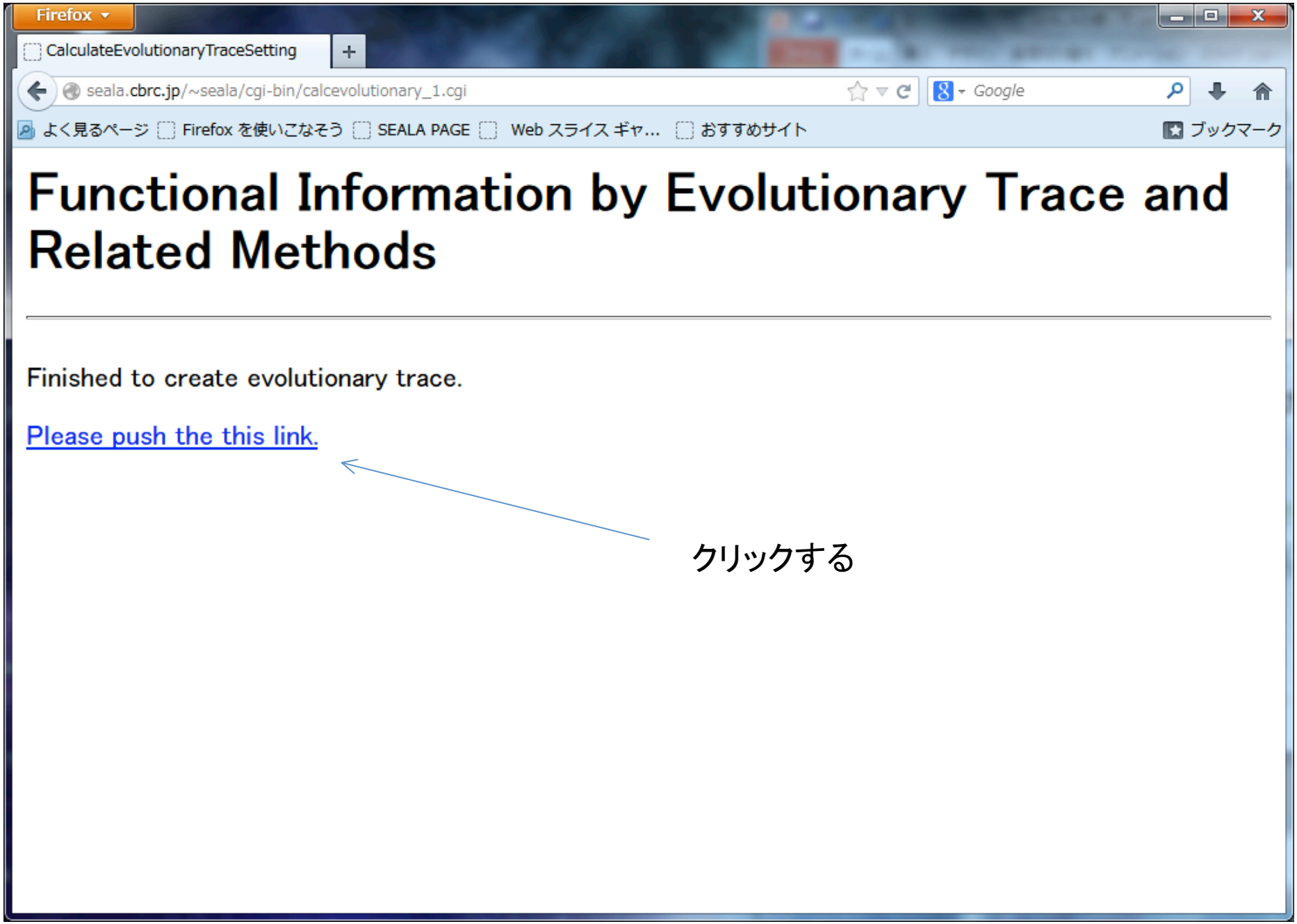

Firefox
CalculateEvolutionaryTrace
seala.cbrc.jp/~seala/calcevolutionary.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Options
Method to Extract Functional Sites[help]
ET(fixed)
ET(fixed)
ET(iterative)
Hybrid ET
Cumulative Relative Entropy
Quantified ET
ET (iterative)を選択
Poiss
nly available for ET(iterative) and Hybrid ET)[help]
poisson correction
Output
Chime/jV[help]


Firefox
CalculateEvolutionaryTrace
seala.cbrc.jp/~seala/calcevolutionary.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
ET(fixed)
Poisson Correction Option(only available for ET(iterative) and Hybrid ET)[help]
poisson correction
Output
Chime/jV[help]
jV
クリックして次の入力画面へ
OK
Reset

2つの入力画面

入力画面2


Firefox
CalculateEvolutionaryTraceSetting
seala.cbrc.jp/~seala/cgi-bin/calcevolutionary_1.cgi
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Output
Output Type[help]
Numerical Table
① デフォルトのNumerical Tableを使用
Gap/No Gap[help]
Gap
Target Sequence[help]
1UJY.pdb
② アラインメント中の配列名
（立体構造に対応、構造ファイル名を
配列名とすること）
③ Submitをクリック
Submit
Reset


Firefox
CalculateEvolutionaryTraceSetting
seala.cbrc.jp/~seala/cgi-bin/calcevolutionary_1.cgi
Google
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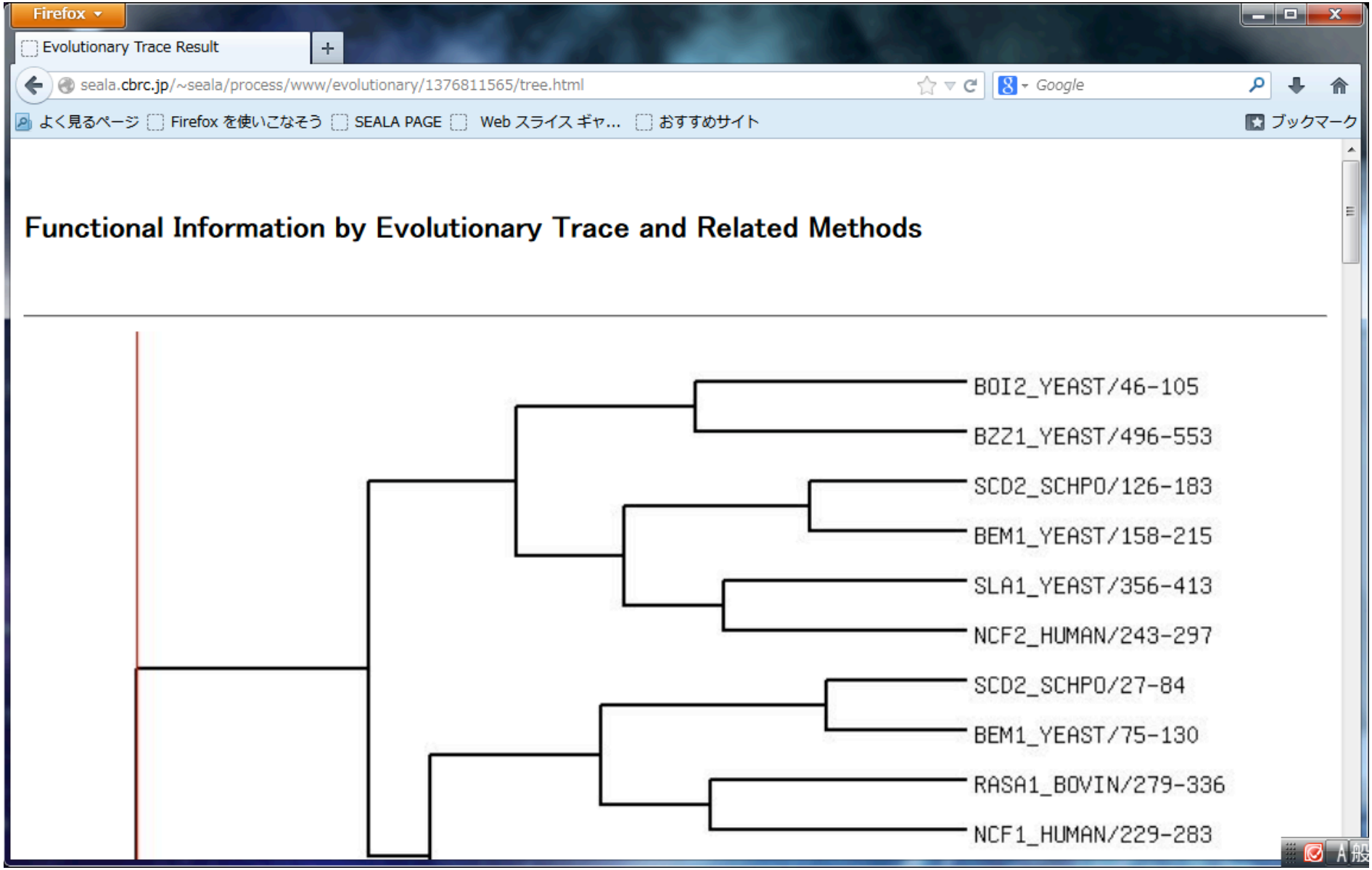
Finished to create evolutionary trace.
Please push the this link.
クリックする

出力画面上部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seala.cbrc.jp/~seala/process/www/evolutionary/1376811565/tree.html
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おすすめサイト
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Functional Information by Evolutionary Trace and Related Methods
BOI2_YEAST/46-105
BZZ1_YEAST/496-553
SCD2_SCHPO/126-183
BEM1_YEAST/158-215
SLA1_YEAST/356-413
NCF2_HUMAN/243-297
SCD2_SCHPO/27-84
BEM1_YEAST/75-130
RASA1_BOVIN/279-336
NCF1_HUMAN/229-283

出力画面下部

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Evolutionary Trace Result

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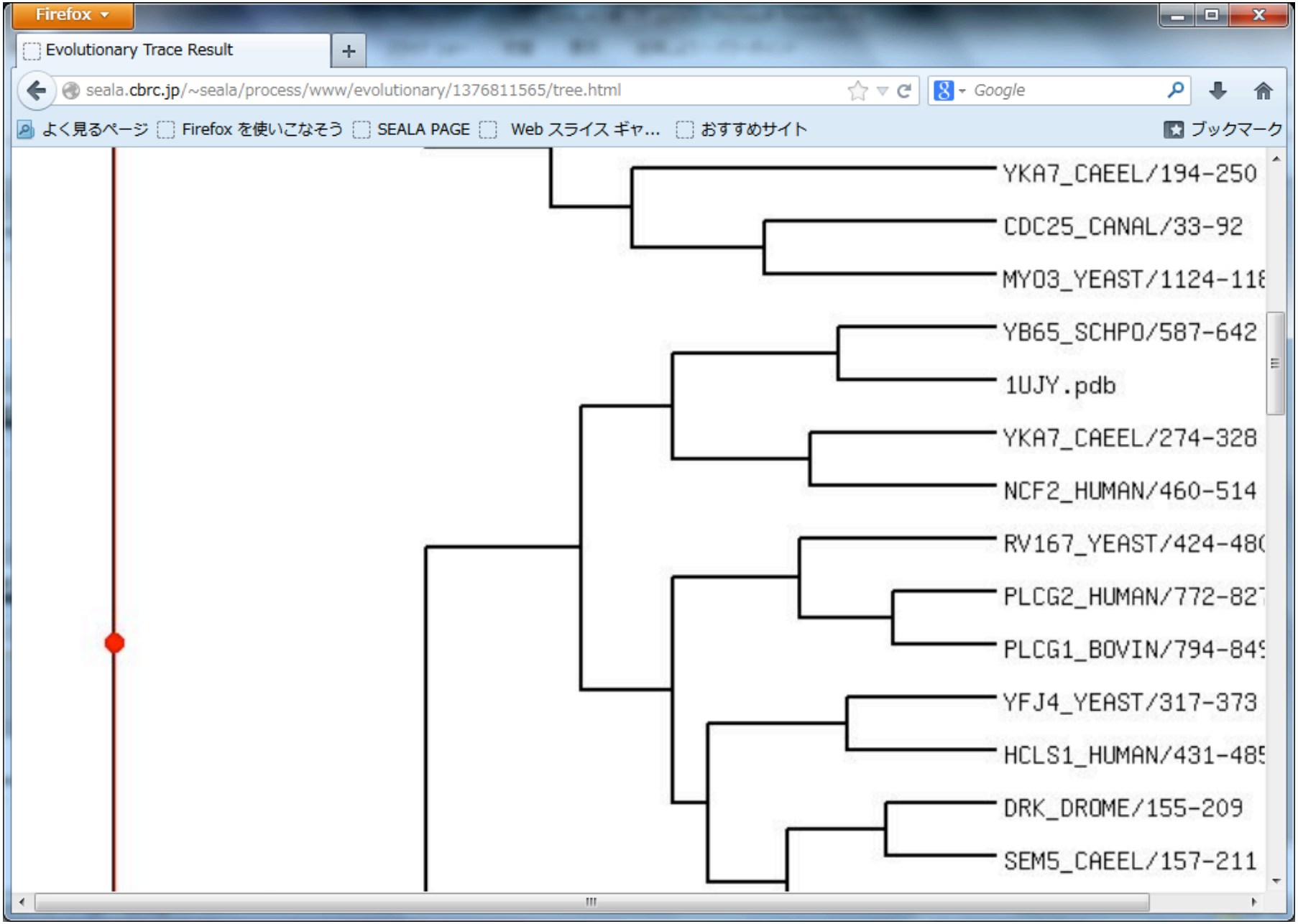
A small ID number indicates that the position of the node is close to the root,
whereas the node with a large ID number is present near the leaf.
Difference of a node indicates the averaged difference between a pair of subclusters
connected at the node, which is calculated in the tree construction by the UPGMA procedure.
The node corresponding to a node ID is mapped on the UPGMA tree by clicking the node ID.
If the difference is clicked, a new window appears where the information about trace residues is shown along
alignment sites.

node id	difference	node id	difference	node id	difference	node id	difference	node id	differenc
1	3.912023	2	3.218876	3	2.813411	4	2.525729	5	2.52572
6	2.525729	7	2.302585	8	2.120264	9	2.120264	10	1.96611
11	1.966113	12	1.832581	13	1.832581	14	1.832581	15	1.71479
16	1.714798	17	1.609438	18	1.609438	19	1.609438	20	1.51412
21	1.427116	22	1.427116	23	1.427116	24	1.272966	25	1.27296
26	1.272966	27	1.203973	28	1.139434	29	1.139434	30	1.13943
31	1.078810	32	1.021651	33	1.021651	34	1.021651	35	1.02165
36	0.916291	37	0.916291	38	0.867501	39	0.867501	40	0.86750
41	0.820981	42	0.820981	43	0.820981	44	0.733969	45	0.69314
46	0.693147	47	0.693147	48	0.693147	49	0.653926	50	0.65392
51	0.616186	52	0.544727	53	0.510826	54	0.478036	55	0.47803

node id :系統樹のnodeに対応
小さいものほどrootに近い

Difference　node idに対応し、そのnode配下にある配列間のdifferenceの平均

Node idを選択すると系統樹上で分割ポイントを表示
系統樹上で赤いバーが接しているnodeが分割ポイント
（最初はルートが分割ポイントになっている）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YKA7_CAEEL/194-250
CDC25_CANAL/33-92
MYO3_YEAST/1124-11
YB65_SCHPO/587-642
1UJY.pdb
YKA7_CAEEL/274-328
NCF2_HUMAN/460-514
RV167_YEAST/424-48
PLCG2_HUMAN/772-82
PLCG1_BOVIN/794-84
YFJ4_YEAST/317-373
HCLS1_HUMAN/431-48
DRK_DROME/155-209
SEM5_CAEEL/157-211

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A small ID number indicates that the position of the node is close to the root, whereas the node with a large ID number is present near the leaf.
Difference of a node indicates the averaged difference between a pair of subclusters connected at the node, which is calculated in the tree construction by the UPGMA procedure.
The node corresponding to a node ID is mapped on the UPGMA tree by clicking the node ID.
If the difference is clicked, a new window appears where the information about trace residues is shown along alignment sites.

1に対応する数字をクリック

node id	difference	node id	difference	node id	difference	node id	difference	node id	difference
1	3.912023	2	3.218876	3	2.813411	4	2.525729	5	2.52572
6	2.525729	7	2.302585	8	2.120264	9	2.120264	10	1.96611
11	1.966113	12	1.832581	13	1.832581	14	1.832581	15	1.71479
16	1.714798	17	1.609438	18	1.609438	19	1.609438	20	1.51412
21	1.427116	22	1.427116	23	1.427116	24	1.272966	25	1.27296
26	1.272966	27	1.203973	28	1.139434	29	1.139434	30	1.13943
31	1.078810	32	1.021651	33	1.021651	34	1.021651	35	1.02165
36	0.916291	37	0.916291	38	0.867501	39	0.867501	40	0.86750
41	0.820981	42	0.820981	43	0.820981	44	0.733969	45	0.69314
46	0.693147	47	0.693147	48	0.693147	49	0.653926	50	0.65392
51	0.616186	52	0.544727	53	0.510826	54	0.478036	55	0.47803
56	0.446287	57	0.446287	58	0.446287	59	0.415515	60	0.41551
61	0.356675								

www.mozilla.com/ja/firefox/central/

Firefox

Evolutionary Trace Result | Evolutionary Trace Result

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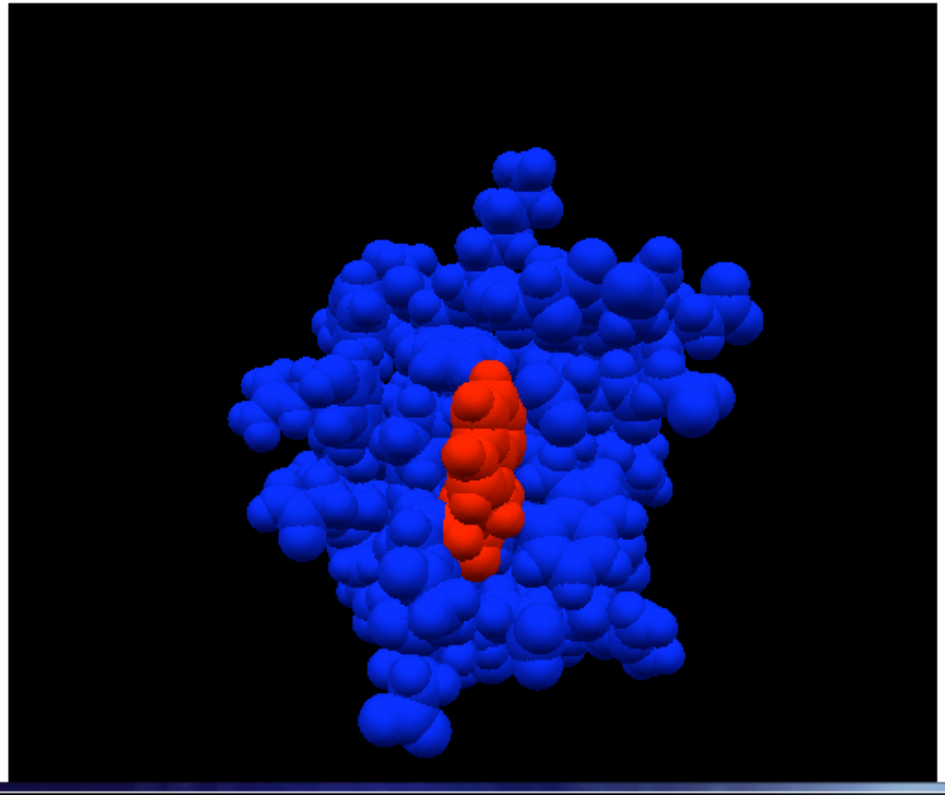

新しいタブに構造が表示

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19	neutral	-	
20	neutral	-	
21	neutral	-	
22	neutral	-	
23	neutral	-	
24	neutral	-	
25	neutral	-	
26	neutral	-	
27	neutral	-	
28	neutral	-	
29	neutral	-	
30	neutral	-	
31	neutral	-	
32	neutral	-	
33	neutral	-	
34	neutral	-	
35	neutral	-	
36	neutral	-	
37	neutral	-	
38	neutral	-	
39	neutral	-	
40	conserved	W	X
41	neutral	-	
42	neutral	-	
43	neutral	-	
44	neutral	-	

① 系統樹の表示されているタブをクリック

Firefox

Evolutionary Trace Result | Evolutionary Trace Result

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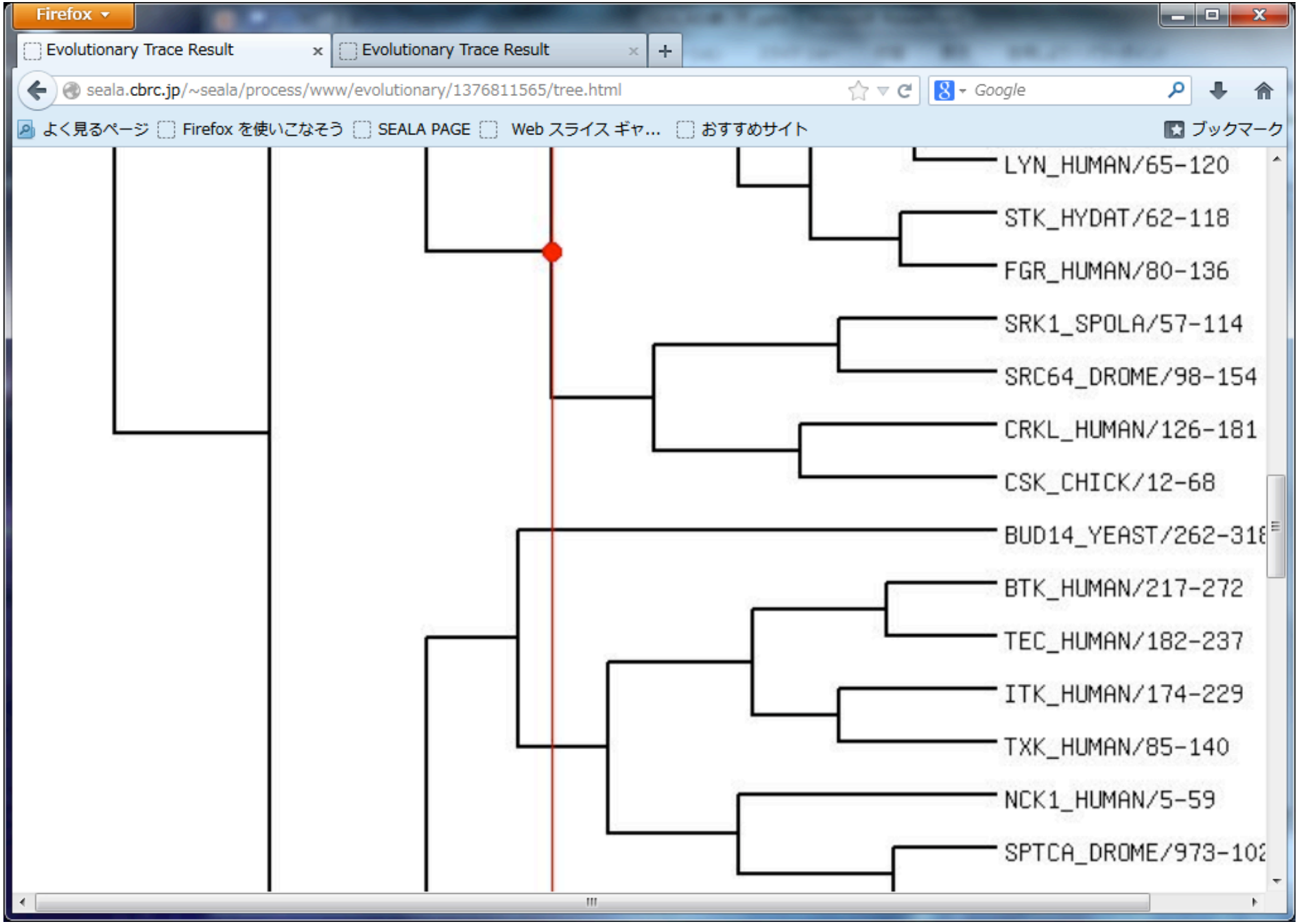
whereas the node with a large ID number is present near the leaf.
Difference of a node indicates the averaged difference between a pair of subclusters connected at the node, which is calculated in the tree construction by the UPGMA procedure.
The node corresponding to a node ID is mapped on the UPGMA tree by clicking the node ID.
If the difference is clicked, a new window appears where the information about trace residues is shown along alignment sites.

② Node id 10をクリック

node id	difference	node id	difference	node id	difference	node id	difference	node id	difference
1	3.912023	2	3.218876	3	2.813411	4	2.525729	5	2.52572
6	2.525729	7	2.302585	8	2.120264	9	2.120264	10	1.96611
11	1.966113	12	1.832581	13	1.832581	14	1.832581	15	1.71479
16	1.714798	17	1.609438	18	1.609438	19	1.609438	20	1.51412
21	1.427116	22	1.427116	23	1.427116	24	1.272966	25	1.27296
26	1.272966	27	1.203973	28	1.139434	29	1.139434	30	1.13943
31	1.078810	32	1.021651	33	1.021651	34	1.021651	35	1.02165
36	0.916291	37	0.916291	38	0.867501	39	0.867501	40	0.86750
41	0.820981	42	0.820981	43	0.820981	44	0.733969	45	0.69314
46	0.693147	47	0.693147	48	0.693147	49	0.653926	50	0.65392
51	0.616186	52	0.544727	53	0.510826	54	0.478036	55	0.47803
56	0.446287	57	0.446287	58	0.446287	59	0.415515	60	0.41551
61	0.356675								


Firefox
Evolutionary Trace Result
Evolutionary Trace Result
seala.cbrc.jp/~seala/process/www/evolutionary/1376811565/tree.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
LYN_HUMAN/65-120
STK_HYDAT/62-118
FGR_HUMAN/80-136
SRK1_SPOLA/57-114
SRC64_DROME/98-154
CRKL_HUMAN/126-181
CSK_CHICK/12-68
BUD14_YEAST/262-318
BTK_HUMAN/217-272
TEC_HUMAN/182-237
ITK_HUMAN/174-229
TXK_HUMAN/85-140
NCK1_HUMAN/5-59
SPTCA_DROME/973-102

② 構造の表示されているタブをクリック

Firefox

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whereas the node with a large ID number is present near the leaf.
Difference of a node indicates the averaged difference between a pair of subclusters connected at the node, which is calculated in the tree construction by the UPGMA procedure.
The node corresponding to a node ID is mapped on the UPGMA tree by clicking the node ID.
If the difference is clicked, a new window appears where the information about trace residues is shown along alignment sites.

①10に対応する数字をクリック

node id	difference	node id	difference	node id	difference	node id	difference	node id	difference
1	3.912023	2	3.218876	3	2.813411	4	2.525729	5	2.52572
6	2.525729	7	2.302585	8	2.120264	9	2.120264	10	1.96611
11	1.966113	12	1.832581	13	1.832581	14	1.832581	15	1.71479
16	1.714798	17	1.609438	18	1.609438	19	1.609438	20	1.51412
21	1.427116	22	1.427116	23	1.427116	24	1.272966	25	1.27296
26	1.272966	27	1.203973	28	1.139434	29	1.139434	30	1.13943
31	1.078810	32	1.021651	33	1.021651	34	1.021651	35	1.02165
36	0.916291	37	0.916291	38	0.867501	39	0.867501	40	0.86750
41	0.820981	42	0.820981	43	0.820981	44	0.733969	45	0.69314
46	0.693147	47	0.693147	48	0.693147	49	0.653926	50	0.65392
51	0.616186	52	0.544727	53	0.510826	54	0.478036	55	0.47803
56	0.446287	57	0.446287	58	0.446287	59	0.415515	60	0.41551
61	0.356675								

Firefox

Evolutionary Trace Result | Evolutionary Trace Result

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Functional Information by Evolutionary Trace and Related Methods

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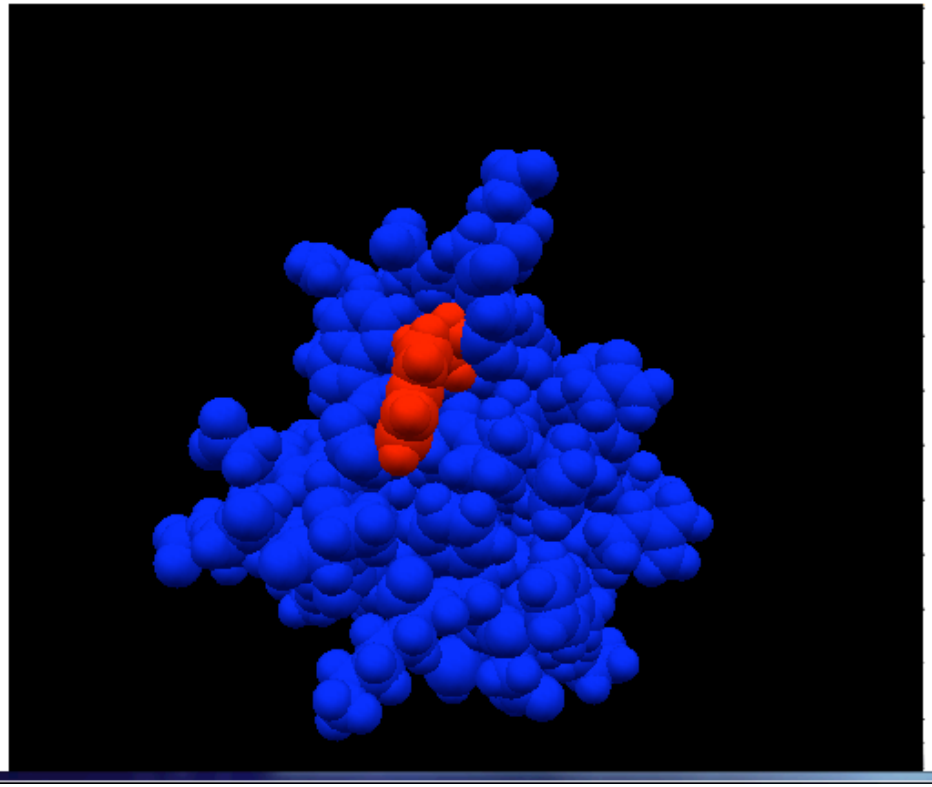

Firefox

Evolutionary Trace Result | Evolutionary Trace Result

seala.cbrc.jp/~seala/process/www/evolutionary/1376811565/10.html

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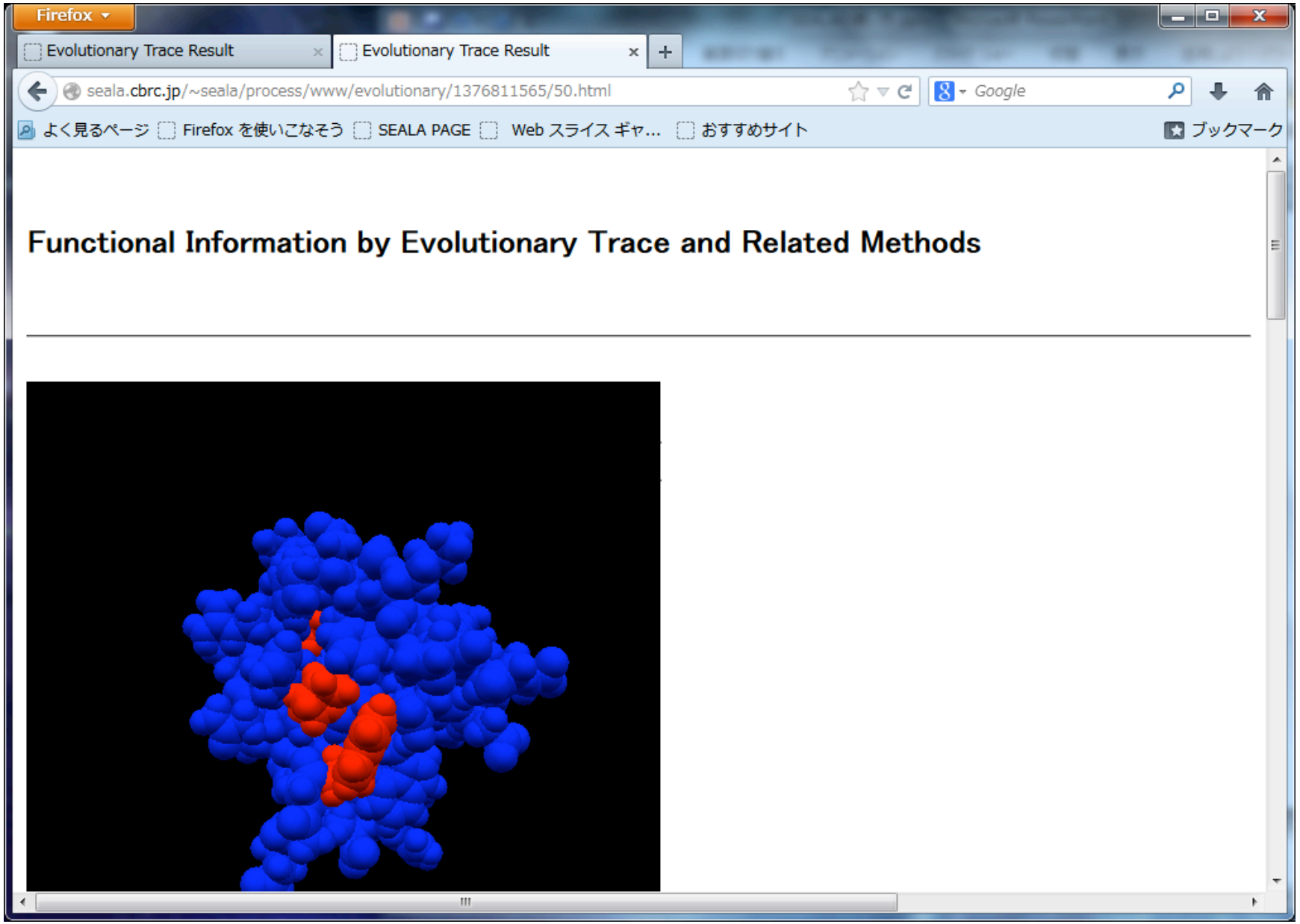
21	neutral	-	-	-	-	-	-	-	-	-	
22	neutral	-	-	-	-	-	-	-	-	-	
23	neutral	-	-	-	-	-	-	-	-	P	
24	neutral	G	G	-	-	-	-	G	G	G	
25	neutral	-	D	-	-	-	-	-	-	D	
26	neutral	-	-	-	-	-	-	-	-	K	
27	neutral	-	-	I	-	-	-	-	-	I	
28	neutral	-	-	-	-	-	-	-	-	-	
29	neutral	-	-	-	-	-	-	V	-	-	
30	neutral	-	-	-	-	-	L	-	-	-	
31	neutral	-	-	-	-	-	-	-	-	-	
32	neutral	-	-	-	-	-	-	-	-	-	
33	neutral	-	-	-	-	-	-	-	-	D	
34	neutral	-	-	-	-	-	-	-	-	-	
35	neutral	-	-	-	-	-	-	D	-	-	
36	neutral	-	-	-	-	-	-	-	-	-	
37	neutral	-	-	-	-	-	-	-	-	-	
38	neutral	-	-	-	-	-	-	-	-	-	
39	neutral	-	-	-	-	-	-	-	-	G	
40	conserved	W	W	W	W	W	W	W	W	W	X
41	neutral	-	-	-	-	-	W	-	-	-	
42	neutral	-	-	-	-	-	-	-	-	-	
43	neutral	-	-	G	-	-	-	-	-	-	
44	neutral	-	-	-	-	-	-	-	-	-	
45	neutral	-	-	-	-	-	-	-	-	N	
46	neutral	-	-	-	-	-	-	-	-	-	
47	neutral	-	-	-	-	-	-	-	-	-	

Node id 50の場合



Node id 54の場合

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Functional Information by Evolutionary Trace and Related Methods

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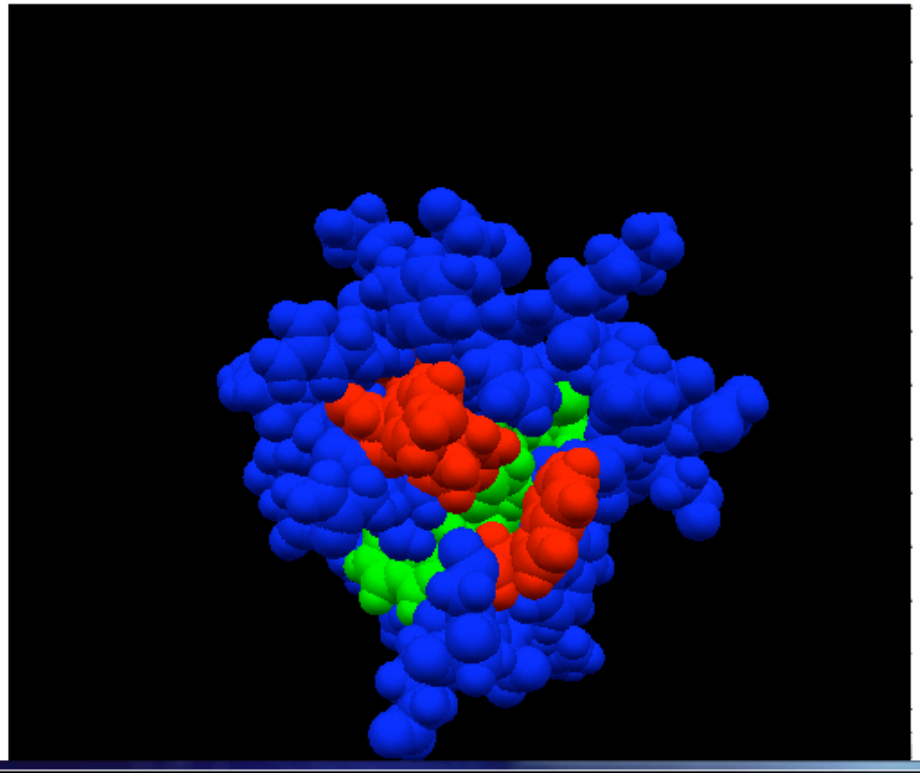

赤: invariant
緑: class-specific

Firefox

Evolutionary Trace Result | Evolutionary Trace Result

seala.cbrc.jp/~seala/process/www/evolutionary/1376811565/54.html

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Functional Information by Evolutionary Trace and Related Methods

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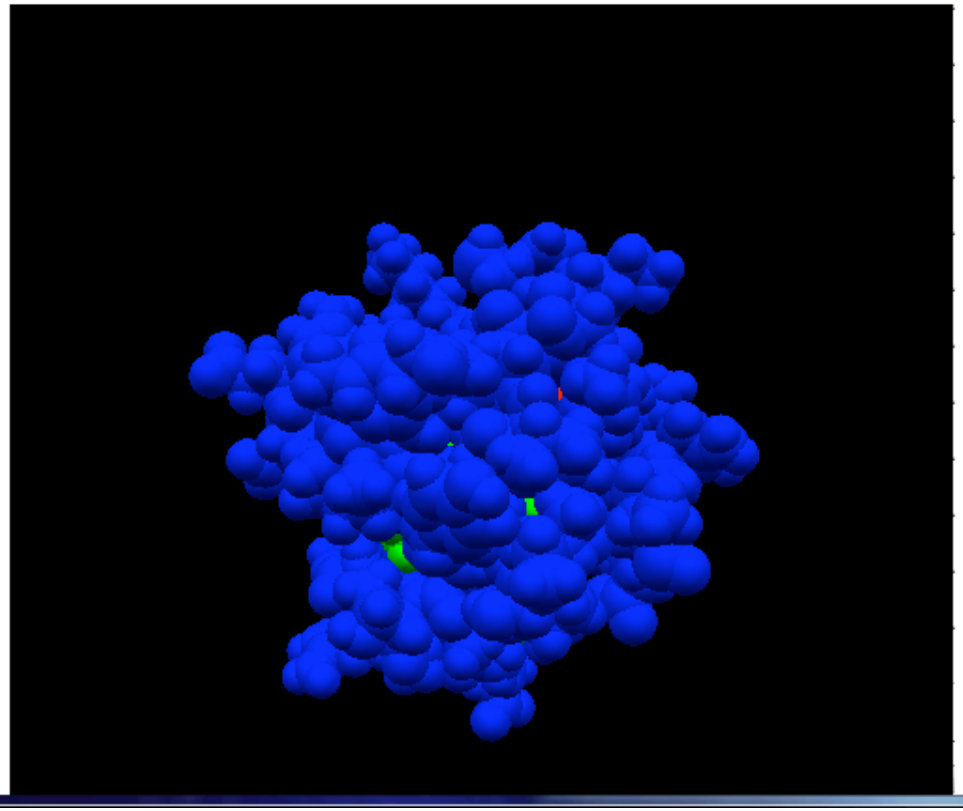

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Evolutionary Trace Result | Evolutionary Trace Result

seala.cbrc.jp/~seala/process/www/evolutionary/1376811565/54.html

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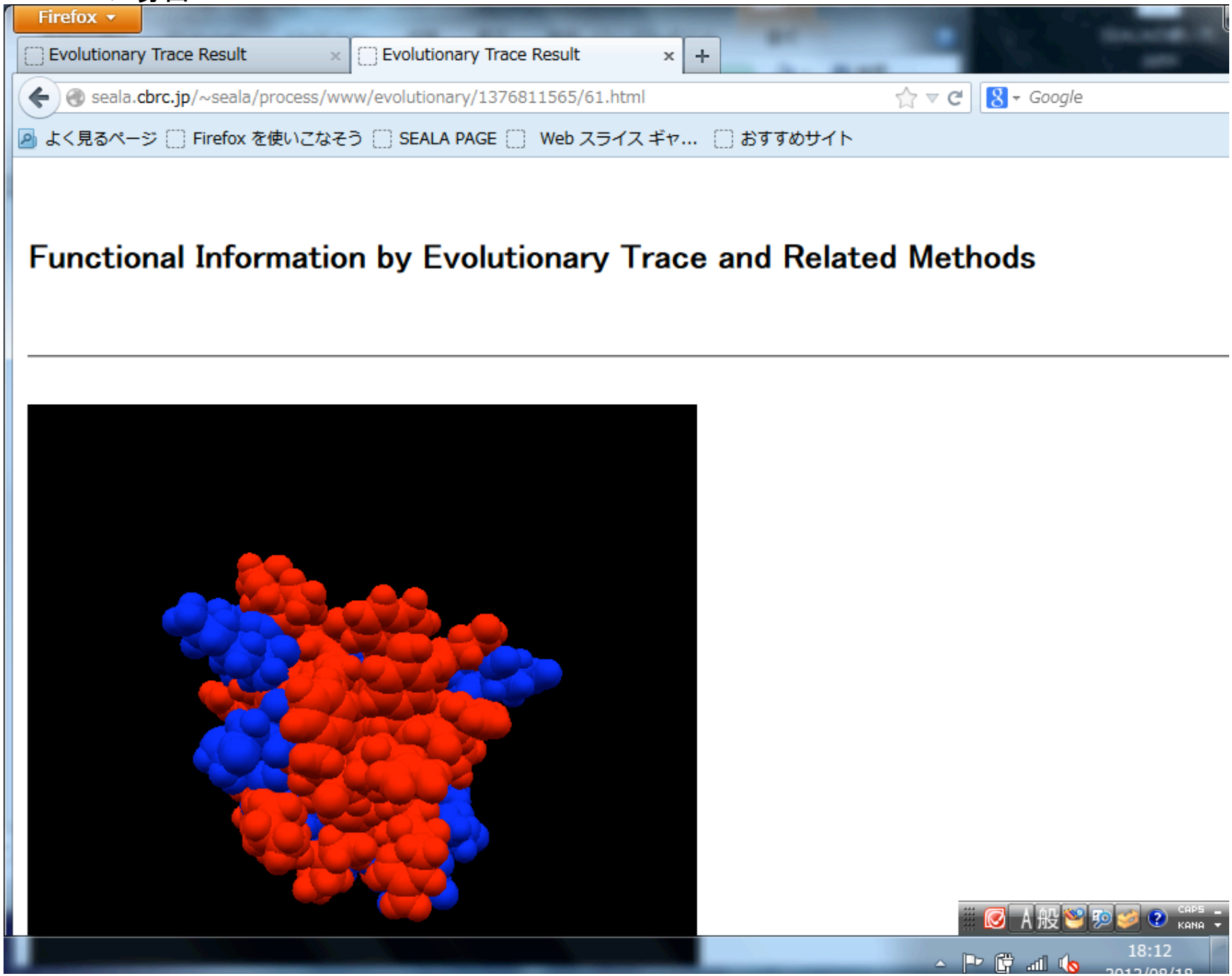
[redacted]

1	neutral	-	-	-	-	-	M	T	-	
2	neutral	-	-	-	L	-	E	-	I	
3	specific	V	V	V	F	V	A	F	V	X
4	neutral	V	Q	-	V	K	-	-	V	
5	conserved	A	A	A	A	A	A	A	A	X
6	neutral	-	L	L	L	L	-	L	L	
7	neutral	Y	-	Y	Y	-	H	Y	Y	
8	neutral	D	D	D	D	D	D	D	-	
9	neutral	-	F	-	F	Y	F	Y	Y	
10	neutral	-	-	-	-	K	-	E	-	
11	neutral	-	P	-	A	A	A	A	-	
12	neutral	-	Q	-	-	-	-	R	I	
13	neutral	-	E	S	G	R	-	-	H	
14	neutral	-	-	-	-	-	-	-	-	
15	neutral	-	-	-	-	-	-	-	-	
16	neutral	-	S	P	-	-	-	-	-	
17	neutral	-	G	R	N	D	D	-	-	
18	neutral	D	E	E	-	E	E	D	D	
19	specific	L	L	V	L	L	L	L	L	X
20	neutral	-	-	-	S	-	S	-	S	
21	neutral	L	F	M	-	F	F	F	F	
22	neutral	-	-	K	-	-	-	-	-	
23	neutral	-	R	K	K	-	-	K	K	
24	neutral	G	G	G	G	-	-	G	G	
25	neutral	-	D	D	E	A	-	E	-	

Node 61の場合


Firefox
Evolutionary Trace Result
Evolutionary Trace Result
seala.cbrc.jp/~seala/process/www/evolutionary/1376811565/61.html
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おすすめサイト
Functional Information by Evolutionary Trace and Related Methods
18:12

（1）　進化トレース法

（2）　累積相対エントロピー法

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ファイル(F) 編集(E) 表示(V) ウィンドウ(W) ヘルプ(H)

1 / 20 100%

しおり

- Evolutionary analysis of functional divergence among chemokine receptors, decoy
  - Introduction
  - Materials and Methods
    - Amino acid sequence data
    - Amino acid sequence alignment and phylogenetic analysis
    - Calculation of the Kullback–Leibler information value
    - Statistical evaluation for bias in the spatial distribution of
    - Residue

frontiers in MICROBIOLOGY

ORIGINAL RESEARCH ARTI

published: 26 July

doi: 10.3389/fmicb.2012.0

Evolutionary analysis of functional divergence amon chemokine receptors, decoy receptors, and viral rece

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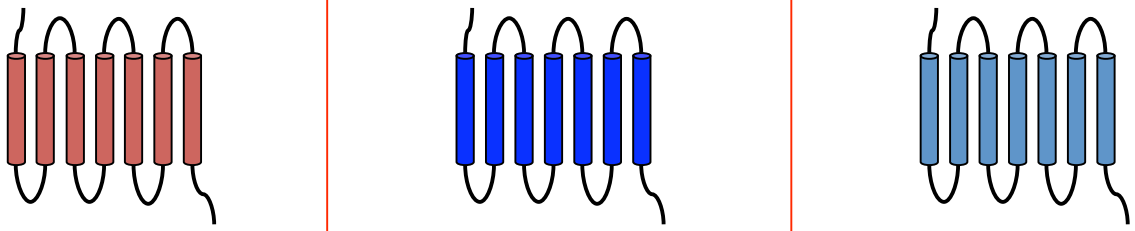
e-mail: daiyasu@ist.osaka-u.ac.jp

Chemokine receptors (CKRs) function in the inflammatory response and homeostasis. Decoy and viral receptors are two types of CKR homologs v functions from those of the typical CKRs. The decoy receptors are able to without signaling. On the other hand, the viral receptors show constitutive si out ligands. We examined the sites related to the functional difference. At fir and viral receptors were each classified into five groups, based on the mol genetic analysis. A multiple amino acid sequence alignment between each g CKRs was then constructed. The difference in the amino acid composition group and the CKRs was evaluated as the Kullback–Leibler (KL) information alignment site. The KL information value is considered to reflect the differenc tional constraints at the site. The sites with the top 5% of KL information selected and mapped on the structure of a CKR. The comparisons with de groups revealed that the detected sites were biased on the intracellular side the sites detected from the comparisons with viral receptor groups were foun extracellular and intracellular sides. More sites were found in the ligand binc

210 x 275 mm

	decoy receptor	chemokine receptor	viral receptor
ligand binding	○	○	△
signaling	×	○	○

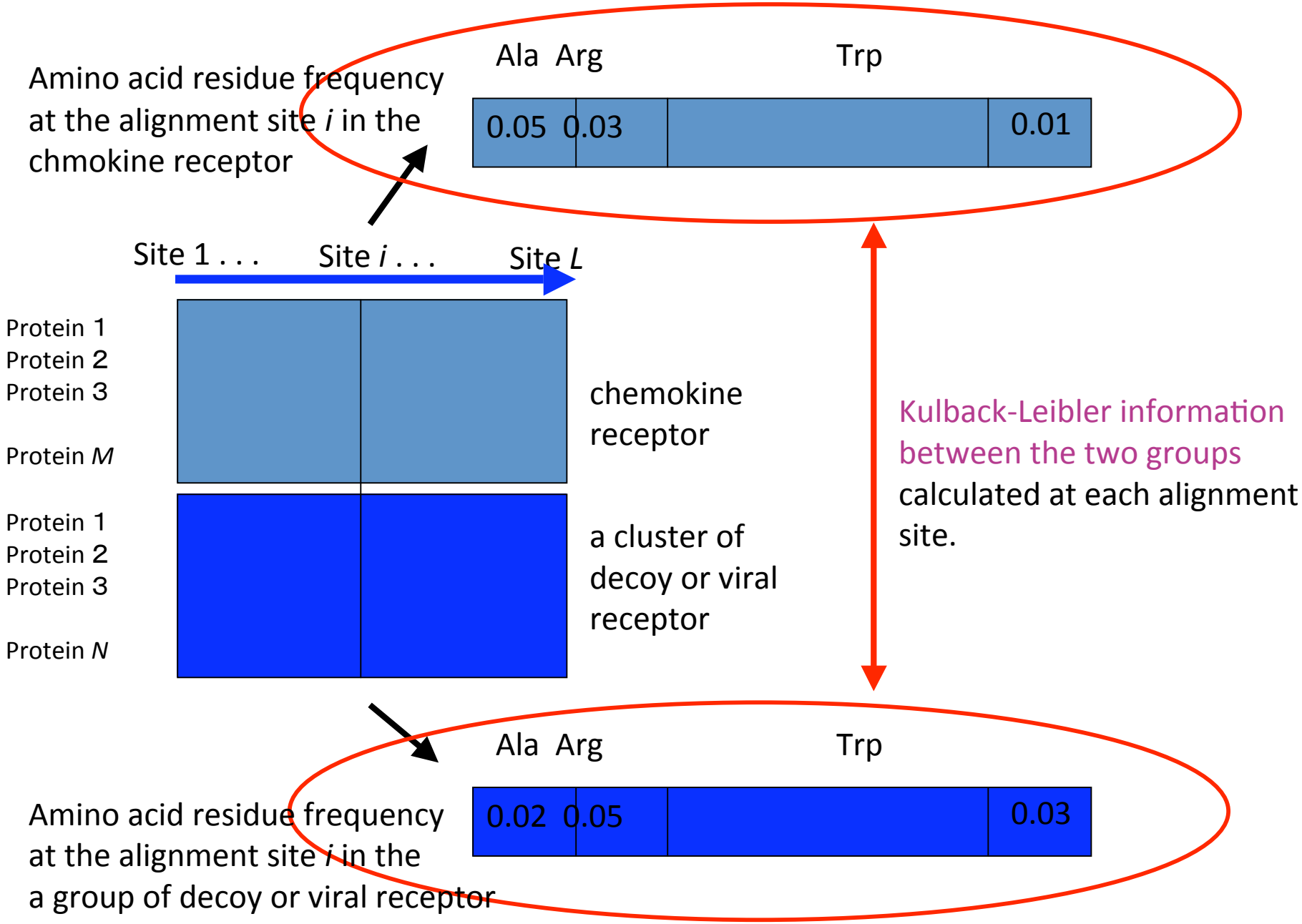


Functional Difference → Difference in Constraints

↓

Difference in Amino Acid Composition

Evaluation of difference between two domains at each alignment site



Estimation of Amino Acid Composition at Each Alignment Site

- Taxonomic Bias

  → Henikoff & Henikoff weight

- Unobserved Residue

  → Pseudocounts adopted in PSI-BLAST

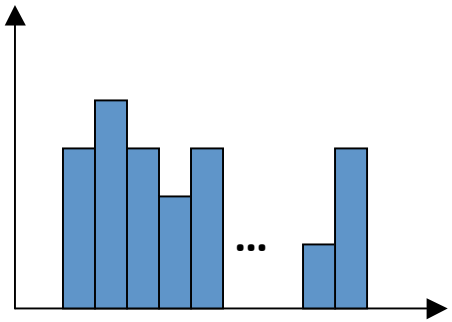
※ It is the same method used for the calculation of PSSM in PSI-BLAST (β = 0.1)

※ BLAST parameter λu was obtained by Newton-Laphson method at each calculation.

※ CRE uses Dirichlet mixture as a prior instead of pseudocount.

The difference between two probability distributions can be quantitatively evaluated with Kullback-Leibler information (KLI).

$p(1)+p(2)+p(3)+\ldots+p(20)=1.0$



$q(1)+q(2)+q(3)+\ldots+q(20)=1.0$

(1) Definition of KLI

$$\sum_{i=1}^{20} p(i) \log \frac{p(i)}{q(i)}$$

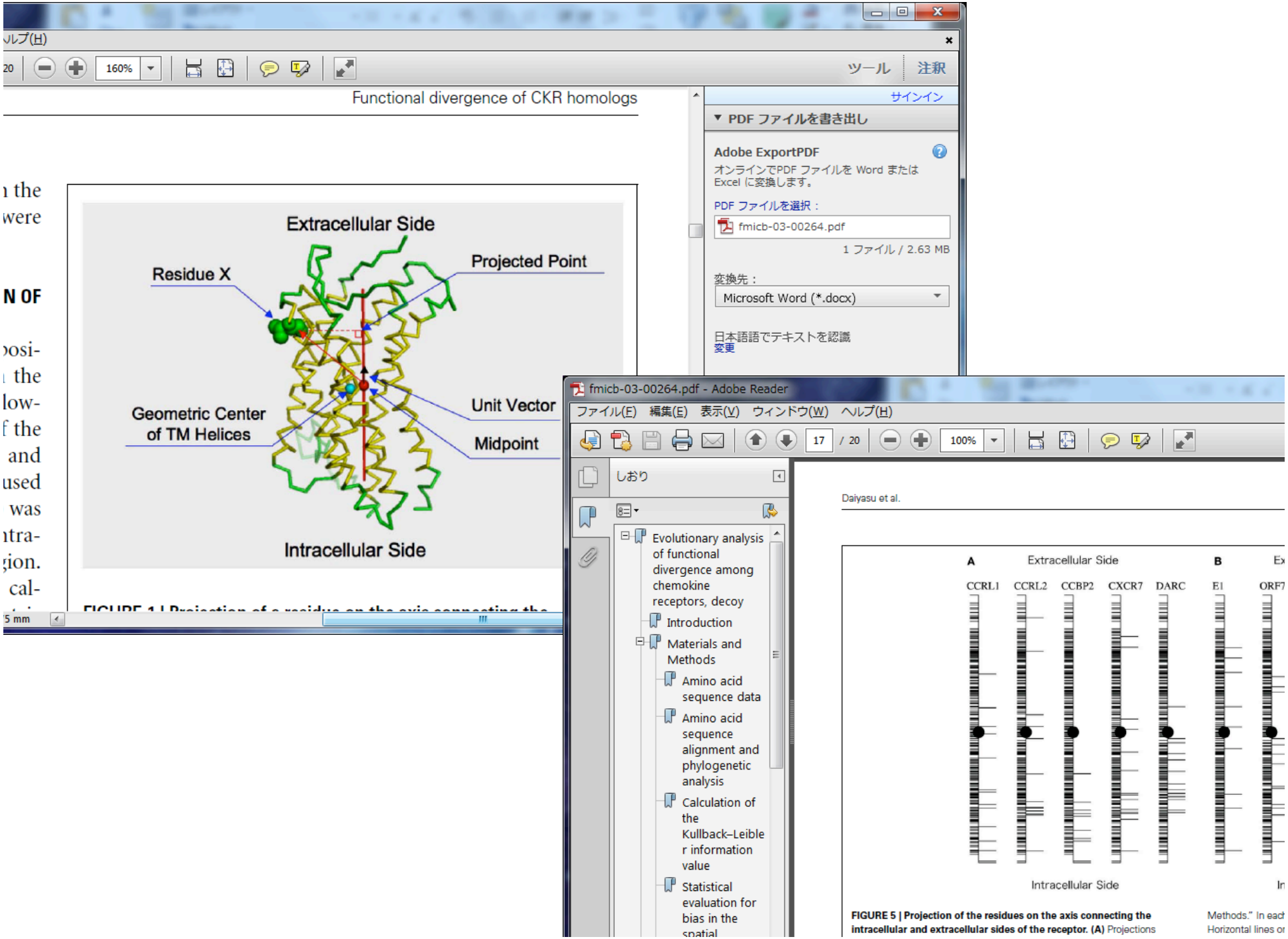
(2) Asymmetry of KLI

$$\sum_{i=1}^{20} p(i) \log \frac{p(i)}{q(i)} \neq \sum_{i=1}^{20} q(i) \log \frac{q(i)}{p(i)}$$

(3) Modified KLI used in this study.

$$\sum_{i=1}^{20} p(i) \log \frac{p(i)}{q(i)} + \sum_{i=1}^{20} q(i) \log \frac{q(i)}{p(i)}$$

Sites with top 5% KLI


Functional divergence of CKR homologs
Extracellular Side
Residue X
Projected Point
Geometric Center of TM Helices
Unit Vector
Midpoint
Intracellular Side
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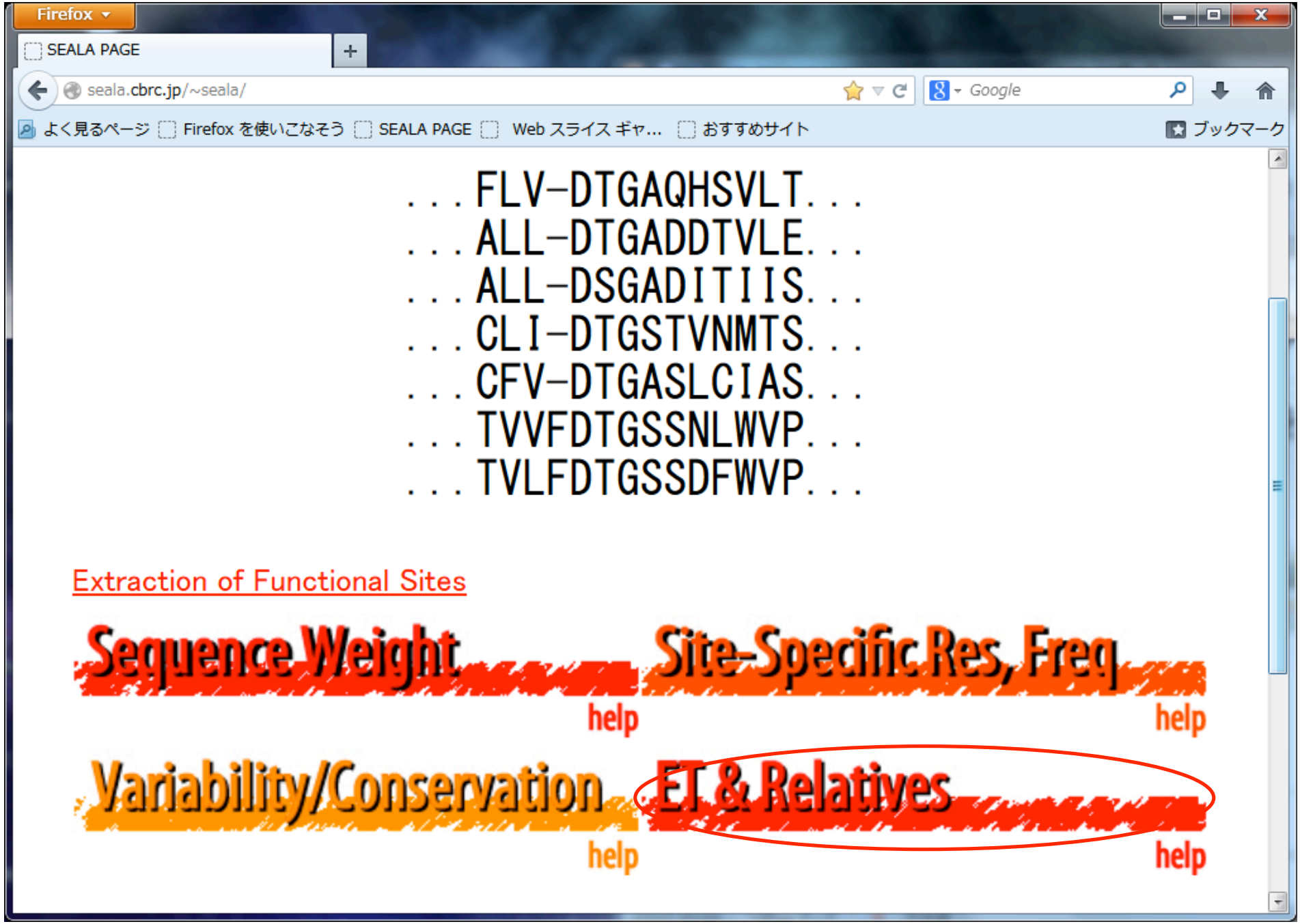
Microsoft Word (*.docx)
日本語語でテキストを認識
変更
fmicb-03-00264.pdf - Adobe Reader
しおり
Evolutionary analysis of functional divergence among chemokine receptors, decoy
Introduction
Materials and Methods
Amino acid sequence data
Amino acid sequence alignment and phylogenetic analysis
Calculation of the Kullback–Leibler information value
Statistical evaluation for bias in the spatial
Daiyasu et al.
Extracellular Side
CCRL1
CCRL2
CCBP2
CXCR7
DARC
E1
ORF7
Intracellular Side
FIGURE 5 | Projection of the residues on the axis connecting the intracellular and extracellular sides of the receptor. (A) Projections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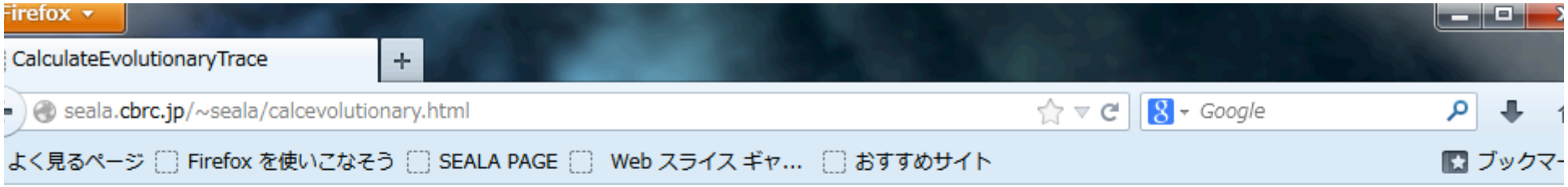
...FLV-DTGAQHSVLT...
...ALL-DTGADDTVLE...
...ALL-DSGADITIIS...
...CLI-DTGSTVNMTS...
...CFV-DTGASLCIAS...
...TVVFDTGSSNLWVP...
...TVLFDTGSSDFWVP...
Extraction of Functional Sites
Sequence Weight
help
Site-Specific Res, Freq
help
Variability/Conservation
help
ET & Relatives
help

入力画面は2つ

1ページ目



Input

Alignment File[help]

参照... CCBP2-CKRall1128v2.aln

① アラインメントと構造の入力はこれまでと同じ

PDB File[help]

参照... 3ODU.pdb

② 機能の異なる二つのグループを指定するファイル

Group Information[help]

参照... CCBP2-CKRall1128v2.CardC

Options

2

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 1
19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34
7 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52
56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89
93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 10
111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126
9 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 1
148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163
66 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181
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424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439
42 443 0

445 446 447 448 449 450 451 452 453 454 455 456 457 458 444

グループファイル

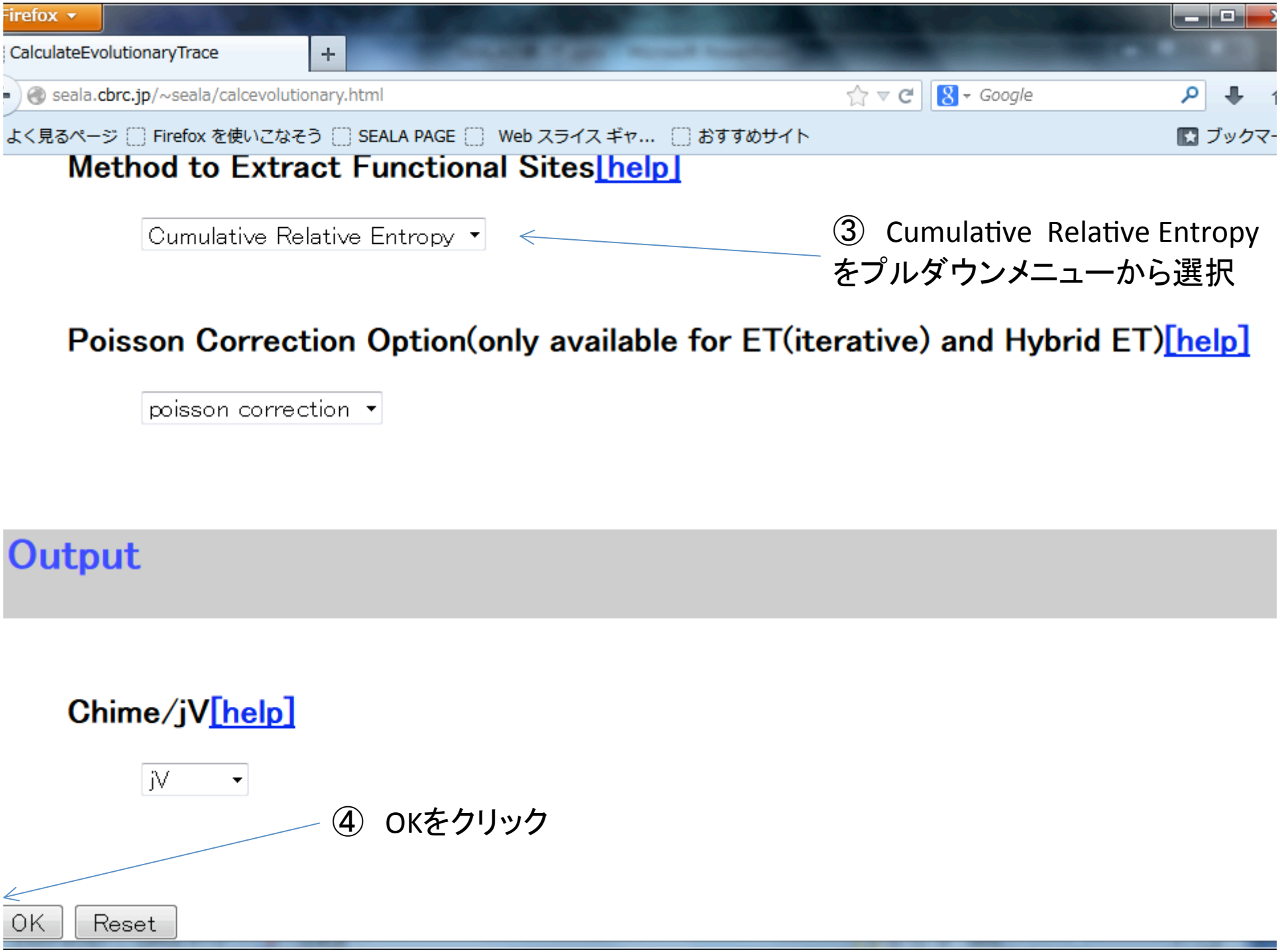
１行目　グループの数　近縁で機能の異なる2グループで見る方法を推奨

２行目　グループ１のアラインメント中の配列の番号 （最初の配列は0番となる。
この行にブランクで区切って配列を入力

3行目　ブランク行

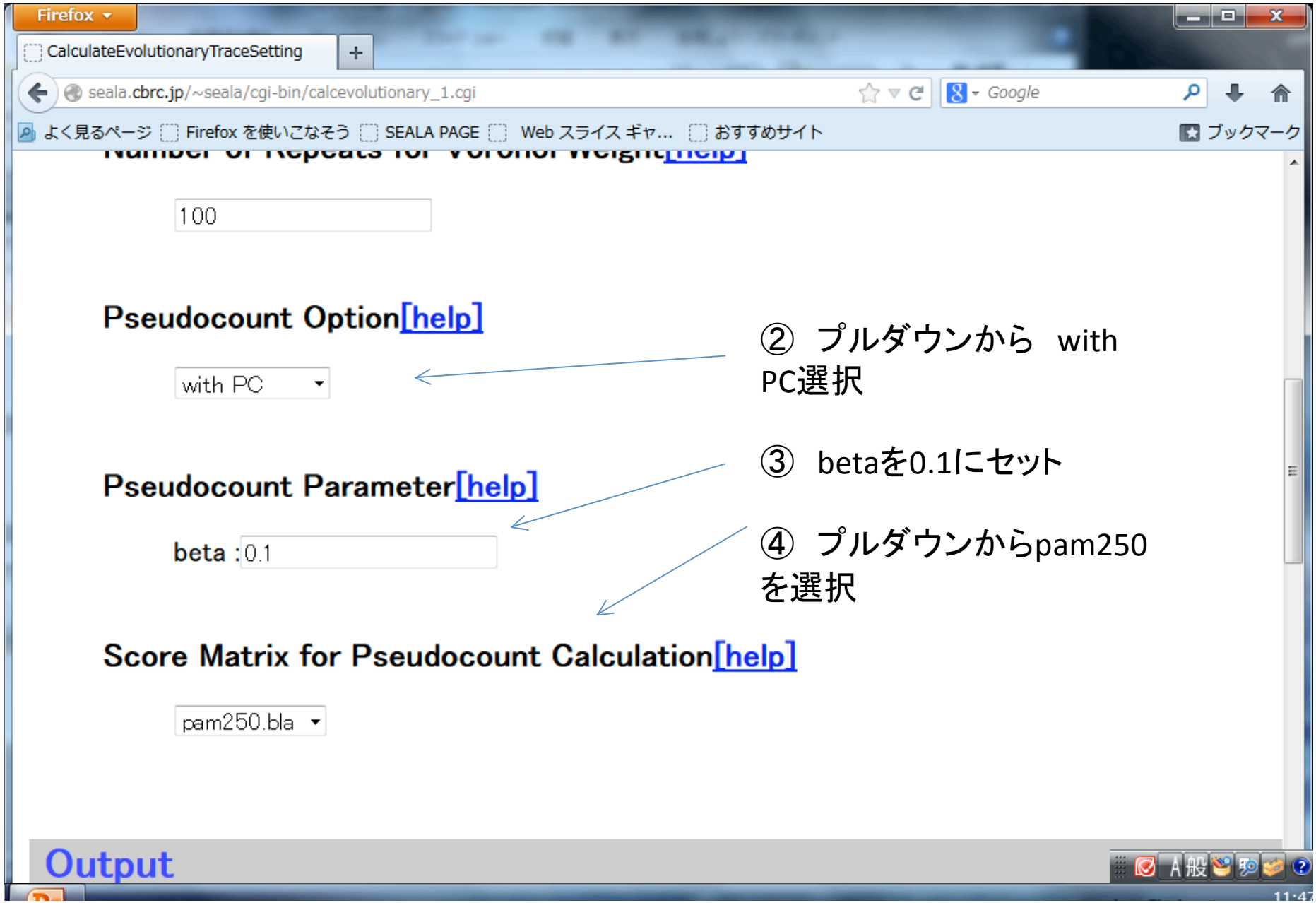
4行目　グループ２のアラインメント中の配列の番号

※　２行目と4行目に，アラインメントの全ての配列が含まれていなくても良い。


Firefox
CalculateEvolutionaryTrace
seala.cbrc.jp/~seala/calcevolutionary.html
Google
よく見るページ
Firefox を使いこなそう
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマー
Method to Extract Functional Sites[help]
Cumulative Relative Entropy
③ Cumulative Relative Entropy
をプルダウンメニューから選択
Poisson Correction Option(only available for ET(iterative) and Hybrid ET)[help]
poisson correction
Output
Chime/jV[help]
jV
④ OKをクリック
OK
Reset

入力画面2枚目

①Henikoff-Henikoffをプルダウンメニューから選択



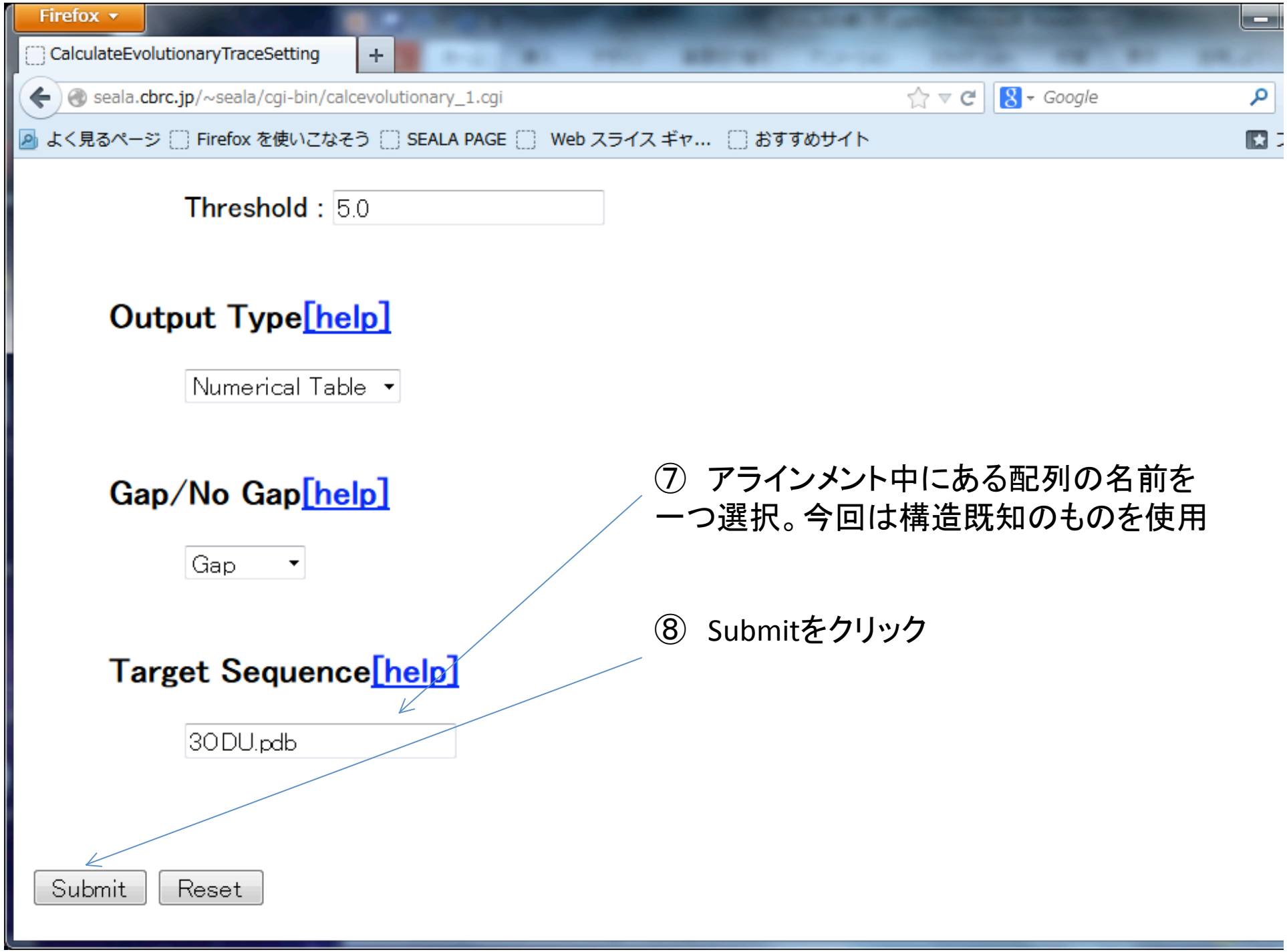
② プルダウンから with PC選択

③ betaを0.1にセット

④ プルダウンからpam250を選択

⑤ デフォルトのScalingを選択

⑥ デフォルトのNumerical Table選択



⑦ アラインメント中にある配列の名前を一つ選択。今回は構造既知のものを使用

⑧ Submitをクリック

Firefox ▾ | Functional Information by Evolution... | +

seala.cbrc.jp/~seala/cgi-bin/calcevolutionary_2.cgi

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Functional Information by Evolutionary Trace an

3ODU.pdb

1	–	−0. 750916
2	–	−0. 750916
3	–	−0. 750916
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15	–	−0. 750916
16	–	−0. 750916
17	–	−0. 750916
18	–	−0. 750916
19	–	−0. 750916
20	–	−0. 750916

Z-score化したKL情報量

Firefox

Functional Information by Evolution...

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787	–	-0.750916
788	–	-0.750916
789	–	-0.750916
790	–	-0.750916
791	–	-0.750916
792	–	-0.750916
793	–	-0.750916
794	–	-0.750916
795	–	-0.750916
796	–	-0.750916
797	–	-0.750916
798	–	-0.750916
799	–	-0.750916
800	–	-0.750916
801	–	-0.750916

3D molecular structureをクリック

3D molecular structure
download pdb file(Please right click, and download the file)
download pdb file whose column for temperature factor is modified with the information about trace residues(see help details)

Firefox

3d structual

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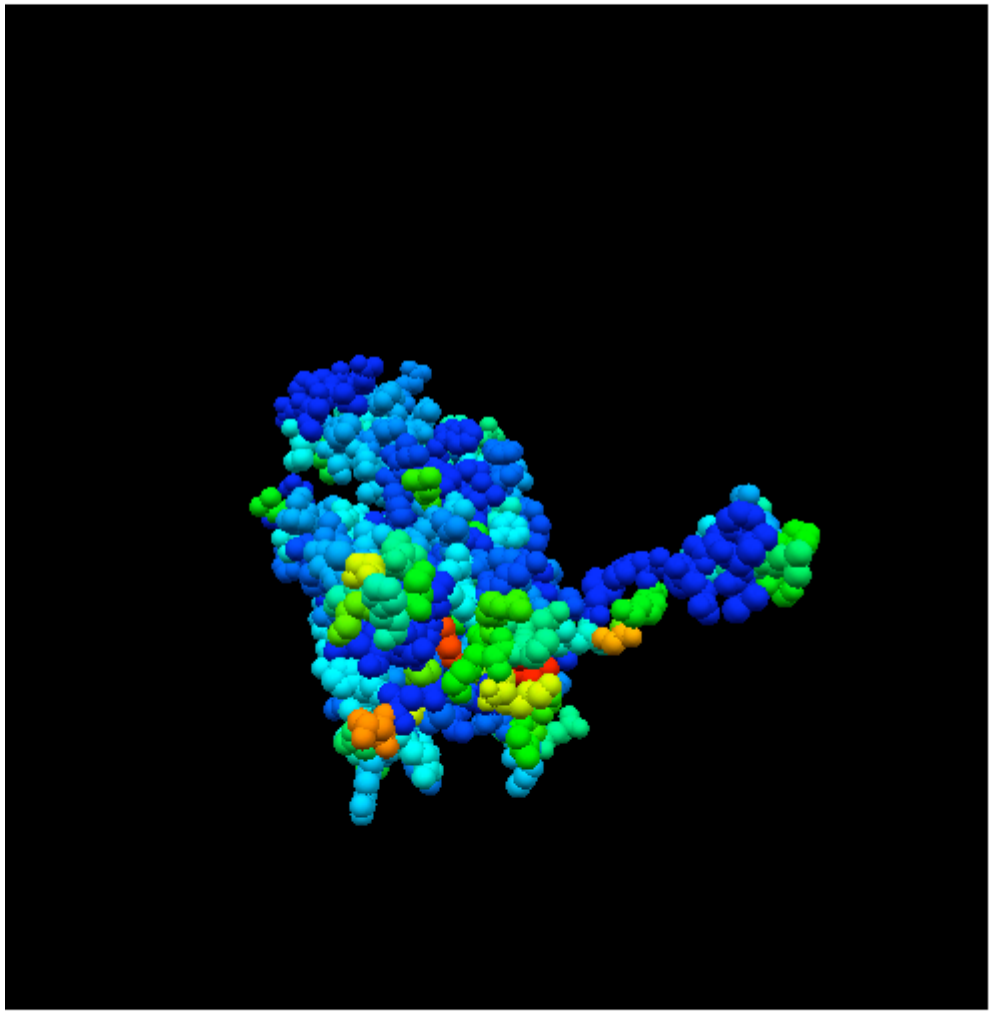

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3d structual

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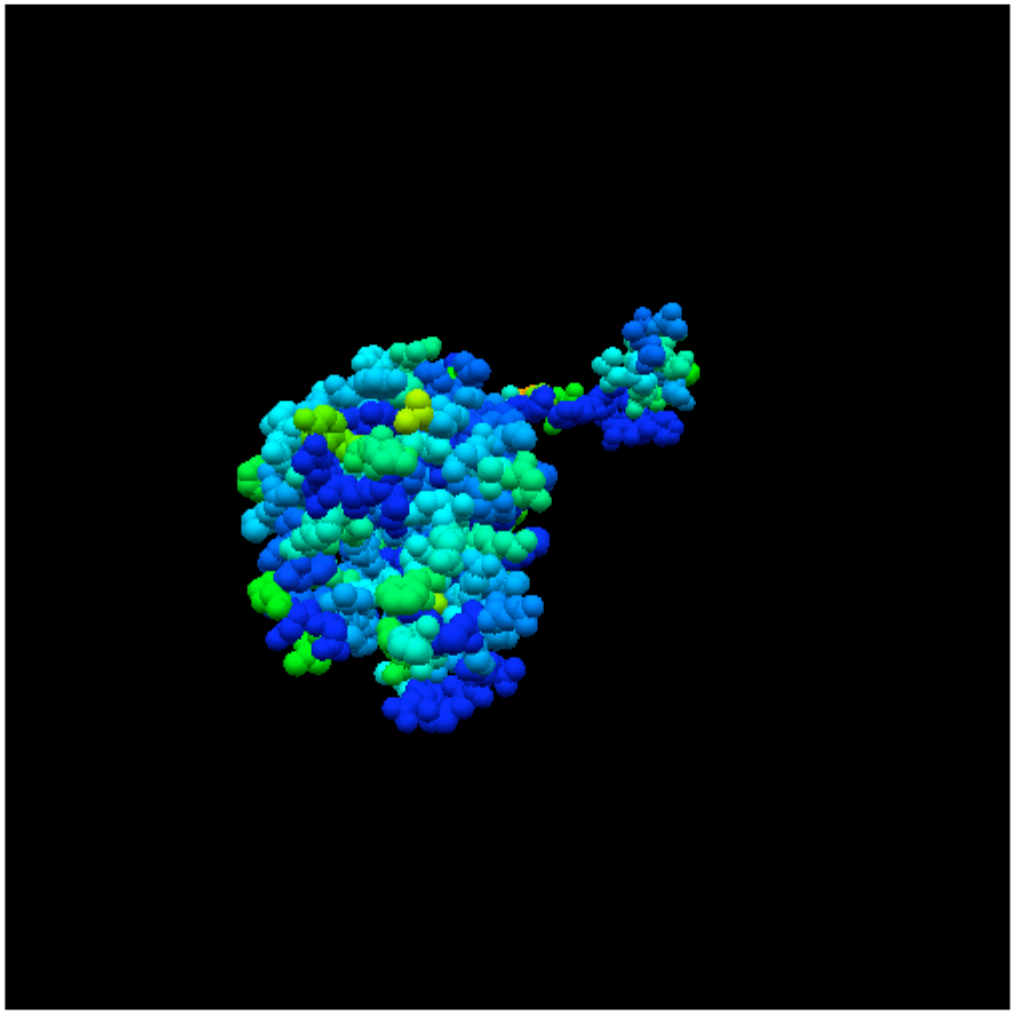
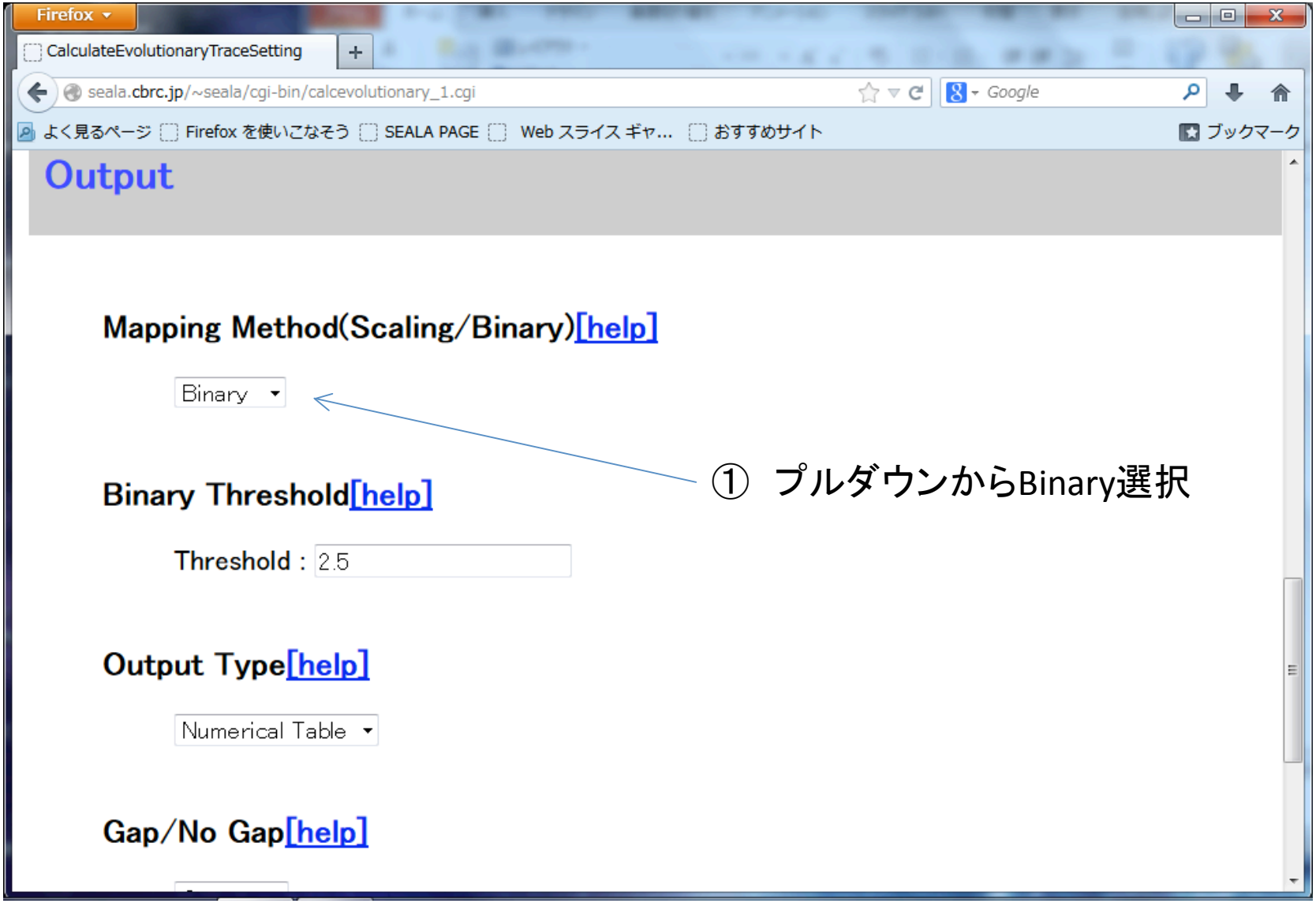


二値化して表示

２ページ目の入力画面を変更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CalculateEvolutionaryTraceSetting
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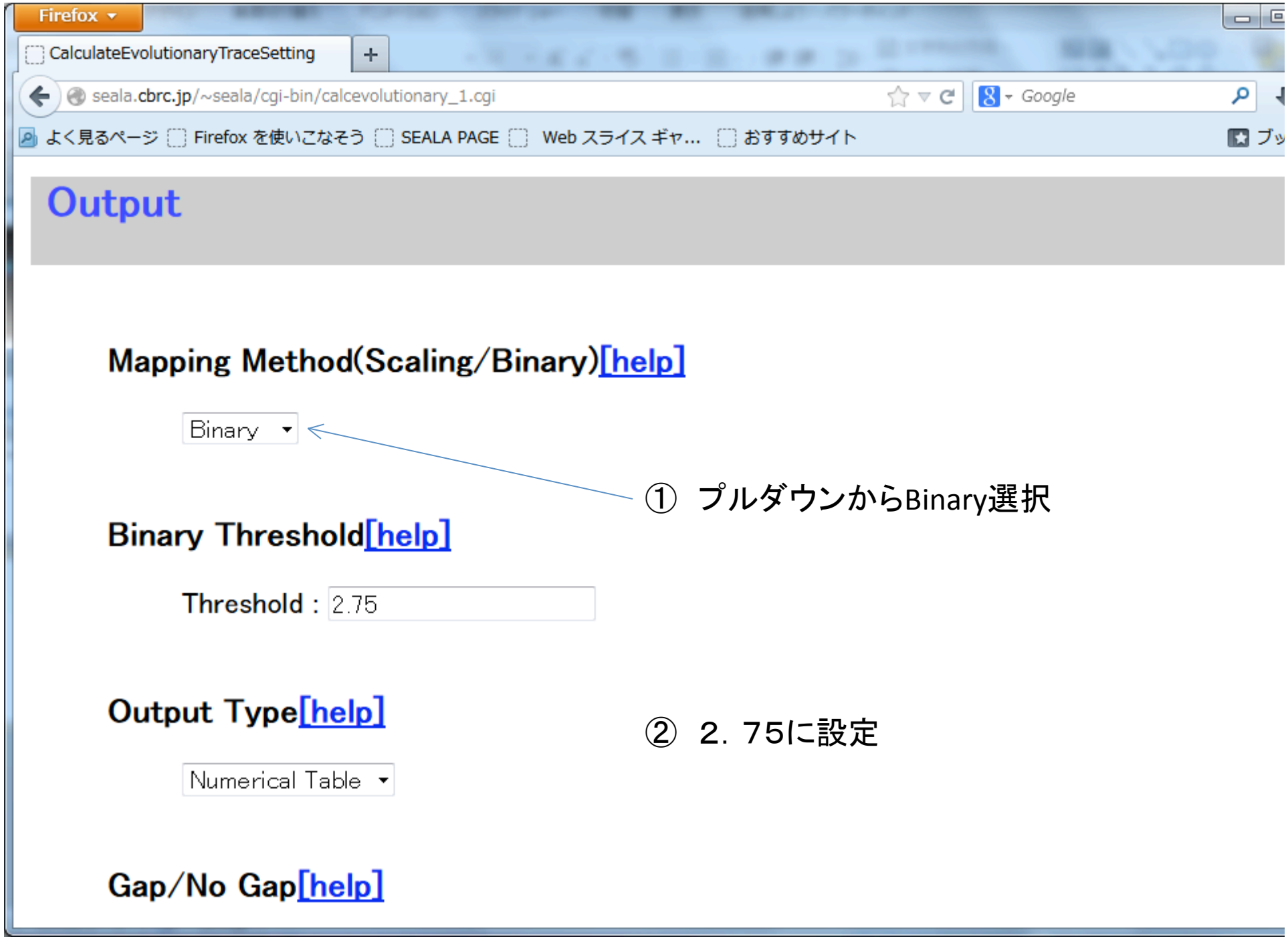
SEALA PAGE
Web スライス ギャ...
おすすめサイト
ブックマーク
Output
Mapping Method(Scaling/Binary)[help]
Binary
Binary Threshold[help]
Threshold : 2.5
Output Type[help]
Numerical Table
Gap/No Gap[help]
① プルダウンからBinary選択



① プルダウンからBinary選択

② ２．７５に設定

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Functional Information by Evolution...

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Functional Information by Evolutionary Trace and Related Methods

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3ODU.pdb

1	-	-0.750916
2	-	-0.750916
3	-	-0.750916
4	-	-0.750916
5	-	-0.750916
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14	-	-0.750916
15	-	-0.750916
16	-	-0.750916

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Functional Information by Evolution...

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798	-	-0.750916
799	-	-0.750916
800	-	-0.750916
801	-	-0.750916

3D molecular structure

download pdb file(Please right click, and download the file)

download pdb file whose column for temperature factor is modified with the information about trace residues(see help details)

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3d structual

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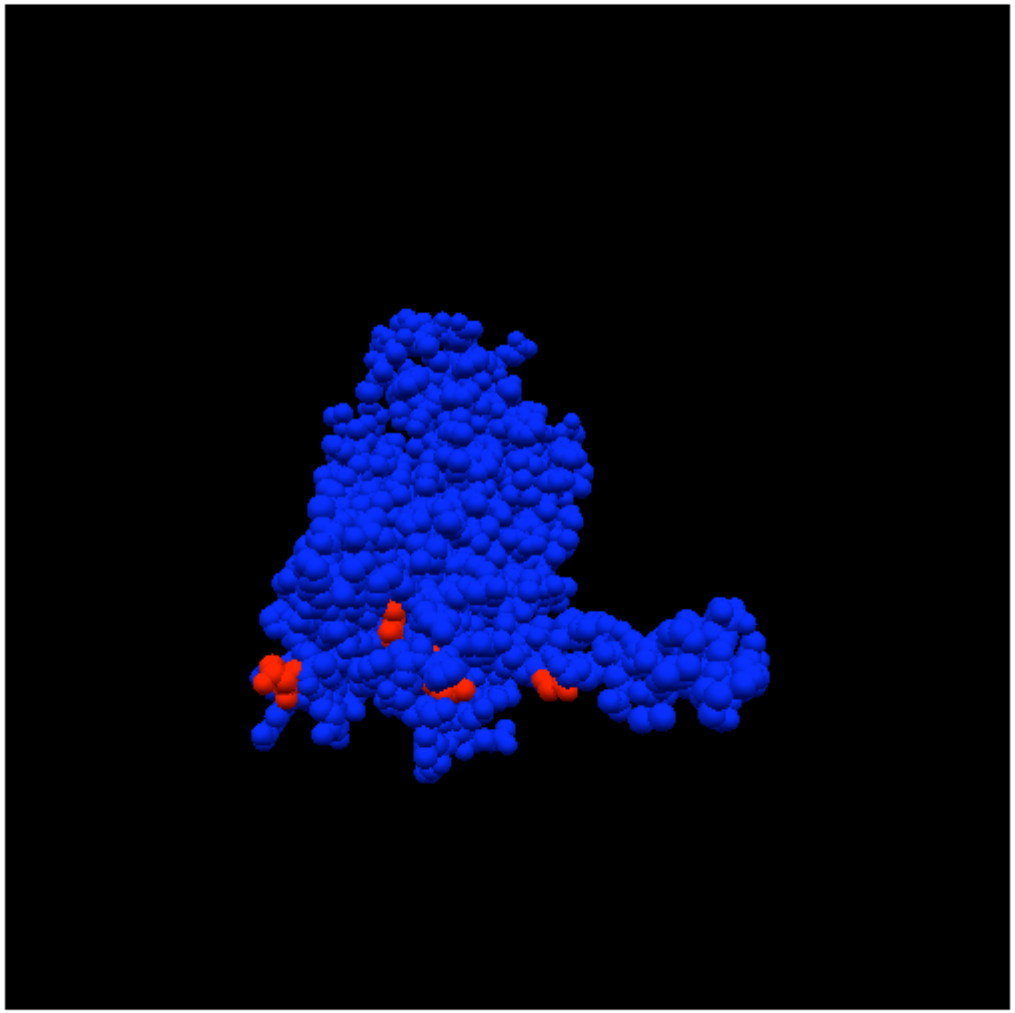

Firefox

3d structual

seala.cbrc.jp/~seala/process/www/evolutionary/1376883903/3d.html

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