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Running a Bioinformatics Help Desk

from drawing colorful plasmid maps to working with HiSeq data

Solved and Unsolved Problems

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Friedrich Miescher Institute

- part of the Novartis Research Foundation
- affiliated institute of Basel University

316 employees

(incl. 96 PhD students, 95 Post Docs)

Epigenetics Growth Control Neurobiology

(7 research groups) (8 research groups)

(8 research groups)

Technology Platforms

Computational Biology – Cell Sorting – Imaging and Microscopy – *C. elegans* Functional Genomics – Histology – Mass Spectrometry – Protein Structure







Computational Biology / Bioinformatics

- member of Swiss Institute of Bioinformatics
- 3 core funded and 2 third party funded FTE
- many interactions with Functional Genomics
- hardware is maintained by IT
- providing support for ~250 scientists
- all services are free
 - "collaborations" → papers
 - "helpdesk"









Bioinformatics Helpdesk

providing support for:

the "average" lab scientist, who wants to:

the "modern" lab scientist, who wants to:

draw plasmids do BLAST searches use Excel



analyze NGS data work genome wide write (Perl) scripts

....and how to bridge the gap?



the "average" lab scientist, struggles with

drawing plasmids

doing BLAST searches

using Excel



drawing plasmids:

the actual problem:

there is no good 'desktop bioinformatics package'

our situation:

package A: - 10 perpetual licenses bought in 2006

- windows only

stuck on version X (does not run on windows 7)

package B: - 20 perpetual licenses bought in 2008

- 3 year support and upgrades

- stuck on version Y

- windows/mac/linux

both packages are ridiculously expensive



drawing plasmids: open source/free alternatives

we have been looking at:

GENtle http://gentle.magnusmanske.de/

Serial Cloner http://serialbasics.free.fr/Serial Cloner.html

pDRAW32 http://www.acaclone.com/

BioEdit http://www.mbio.ncsu.edu/BioEdit/BioEdit.html

GeneCoder http://www.algosome.com

Workbench http://www.ncbi.nlm.nih.gov/tools/gbench/

Ape http://biologylabs.utah.edu/jorgensen/wayned/ape/

UGene http://ugene.unipro.ru/

Has anybody experience with these or other open source/free packages?



drawing plasmids:

what about EMBOSS ?
(we offer most EMBOSS tools in our Galaxy server)

The tools 'cirdna' and 'lindna' produce reasonable maps of DNA constructs.....but the data needs to be in 'cirp' and 'linp' format, respectively.

How do I transform a genbank file to 'cirp' format?

we have no satisfying solution



doing BLAST searches

the actual problem: people are struggling using web resources

running training courses internal wiki pages / FAQ



using Excel

the actual problems:

- people have no statistics understanding
- "Excel"



no help provided

running training courses





promoting the use of R



the "modern" lab scientist, struggles with

writing (Perl) scripts

analyzing NGS data

work genome wide

simple solution: running introductory and advanced training courses in R



running R training courses

- R is a decent scripting language
- we can teach them statistics on the side
- they can start using Bioconductor

we currently re-implement our (perl based) NGS pipeline in a new Bioconductor package: "QuasR"

...but one problem remains: people want to display their data in a genome browsers



genome browsers

we use a combination of:

R/Bioconductor: GenomeGraphs, new package Gviz

web resources: ensembl - too slow

UCSC - S. pombe is missing

(we don't have the resources to run a local mirror)

local on desktop: IGV and IGB

Galaxy "Trackster"

Has anybody a perfect solution?



Bridging the Gap

the "average" lab scientist

| Colay / INT-e-bit | Colay / INT-e-b



Galaxy / FMI-Xenon1

Options

Analyze Data

Workflow Shared Data

b Visualization

Admin

=PAPOLA PE=1 SV=4

Help

History

Tools

>PAPOA_HUMAN_1 Poly(A) polymerase alpha OS=Homo sapiens GN=PAPOLA PE=1 SV=4 MPFPVTTOGSOOTOPPOKHYGITSPISLAAPKETDCVLTOKLIETLKPFGVFEEEELOR

Get Data

Text Manipulation

FASTA manipulation

FASTQ manipulation

Filter and Sort

Join, Subtract and Group

Unix Tools

Convert Formats

Extract Features

Operate on Genomic Intervals

Statistics

Graph/Display Data

Multiple regression

Multiple Alignments

EMBOSS TOOLS

EMBOSS search tools

EMBOSS sequence manipulation tools

GALAXY NGS TOOLS

NGS: Peak Calling

FMI TOOLS

FMI: Bioinformatics-Support

FMI: Functional Genomics

FMI: DNA Restriction Digest

FMI: DeepSeqRepository

FMI: qPCR

FMI: Thoma-lab

FMI: Schuebeler-lab

FMI: Roska-lab

Workflows

Tools

NLPQSVIENVGGKIFTFGSYRLGVHTKGADIDALCVA
KDLRAVEEAFVPVIKLCFDGIEIDILFARLALQTIPE
CRVTDEILHLVPNIDNFRLTLRAIKLWAKRHNIYSNI
IASTLVHKFFLVFSKWEWPNPVLLKQPEECNLNLPVW
NSTYNVSVSTRMVMVEEFKQGLAITDEILLSKAEWSK
EKQRLEWVGLVESKIRILVGSLEKNEFITLAHVNPQS
KKTENSENLSVDLTYDIQSFTDTVYRQAINSKMFEVD
KKKKHSTEGVKLTALNDSSLDLSMDSDNSMSVPSPTS
TAASVTNIQATEVSVPQVNSSESSGGTSSESIPQTAT
PPPRSSGNAATSGNAATKIPTPIVGVKRTSSPHKEES
DKTEAKEQLDTETSTTQSETIQTAASLLASQKTSSTD

LSDIPALPANPIPVIKNSIKLRLNR

>PAPOA_HUMAN_2 Poly(A) polymeras CESF*PPRAASRPSPPRSTTASPAPSAWPPPR ES*SWAS*TTW*RSGSERSARARTCPRA*SRT PDTWTEATSSPASTTS*SCRRR*RT*EPWRRP TWT*ETTAC*RTWTSDASEA*TAAE*PTRSCT WASWAA*AGPCWWPEPASCTPTPSPAPWCTSS TPE*TPATDTT*CPSSPPPTPSRTAPTT*A*A CSRPPTSSRSTSTTSCCWPAPPPRSRDWSGWA SPPPRRTPTRRSSEPCG*SAWCSRRPRTART* *RSPPCT*RESSCTSCCPTTCCRRRSTAPRA PPRPAP*TAAAAARAETAPPPP**PPPA*DTSR

PPRPAP*TARAAARAETAPPPP
SPPSAPPSPP*AEW*AAPDW*
PRRPRPRRTRPARTPTAWP*AI
*ATSPPCPPTPSP*SRTASS*I
>PAPOA_HUMAN_3 Poly(A)
ALPRDHPGQPADPAPPEALRHI
NPDPGQAEQPGEGVDQRDQRE(
QTRGQKRLLHQLLRQAEAAGGC
PGPERRQPAEEPGHQMHQKPEI
GLPGRRELGHAGGQNLPAVPQI
PQSEPQRQIPPDAHHHPRLPPI

GUI RE MP PR TS CG AS RA MT PA

Display

VRGPQLLPEVQALHRAAGQRPHREAETGVGGPGGEQDQNPGGQPGEERVHHPGPREPPEL
PRPQGEPRQGGVQNHVGDRPGVQEDREQREPERGPDLRHPELHRHRVQTGHQQQDVRGGH
EDRRHAREEKAAAPAAAQPRAAEEEEAQHRGREADRPERQQPGPEHGQRQQHERAQPHQR
HQDQPPEQQRQQPGQKQPRPRDRRQRDQHPGHRGERAPGEQQREQRRHQQREHPPDRHP
ARHQPPPQAHREQSGEQHQTGEPPPQKQRQRRHQRQRRHQDPHPHRGREENQQPPQGGEP
QEDQDRGGRDQRRQLPGPERPRQDRGQGAAGHRDQHHPERDHPDRRQPAGQPEDQHRP

ERHPRPARQPHPRDQEQHQAETEQX

>PAPOA_HUMAN_4 Poly(A) polymerase alpha OS=Homo sapiens GN=PAPOLA PE=1 SV=4
SVQSQLDAVLDHGDGVGGQGGDVAQVGAAGLLAGQQAGGGLDGLALGGAGLGVQLLLGLG
LVVAAQGQAVGVLAGLVLLGLGLLGALLLVGAAGSLHAHDGGGDLGGGVAAGGGVAAASG
GGVHQSGAAHHSAHGGLGGGAGGLGGGLGDALAAGAAALAAVHLGHAHGGLDVGHAG
GGHGGGAVSALAAAAAVQGAGLGGAGGAGHAHAVVAVHAQVQAAVVQGGQLHALGAVLL
LLLQHVVGQQLVQLLSLHVHGGDLHVHLEHLAVDGLSVHGVGEALDVVGQVHAQVLAVLG
LLEHOADHPHGSELLLVGVLLGGGEALGVHVGOGDELVLLOAAHODSDLALHOAHPLOSL

0 14.4 Kb Long Beach 7: Tabular-to-FASTA on @ 1 X data 5 🚫 6: Tabular-to-FASTA on 👁 🛭 🛭 data 5 @ 0 X 5: Select on data 4 O 1/ XX 4: FASTA-to-Tabular on data 3 @ 0 X 3: transeg on data 2 6 seauences format: fasta, database: ? (2) E >PAPOA_HUMAN_1 Poly(A) polymerase alph MPFPVTTOGSOOTOPPOKHYGITSPISLAAPKETDCVL RILILGKLNNLVKEWIREISESKNLPQSVIENVGGKIF PRHVDRSDFFTSFYDKLKLOEEVKDLRAVEEAFVPVIK DLDLRDDSLLKNLDIRCIRSLNGCRVTDEILHLVPNIC LGFLGGVSWAMLVARTCOLYPNAIASTLVHKFFLVFSK) 4 b 2: backtranseg on data 1 @ 0 X 1: P51003

why are we using Galaxy

- open source
- we can modify the tools
- we can add our own tools
 (we offer our own NGS pipeline tools, and have disabled the provided Galaxy NGS tools/wrapper)
- the "Galaxy" community is big and part of a wider community: "GenomeSpace", "GMOD"
- it is simple to install and maintain
- you can adjust the set-up according your needs
- it is easy to track what people are doing



we are using Galaxy for:

- microarray analysis (wrapped R/Bioconductor scripts)
- NGS analysis (wrapped perl scripts)
- EMBOSS
- file format conversion
- genomic interval operations
- providing a GUI for 'helpdesk' scripts

Galaxy is a stepping stone

 people learn how to built workflows instead of pressing red buttons



Galaxy does not solve all your problems

- there are no plasmid drawing tools
- built in genome browser ("Trackster") is Beta
- it does not replace the 'Bioinformatician'
 - do not offer tools you don't understand
- it does not replace the 'sys-admin'
 - if your tool does not run on the command line, it won't run in Galaxy
 - 'big data' needs 'big toys'
- it is simple to install and maintain....but it does need maintenance!



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