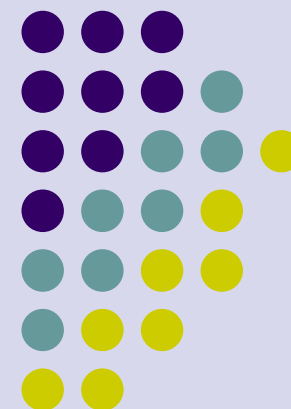


# Présentation de la plate-forme BacTrans<sup>2</sup>

- Equipe ComBi du LINA
- Sylvain Demey

<http://www.sciences.univ-nantes.fr/lina/bioserv/>

[Sylvain.Demey@univ-nantes.fr](mailto:Sylvain.Demey@univ-nantes.fr)





# PLAN

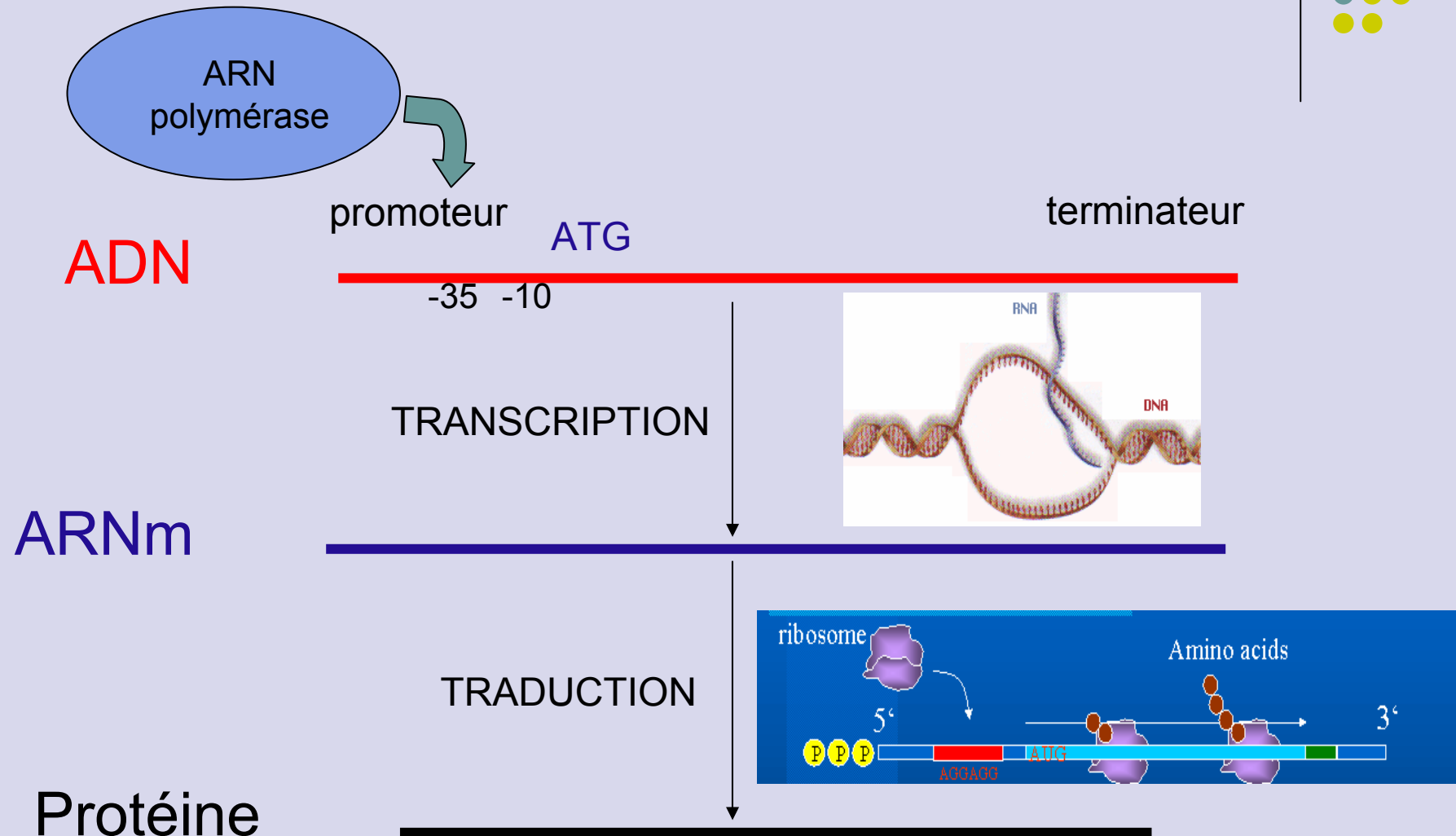
- Introduction
- Le Contexte Biologique du Projet
- La Plate-forme et son utilisation
- La fonctionnalité 'Statistiques'
- Conclusion-Perspectives



# Introduction

- Idée née en Janvier 2002 d'une collaboration informelle entre l'UMR Recherche en Biocatalyse du Laboratoire des Biotechnologies de l'Université de Nantes et l'équipe ComBi du LINA
- Axée sur l'inférence de connaissances sur les promoteurs forts des génomes bactériens pour aider les biologistes à étudier ces promoteurs

# Le Contexte Biologique du Projet

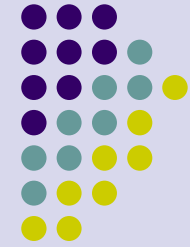


# Le Contexte Biologique du Projet (suite)



- But : Donner aux biologistes les caractéristiques complètes des gènes à promoteurs forts des génomes bactériens et des outils d'analyses
- Travail d'abord réalisé sur *Thermotoga maritima* puis étendu à 30 autres procaryotes
- Caractéristiques → 23 critères relatifs :
  - aux signaux de transcription, de traduction
  - aux structures secondaires prédites, relatives à certaines régions des ARNm concernés
  - à la stabilité de ces molécules.

# Le Contexte Biologique du Projet (suite)



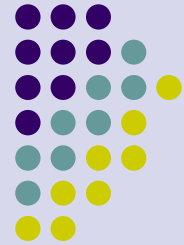
- *Aquifex aeolicus*-----80°C
- *Bacillus subtilis*-----37°C
- *Borrelia burgdorferi*-----37°C
- *Brucella melitensis*-----35°C
- *Chlamydomophila pneumoniae*-----35°C
- *Clostridium perfringens*-----37°C
- *Deinococcus radiodurans*-----30°C
- *Escherichia coli* k12-----37°C
- *Haemophilus influenza*-----37°C
- *Helicobacter pylori*-----37°C
- *Mycobacterium leprae*-----30°C
- *Mycobacterium tuberculosis*----37°C
- *Neisseria meningitidis*-----37°C
- *Oceanobacillus iheyensis*-----<15°C
- *Pseudomonas aeruginosa*-----55°C
- *Pyrococcus abyssi*-----95°C
- *Pyrococcus horikoshii*-----98°C
- *Rickettsia prowazekii*-----35°C
- *Salmonella typhimurium*-----37°C
- *Shewanella oneidensis*-----22°C
- *Sinorhizobium meliloti*-----31°C
- *Staphylococcus aureus*-----37°C
- *Streptococcus pneumoniae*-----37°C
- *Streptomyces coelicolor*-----30°C
- *Thermoanaerobacter tengcongensis*-75°C
- *Thermotoga maritima*-----80°C
- *Treponema pallidum nichols*----18°C
- *Vibrio cholerae*-----37°C
- *Xanthomonas campestris*-----28°C
- *Yersinia pestis*-----28°C



# La Plate-forme

- Développée sur Bioserv (serveur financé par Ouest-Génopole)
- Réalisée dans le but d'une large utilisation par les biologistes étudiant les Procaryotes
- Fonctions:
  - Regrouper les connaissances sur les promoteurs forts
  - Mettre à disposition des outils d'analyses

# La Plate-forme et son utilisation



The screenshot shows a web browser window with the address bar displaying `http://193.52.99.6/~demey/v1.0/`. The page content is as follows:

oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

[New User](#) [Log On](#) [Help](#)

Presentation

To begin you can: [log on](#) or [create a new account](#)

Acknowledgements

BacTrans<sup>2</sup> was created by:  
[G.Blin](#)(1), [A.Drazek](#)(2), [G.Herry](#)(2), [C.Sinoquet](#)(3) and [S.Demey](#)(4)

University of Nantes - FRANCE

Laboratoire Informatique de  
Nantes Atlantique

(1) Phd Student in Bioinformatics  
(2) Master Student  
(3) Associate Professor  
(4) Engineer in Bioinformatics

FeedBack

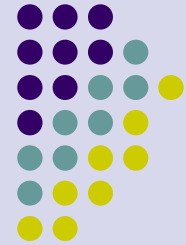
Suggestions on how to improve BacTrans<sup>2</sup> are heartily welcomed !  
Please email [Sylvain.Demey@univ-nantes.fr](mailto:Sylvain.Demey@univ-nantes.fr)

oO~ BacTrans<sup>2</sup> ~Oo

Two red arrows point to the 'New User' and 'Log On' links.



# La Plate-forme: création d'un compte



oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

[Home](#) [Help](#)

---

Create a New Account

Please fill out the following informations:


Login

Password

Check

Pass

E-mail

Create a New Account 

NB : a confirmation of your subscribe will be sent to you.

---

oO~ BacTrans<sup>2</sup> ~Oo

# La Plate-forme: 'log on'



oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

New User Log On Help

Presentation

To begin you can: [log on](#)

Acknowledgements

BacTrans<sup>2</sup> was created by:  
[G.Blin](#)(1), [A.Drazek](#)(2), [C.](#)

University of Nantes - FI  
Laboratoire Informatique  
Nantes Atlantique

(1) Phd Student in Bioinformatics  
(2) Master Student  
(3) Associate Professor  
(4) Engineer in Bioinformatics

FeedBack

Suggestions on how to improve BacTrans<sup>2</sup> are heartily welcomed !  
Please email [Sylvain.Demey@univ-nantes.fr](mailto:Sylvain.Demey@univ-nantes.fr)

oO~ BacTrans<sup>2</sup> ~Oo

Invite

Entrez le nom et le mot de passe pour "Restricted Area" à <http://193.52.99.6>

Utilisateur : demey

Mot de passe : \*\*\*\*\*

☐ Utiliser le gestionnaire de mots de passe pour se souvenir de ce mot de passe.

OK Annuler

UNIVERSITE DE NANTES

lina LABORATOIRE D'INFORMATIQUE  
DE NANTES ATLANTIQUE

# La Plate-forme: la page centrale



oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)


Logout Help


---

CREATE

Create a .rna file

Create a New Session

  
Filter


  
Create


---


Current Sessions


Sessions	Informations
Session 1	Creation Date : Temperature in C° : Expiration Date :
Session 2	


Outils →


 Fold


 Classify

 Compare

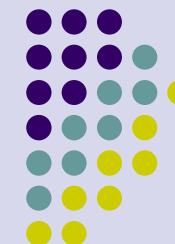
 Statistics

 Tool Box

 Delete

 Extend

# La Plate-forme: 'Filter'



http://193.52.99.6/~demey/v1.0/secure/Filter.cgi?identifiant=demey

oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

back Help

---

## Filter

---

### input files

Choose genbank input file

Choose genome input file

Choose operon input file

Choose filter input file

☒ Parse whole genome with operon file  
☐ Parse genome with filter file

---

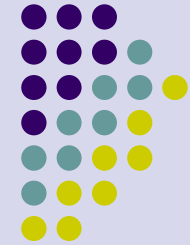
### Constraint Settings

☒ Not use the UP constraint  
☐ Use the UP constraint

  
 Set to Default constraints


	Searched pattern	Maximal Hamming distance	
UP	nnaaawwtwttnnaaaannn	4	(*)
-35 Box	ttgac	3	
-10 Box	tataat	2	

# La Plate-forme: 'Filter'(suite)



Constraint Settings

☒ Not use the UP constraint  
☐ Use the UP constraint

  
Set to Default constraints


	Searched pattern	Maximal Hamming distance	
UP	nnaaawwtwttnnaaaannn	4	(*)
-35 Box	ttgac	3	
-10 Box	tataat	2	
Shine Dalgarno	ggagg	0	

(\*) We considered just Maximal Hamming distance for UP left

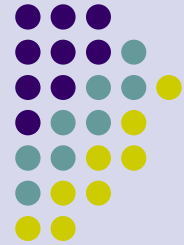
	Minimal Distance between	Maximal Distance between
UP and -35 Box	0	15
-35 Box and -10 Box	15	20
-10 Box and Shine Dalgarno	0	200
Shine Dalgarno and Start codon	2	10

5'Utr length threshold for considering whether 5'Utr region is short or long :

Cut RNA downstream start codon at length  if 5'Utr region is long.

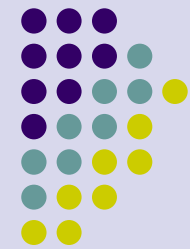
  
Filter

# La Plate-forme: 'Filter'(suite)



```
/gene/ TM1016 1
  /5'UTR length/ 14
  /global error score/ 5.0
  /UP left errors/ 2
  /UP right errors/ 2
  /errors (-35 box)/ 1
  /errors (-10 box)/ 1
  /errors (SD box)/ 0
  /distance UP,-35 box/ 3
  /distance -35 box,-10 box/ 17
  /distance -10 box, Shine-Dalgarno/ 8
  /distance Shine-Dalgarno, start codon/ 9
  /positions for UP w.r.t. +1 transcript./ -61 -40
  /positions for -35 box w.r.t. +1 transcript./ -36 -32
  /positions for -10 box w.r.t. +1 transcript./ -14 -9
  /positions for Shine-Dalgarno box w.r.t. +1 transcript./ 1 5
  /position for start codon w.r.t. +1 transcript./ 15
  /-35 box/ ttgaa
  /tataBox/ tttaat
  /Shine-Dalgarno box/ ggagg
  /start codon/ atg
  /leftContext Shine-Dalgarno box/ tagcc
  /rightContext Shine-Dalgarno box/ tgatg
  /leftContextStartCodon/ gtgag
  /rightContextStartCodon/ tatag
  ggagggtgatgtgagatgtatagagataaaaattgcaaaaattatcgggtactgtcttttcggcattgacagtacttccactt
```

# La Plate-forme : création de session



oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)


Logout Help


---

CREATE

Create a .rna file

Create a New Session






Filter


Create


---


Current Sessions


Sessions	Informations
Session 1	Creation Date : Temperature in C° : Expiration Date :
Session 2	

















Fold

Classify

Compare

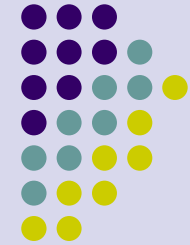
Statistics

Tool Box

Delete

Extend

# La Plate-forme : création de session (suite)



http://193.52.99.6/~demey/v1.0/secure/creer\_session.cgi?id=demey

New session creation - demey

if you wish a file with an optimal RNA selection click on:

[Optimal RNA Selection](#) ←



OR:


select a file .rna (create with "Filter")

mas\_fv\_ss\_escherichia\_coli\_k12\_3\_2\_0\_15\_20\_0\_200\_2\_10\_70\_10\_13\_09\_05.rna

select a temperature

37

[SUBMIT QUERY](#)

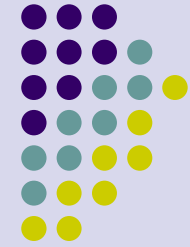


[back](#)

oO~ BacTrans<sup>2</sup> ~Oo



# La Plate-forme : création de session (suite)



http://193.52.99.6/~demey/v1.0/secure/selection.cgi?identifiant=demey

OK

## OPTIMAL RNA SELECTION


select a file .ud

ud\_escherichia\_coli\_k12\_3\_2\_0\_15\_20\_0\_200\_2\_10\_70\_10\_13\_09\_05.ud

select a .ma file

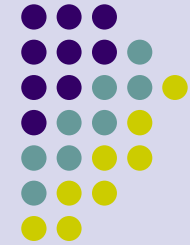
mas\_escherichia\_coli\_k12\_3\_2\_0\_15\_20\_0\_200\_2\_10\_70\_10\_13\_09\_05.ma

RUN

  
back

oO~ BacTrans<sup>2</sup> ~Oo


# La Plate-forme : création de session (suite)



http://193.52.99.6/~demey/v1.0/secure/creer\_session.cgi?id=demey

**New session creation - demey**


if you wish a file with an optimal RNA selection click on:



OR:

select a file .rna (create with "Filter")

select a temperature



back

oO~ BacTrans<sup>2</sup> ~Oo










# La Plate-forme : Les Outils

*Current Sessions*

Sessions	Informations
Session 1	
Session 2	

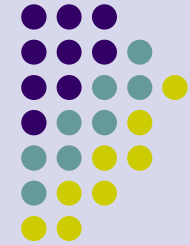
  

Creation Date :	05/10/11
Temperature in C° :	37
Expiration Date :	05/10/31

						
Fold	Classify	Compare	Statistics	Tool Box	Delete	Extend

oO~ BacTrans<sup>2</sup> ~Oo

# La Plate-forme : 'Fold'



oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

sessions manager Help

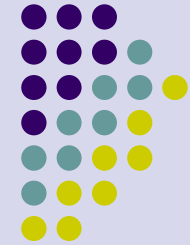
Gène *ftsX* Version 1 Suboptimal 1/12 - Température : 37°C

+ yaeB  
+ b1590  
+ uidB  
+ sodC  
+ nuoK  
+ b1680  
+ sgaE  
+ ccmE  
+ dsbE  
+ ccmH  
+ thiH  
+ ninE  
+ yegO  
+ ydjs  
+ nrfD  
+ phnI  
+ hybE  
+ glpC  
+ b2100  
+ nirD  
+ ftsX  
version 1

Local Save

oO~ BacTrans<sup>2</sup> ~Oo

# La Plate-forme : 'Fold'(suite)



oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

sessions manager Help

+ yaeB  
+ b1590  
+ uidB  
+ sodC  
+ nuoK  
+ b1680  
+ sgaE  
+ ccmE  
+ dsbE  
+ ccmH  
+ thiH  
+ ninE  
+ yegO  
+ ydjS  
+ nrfD  
+ phnI  
+ hybE  
+ glpC  
+ b2100  
+ nirD  
+ ftsX  
version 1

Red : Shine Dalgarno - Blue : Start Codon

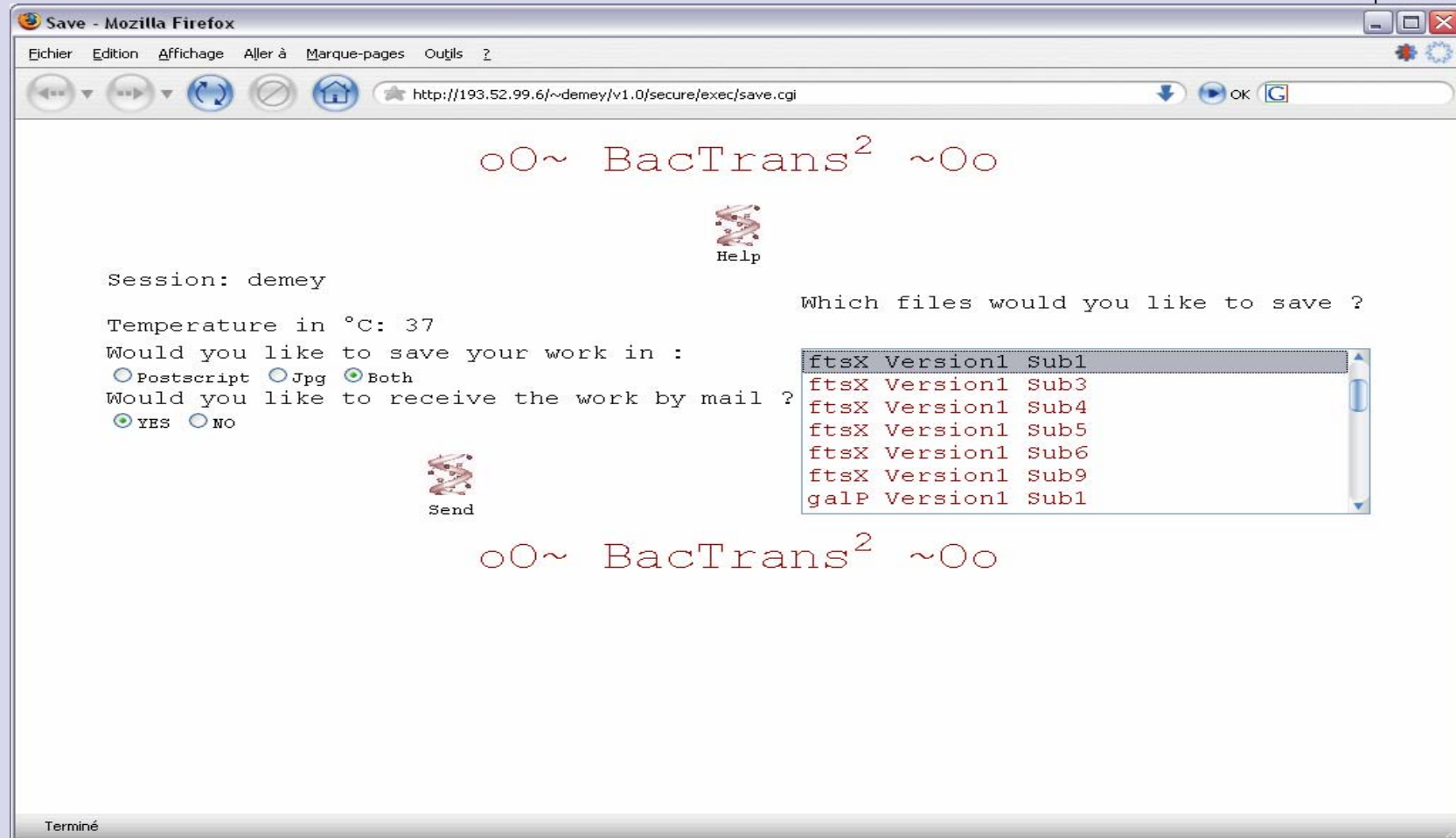
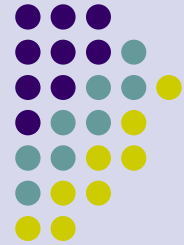
Select directly the th suboptimal

Next

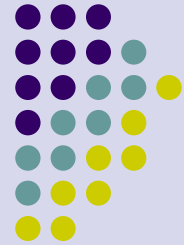
Local Save

oO~ BacTrans<sup>2</sup> ~Oo

# La Plate-forme : 'Fold'(suite)



# La Plate-forme : 'Classify'



http://193.52.99.6/~demey/v1.0/secure/exec/calcclassify.cgi?selection=demey\_1\_37\_051011.rna&nom=c

oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

sessions manager Help

- + bl680
- + sgaE
- + ccmE
- + dsbE
- + ccmH
- + thiH
- + ninE
- + yegO
- + ydjS
- + nrfD
- + phnI
- + hybE
- + glpC
- + b2100
- + nirD
- + ftsX
- Version1

The significative elements for ftsX\_1 are  
ftsX\_1\_04 (-37.30) ,ftsX\_1\_06 (-37.30) ,ftsX\_1\_01  
(-38.00)

Element	Value
ftsX_1_01	-38.00
ftsX_1_02	-37.30
ftsX_1_03	-37.30
ftsX_1_05	-37.30
ftsX_1_06	-37.30
ftsX_1_04	-37.30

The maximal number of significative elements for  
ftsX\_1 is 6  
3 significative elements for ftsX\_1 have been  
extracted

Local Save Server-Side Save

oO~ BacTrans<sup>2</sup> ~Oo



# La Plate-forme : 'Compare'

## Compare

### input files

Choose the first file in fasta format

Choose the second file in fasta format

### Constraint Settings

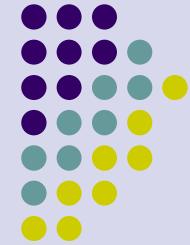
maximal length difference

minimal homology threshold

(\*) We use bl2seq from BLAST, developed by Altschul, Madden, Schaeffer, Zhang, Miller, Lipman (NCBI)



# La Plate-forme : 'Compare'(suite)



oO~ BacTrans<sup>2</sup> ~Oo

---

Result of Comparison

---

Query= PAB2026 (387 letters)

>PAB2026

Length = 387

Score = 753 bits (1944), Expect = 0.0  
Identities = 387/387 (100%), Positives = 387/387 (100%)

Query: 1 MPTNVTAEYLAEEEEYRNAKTIPEKIRALEKMYALVPKHGTEKRLQIKRKLAEIRKEL 60  
MPTNVTAEYLAEEEEYRNAKTIPEKIRALEKMYALVPKHGTEKRLQIKRKLAEIRKEL  
Sbjct: 1 MPTNVTAEYLAEEEEYRNAKTIPEKIRALEKMYALVPKHGTEKRLQIKRKLAEIRKEL 60

Query: 61 EKQFQQRKGGGYS LAVKKEGAAQIVLVGLPNVKGSELLRALTGVDVESADYPTTTEPIP 120  
EKQFQQRKGGGYS LAVKKEGAAQIVLVGLPNVKGSELLRALTGVDVESADYPTTTEPIP  
Sbjct: 61 EKQFQQRKGGGYS LAVKKEGAAQIVLVGLPNVKGSELLRALTGVDVESADYPTTTEPIP 120

Query: 121 AMNMYKDVQIQLVVEVPLIEGAALGKMGQPQLLAVIRNADAIATVIDLSEDPKQMKILL 180  
AMNMYKDVQIQLVVEVPLIEGAALGKMGQPQLLAVIRNADAIATVIDLSEDPKQMKILL  
Sbjct: 121 AMNMYKDVQIQLVVEVPLIEGAALGKMGQPQLLAVIRNADAIATVIDLSEDPKQMKILL 180

Query: 181 REFERAGIKVNRPRRIEIRRTPSGGIVINGIENIKGDINEVHKMLREEKIHSAEITVRE 240  
REFERAGIKVNRPRRIEIRRTPSGGIVINGIENIKGDINEVHKMLREEKIHSAEITVRE  
Sbjct: 181 REFERAGIKVNRPRRIEIRRTPSGGIVINGIENIKGDINEVHKMLREEKIHSAEITVRE 240

Query: 241 PVTLEDADALDESLVKKAI I IANKGDAPGSKDNYEKLKAYGERFRKIIPVSAKKRINL 300  
PVTLEDADALDESLVKKAI I IANKGDAPGSKDNYEKLKAYGERFRKIIPVSAKKRINL  
Sbjct: 241 PVTLEDADALDESLVKKAI I IANKGDAPGSKDNYEKLKAYGERFRKIIPVSAKKRINL 300

Query: 301 DAVKEALYDVAEIIIRVFTKSPGEEPATPPIALKRGSTVLDVAERIHKDLVKNFYARVWG 360  
DAVKEALYDVAEIIIRVFTKSPGEEPATPPIALKRGSTVLDVAERIHKDLVKNFYARVWG  
Sbjct: 301 DAVKEALYDVAEIIIRVFTKSPGEEPATPPIALKRGSTVLDVAERIHKDLVKNFYARVWG 360

Query: 361 KSVKFPQQRVGPDPHVLEDGDI IVEIHAR 387  
KSVKFPQQRVGPDPHVLEDGDI IVEIHAR  
Sbjct: 361 KSVKFPQQRVGPDPHVLEDGDI IVEIHAR 387

Lambda K H 0.316 0.136 0.378 Gapped Lambda K H 0.267 0.0410 0.140 Matrix: BLOSUM62 Gap Penalties: Existence: 11, Extension: 1 Number of Hits to

DAVKEALYDVAEIIIRVFTKSPGEEPATPPIALKRGSTVLDVAERIHKDLVKNFYARVWG  
Sbjct: 298 DAVKEALYDVAEIIIRVFTKSPGEEPATPPIALKRGSTVLDVAERIHKDLVKNFYARVWG 357

Query: 361 KSVKFPQQRVGPDPHVLEDGDI 381  
KSVKFPQQRVGPDPHVLEDGDI  
Sbjct: 358 KSVKFPQQRVGPDPHVLEDGDI 378

Lambda K H 0.316 0.136 0.378 Gapped Lambda K H 0.267 0.0410 0.140 Matrix: BLOSUM62 Gap Penalties: Existence: 11, Extension: 1 Number of Hits to  
DB: 777 Number of Sequences: 0 Number of extensions: 13 Number of successful extensions: 6 Number of sequences better than 10.0: 1 Number of HSP's better  
than 10.0 without gapping: 1 Number of HSP's successfully gapped in prelim test: 0 Number of HSP's that attempted gapping in prelim test: 0 Number of HSP's  
gapped (non-prelim): 1 length of query: 387 length of database: 378 effective HSP length: 30 effective length of query: 357 effective length of database: 348 effective  
search space: 124236 effective search space used: 124236 T: 11 A: 40 X1: 16 (7.3 bits) X2: 38 (14.6 bits) X3: 64 (24.7 bits) S1: 24 (13.8 bits) S2: 24 (13.9 bits)

Query= PAB1296 (309 letters)

>PAB1296

Length = 387

Score = 20.8 bits (42), Expect = 0.055  
Identities = 11/47 (23%), Positives = 22/47 (46%)

Identities < threshold of minimal homology

Query= PAB1296 (309 letters) Lambda K H 0.320 0.139 0.383 Gapped Lambda K H 0.267 0.0410 0.140 Matrix: BLOSUM62 Gap Penalties: Existence: 11,  
Extension: 1 Number of Hits to DB: 109 Number of Sequences: 0 Number of extensions: 4 Number of successful extensions: 0 Number of sequences better than  
10.0: 0 Number of HSP's better than 10.0 without gapping: 0 Number of HSP's successfully gapped in prelim test: 0 Number of HSP's that attempted gapping in  
prelim test: 0 Number of HSP's gapped (non-prelim): 0 length of query: 309 length of database: 177 effective HSP length: 23 effective length of query: 286 effective  
length of database: 154 effective search space: 44044 effective search space used: 44044 T: 11 A: 40 X1: 16 (7.4 bits) X2: 38 (14.6 bits) X3: 64 (24.7 bits) S1:  
20 (12.1 bits) S2: 20 (12.3 bits)

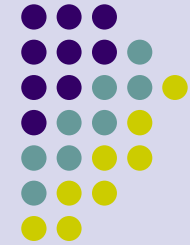
Query= PAB1296 (309 letters)

>PAB1296

Length = 309

Score = 596 bits (1537), Expect = e-175  
Identities = 309/309 (100%), Positives = 309/309 (100%)

# La fonctionnalité 'Statistiques'



oO~ BacTrans<sup>2</sup> ~Oo

Version 1.0 (2005-09-21)

[sessions manager](#) [Help](#)

---

## Statistical Analysis

---

- Menu -

- [Parameters to create new statistics files](#)
- [Statistics files List](#)
- [Graphs for Intra Genomic Analysis](#)
- [Graphs for Inter Genomic Analysis](#)

---

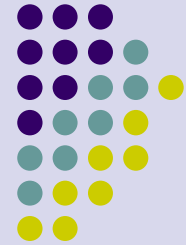
- Parameters to create new statistics files -

demey\_1\_37\_051011.rn:

---

- Statistics files -

# La fonctionnalité 'Statistiques' (suite)



## - Menu -

- [Parameters to create new statistics files](#)
- [Statistics files List](#)
- [Graphs for Intra Genomic Analysis](#)
- [Graphs for Inter Genomic Analysis](#)

## - Parameters to create new statistics files -

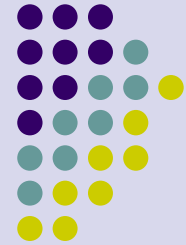
demey\_1\_37\_051011.ma

## - Statistics files -

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[Escherichia coli at5 demey 1 37 051011.ma](#)  
[Escherichia coli energ T37 demey 1 37 051011 first structures.ma](#)  
[Escherichia coli err-10 demey 1 37 051011.ma](#)  
[Escherichia coli err-35 demey 1 37 051011.ma](#)  
[Escherichia coli free T37 demey 1 37 051011 first structures.ma](#)  
[Escherichia coli frans demey 1 37 051011.ma](#)  
[Escherichia coli gcSC demey 1 37 051011.ma](#)  
[Escherichia coli gcSD demey 1 37 051011.ma](#)  
[Escherichia coli gcpair T37 demey 1 37 051011 first structures.ma](#)  
[Escherichia coli haim hcpair T37 demey 1 37 051011 first structures.ma](#)

# La fonctionnalité 'Statistiques' (suite)



- *Graphs for Intra Genomic Analysis* -  
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- *Correlation graphs* - Choose a matrix

- *Start Codon Class graphs* - Choose a file

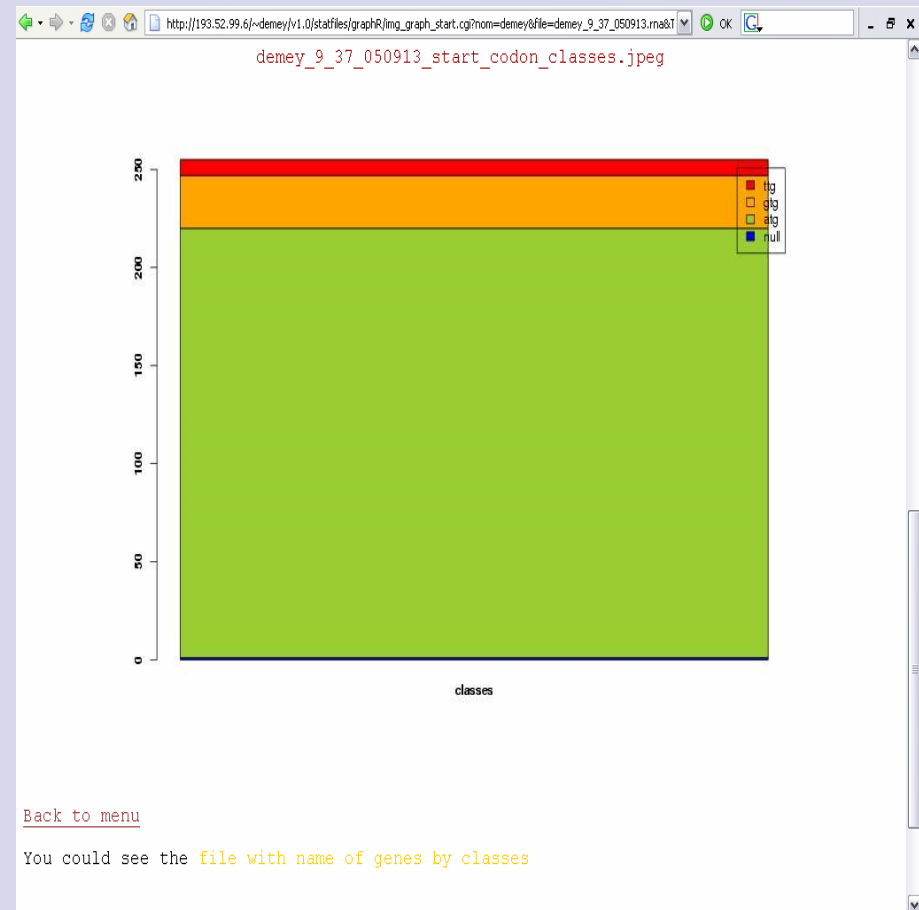
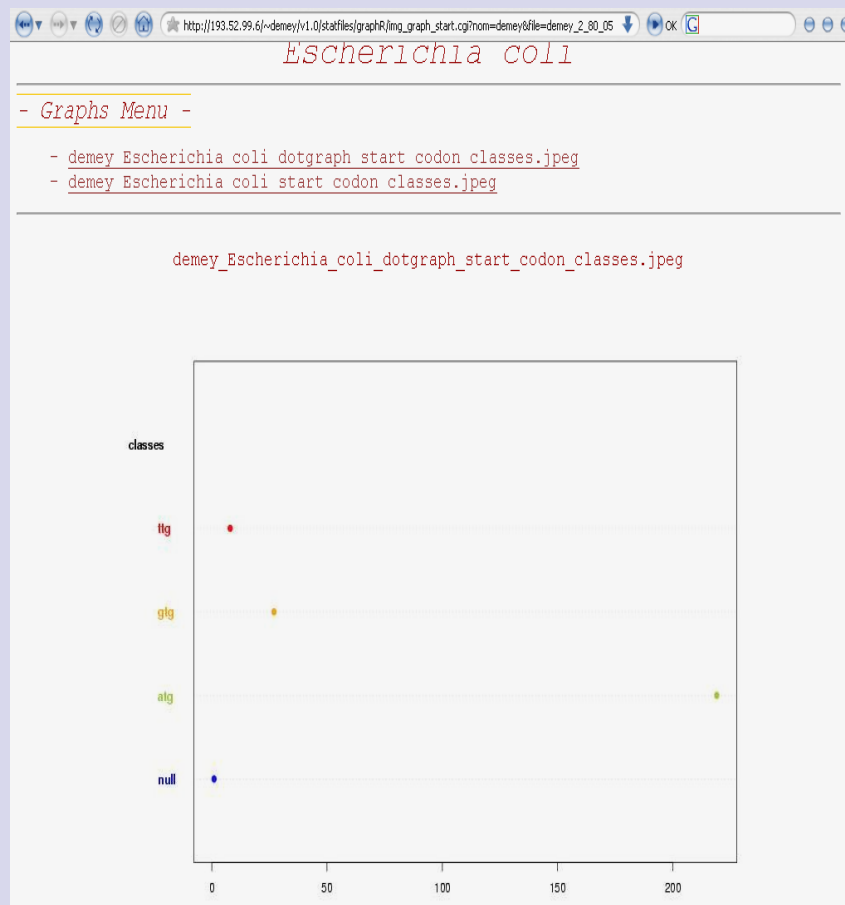
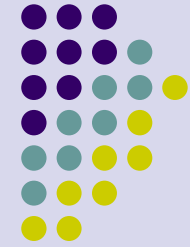
- *Hairpin Distribution graphs* - Choose a file

- *Transcription force class graphs* - Choose a file

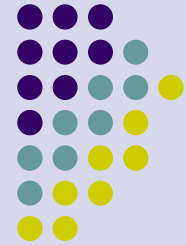
- *Interference class graphs* - Choose a file

- *Graphs for Inter Genomic Analysis* -  
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# La fonctionnalité 'Statistiques' : exemple de graphiques du point de vue Intra Génomique



# La fonctionnalité 'Statistiques' (suite)



- *Graphs for Inter Genomic Analysis* -

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- *free energy variation graph* - use all your session files

- *UTR length variation graph* - use all your session files

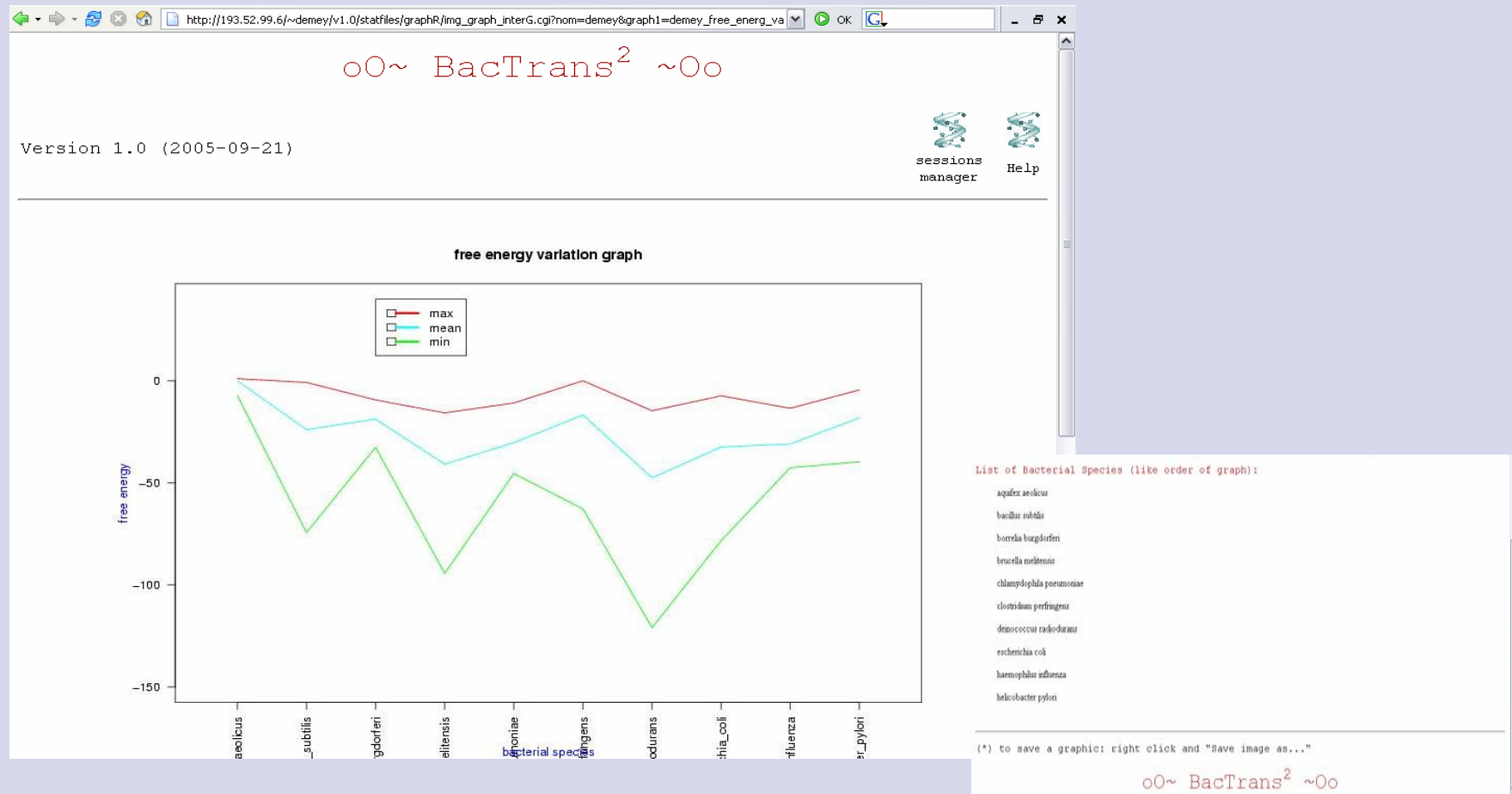
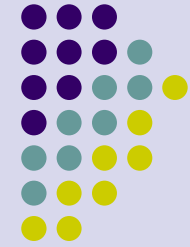
- *GC paired percent variation graph* - use all your session files

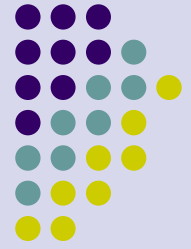
- *AT percent variation graph* - use all your session files

- *Free Bases percent variation graph* - use all your session files

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# La fonctionnalité 'Statistiques': exemple de graphiques du point de vue Inter Génomique

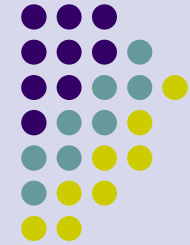




# Conclusion-Perspectives

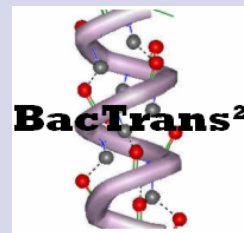
- Finaliser la plate-forme
  - Automatisation de certaines tâches
  - Etudes statistiques pour valider la plate-forme
  - La mettre à disposition
- La soumettre aux biologistes
  - Ajout de nouvelles espèces à leurs demandes
  - Développer de nouveaux outils suivant leurs besoins
- → Plate-forme évolutive





Merci de votre attention

~o0 BacTrans<sup>2</sup> 0o~



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