

Comunicação gráfica  
com Inteligência Artificial:

# O Poster

Marco Soares, designer

# Objetivos de uma boa apresentação científica

**1.**

Comunicar a  
Ciência de forma  
clara

**2.**

Deixar uma impressão  
duradoura no público

**3.**

Melhorar a  
reputação do  
cientista

# O que faz uma boa apresentação científica em Poster?

1

Ter um aspeto visual **cativante que desperte a atenção** e que induza à leitura.

2

Ter mensagens **claras e informativas** , bem estruturadas e de fácil entendimento.

3

Grande **capacidade de síntese** mas que ao mesmo tempo diga o essencial e deixe uma mensagem clara.

# Cores

## Significado

Elegância  
Mistério  
Morte

Tranquilidade  
Segurança  
Harmonia

Esperança  
Saúde  
Natureza

Alegria  
Luz  
Alerta

Paixão  
Poder  
Força

Vitalidade  
Juventude  
Energia

Paz  
Pureza  
Clareza



POLÍCIA

POLÍCIA



FARMÁCIA





sure we can

TNT

TNT

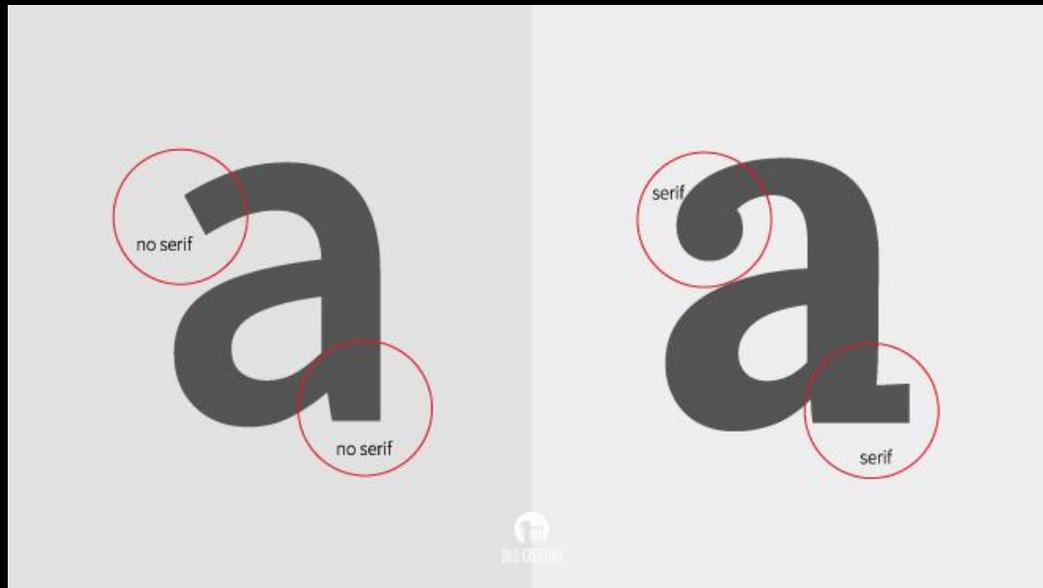
pak 5 000



McDonald's

# Tipografia

## Tipos



# Tipografia

## Tipos

A casa que os Maias vieram habitar em Lisboa, no outono de 1875, era conhecida na vizinhança da rua de S. Francisco de Paula, e em todo o bairro das Janelas Verdes, pela casa do Ramalhete ou simplesmente o Ramalhete.

- *Os Maias, Eça de Queiroz*

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# Tipografia

## Alinhamento

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- *Os Maias, Eça de Queiroz*

# Tipografia

## Famílias

# Open Sans

Light

*Light Italic*

Regular

*Italic*

**Semibold**

***Semibold Italic***

**Bold**

***Bold Italic***

**Extrabold**

***Extrabold Italic***

# Tipografia

## Tamanhos

And you will read this last

**You will read  
this first**

And then you will read this

Then this one

# Tipografia

Famílias / Tamanhos

6 PM TIL LATE

# WE LOVE LIVE MUSIC

EVERY SUNDAY

FREE ENTRY  
TIL 9PM

ON THE DECK / AUGUST

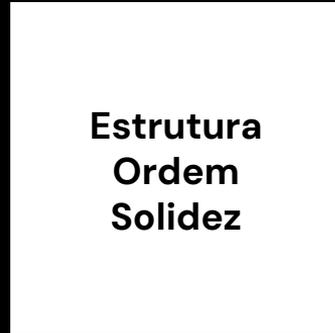
05 ALICE JAZZ • 12 SILENT JAM  
19 TRACE WARS • 26 BIG TIMES SOUND

FREE BBQ 6PM • DRINK SPECIALS  
\$10 BEER JUGS • POOL COMP FROM 7PM

TERMS & CONDITIONS MAY APPLY

# Formas

## Psicologia das Formas



**Quadrado**



**Círculo**



**Triângulo**



**Orgânico**

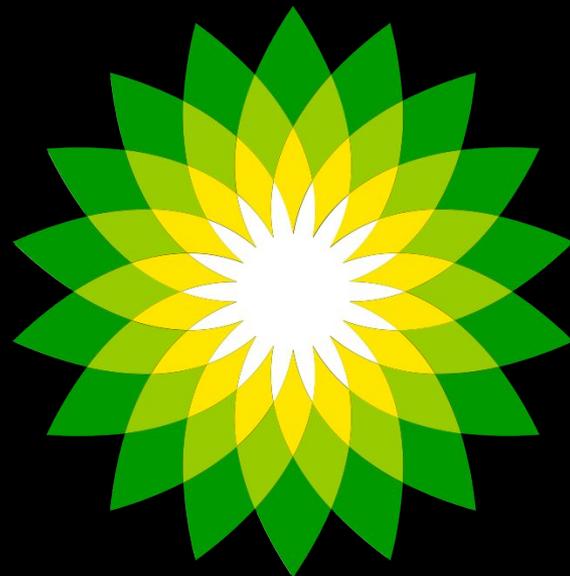
Forma

Cultura

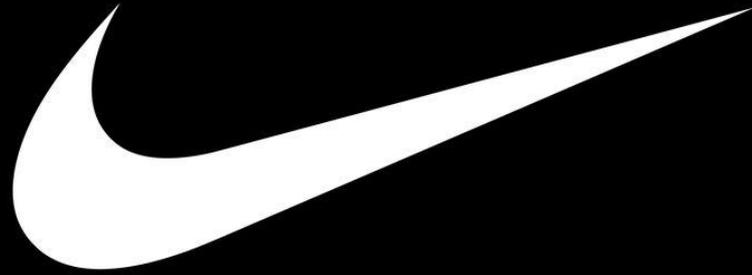


**Forma**

**Cultura**



**Forma**  
**Cultura**



LiGHT

The image features the word "LiGHT" in a stylized, outlined font against a black background. The letter 'L' is a simple outline. The lowercase 'i' has a solid yellow dot above it. The uppercase 'G' is filled with a yellow-to-black gradient, with a circular shadow effect behind it. The uppercase 'H' and 'T' are also simple outlines. The lowercase 'h' is filled with a yellow-to-black gradient, matching the 'G'. The uppercase 'T' is an outline with a yellow-to-black gradient fill on its right side.

**Poster**

# Estrutura

## Formato IMRaD

### Introduction

Apresenta os antecedentes e o objetivo da investigação.

### Results

Apresentação das conclusões, sem qualquer explicação ou comentário sobre as mesmas.

### Methods

Conceção da investigação, contexto da investigação, número de pessoas incluídas no estudo e forma como foram seleccionadas.

### Discussion

Indica de forma concisa o que se pode concluir do estudo e as suas implicações.

# Estrutura

## Simplicidade e Equilíbrio

Diferenciação entre as diferentes áreas.

Uso da tipografia para uma boa hierarquização da informação.

Usar cores como códigos quer de identificação, quer de diferenciação.



# A drop in the ocean?

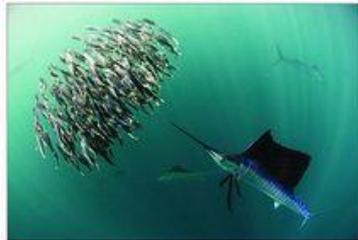
## How many marine species remain undiscovered?

Most species are not known to science<sup>1,2</sup>. This has important consequences for conservation. Recently discovered species have been overwhelmingly identified in biodiversity hotspots<sup>3</sup>, places with areas of extensive habitat loss. As-yet-unknown species are likely to be similarly situated – and similarly threatened with extinction<sup>4</sup>. Determining how many of these species there are is therefore a crucial step in setting international conservation priorities<sup>5</sup>.



### Approach

Recent efforts at estimating the numbers of species remaining have focused on extrapolating existing data over time, in the belief that the numbers of new species per time period will diminish as the group of unknown species shrinks<sup>6,7</sup>. However, these approaches have overlooked the importance of the taxonomists who describe species. As their numbers have increased over the last 250 years, so to have the numbers of species described<sup>8</sup>.



A school of Indo-Pacific parrotfish following bait fish off the coast of Mexico

**Taxonomic effort**  
In fisheries ecology, raw fish catches are scaled by the effort taken to obtain them, producing catch per unit effort (CPUE). Here, using methods developed for terrestrial ecology<sup>9</sup>, we model the rate at which taxonomists catch previously unknown species, to estimate how many marine species remain undiscovered.

**What's in a name?**  
To predict the total number of species in a taxon, we need to first determine how many valid species have already been described. This is surprisingly onerous, as different taxonomists inadvertently give different names to the same species, causing considerable redundancy.

**Data sources**  
To overcome these problems of synonymy, this study will aggregate data from multiple sources, including GBIF and WoRMS, FishBase and AlgaeBase, as well as an original dataset developed by Roberts et al.<sup>10</sup> From these sources, representative genera where synonymy problems have been largely resolved will be selected and modelled.



### Future Directions

The purpose of this study is to estimate how many marine species are presently unknown to science. However, when setting international conservation priorities, we need to understand not just how many missing species there are, but also where they are likely to be found.

By using range data collected for this study, we will additionally model where those missing species may reside. Our results may suggest new conservation priorities in new areas. We may even discover that some of our hotspots are in the wrong place.

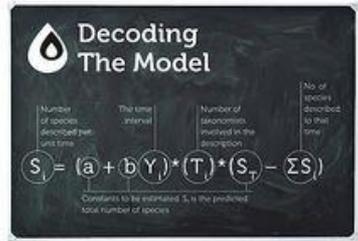


### Expected Results

In line with the results from the terrestrial applications of this model for flowering plants and angiosperms<sup>11</sup>, we would expect to see a marked increase in the numbers of species described over time and a concurrent increase in numbers of taxonomists.

This would fatally undermine any modelling of total species numbers that assumes the rate will slow. Instead, the number of species per taxonomist would increase rapidly initially, before declining as the pool of unknown species begins to dry up.

The models would likely predict that comparatively few marine organisms living in shallow waters close to areas of human habitation remain unknown, whereas significant proportions of their deeper-dwelling or remote counterparts have yet to be discovered.



**Acknowledgements:** The author thanks Louise Bales and Stuart Reynolds for their input, feedback and advice. **Further information:** <http://www.york.ac.uk/inst/steve/steve588/>

1. May, RM. How Many Species Are There on Earth? Science (2002) 298: 949-950.  
2. Wilson, EO. The Diversity of Life. (Princeton: 2002).  
3. Myers, B. Biodiversity Hotspots for Conservation Priorities. Nature 403: 803-806 (2000).  
4. Drake, LA, Roberts, ST, & Brown, CL. How Many Species of Flowering Plants are Missing? Proceedings of the Royal Society B: Biological Sciences (2008).  
5. Drake, LA, & Brown, CL. Describing the Number of Species from the Discovery of New Ones. Biol. J. Linn. Soc. (2007).  
6. Wilson, EO. Conservation: The Enduring Value of Biodiversity. Conservation Biology: Integrating the Natural and Human Sciences. Academic Press (2001) pp. 205-215.  
7. Roberts, ST, & Drake, LA. Describing the Number of Species from the Discovery of New Ones. Biol. J. Linn. Soc. (2007).  
8. Roberts, ST, & Drake, LA. Describing the Number of Species from the Discovery of New Ones. Biol. J. Linn. Soc. (2007).  
9. Pimm, SL, & Drake, LA. Describing the Number of Species from the Discovery of New Ones. Biol. J. Linn. Soc. (2007).  
10. Roberts, ST, & Drake, LA. Describing the Number of Species from the Discovery of New Ones. Biol. J. Linn. Soc. (2007).  
11. Pimm, SL, & Drake, LA. Describing the Number of Species from the Discovery of New Ones. Biol. J. Linn. Soc. (2007).

# Estrutura

## Simplicidade e Equilíbrio

Uso de **gráficos** limitado mas simples e legíveis.

Áreas **vazias** para que a informação “respire”.

Utilização de **ícones** para evitar texto.

# TITLE OF YOUR RESEARCH

First name Last name<sup>1</sup>

<sup>1</sup> Affiliation

## Introduction

Start by providing background context and briefly explain the topic or problem you are addressing. This helps set the stage for your research and provides a foundation for understanding the significance of your work. Explain why your research is important and why it is relevant to the field or discipline. Discuss any gaps or limitations in existing knowledge or previous studies and highlight the potential impact or benefits of your research.

### Aim

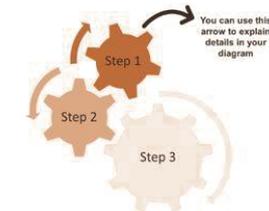
In the aim section of your research poster, succinctly state your research question and objectives, outlining what you intend to investigate or achieve. This section should provide a clear direction for your study, highlighting its purpose and significance in a concise manner.

## Methods

Use this space to describe the methodology section of your research. Briefly discuss the rationale behind your chosen design and how it aligns with your research question or objective. Describe the characteristics of the participants or sample involved in your study.

### Methods subheading

- You might want to use bullet points
- Or maybe use the boxes for images.
- Begin by explaining the overall design of your study.



### Contact information:

E-mail:  
K:

## Results

In the results section of a poster presentation, you should aim to present your core findings in a clear and organized manner.

Make sure you include into your results:

- **Data Presentation:** Use graphs, tables, or figures to present your data visually. Ensure these elements are well-labeled and can stand alone in conveying the results.
- **Key Findings:** Highlight the most important results of your study. This might include significant statistical outcomes, trends, or patterns observed in the data.
- **Brevity and Clarity:** Keep explanations concise. Use bullet points or numbered lists to make the information digestible.
- **Contextualize Results:** Briefly relate your results back to your research question or hypothesis to help viewers connect how the data answers the initial inquiry.
- **No Interpretation:** The results section should be free from analysis or interpretation. Stick to what the data shows, leaving analysis for the discussion or conclusion section.

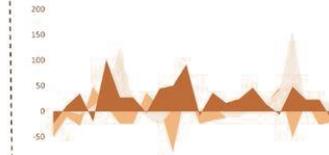


Figure 3: Insert a caption for your figure here.

You can use this space to clarify some more details about your results.

Table 1: Insert a caption for your table here.

	Mild	Moderate	Severe
1	30.35%	28.40%	26.85%
2	17.28%	20.99%	23.15%
3	12.65%	9.57%	9.88%

## Conclusion

The conclusion of a poster presentation should succinctly synthesize the main findings or contributions of your research. It's important to, briefly restate the research question and the answers your work provides, emphasizing the most significant results. And discuss the broader implications of your findings for the field of study or potential practical applications.

### Future Work

- Acknowledge any limitations of the study and suggest areas for future research.
- If applicable, end with a call to action, encouraging viewers to consider the changes recommended by your research or to explore the topic further.

### References

- 1. Smith, J. A., & Lee, B. (2021). Advances in solar panel efficiency: A ten-year review. *Journal of Renewable Energy*, 36(1), 123-135.
- 2. Chen, M., Taylor, S., & Evans, A. (2018). Harnessing wind power: Innovation in turbine technology. *Energy Innovation*, 1(2), 98-110.
- 3. Davis, P. J., & Clark, T. (2020). From data to insights: The importance of technology. *International Journal of Information Management*, 45(1), 100-105.



# Elementos Gráficos

## Boas ilustrações e gráficos são essenciais

Usar gráficos, fotografias ou ilustrações para mostrar a experiência ou o sistema de estudo em ação e para explicar conceitos abstratos.



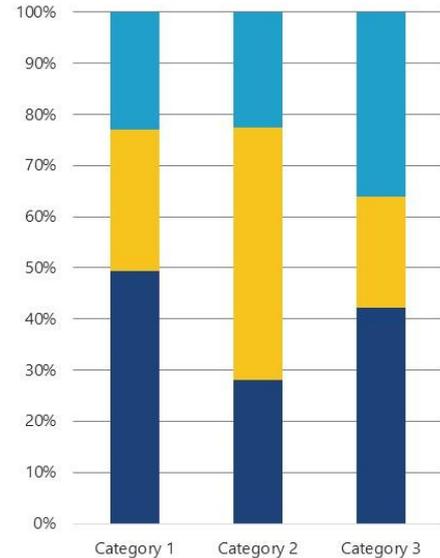
# Elementos Gráficos

## Usar gráficos para mostrar resultados

As tabelas são difíceis de digerir pelo público, mas se tiver de usar, deve ser simplificada.

## Rotular os eixos dos gráficos com as unidades

Identificar os componentes importantes e incluir legendas.



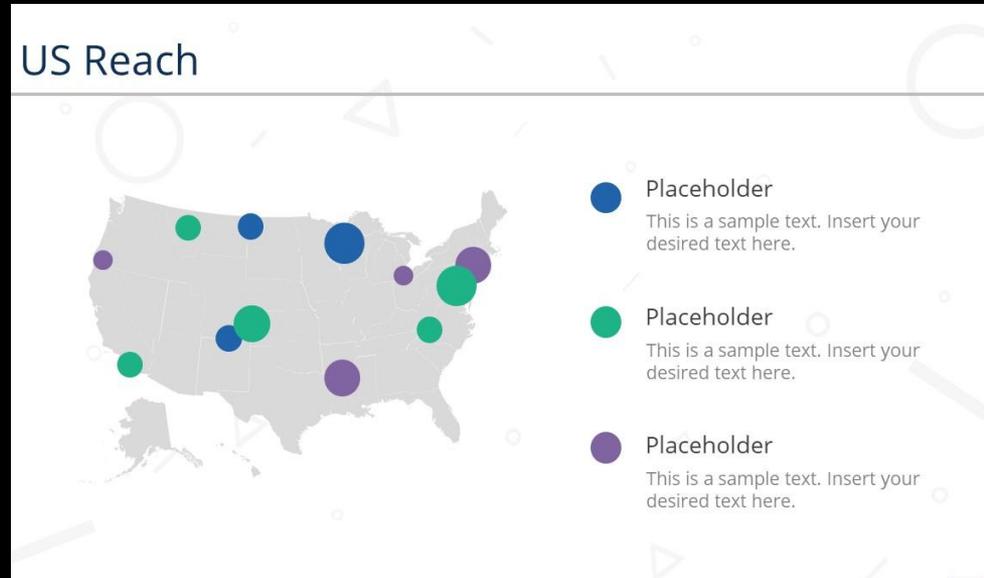
# Elementos Gráficos

## Explicar todos os elementos de um gráfico

Incluindo os eixos, o significado das cores e dos marcadores e os padrões nos dados.

## Simplificar os gráficos

Se necessário, fazer novas versões mais simplificadas e suficientemente grandes para serem vistas ao longe.





# Elementos Gráficos

## Infografia

É uma união entre informação e recursos gráficos para facilitar ao máximo a comunicação.



# Elementos Gráficos

## Infografia

É uma união entre informação e recursos gráficos para facilitar ao máximo a comunicação.

É um recurso muito utilizado em revistas, jornais e livros didáticos.

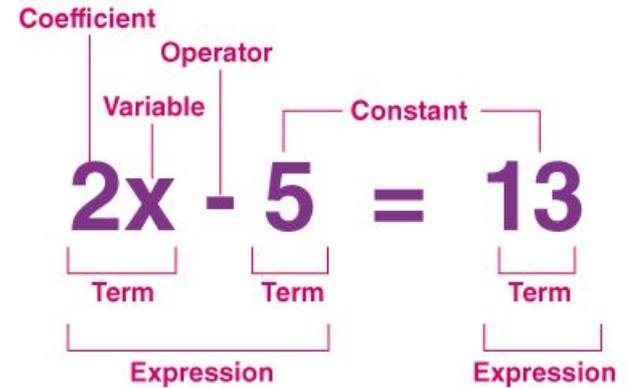


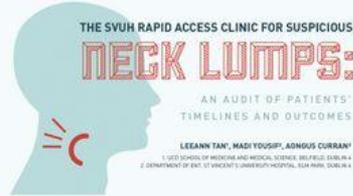
# Elementos Gráficos

## Equações

### Dedicar algum tempo a explicar as equações e as fórmulas

Incluir caixas de texto para explicar as variáveis e os termos matemáticos e colocá-las por baixo de cada termo da equação





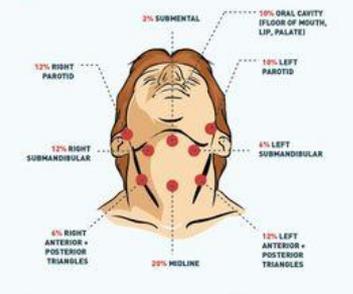
## BACKGROUND & OBJECTIVES

The Rapid Access Clinic for patients with suspicious neck lumps was set up at St Vincent's University Hospital in order and the speedy diagnosis of malignancy in patients with Head & Neck Cancer. This is the first clinic of its kind for Head & Neck Cancer in Ireland. The aim of this audit was to evaluate the clinic's output and analyse new referrals to the clinic in a 6-month period with considerations for patients' timelines and outcomes.

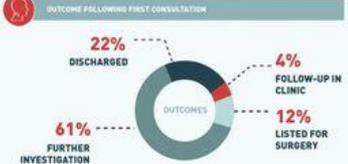
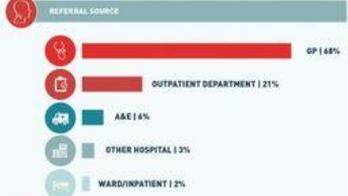
## METHODOLOGY

A retrospective cohort of **new referrals** seen in the Rapid Access Neck Lump Clinic was identified from clinic lists over a period of **6 months** between September 2012 and January 2013. Of the 73 patients identified 10 did not attend the first consultation at the clinic and hence were excluded from the study, giving a final sample of **43 patients**. Audit data was obtained from clinical notes via a **retrospective chart review**. Patients' demographics, referring diagnosis, timelines, and outcomes were recorded and data analysed in Excel® (Microsoft, Redmond, WA, USA).

## RESULTS



\* 14 out of the 43 patients in the study cohort presented with NO LUMPS



## DISCUSSION & CONCLUSION

Waiting times for patients to be seen (average 44 days) and to obtain routine investigations is unacceptable (the NICE guidelines on cancer services "Improving Outcomes in Head and Neck Cancers" recommends that all cancer referrals be seen within 2 weeks). There is evidence in the literature that the "one-stop neck lump assessment clinic" model (in a broadly similar fashion to one-stop triple assessment breast clinics) offers the opportunity to eliminate many of the delays along the diagnostic pathway as seen in this audit, hence the implementation of such a service considering resources permitting. The malignancy pick-up rate of 3%, which is significantly lower than in comparable studies<sup>1,2</sup> may be partially explained by a high number of inappropriate "urgent" referrals, the extent of which will need further investigation and addressing, however more encouragingly this could also allude to the team's clinical acumen in discerning worrying clinical presentations that show up through alternative admission pathways e.g. other routine ENT clinics or A&E referrals.

1. Mawardi H, et al. (2008) Head and Neck Cancer: A Practical Approach. Oxford: Blackwell.  
2. Mawardi H, et al. (2008) Head and Neck Cancer: A Practical Approach. Oxford: Blackwell.  
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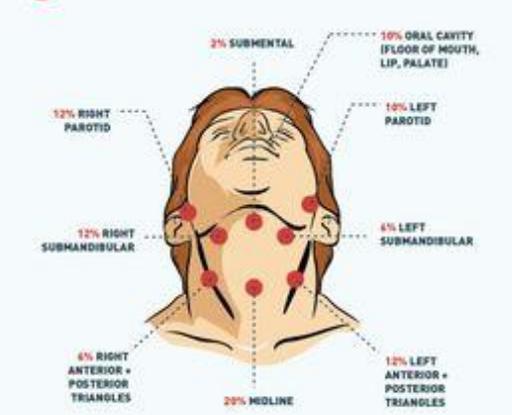
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## RESULTS



## SITE OF LUMP\*



\* 14 out of the 43 patients in the study cohort presented with NO LUMPS



## TIMELINES



## DIAGNOSES (OP 2+ HEAD AND NECK LUMPS)



## DISCUSSION & CONCLUSION

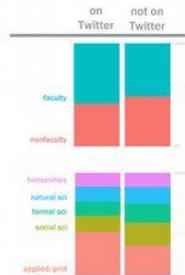
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# prevalence and use of Twitter among scholars

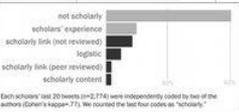


no one rank ( $\chi^2=11.2$ ,  $df=4$ ,  $p=.12$ ) or discipline ( $\chi^2=2.4$ ,  $df=1$ ,  $p=.02$ )<sup>\*</sup> is significantly over-represented on Twitter:

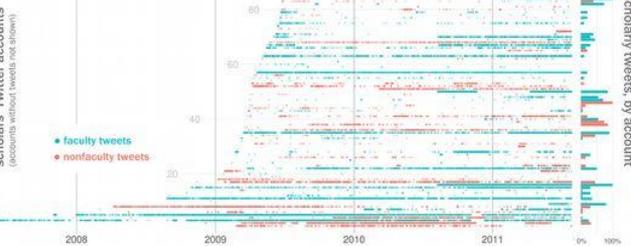


<sup>\*</sup>We use .01 significance level due to the high n and large number of tests.

## scholars tweet about their scholarship



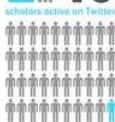
Each scholar's last 20 tweets (n=2,774) were independently coded by two of the authors (Cohen's kappa=.77). We counted the last four codes as "scholarly."



code + details available at <https://github.com/jasonpriem/Sun-Twitter-study>

presented at Metrics 2011 Symposium on Informetric and Scientometric Research

1 in 40 scholars active on Twitter



5 tweets per week

percent of tweets that are scholarly:

nonfaculty: 15%  
faculty: 30%

## method

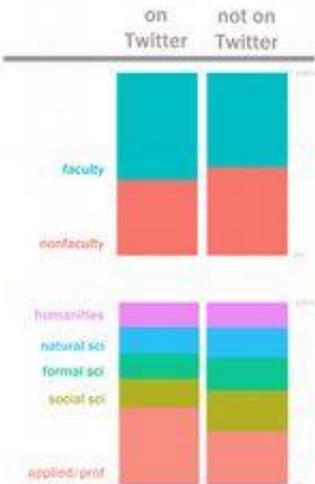
We selected five diverse, representative US and UK universities. Using manual searches of department web pages, we compiled a list of all the scholars (defined as fulltime faculty, postdocs, or doctoral students) at each one, yielding a sample of 8,826.

We then used the Twitter user/search APIs to find Twitter user profiles that matched our scholars' names. 3,019 scholars returned more than 20 potential name matches; this "common-name group" was removed from the sample. The remaining scholars returned 17,177 Twitter accounts; around half of these had no identifying information and were discarded. For the remaining 8,038 accounts, we used a combination of automatic scripts and manual inspection to make positive matches between scholars and accounts, considering evidence from departmental webpages and the Twitter profile fields for name, location, description, URL, vname, and picture.

This gave us a list of 230 scholars with confirmed Twitter accounts; this number is certainly an undercount, since many accounts did not have enough information for a positive ID. We then returned to the Twitter APIs to gather all the public tweets for these users.

## scholarly Twitter use is growing

no one rank ( $\chi^2=11.2$ ,  $df=4$ ,  $p=.12$ ) or discipline ( $\chi^2=2.4$ ,  $df=1$ ,  $p=.02$ )<sup>\*</sup> is significantly over-represented on Twitter:



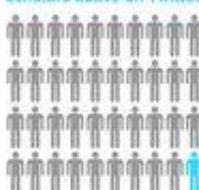
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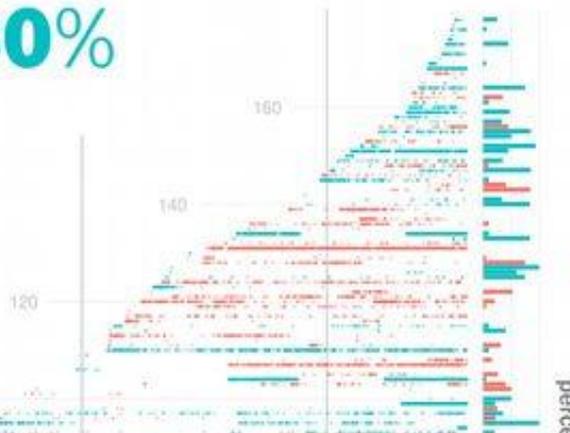
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## scholarly Twitter use is growing



perce

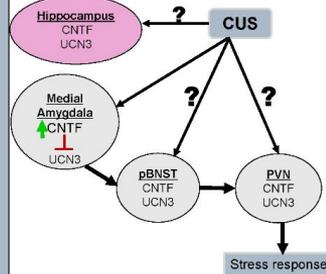
## Introduction

Post-traumatic Stress Disorder (PTSD) is characterized by fear extinction deficit; chronic stress worsens this deficit. Using a Chronic Unpredictable Stress (CUS) model, we previously found that CUS increased fear extinction deficit in female mice and knockout of Ciliary Neurotrophic Factor (CNTF) attenuated it. The amygdala, specifically the medial amygdala, is strongly associated with fear conditioning and extinction. CUS increased CNTF and reduced Urokinase 3 (UCN3) in the medial amygdala, suggesting CNTF-mediated UCN3 inhibition may be involved in CUS-induced deficit of fear extinction. The medial amygdala connects to the hypothalamic paraventricular nucleus (PVN) via posterior bed nucleus of stria terminalis (pBNST) and mediates the stress response (Fig. 1). The objective of this project is to determine whether CUS affects CNTF, UCN3, and CNTF-related cytokine leukemia inhibitory factor (LIF) and interleukin-6 (IL-6) in the pBNST and hypothalamic PVN. Hippocampal CNTF expression was also examined as a brain region outside of the medial amygdala-pBNST-hypothalamic PVN circuitry.

## Methods

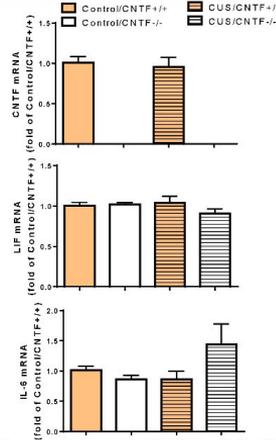
**Animal:** adult female CNTF<sup>+/+</sup> and CNTF<sup>-/-</sup> mice.  
**Experimental design:** 4 groups with 5 mice/group. CNTF<sup>+/+</sup> and CNTF<sup>-/-</sup> mice were treated with 4 weeks of CUS or control handling. At the end, fresh brain were collected. The hypothalamic PVN, pBNST and hippocampus were punched out from 600-700 um cryostat frozen sections.  
**CUS:** CUS was applied for 4 weeks. It includes 7 pairs of environmental and social stressors without food and water deprivation with one pair per day. 1 h on an orbital shaker (100 rpm)+12 h damp bedding on day 1; 30 min immobilization in 50 ml Falcon tube+12h in a tilted cage (45°) on day 2; 1 h exposure to overcrowding by placing four mice in a plastic box (10x10x5cm) with ventilation holes+1 h cage shaking on day 3; 30 min immobilization+12 h tilted cage on day 4; 1 h exposure to overcrowding+12 h damp bedding on day 5; 1 h cage shaking+12 h tilted cage on day 6; and 30 min immobilization+24 h light on (no dark period) on day 7. The control mice will be handled daily for 4 weeks.  
**RNA extraction and RT-qPCR:** RNA was extracted from tissue using QIAGEN Rneasy mini kit.  
**Western blotting:** BCA assay was performed to analyze protein concentration. 10% SDS gel was used to run the protein samples. UCN3 (Santa Cruz, SC-517449), Actin (Cell Signaling, 4970), and HPR-conjugated 2<sup>nd</sup> antibodies (Cell Signaling, 7074, 7076).  
**Statistical analysis:** one-way ANOVA followed by Bonferroni multiple comparison or 2-tailed T test. p<0.05 was defined as significant difference.

## The medial amygdala-pBNST-hypothalamic PVN circuitry



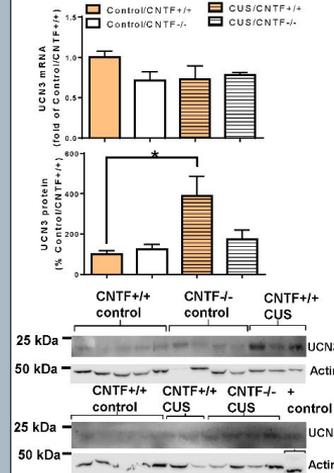
**Figure 1.** The brain circuitry for stress response. This project focuses on CNTF and UCN3 in the pBNST and PVN. Hippocampus served as a negative control.

## pBNST mRNA



**Figure 2.** CUS did not affect CNTF, LIF and IL-6 mRNA expression in the pBNST. N=5, 5, 5, 4 mice/group.

## pBNST UCN3 mRNA and protein



**Figure 3.** CUS increased UCN3 protein expression in the pBNST. N=5, 5, 5, 4 mice. p<0.05

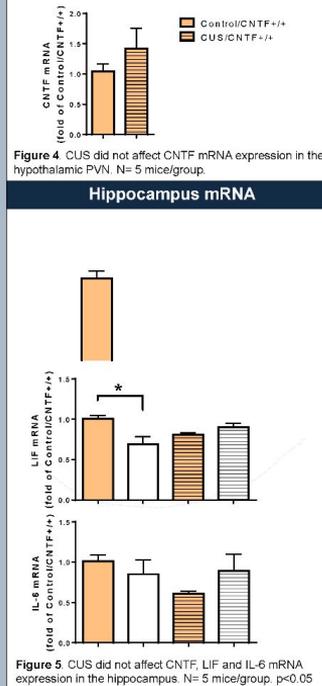
## Conclusion

- In the pBNST, CUS did not affect CNTF and UCN3 mRNA expression. However, UCN3 protein was upregulated by CUS in CNTF<sup>+/+</sup> but not CNTF<sup>-/-</sup> mice, suggesting CNTF inhibits UCN3 expression, possibly through post-transcriptional mechanism.
- CUS did not alter LIF and IL-3 in the pBNST.
- CUS did not alter CNTF mRNA expression in the PVN. Further study will measure UCN3 mRNA and protein in the PVN.
- NO CUS effect on CNTF, LIF and IL-6 mRNA in the hippocampus.

## Acknowledgements

I want to thank Dr. Cuihong Jia for her supervision and support. Special thanks to Chiharu Lovins, Donald Lovins, Shantaya Jones, Dr. Matt Keasey and Dr. Theo Hagg for their guidance and encouragement. Finally, I would like to thank the ETSU Biomedical Science Department for the wonderful opportunity.

## Hypothalamic PVN mRNA



**Figure 4.** CUS did not affect CNTF mRNA expression in the hypothalamic PVN. N= 5 mice/group.

**Figure 5.** CUS did not affect CNTF, LIF and IL-6 mRNA expression in the hippocampus. N= 5 mice/group. p<0.05

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

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## Introduction

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

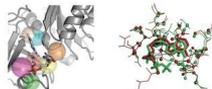


In red, Sex-Hormone Binding Globulin (PDB 1LHU) and in green, Estrogen Nuclear Receptor (PDB 1GK7) both bound to estradiol.

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 propensity can also be harnessed to 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<sup>1</sup>



Binding site atoms  
IsoCleft<sup>2</sup>

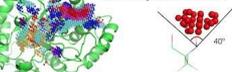


Pseudo-Centers  
+ surface patches  
CavBase<sup>3</sup>



Sequence order independent  
COIPPA<sup>4</sup>

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

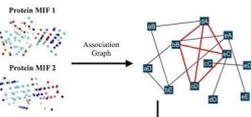


At each grid intersection, 6 probes evaluate the presence of intermolecular interactions using a coarse-grain distance based potential and an atom-probe interaction matrix.

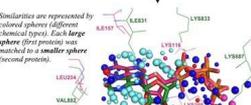
Molecular Interaction Fields  
isoMIF<sup>5</sup>

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.



Similarities are represented by colored spheres (different chemical classes). In a larger sphere (first protein) was matched to a smaller sphere (second protein).

Then & Keresch algorithm then superimposition based on matched probes

Shared H-bond donor and acceptors

## 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<sup>5</sup> across different datasets. This was evaluated with ROC curves across 4 datasets used to benchmark other similar methods.

AUC averaged across 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.

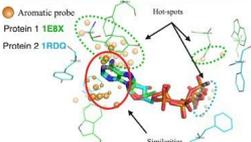
Sequence Identity Threshold	isoMIF				Sequence	No. of entries
	PDBbind	scPDB	PDBbind	scPDB		
100 %	0.93	0.87	0.81	0.68	1415	3809
35 %	0.86	0.82	0.63	0.58	773	3038
25 %	0.84	0.82	0.59	0.56	599	2699
15 %	0.79	0.79	0.51	0.50	414	2292

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.



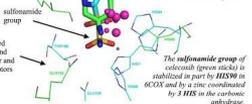
MIF similarities (circled red - opaque spheres) and hot-spots (circled black - semi-transparent spheres) can be identified at scale for multiple targets and guide the design of more selective inhibitors.

### 2. Drug repurposing.

Cyclooxymase-2 (cCOX) bound to celecoxib an approved drug (Celebra)

compared to 400 binding sites

Carbonic anhydrase 1R2J6 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<sup>6</sup>.



The sulfonamide group of celecoxib (green stick) is substituted in part by H2N in cCOX and by a zinc coordinated by 2 H2S in the carbonic anhydrase.

Found by IsoMIF

Tacetoph (Pinar) removed from phase III clinical trials for hypertensive side-effects

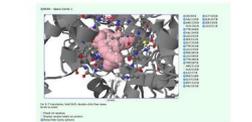


Query PDB 3D8D Cholesteryl ester transfer protein

From 8077 entries in the scPDB dataset, 4 entries within the 20 top hits (z-score between 3.67 and 3.44) were found by IsoMIF and also predicted by Xie et al.<sup>7</sup> as potential off-targets of atorvastatin that could explain hepatotoxic side-effect through R4AS modulation

## Online Interface

IsoMIF Finder is an online interface developed 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 cavity 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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# Inteligência Artificial



... commentary in snack-sized mouthfuls

"I want AI to do my laundry and dishes so that I can do art and writing, not for AI to do my art and writing so that I can do my laundry and dishes."

Author and videogame enthusiast **Joanna Maciejewska** nails it (although bathroom cleaning goes ahead of laundry and dishes)

"I'm sure I deserve a lot of criticism"



Imagem gerada por IA de uma série de stills #aicinema chamada "Vinyl Vengeance" de Julie Wieland (criada usando o Midjourney)



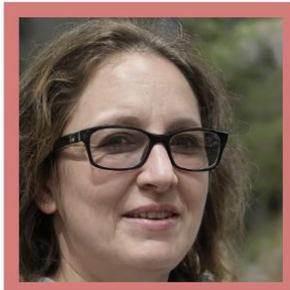
# Test Yourself: Which faces were made by A.I.?

New York Times, by Stuart A. Thompson – Jan. 19, 2024



<https://www.nytimes.com/interactive/2024/01/19/technology/artificial-intelligence-image-generators-faces-quiz.html>

## Top photos identified as “real” in the study



× A.I.

93% got it wrong



× A.I.

92% got it wrong



× A.I.

90% got it wrong



✓ Real

90% got it right



× A.I.

89% got it wrong

## Top photos identified as “A.I.” in the study



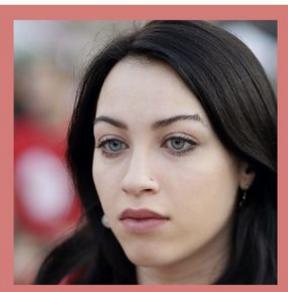
× Real

90% got it wrong



× Real

86% got it wrong



× Real

84% got it wrong



✓ A.I.

82% got it right

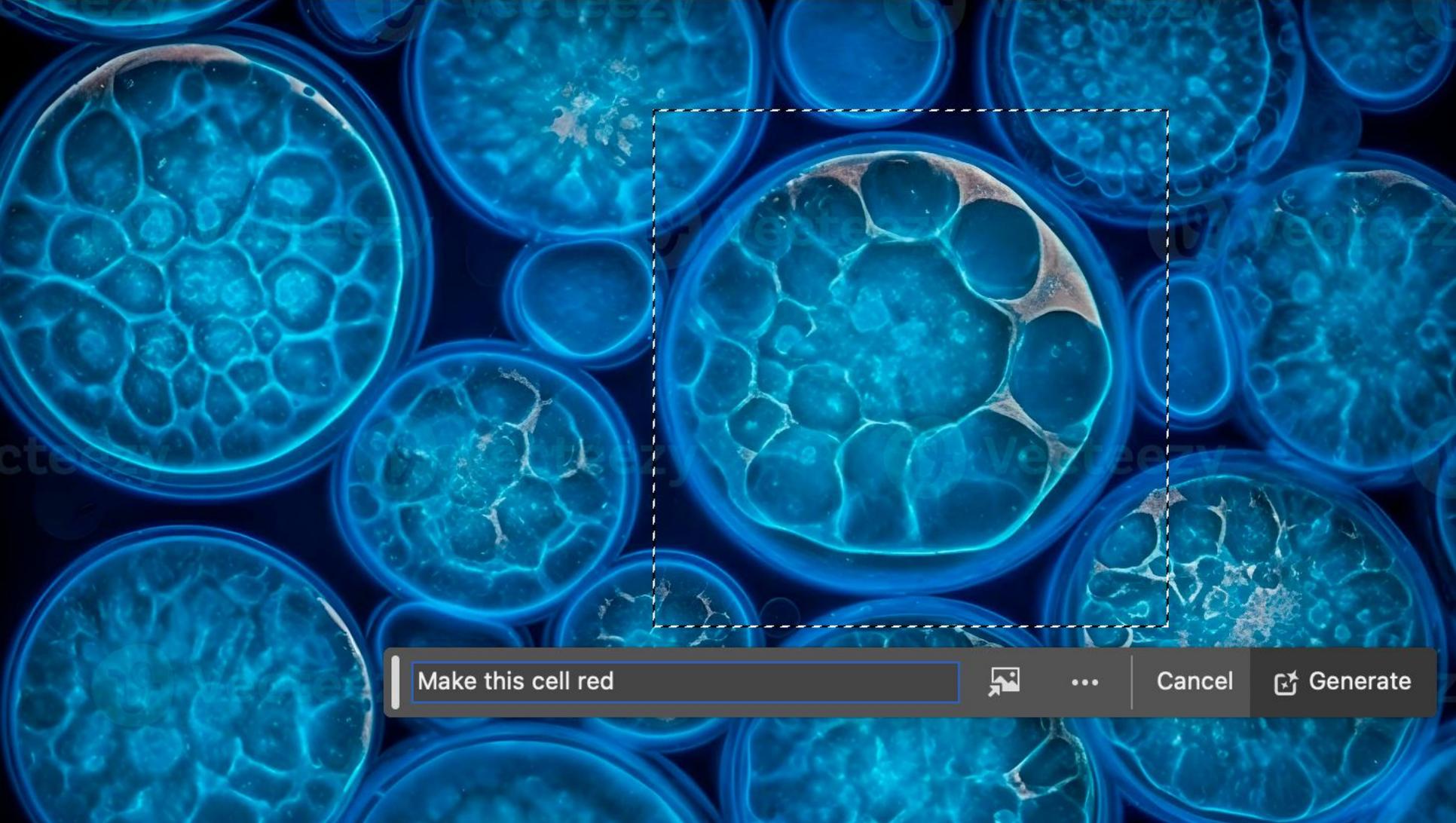


× Real

79% got it wrong



Células ao microscópio. Rede neural gerada por IA através de Pro Photo



Make this cell red



Cancel

Generate



Make this cell red



1/3



Generate





Make this cell red



2/3



Generate





Make this cell red



3/3



Generate



# Concept Design

Aplicação de imagem gerada por IA para apresentação de Concept Design na Arquitetura, aplicando conceitos de sustentabilidade e Ambiente.

Imagem gerada usando Midjourney



# Resumir texto

A IA é uma excelente ferramenta para resumir texto e assim torná-lo mais “apetecível” de ler

teacher, played by Ted Danson's real-life wife, Mary Steenburgen), or the revelation that both Roberto Clemente and Clara “Where’s the Beef” Peller have finally passed the afterlife test, or Gen the Judge’s East Dillon Lions T-shirt, or how Jeff the Doorman gets a little bored of frogs after a while, or the final appearance of Brent Norwalk (overheard asking one of the afterlife testers, “But what if she’d legitimately be prettier if she smiled?”). But it’s time to let go and move on. I’ve enjoyed spending time with you all, talking about this wonderful sitcom. See you in another life, brothers and sisters ... and Janets.

← Article text

Summarize the article above. | ← Text prompt

ChatGPT may produce inaccurate information about people, places, or facts. [ChatGPT May 12 Version](#)

e ChatGPT

ChatGPT can make mistakes. Check important info.

F9

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**Obrigado ■**