Poster Skills & Visual Knowledge Mobilization Workshop

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FGSR SRI workshops
Regina, SK
26 June 2025

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Fighting Superbugs!

University of Regina

What are the roles of posters in academic communications?

Disclaimer!
SciCom (Posters included) is a form of art

- There is no single recipe for success

- Breaking with tradition can pay off, **but** may often revile and repel, rather than amaze and astound.

➢ Don’t drastically depart from traditional guidelines in your field unless you have prior knowledge and experience – experiment with you peers/mentors first!

What do you notice?

What are the important elements for a successful poster presentation?

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What are the important elements for a successful poster presentation?

- When it comes to posters, style, format, color, readability, attractiveness, and ‘stage presence’ all count.

➢ Take the time to get things right.

Before starting

- Keep your audience in mind:
  - Is it a general audience?
  - Broad scientific audience?
  - Specialists?

- Check on conference site about poster dimensions.

- Focus on a single story.

Content

Content

Title: Write a succinct, but attention-grabbing, title. Don't agonize if it is not splashy!

Authorship: Correctly acknowledge all contributing authors and their institutional affiliations.

Background

- Setup your story by establishing the knowledge gap and your hypothesis.
- Use images or models.

Hypothesis and objectives

Methods

- Demonstrate why you chose this approach or how your approach is unique.
- For standard protocols, just state the name of the technique. For unique protocols, avoid technical details (use handouts or link to details).
- Use flow-charts, models, or graphics, as much as possible.

Results

- Use data that are relevant to the story and no more.
- Use active, not passive, voice.
- Keep graphics clean, simple, and easily understood (no unnecessary gridlines).

Conclusions and Future Directions

- Use clear and succinct language.
- Use same image as in the background to fill the gap (if possible).
- Use bullet points sparingly.

Acknowledgements, References, and Funding

- List only key references. Correctly acknowledge collaborators and all funding sources.

Rule 1: The Title Is Important

- The title is a good way to sell your work – it should make them want to come and visit.
- The title is your equivalent of a newspaper headline—short, sharp, compelling, and comprehensible to a broad audience.
- The title might pose a decisive question, define the scope of the study, or hint at a new finding.

Do’s and Don’ts: Title

- DON'T write an overlong title. Save it for your abstract. Avoid excess jargon, colons, and too cute phrases.

- DO keep your title short, snappy, and on target. The title needs to highlight your subject matter, but need not state all your conclusions, after all.

Do’s and Don’ts: Title

- DON'T make the title type size too large or too small or all capital letters.

- DO make your title large enough to be read easily from a considerable distance (say, 10-20 feet). The title should span the width of the poster but should not occupy more than two lines.

Do’s and Don’ts: Title section

- DON’T leave people wondering about who did this work.
- DO put the names of all authors and institutional affiliations just below (or next to) your title. It’s a nice touch to supply first names rather than initials.
- Don't use the same large type size as you did for the title; use something smaller and more discreet.

Rule 2: Sell Your Work in Ten Seconds

- Some conferences will present hundreds of posters; you will need to fight for attention.

- **Prepare an elevator pitch**: A very quick summary of the critical question behind your work and your main finding(s). The goal is to **spark interest!**

Rule 3: Layout and Format Are Critical

- Guide the passerby's eyes from one succinct frame to another in a logical fashion from beginning to end.

➢Usually left to right – top to bottom.

- Look for appropriate templates as a starting point: Don't re-invent the wheel!

- Never use less than a size 24-point font, and make sure the main points can be read at eye level.

Do’s and Don’ts: Layout & Format

- DON’T use too small font. This is the single most common error. Never, ever, use 10- or 12-point type.

- DO use a typesize that can be read easily at a distance of ~4 feet or better.
  Not enough space to fit all your text? Then shorten your text!

Do’s and Don’ts: Layout & Format

- DON’T pick a font that's a pain to read. Please, don’t get too creative in your font selections.

- DO select a highly legible font.

Do’s and Don’ts: Layout & Format

- DON'T vary the font sizes and/or types excessively throughout the poster.
  For example, don’t use something different for every bit of text and graphics.

- DO design your poster as if you were designing the layout for a magazine or newspaper. Select fonts and sizes that work together well. Strive for **consistency**, **uniformity**, and a clean, readable look.

Do’s and Don’ts: Layout & Format

- DON'T make your reader jump all over the poster area to follow your presentation. Don’t segregate your text, figures, and legends in separate areas.

- DO lay out the poster segments in a logical order, The best way to set up this pattern is **columnar format**, so the reader proceeds vertically first, from top to bottom, then left to right.

Do’s and Don’ts: Layout & Format

- DON'T use distracting colors. Colors attract attention but can equally well detract from your message when misused. Use color with deliberation; avoid using it for its own sake.

- DO use color in a way that helps to convey additional meaning.
  - For borders, select colors that draws attention but doesn’t overwhelm.
  - For artwork, make sure that the colors actually mean something and serve to make useful distinctions.
  - Be mindful of color contrast when choosing colors; never place isoluminous colors in close proximity (dark red on navy blue, etc.),
  - Remember that a lot of people out there happen to be red/green colorblind.

Rule 4: Content Is Important, but Keep It Concise

- Everything on the poster should help convey the message – Avoid redundancy!

- Use illustrations (chart, graph, or model) to transform complex data into a coherent and convincing story.
- Allow a figure to be viewed in both a superficial and a detailed way.
  - A graph could provide a bold trend line (with its interpretation clearly and concisely stated), and also have many detailed points with error bars.
  - Add a **take home message in each data panel**.

- Have a **clear and obvious set of conclusions**—this is where the passerby's eyes will wander first!

Content: Use clear, brief, jargon-free terms to explain

1. The scientific problem in mind (what's the question?)
2. Its significance (why should we care?)
3. How your experiment addresses the problem (what's your strategy?)
4. The experiments performed (what did you actually do?)
5. The results (what did you actually find?)
6. The conclusions (what did you think it all means?)
7. Caveats (and reservations) and/or future prospects (where do you go from here ?)

Do’s and Don’ts: Content

- DON'T write your poster as one long, rambling thread.

- DO break your poster up into sections. Label all the sections with titles.

Do’s and Don’ts: Content

- DON’T expect anyone to spend more than 5 min at your poster. If you can't clearly convey your message pictorially in less time than this, chances are you haven't done the job properly.

- DO get right to the heart of the matter and remember the all-important KISS Principle!

Do’s and Don’ts: Content

- DON'T waste lots of precious space on experimental details (**skip a complete Materials and Methods section**). Don't display all results. Don't ever supply long tables. And don't lift long sections of text directly from some manuscript.
  A poster is not a worked-over manuscript.

- DO recall that a poster should be more **telegraphic in style**, and also far more accessible. Stress experimental strategy, **key** results, and your conclusions. Convey the Big Picture.

Do’s and Don’ts: Content

- DON'T leave prospective readers hanging or assume they're all experts. They're not.

- DO consider adding anything that would help teach your readers what they need to know to understand and appreciate your work. Use graphics.

Do’s and Don’ts: Content

- DON'T leave out the acknowledgments.

- DO remember that it never hurts to give credit where it's due, including your sources of financial support and everyone who helped you to get this work done.

Do’s and Don’ts: Content

- DON'T leave out the references

- DO provide parties with routes into the literature and supply a context for your work.
  Poster references need not be as extensive as those in papers.
  If your poster work or work closely related to it has already been published, display the citation(s).

Rule 5: Good Posters Have Unique Features Not Pertinent to Papers

- A poster requires you to distill the work, yet not lose the message or the logical flow.
- Posters need to be viewed from a distance but can take advantage of your presence – do not follow the same rules re: captions and table titles, etc.
- Posters can be used as a distribution medium for associated papers, supplementary information, etc. – Use QR code when relevant but **be careful with what you share**
- Posters allow you to be more **speculative**.
- Posters may show Your Personality!

Rule 6: The Impact of a Poster Happens Both During and After the Poster Session

- The right presenter–audience interaction is required to achieve maximum impact.
- Work to get a crowd by being engaging; one engaged viewer will attract others.
- Don’t badger people, let them read.
- **Work all the audience at once**, do not leave visitors waiting for your attention.
- Make eye contact with every visitor.

Rule 6: The Impact of a Poster Happens Both During and After the Poster Session

- Make it easy for a conference attendee to contact you afterward.
- Follow up with people who come to the poster (*Take note of who came to your poster*).
- As the host of the work presented on the poster, be attentive, open, and curious, and self-confident but never arrogant and aggressive.
- Leave the visitors space and time—they can “travel” through your poster at their own discretion and pace. If a visitor asks a question, talk simply and openly about the work.

Do’s and Don’ts: Presentation

- DON'T leave everything until the last minute.
- DO start putting your poster together early.

- DON'T become so engrossed in conversation with any single individual preventing others from viewing your poster.
- DO try to stay close by, but off to the side just a bit, so that passers-by can see things also so that you don't block the vision of people already gathered.

- DON'T badger the nice people who come to read your poster.
- DO give them some space. If they engage you with a question, then that is your opening. Conversely, don't ignore people who look as though they may have questions.

Other presentation tips

- Identify questions that will be asked and think of answers in advance.
- Plan for interruptions during talk.
- Plan for other poster presenters also talking around you adding to room noise.
- Prepare by being confident, enthusiastic, and audible.

Before, during, and after your poster session

- Invite relevant attendees to your poster by emailing in advance or while at the meeting.
- Use it to connect with future employers and advisors.
- If you have movies (or 3D data), plan to have an iPad to show them.
- Take a picture with your poster and promote on social media with conference hashtag (Don’t post sensitive/unpublished work**!**).
- Have water, tea, lozenges handy.
- Take quick notes on attendee names and send personalized thank you notes.
- Connect with visitors on LinkedIn/X.
- Display your poster in your department hallway for local colleagues to see your work.

Final notes

- Proof-read before printing. Have at least two colleagues give you feedback. Get approval from your supervisor.

- Good posters and their presentations can improve your reputation, both within and outside your working group and institution, and may also contribute to a certain scientific freedom.

- Poster prizes count when peers look at your resume.

Now, some examples…

PIGS IN SPACE: EFFECT OF ZERO GRAVITY AND AD LIBITUM FEEDING ON WEIGHT GAIN IN CAVIA PORCELLUS

Colin B. Purrington
6673 College Avenue, Swarthmore, PA 19081 USA

ABSTRACT:

One ignored benefit of space travel is a potential elimination of obesity, a chronic problem for a growing majority in many parts of the world. In theory, when an individual is in a condition of zero gravity, weight is eliminated. Indeed, in space one could conceivably follow ad libitum feeding and never even gain an gram, and the only side effect would be the need to upgrade one's stretchy pants("exercise pants"). But because many diet schemes start as very good theories only to be found to be rather harmful, we tested our predictions with a long-term experiment in a colony of Guinea pigs (Cavia porcellus) maintained on the International Space Station. Individuals were housed separately and given unlimited amounts of high-calorie food pellets. Fresh fruits and vegetables were not available in space so were not offered. Every 30 days, each Guinea pig was weighed. After 5 years, we found that individuals, on average, weighed nothing. In addition to weighing nothing, no weight appeared to be gained over the duration of the protocol. If space continues to be gravity-free, and we believe that assumption is sound, we believe that sending the overweight — and those at risk for overweight — to space would be a lasting cure.

INTRODUCTION:

The current obesity epidemic started in the early 1960s with the invention and proliferation of elastane and related stretchy fibers, which released wearers from the rigid constraints of clothes and permitted monthly weight gain without the need to buy new outfits. Indeed, exercise today for hundreds of million people involve only the act of wearing stretchy pants in public, presumably because the constrictive pressure forces fat molecules to adopt a more compact tertiary structure (Xavier 1965).

Luckily, at the same time that fabrics became stretchy, the race to the moon between the United States and Russia yielded a useful fact: gravity in outer space is minimal to nonexistent. When gravity is zero, objects cease to have weight. Indeed, early astronauts and cosmonauts had to secure themselves to their ships with seat belts and sticky boots. The potential application to weight loss was noted immediately, but at the time travel to space was prohibitively expensive and thus the issue was not seriously pursued. Now, however, multiple companies are developing cheap extra-orbital travel options for normal consumers, and potential travelers are also creating news ways to pay for products and services that they cannot actually afford. Together, these factors open the possibility that moving to space could cure overweight syndrome quickly and permanently for a large number of humans.

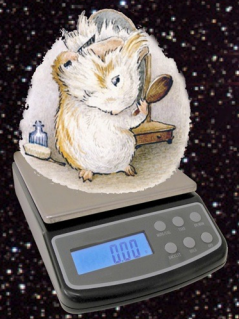
We studied this potential by following weight gain in Guinea pigs, known on Earth as fond of ad libitum feeding. Guinea pigs were long envisioned to be the "Guinea pigs" of space research, too, so they seemed like the obvious choice. Studies on humans are of course desirable, but we feel this current study will be critical in acquiring the attention of granting agencies.

MATERIALS AND METHODS:

One hundred male and one hundred female Guinea pigs (Cavia porcellus) were transported to the International Space Laboratory in 2010. Each pig was housed separately and deprived of exercise wheels and fresh fruits and vegetables for 48 months. Each month, pigs were individually weighed by duct-taping them to an electronic balance sensitive to 0.0001 grams. Back on Earth, an identical cohort was similarly maintained and weighed. Data was analyzed by statistics.

RESULTS:

Mean weight of pigs in space was 0.0000 +/- 0.0002 g. Some individuals weighed less than zero, some more, but these variations were due to reaction to the duct tape, we believe, which caused them to be alarmed push briefly against the force plate in the balance. Individuals on the Earth, the control cohort, gained about 240 g/month ($p = 0.0002$). Males and females gained a similar amount of weight on Earth (no main of effect of sex), and size at any point during the study was related to starting size (which was used as a covariate in the ANCOVA). Both Earth and space pigs developed substantial dewlaps (double chins) and were lethargic at the conclusion of the study.



CONCLUSIONS:

Our view that weight and weight gain would be zero in space was confirmed. Although we have not replicated this experiment on larger animals or primates, we are confident that our result would be mirrored in other model organisms. We are currently in the process of obtaining necessary human trial permissions, and should have our planned experiment initiated within 80 years, pending expedited review by local and Federal IRBs.

ACKNOWLEDGEMENTS:

I am grateful for generous support from the National Research Foundation, Black Hole Diet Plans, and the High Fructose Sugar Association. Transport flights were funded by SPACE-EXES, the consortium of wives divorced from insanely wealthy space-flight startups. I am also grateful for comments on early drafts by Mañana Athletic Club, Corpus Christi, USA. Finally, sincere thanks to the Cuy Foundation for generously donating animal care after the conclusion of the study.

LITERATURE CITED:

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Sekulić, S.R., D. D. Lukač, and N. M. Naumović. 2005. The Fetus Cannot Exercise Like An Astronaut: Gravity Loading Is Necessary For The Physiological Development During Second Half Of Pregnancy. Medical Hypotheses. 64:221-228

Xavier, M. 1965. Elastane Purchases Accelerate Weight Gain In Case-control Study. Journal of Obesity. 2:23-40.

Classical Torques on Gravity Probe B Gyros

Alex Silbergleit, Mac Keiser, Yoshimi Ohshima

1. Classification of Torques

Rotor and housing: electrodes seen

– Support dependent (SD) - torques caused by suspension system operation

– Support independent (SI) - torques caused by anything else

Support Dependent Torques:
– Caused by residual accelerations (difference of squares of electrode voltages)
– Caused by preload accelerations (sum of squares of electrode voltages)

Support Independent Torques:
– Housing - fixed
– Inertially fixed

SD & SI housing-fixed – by Gyro Position:
– Nominal (gyro centered, its spin and S/C roll axes aligned)
– Misaligned (centered, spin axis not exactly along roll)
– Miscentered (spin & roll axes aligned, gyro not exactly centered)

No misaligned position housing-fixed SI torques known/detected

Small parameters: gap/rotor radius=1.7×10^{-4}; asphericity/radius~10^{-5}; miscentering/gap=3×10^{-4}, D.C.; miscentering/gap=3×10^{-5}, at roll freq.; $\Delta I/I < 4\times10^{-5}$; average spin-to-roll axis misalignment = 5×10^{-5};

2. Torque Theory

Systematic theory of electrostatic **Support Dependent** torques complete to lowest order in small parameters is developed

- 2 independent derivations based on: a) direct torque calculation, and b) energy conservation+ symmetry lead to the same results
- 'Magic' general formula

Torque = (position factor) x (torque coefficient) x $(V_{+}^{2} - V_{-}^{2})$

- Position factor = 1, nominal; = NS or EW misalignment, misaligned; = miscentering/gap ratio, miscentered position torques
- Torque coefficient, K_{-}, depends on the rotor asphericity (deviation from perfect sphere) only. Total 15 torque coefficients, only 6 are involved in (most contributing) nominal and misaligned position torques
- V_{+}, V_{-} are voltages of opposite electrodes of one of 3 electrode pairs

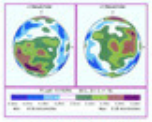
- No general theory of **SI** torques available, due to various physical origin (electrostatic, magnetic, differential damping torques, etc.)
- Expression for each **SI** torque is derived separately
- Examples of **SI** torques: direct gravity gradient torque; torque due to coupling of London moment with local shield; torque due to residual gas pressure (largest of SI torques)

3. Pre-Flight Estimates of Classical Drift

Based on torque theory, requirements, ground measurements and best parameter estimates when measurements not available

Example: torque coefficients

- Three flight-class coated rotors anodized to carefully measure their shape (up to $l=16$ in terms of spherical harmonics)
- All 15 torque coefficients computed from found rotor shape coefficients for every position of the spin axis in the body of each rotor
- Range for each torque coefficient was thus established and used in the **Support Dependent** torque estimates



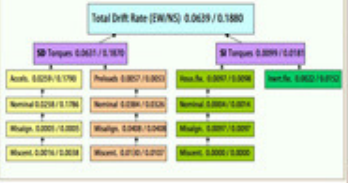
Measured surface map of flight uncoated rotor

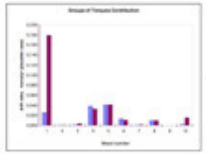
Total drift rate due to classical torques is computed for each gyro through its Error Tree, an Excel Workbook with

- >120 input parameters (mechanical, electrical, and magnetic parameters of the rotor; various S/C parameters, such as orbital ones; torque coefficients; preload accelerations, etc.)
- residual accelerations by formulas from input parameters
- >100 individual torques grouped according to their classification by formulas from input parameters and residual accelerations
- drift rates in 2 inertial directions, EW and NS

4. Pre-Flight Estimates - II

Top Sheet of Pre-Flight Error Tree for Gyro 4 (Unsupported Gyro 1; Drift Rate in *marc-sec/year*)

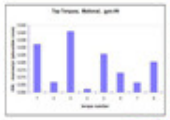




Contributions of the above groups of torques:
BLUE – EW
PINK - NS

5. Pre-Flight Estimates - III

Important result: not more than 8 torques contribute >99% of classical drift rate for **each** gyroscope **in either** of the directions (list/magnitude of torques varies slightly depending on the gyro and direction)



Top Torques, Gyro 4, EW (99.98% of drift)

1.	SD, PD, MoP, D.C. preloads	0.041 mas/yr
2.	SD, PD, NP, preload difference @ roll	0.032 mas/yr
3.	SD, AD, NP, gravity grad. perp roll axis	0.026 mas/yr
4.	SD, PD, MoP, D.C. prel.× misc. at roll	0.013 mas/yr
5.	SI, HF, MoP, LM-coupling to loc. shield	0.007 mas/yr
6.	SI, HF, MoP, resid. gas press. + asymm.	0.007 mas/yr
7.	SI, IF, direct gravity gradient	0.002 mas/yr
8.	SD, PD, NP, preloads×gravity gradient	0.002 mas/yr

Legend: PD / AD = Acceleration / Preload Dependent; HF / IF = Housing- / Inertially-Fixed
NP / MaP / McP = Nominal / Misaligned / Miscentered Position

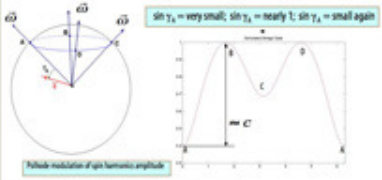
Pre-flight estimates of classical drift rate, *marc-sec/year*

	G1	G2	G3	G4
EW	0.055	0.055	0.068	0.064
NS	0.105	0.086	0.172	0.188

6. Post-Flight Estimates of Classical Drift

In work currently. Are obtained using on-orbit measurements and calibrations

Example 1: Flight Measurement of Rotor Mass Unbalance (MU). MU=distance between center of mass and geometrical center (fixed in body). Spin axis moves in the body along polhode path modulating gyro position signal at spin frequency. MU contributes up to 50% to all odd harmonics torque coefficients



	G1	G2	G3	G4
Pre-Flight	18.8	14.5	16.8	13.5
In-Flight	10.1	6.6	4.0	8.9

Measured MU, in *nm*

7. Post-Flight Estimates - II

Example 2: Flight Calibrations of Torque Coefficient K_1. Coefficient K_1 governs one of the top torques due to preload difference at roll frequency. In flight but **before** science this torque was used to align gyro spin axes with the direction to the Guide Star, for which the difference at roll was strongly enhanced. It was deliberately enhanced once again **after** science for precise calibration. Both times the measurement scheme was: detect the (large) drift rate, compute the torque from it, and, knowing voltages, find K_1 using 'magic' formula of chart 2. Calibration values (essentially more accurate than spin alignment ones) turn out 10 (or more!) times smaller than the conservative pre-flight estimates

Measured K_1, in *pf/rad*

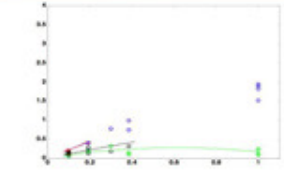
	G1	G2	G3	G4
Pre-Flight Estim.	-0.0682	-0.0964	-0.0872	-0.0859
Spin Axis Align., before science	-0.0061	-0.0022	-0.0184	-0.0057
Calibration, after science	-0.0008	-0.0108	-0.0183	-0.0072

After refining all the torque parameters incorporating all the relevant flight data, recalculate classical drift rate by scaling pre-flight results
- By groups of torques, or
- By top torques

Current estimates (to be sharpened) of classical drift error in the experiment results are <1 mas/yr for gyros 1,3, 4; <2 mas/yr for gyro 2 (both directions) – ALL torques, EXCEPT just one…

8. Misalignment Torque: Patch Effect

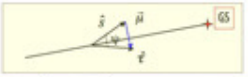
Anomalously large drift rate detected in post-flight calibrations with spin-to-roll axis misalignment deliberately enhanced (from ~10 *as* up to several degrees). It grows with the misalignment in a non-linear way, but is linear for smaller misalignments within few tens of a degree (fit to measured drift rate below)
- Proportionality coefficient up to 1 – 3 *as/(deg*day)*
- Drift direction perpendicular to the misalignment
- Thus fully separable from relativistic drift fixed in the inertial space



Explanation: Patch Effect Electrostatic potential on rotor and housing surfaces may be not uniform due microcrystal structure, or dipole surface layer, etc. (patch effect). Due to patches and relative motion of rotor and housing (gyro spin, S/C roll in the inertial space), electrostatic torques on rotor are generated.

9. Patch Effect: Modeling

Complete Theory of Patch Effect Torque is developed. Potential distributions on the rotor and housing surfaces are characterized by constant coefficients of their spherical harmonics expansions in the rotor- and housing-fixed frames, respectively. By rotating the first frame to the second one, we solve the electrostatic boundary value problem in the gap, compute electrostatic energy (to lowest order in gap/radius ratio), and vary it in three independent angles (spin phase, roll phase and the misalignment) to get all the torques. The 1st torques is spin-up/down and averages out over spin period, the 2nd is also mainly spin-up/down one (small misalignment!). The 3rd is responsible for the observed drift and should be taken out of the signal



Unit vectors of spin, $\hat{s}$, and roll, $\hat{\tau}$, axes, misalignment vector, $\vec{\mu}$, and misalignment angle, ψ. To lowest order, $\psi = \mu$.

Gyro Spin Motion Equation (roll averaged model to linear order in μ.)

$$\frac{ds_{NS}}{dt} = r_{NS} + k(t)[\tau_{EW}(t) - s_{EW}(t)]$$

$$\frac{ds_{EW}}{dt} = r_{EW} - k(t)[\tau_{NS}(t) - s_{NS}(t)]$$

W. W. Hansen Experimental Physics Laboratory • Stanford University, Stanford, CA 94305-4085 • http://einstein.stanford.edu

This research supported by NASA on contract NAS8-39225

IsoMIF: detection of molecular interaction field similarities. Online interface and applications.

Matthieu Chartier & Rafael Najmanovich

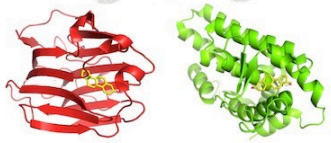
Département de Biochimie, Faculté de médecine et des sciences de la santé, Université de Sherbrooke, Québec

bcb.med.usherbrooke.ca

Groupe de Recherche NAJMANOVICH Research Group

Introduction

Two proteins **with no sequence or structural similarities** can bind identical ligands.

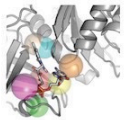


In red, Sex-Hormone Binding Globulin (PDB 1LHU) and in green, Estrogen Nuclear Receptor (PDB 1QKT) both bound to estradiol.

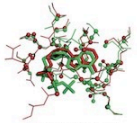
This dual **molecular function** can result from **convergent evolution** and allows the complexity of biological processes with minimal biological elements. Multiple targets able to bind one molecule can be a problem when a drug binds unintended targets and cause **adverse side effects**. This promiscuity can also be harnessed in **polypharmacological strategies**.

How can we detect similarities responsible for the recognition of identical ligands regardless of sequence or fold?

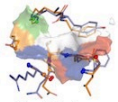
Binding site similarities



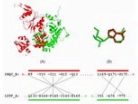
Micro-Environments
PocketFEATURE[1]



Binding site atoms
IsoCleft[2]



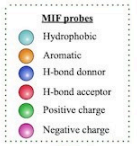
PseudoCenters
+ surface patches
CavBase[3]



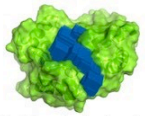
Sequence order independant
Cα alignments
SOIPPA[4]

The IsoMIF Method

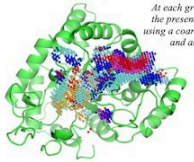
We developped IsoMIF[5], that calculates Molecular Interaction Fields (MIFs) **in the volume of protein cavities** and can then compare two MIFs to find similarities: **intermolecular interactions in geometrically equivalent positions**.



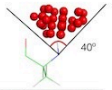
*A **regular grid** is built in the **volume of cavities**, here with a resolution of 0.5Å.*



*At each grid intersection, **6 probes** evaluate the presence of **intermolecular interactions** using a coarse-grain distance based potential and an **atom-probe interaction matrix**.*

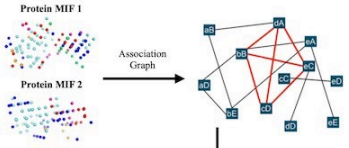


Molecular Interaction Fields
IsoMIF[5]



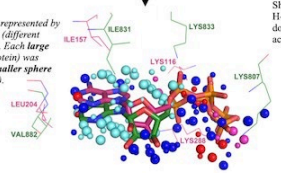
The directionality of interactions is considered for H-bonds and aromatic interactions.

IsoMIF can find similarities regardless of sequence or fold



The protein structures and bound ligands are **superimposed based on the MIF similarities found**. Residues underlying the similarities can be identified using PyMOL.

Bron & Kerbosch algorithm then superimposition based on matched probes



*Similarities are represented by colored spheres (different chemical types). Each **large sphere** (first protein) was matched to a **smaller sphere** (second protein).*

Validation

How well can IsoMIF find as more similar proteins bound to same ligands than others bound to different ligands?

We **evaluated the performance** of IsoMIF[5] accross different datasets. This was evaluated with ROC curves accross 4 datasets used to benchmark other similar methods.

AUC averaged accross 4 datasets for similar methods			
IsoMIF	**eMatchSite**	**SiteEngine**	**PocketMatch**
0.82 ± 0.04	0.80 ± 0.15	0.73 ± 0.16	0.60 ± 0.10

To **control** for similarities that emerged from **divergent evolution**, we measured AUCs using **increasingly stringent local sequence identity thresholds** to **remove trivial cases** on larger datasets.

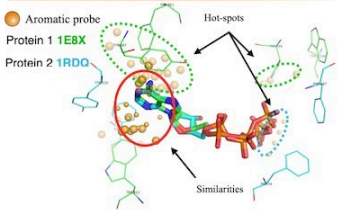
	IsoMIF		Sequence		Nb. of entries	
Sequence redundancy threshold	**PDBbind**	**scPDB**	**PDBbind**	**scPDB**	**PDBbind**	**scPDB**
100 %	0.93	0.87	0.81	0.68	1415	3809
35 %	0.86	0.82	0.63	0.58	773	3038
25 %	0.84	0.82	0.59	0.56	599	2699
15 %	0.79	0.79	0.51	0.50	414	2292

Limitations exist with our approach:

- **Availability of protein structures** and their conformations.
- **True-positive definition** used: bound to same ligand is simplistic.
- One ligand can bind with **different binding modes**.

Applications

1. Rational drug design.

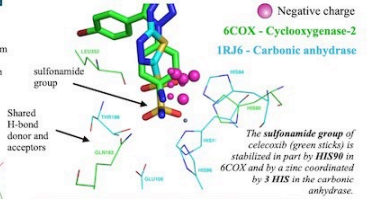


*MIF **similarities** (circled red - opaque spheres) and **hot-spots** (dashed circles - semi-transparent spheres) can be identified at scale for multiple targets and guide the design of more **selective inhibitors**.*

2. Drug repurposing.

Cyclooxygenase-2 (6COX) bound to **celecoxib** an approved drug (Celebrex) — compared to — 400 binding sites

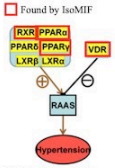
Carbonic anhydrase 1RJ6 was found as 5th top hit (z-score: 1.82). Celecoxib was reported to be a **potent carbonic anhydrase inhibitor** and proposed as a treatment for glaucoma[6].



*The **sulfonamide group** of celecoxib (green sticks) is stabilized in part by **HIS90** in 6COX and by a zinc coordinated by **3 HIS** in the carbonic anhydrase.*

3. Prevention of side-effects

Torcetrapib (Pfizer) removed from phase III clinical trials for **hypertensive side-effects**

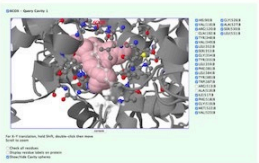


Query PDB 2OBD
Cholesterylester transfer protein

*From 8077 entries in the scPDB dataset, 4 entries within the 20 top hits (z-score between 3.07 and 5.44) were found by IsoMIF and also predicted by Xie et al.[7] as potential off-targets of torcetrapib that **could explain hypertensive side-effects** through **RAAS modulation**.*

Online Interface

IsoMIF Finder[8] is an online interface **developped for non-technical users**. It allows the comparison of user defined query cavities to 4 ensembles of pre-calculated MIFs or to user defined cavities.



*The screenshot shows how the **user can crop the cavities** found for the query protein. This allows MIFs to be calculated in regions of interest and increase relevance of the results.*

Perspectives

400 binding sites bound to drugs — compared to — PDB PROTEIN DATA BANK

A comparison of 400 binding sites bound to small molecules mapped in drugbank to a non-redundant dataset of the PDB (14082 cavities) will help identify potential new **drug repurposing avenues** or clues for the **mechanism of observed drug side effects**.

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6. Weber *et al.* (2004). *Journal of Medicinal Chemistry*, 47(3), 550–557
7. Xie *et al.* (2009). *PLoS Computational Biology*, 5(5), e1000387
8. **Chartier** *et al.* (2015). *Bioinformatics* (Oxford, England), btv616

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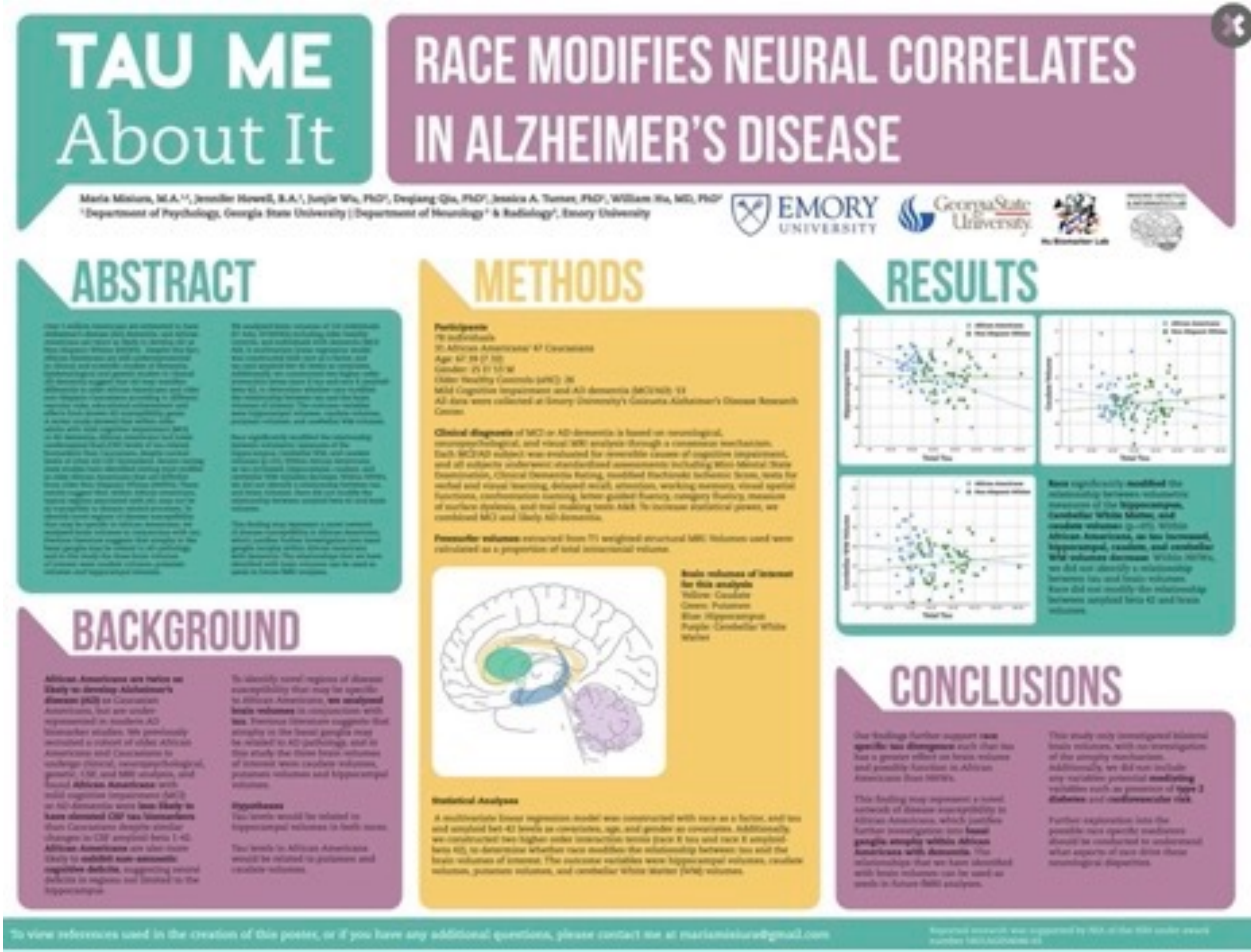
TAU ME
About It
RACE MODIFIES NEURAL CORRELATES IN ALZHEIMER'S DISEASE
Maria Misiura, M.A.1,2, Jennifer Howell, B.A.1, Junjie Wu, PhD2, Deqiang Qiu, PhD3, Jessica A. Turner, PhD1, William Hu, MD, PhD2
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EMORY UNIVERSITY
Georgia State University
ABSTRACT
BACKGROUND
METHODS
Brain volumes of interest for this analysis
Yellow: Caudate
Green: Putamen
Blue: Hippocampus
Purple: Cerebellar White Matter
Statistical Analyses
RESULTS
Total Tau
CONCLUSIONS
To view references used in the creation of this poster, or if you have any additional questions, please contact me at mariamisiura@gmail.com

miR-218 Function in Determining Spinal Cord Motor Neuron Identity

Karen P. Thiebes[1], Heejin Nam[4], Xiaolu A. Cambronne[2], Rongkun Shen[2], Stacey M. Glasgow[5], Richard H. Goodman[2], Jae W. Lee[1,2,3]*, Seunghee Lee[4,*], & Soo-Kyung Lee[1,2,3]*

1Pediatric Neuroscience Research Program, Papé Family Pediatric Research Institute, Department of Pediatrics, 2Vollum Institute, 3Department of Cell and Developmental Biology, Oregon Health & Science University, Portland, OR 97239, USA; 4College of Pharmacy and Research Institute of Pharmaceutical Sciences, Seoul National University, Seoul 151-742, Korea; 5Center for Cell and Gene Therapy, Baylor College of Medicine, One Baylor Plaza, Houston, TX 77030, USA

INTRODUCTION

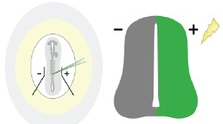
While microRNAs have emerged as an important component of gene regulatory networks, how microRNAs collaborate with transcription factors in the gene network that determines neuronal cell fate remains unclear. Here we show that in the developing spinal cord, the expression of miR-218 is directly upregulated by the Isl1-Lhx3 complex, which drives motor neuron fate. Inhibition of miR-218 suppresses the generation of motor neurons in chick neural tube and mouse embryonic stem cells, suggesting that miR-218 plays a crucial role in motor neuron differentiation. Our unbiased RISC-trap screens, in vivo reporter assays, and expression studies revealed that miR-218 directly represses transcripts that promote developmental programs for interneurons and neural progenitors. In addition, miR-218 activity is required for Isl1-Lhx3 to effectively induce motor neurons and suppress interneuron fates. Together, our studies uncovered an essential role for miR-218 as a downstream effector of the Isl1-Lhx3 complex in establishing motor neuron identity.

METHODS

Isl1-Lhx3 ESC miRNA Array and Small RNA Quantitative RT-PCR
The generation and differentiation of Isl1-Lhx3 ESCs was previously described (Lee et al. 2012). The miRNA array assays were performed with TaqMan® Array Rodent MicroRNA Card A (Life Technologies).

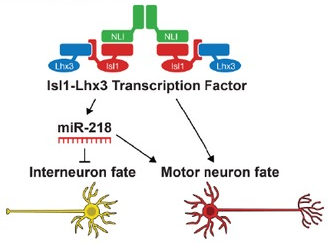
RISC-trap, RNA Extraction and Quantitative RT-PCR
RISC-trap experiments and data analyses were performed as previously described (Cambronne et al. 2012), except that reads for each gene were counted by HTSeq (Simon.Huber.2013_HTSeq A Python framework to work with high-throughput sequencing data_BioRxiv002824).

***In Ovo* Electroporation**
Expression constructs were injected into the lumens of chick embryonic spinal cords at HH stages 12-14 (Hamburger and Hamilton 1951). Electroporation was performed using a square wave electroporator (BTX) as previously described (Nakamura and Funahashi 2001). Incubated chicks were harvested and analyzed at HH stages 17-30, fixed in 4% paraformaldehyde, and cryosectioned at 12 um.



CONCLUSIONS

Summary
- miR-218 is expressed and active in developing spinal cord motor neurons
- Isl1-Lhx3 directly binds and upregulates miR-218-1 and miR-218-2 genes
- miR-218 is essential for the generation of motor neurons from ESCs
- miR-218 inhibits expression of genes that are important for neural progenitors and interneurons



RESULTS

miR-218 Expression

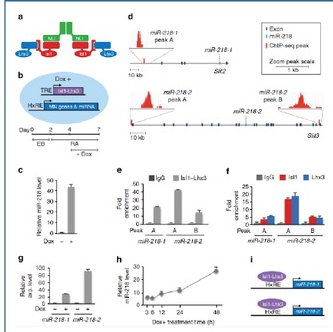


Figure 1. miR-218 is upregulated by Isl1–Lhx3 in motor neurons

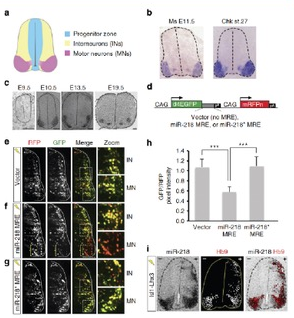


Figure 2. miR-218 is expressed in developing motor neurons

miR-218 is Essential for Motor Neuron Fate Specification

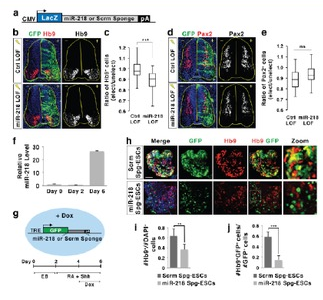


Figure 3. miR-218 is important for ESC motor neuron differentation

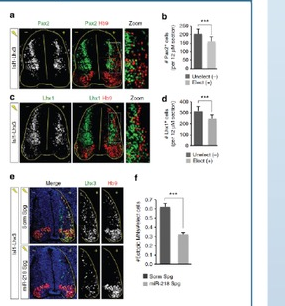


Figure 4. miR-218 is important for spinal cord motor neuron differention

miR-218 Target Identification

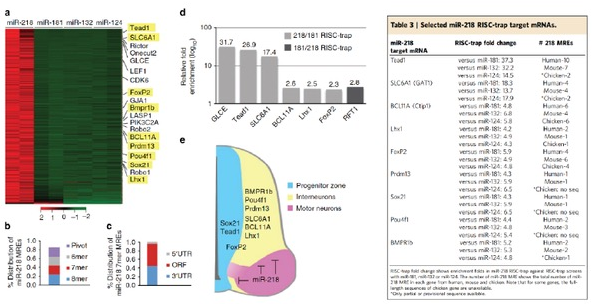


Figure 5. miR-218 targets neural progenitor and interneuron mRNAs

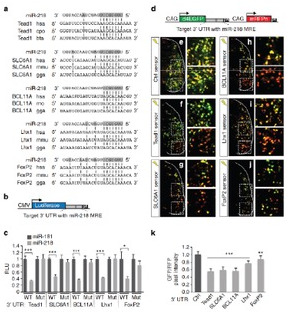


Figure 6. miR-218 *in vitro* target validation

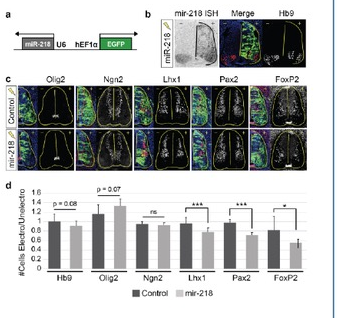


Figure 7. miR-218 *in vivo* target validation

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ACKNOWLEDGEMENTS

We are grateful to Drs. Fred H. Gage and Xinwei Cao for the miRNA sensor vector; to Dr. Greg Smith for creating the ImageJ GFP/RFP pixel intensity analysis script; Younjung Park for the excellent technical support; to Lee laboratory members for discussions. This research was supported by grants from NIH/NINDS (R01 NS054941) (to S.-K.Lee), NIH/NIDDK (R01 DK064678) (J.W.Lee), NIH/NIMH (R01 MH094416) (to R.H.Goodman) and Research Institute of Pharmaceutical Sciences, POSCO TJ Park Science Fellowship, Basic Science Research Program (2012R1A1A1001749) and Bio & Medical Technology Development Program (2012M3A9C6050508) of the National Research Foundation (NRF) funded by the Korean government (MEST) and National R&D Program for Cancer Control, Ministry of Health & Welfare, Republic of Korea (1220120) (to S.Lee).

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Poor — 1 0

2 0

Fair — 3 0

4 0

Excellent — 5 0

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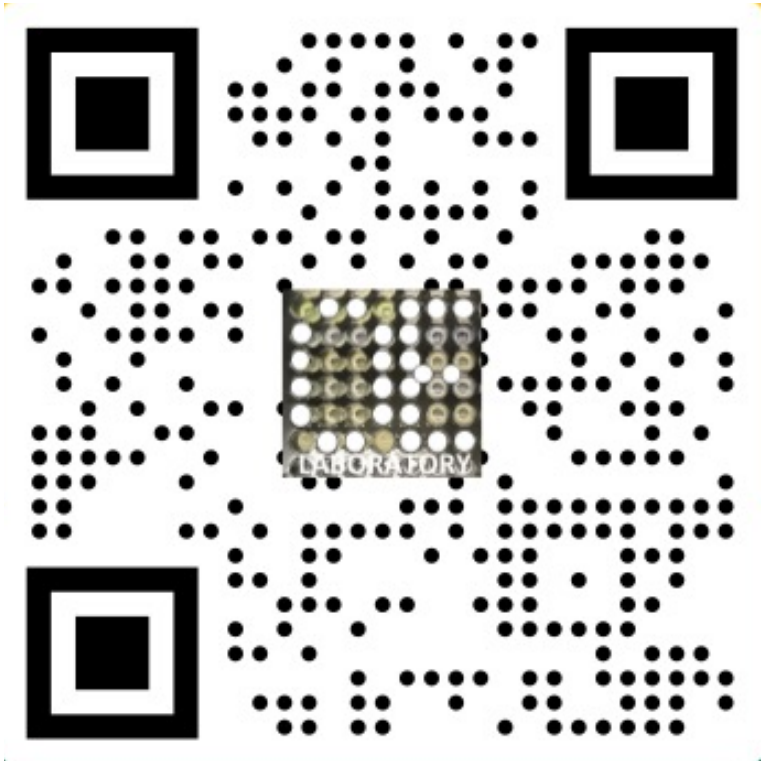

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Resources

- Erren TC, Bourne PE (2007) Ten simple rules for a good poster presentation. PLoS Comput Biol 3(5): e102. doi:10.1371/journal.pcbi.0030102

- Block-1996-biophysical journal-Do's and Don'ts of Poster presentation