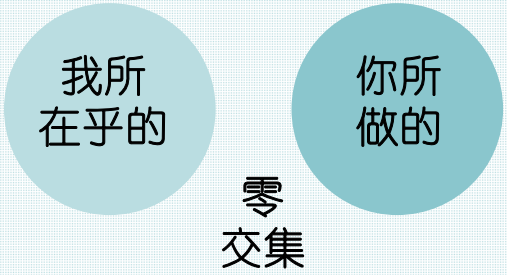
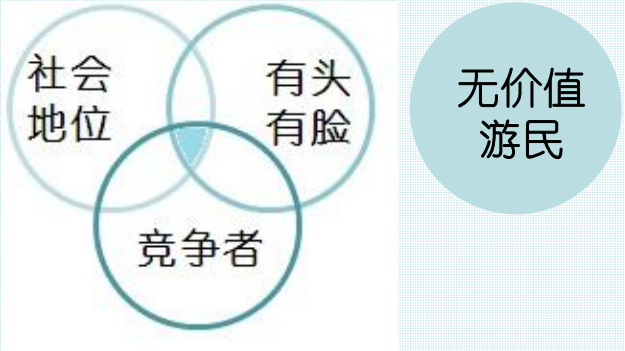
数据可视化

——如何在论文中画出漂亮的插图

四川大学图书馆
制作： 魏丽敏

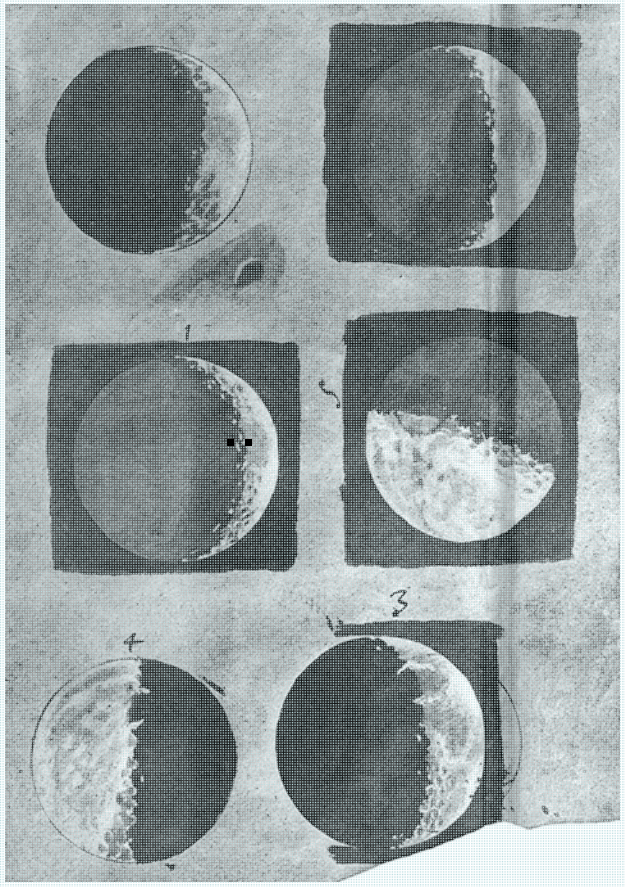


“坦白说，亲爱的，我一点也不在乎。”
——白瑞德，《乱世佳人》，1939



“你根本不能明白，我本可以获得社会地位，我本可以是个竞争者，我本可以是任何有头有脸的人而不是一个毫无价值的游民！”
——特里●马洛伊，《码头风云》，1954

日常生活中的数据可视化



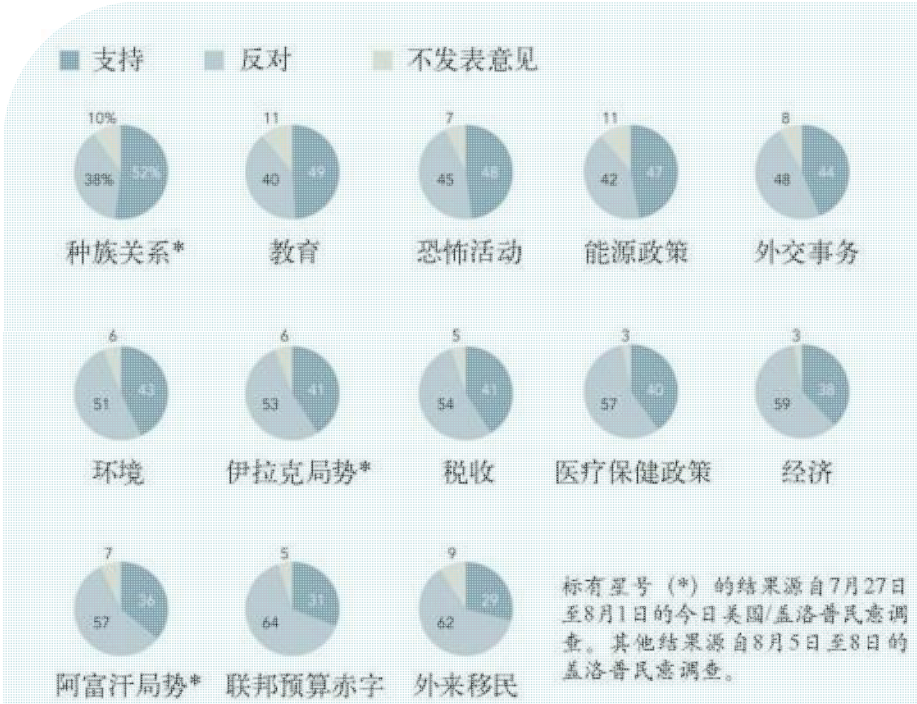
伽利略于1616年关于月亮周期的绘图

月亮周期的摄像图

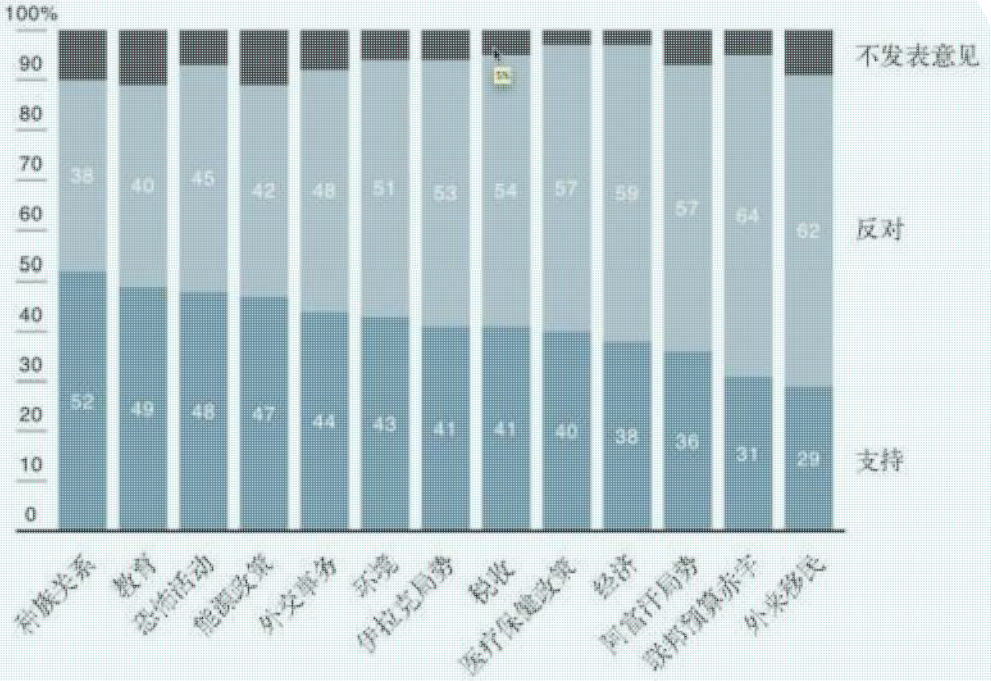
日常生活中的数据可视化

巴拉克•奥巴马的支持率

近期民意调查显示，民众对巴拉克•奥巴马在种族关系问题上的举措持有52%的支持率。这也是以下13个问题中他唯一获得多数支持的举措。在其中8个问题上他都获得了多数反对。



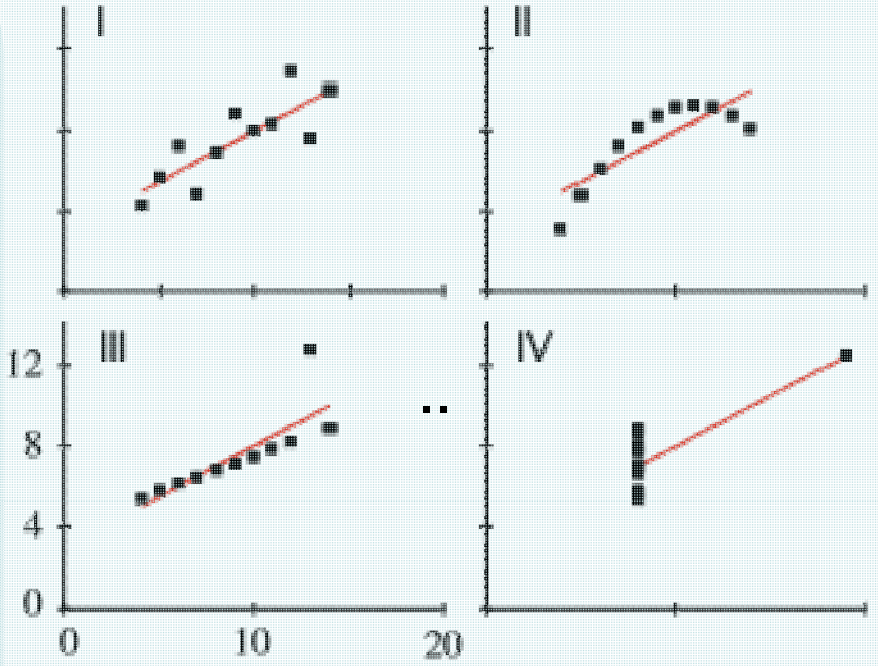
系列饼图



堆叠式柱形图

日常生活中的数据可视化

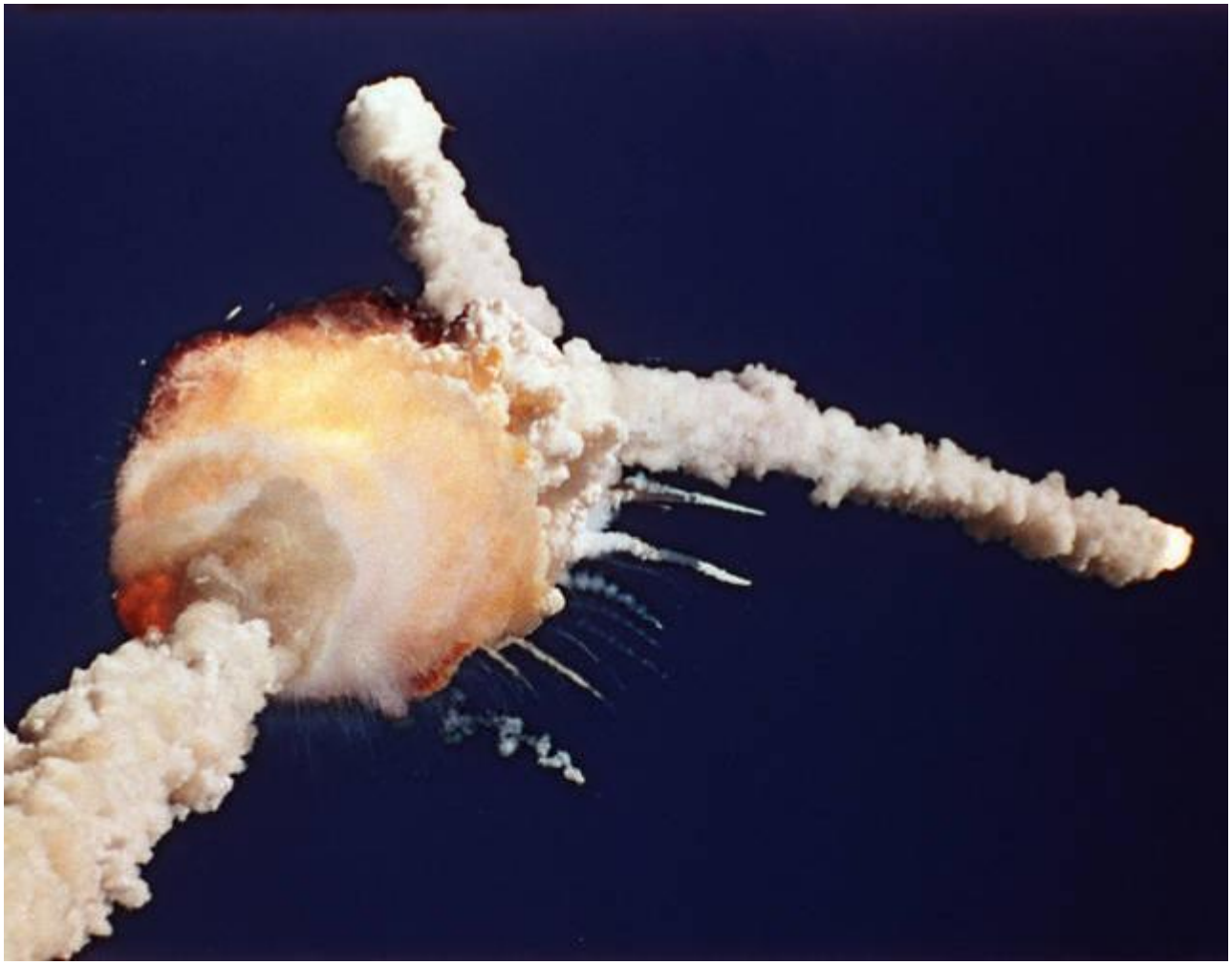
1	2	3	4
10.0, 8.04	10.0,9.14	10.0, 7.46	8.0, 6.58
8.0, 6.95	8.0,8.14	8.0, 6.77	8.0, 5.76
13.0, 7.58	13.0,8.74	13.0,12.74	8.0, 7.71
9.0, 8.81	9.0,8.77	9.0, 7.11	8.0, 8.84
11.0, 8.33	11.0,9.26	11.0, 7.81	8.0, 8.47
14.0, 9.96	14.0,8.10	14.0, 8.84	8.0, 7.04
6.0, 7.24	6.0,6.13	6.0, 6.08	8.0, 5.25
4.0, 4.26	4.0,3.10	4.0, 5.39	19.0,12.50
12.0,10.84	12.0,9.13	12.0, 8.15	8.0, 5.56
7.0, 4.82	7.0,7.26	7.0, 6.42	8.0, 7.91
5.0, 5.68	5.0,4.74	5.0, 5.73	8.0, 6.89



4个数据集的数字表示

4个数据集的图形标识

科学研究中的数据可视化



1986年1月28日美国挑战者号航天飞机升空后

原因

低温（零下7度）

火箭密封胶圈失灵

导致燃料泄漏

支持延期发射的数据表格

HISTORY OF O-RING DAMAGE ON SRM FIELD JOINTS

	SRM No.	Cross Sectional View: Erosion Depth (in.)	Cross Sectional View: Perimeter Affected (deg)	Cross Sectional View: Nominal Dia. (in.)	Top View: Length Of Max Erosion (in.)	Top View: Total Heat Affected Length (in.)	Clocking Location (deg)
61A LH Center Field**	22A	None	None	0.280	None	None	36°--66°
61A LH CENTER FIELD**	22A	NONE	NONE	0.280	NONE	NONE	338°-18°
51C LH Forward Field**	15A	0.010	154.0	0.280	4.25	5.25	163
51C RH Center Field (prim)***	15B	0.038	130.0	0.280	12.50	58.75	354
51C RH Center Field (sec)***	15B	None	45.0	0.280	None	29.50	354
41D RH Forward Field	13B	0.028	110.0	0.280	3.00	None	275
41C LH Aft Field*	11A	None	None	0.280	None	None	--
41B LH Forward Field	10A	0.040	217.0	0.280	3.00	14.50	351
STS-2 RH Aft Field	2B	0.053	116.0	0.280	--	--	90

*Hot gas path detected in putty. Indication of heat on O-ring, but no damage.
**Soot behind primary O-ring.
***Soot behind primary O-ring, heat affected secondary O-ring.

Clocking location of leak check port - 0 deg.

OTHER SRM-15 FIELD JOINTS HAD NO BLOWHOLES IN PUTTY AND NO SOOT NEAR OR BEYOND THE PRIMARY O-RING.

SRM-22 FORWARD FIELD JOINT HAD PUTTY PATH TO PRIMARY O-RING, BUT AND NO SOOT BLOWBY. OTHER SRM-22 FIELD JOINTS HAD NO BLOWHOLES IN PUTTY.

1. 没有提供任何温度数据
2. 没有对损坏程度定量
3. 没有评估温度与胶圈损坏的关系

BLOW BY HISTORY

SRM-15 WORST BLOW-BY
- 2 CASE JOINTS (80°), (110°) ARC
- MUCH WORSE VISUALLY THAN SRM-22

SRM 22 BLOW-BY
- 2 CASE JOINTS (30-40°)

SRM-13A, 15, 16A, 18, 23A 24A
- NOZZLE BLOW-BY

HISTORY OF O-RING TEMPERATURES (DEGREES-F)

MOTOR	MBT	AMB	O-RING	WIND
DM-1	68	36	47	10 MPH
DM-2	76	45	52	10 MPH
QM-3	72.5	40	48	10 MPH
QM-4	76	48	51	10 MPH
SRM-15	52	64	53	10 MPH
SRM-22	77	78	75	10 MPH

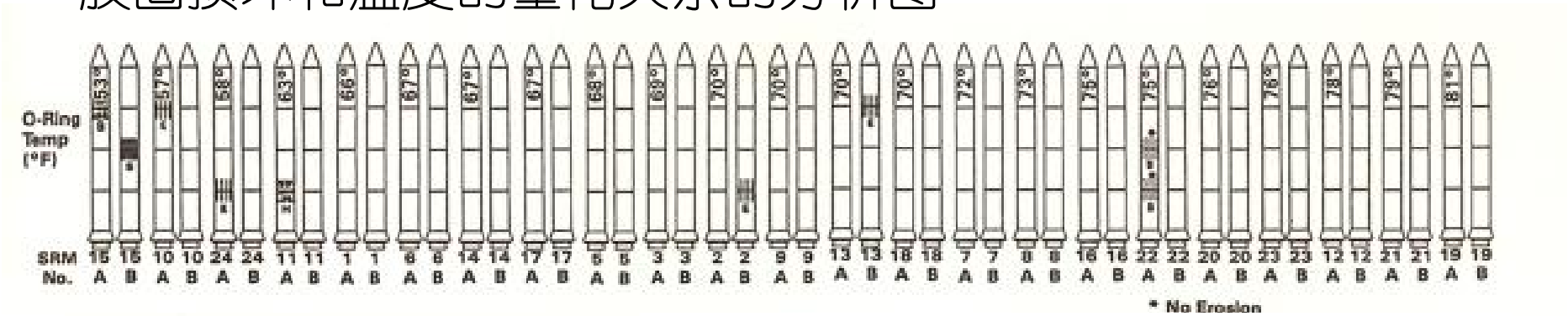
1. 只列出2次胶圈损坏（没有定量）时的温度数据
2. 遗漏了其余22次发射的数据（其中7次有损坏，17次没有）

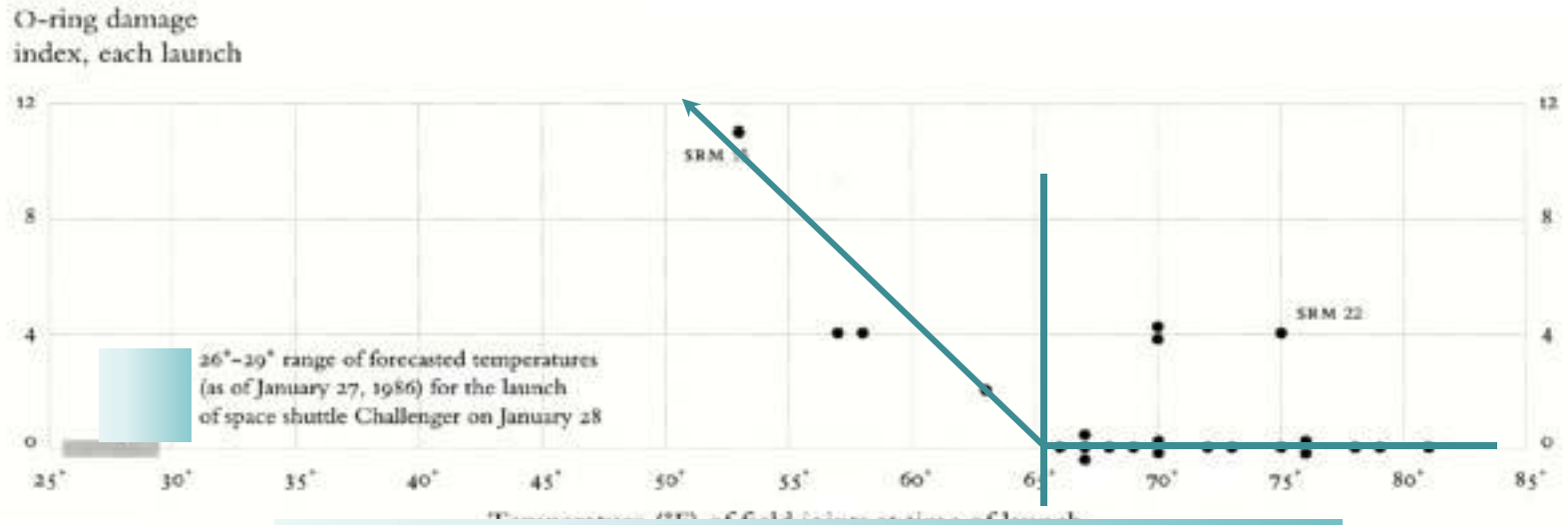
由Morton Thiokol传真到 NASA的13页纸中的2页

胶圈损坏和温度的量化关系的分析表

Flight	Date	Temperature °F	Erosion incidents	Blow-by incidents	Damage index	Comments
51-C	01.24.85	53°	3	2	11	Most erosion any flight; blow-by; back-up rings heated.
41-B	02.03.84	57°	1		4	Deep, extensive erosion.
61-C	01.12.86	58°	1		4	O-ring erosion on launch two weeks before Challenger.
41-C	04.06.84	63°	1		2	O-rings showed signs of heating, but no damage.
1	04.12.81	66°			0	Coolest (66°) launch without O-ring problems.
6	04.04.83	67°			0	
51-A	11.08.84	67°			0	
51-D	04.12.85	67°			0	
5	11.11.82	68°			0	
3	03.22.82	69°			0	
2	11.12.81	70°	1		4	Extent of erosion not fully known.
9	11.28.83	70°			0	
41-D	08.30.84	70°	1		4	
51-G	06.17.85	70°			0	
7	06.18.83	72°			0	
8	08.30.83	73°			0	
51-B	04.29.85	75°			0	
61-A	10.30.85	75°		2	4	No erosion. Soot found behind two primary O-rings.
51-I	08.27.85	76°			0	
61-B	11.26.85	76°			0	
41-G	10.05.84	78°			0	
51-J	10.03.85	79°			0	
4	06.27.82	80°			?	O-ring condition unknown; rocket casing lost at sea.
51-F	07.29.85	81°			0	

胶圈损坏和温度的量化关系的分析图





失事的教训：

1. 没有正确估价以前发射中胶圈损坏的原因
2. 没能说明低温与胶圈损坏的因果关系
3. 没有有效地提出证据，图表缺乏说服力

Tufte教授绘制的演示低温如何摧毁O形密封圈

什么是可视化

通过电脑对数据进行交互的可视表达以增强认知

是一个生成图形图像的过程

- 形成某个物体的感知图像
- 强化认知理解

目的是洞悉而非图像

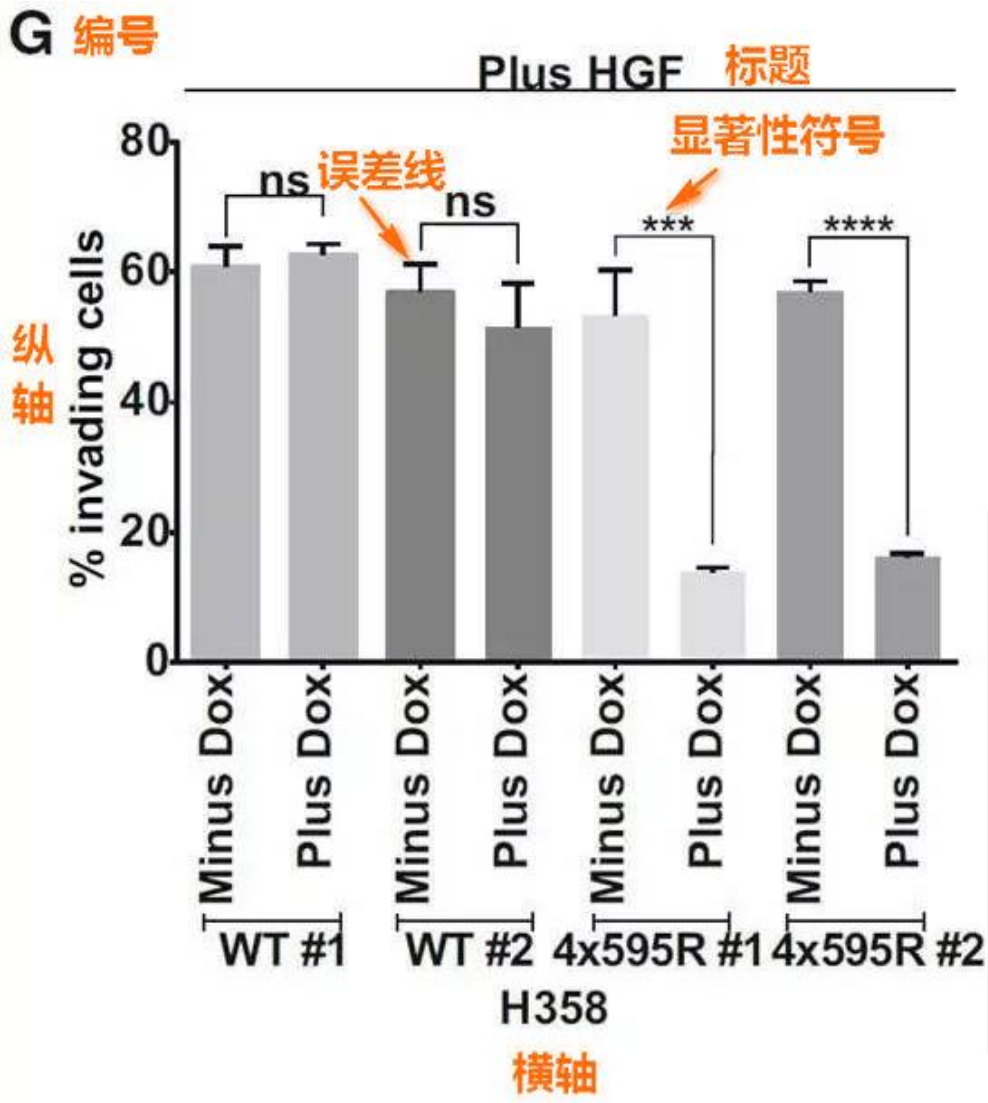
- 发现，决策，解释，分析，探索，学习

图表帮助你

分析数据的本质和内在规律

巧妙地展示有意义的数据
防止对数据的曲解
鼓励读者比较不同的数据
吸引读者注意数据的实质
与数据统计和文字描述有机地整合

1. 统计图



编号：用A、B、C、D编号及相应图注

标题：明白图片内容。

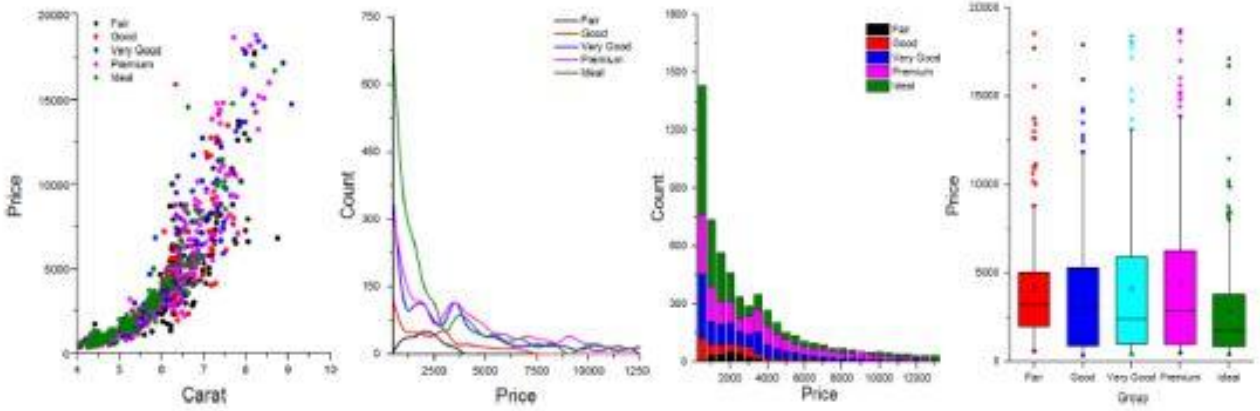
纵轴：多是数值，注明单位。

横轴：分组写清组名，数字注明单位。

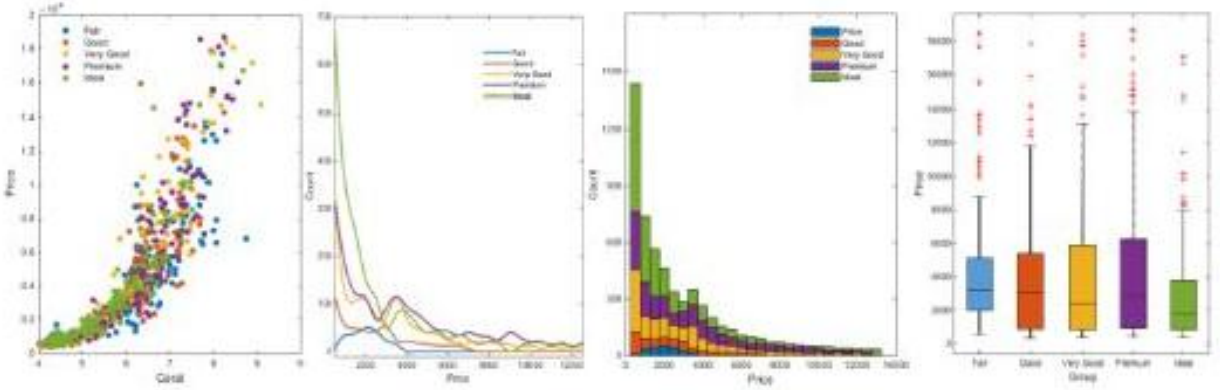
误差线：标准差或标准误。

显著性符号：用*/**/***代表

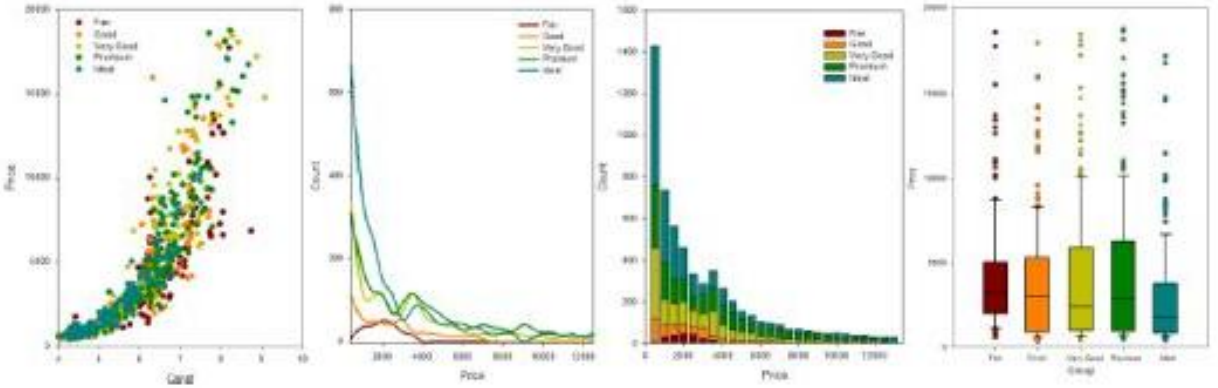
Origin



Matlab

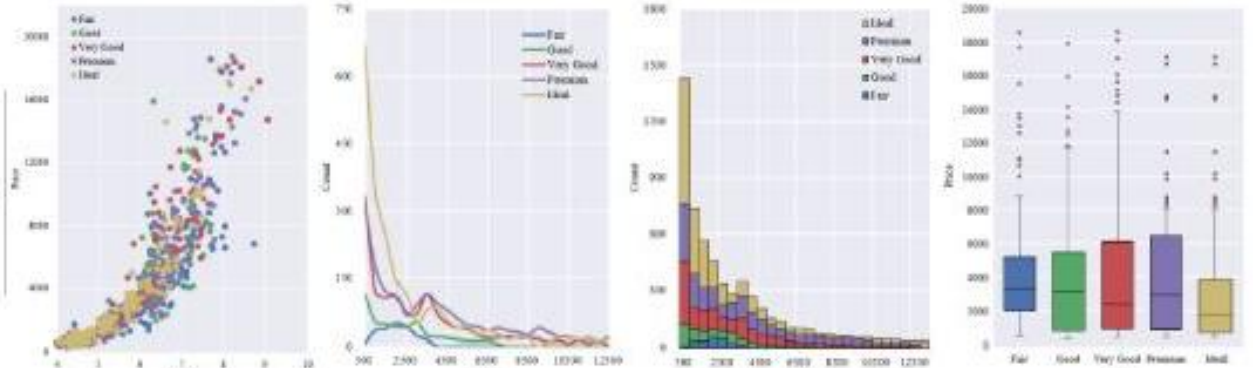


Sigmaplot



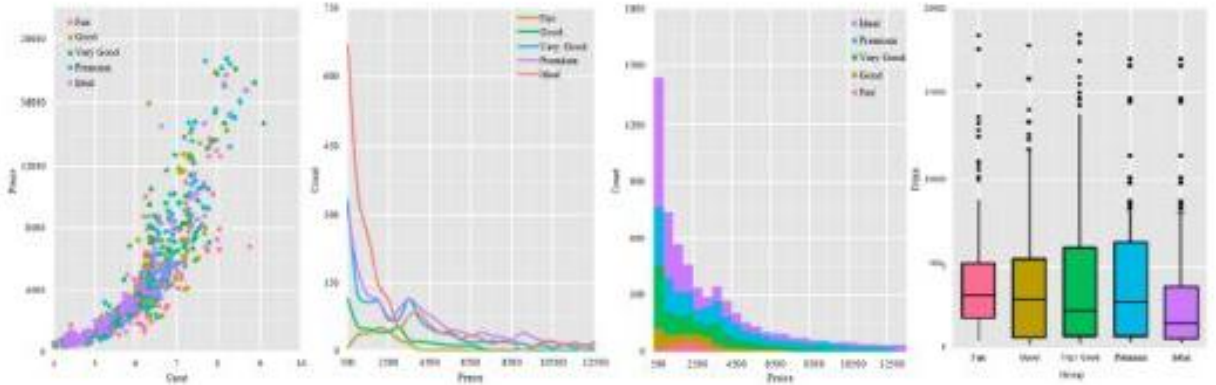
Python

Matplotlib, Seaborn
ggplot, Plotly,
geoplotlib

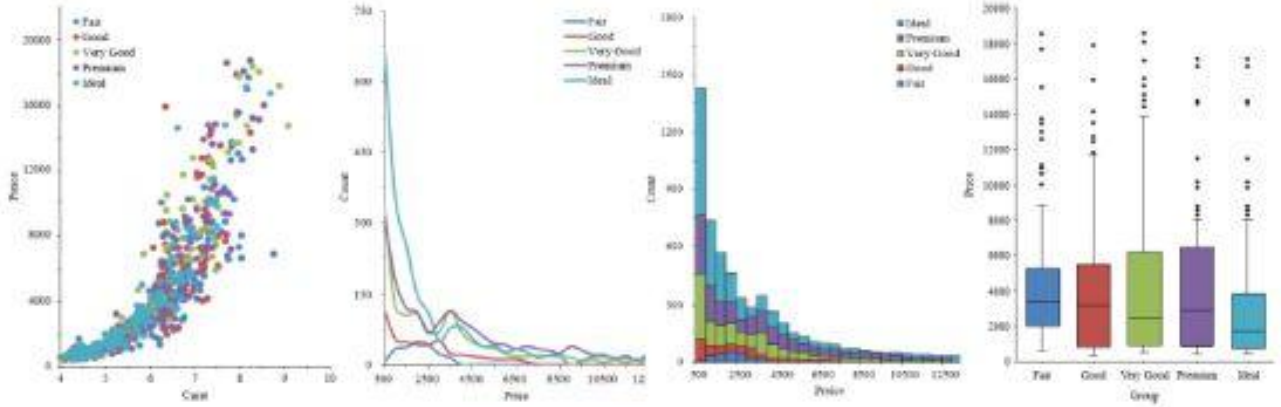


R

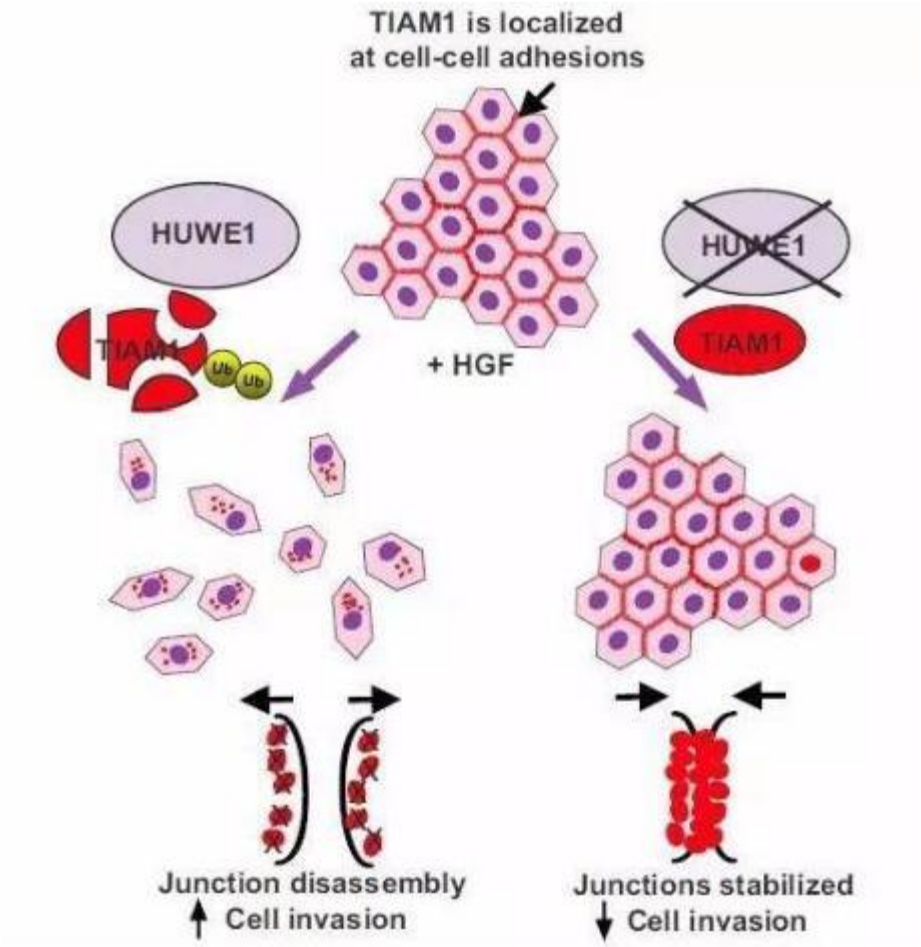
ggplot2, lattice, Plotly



Excel

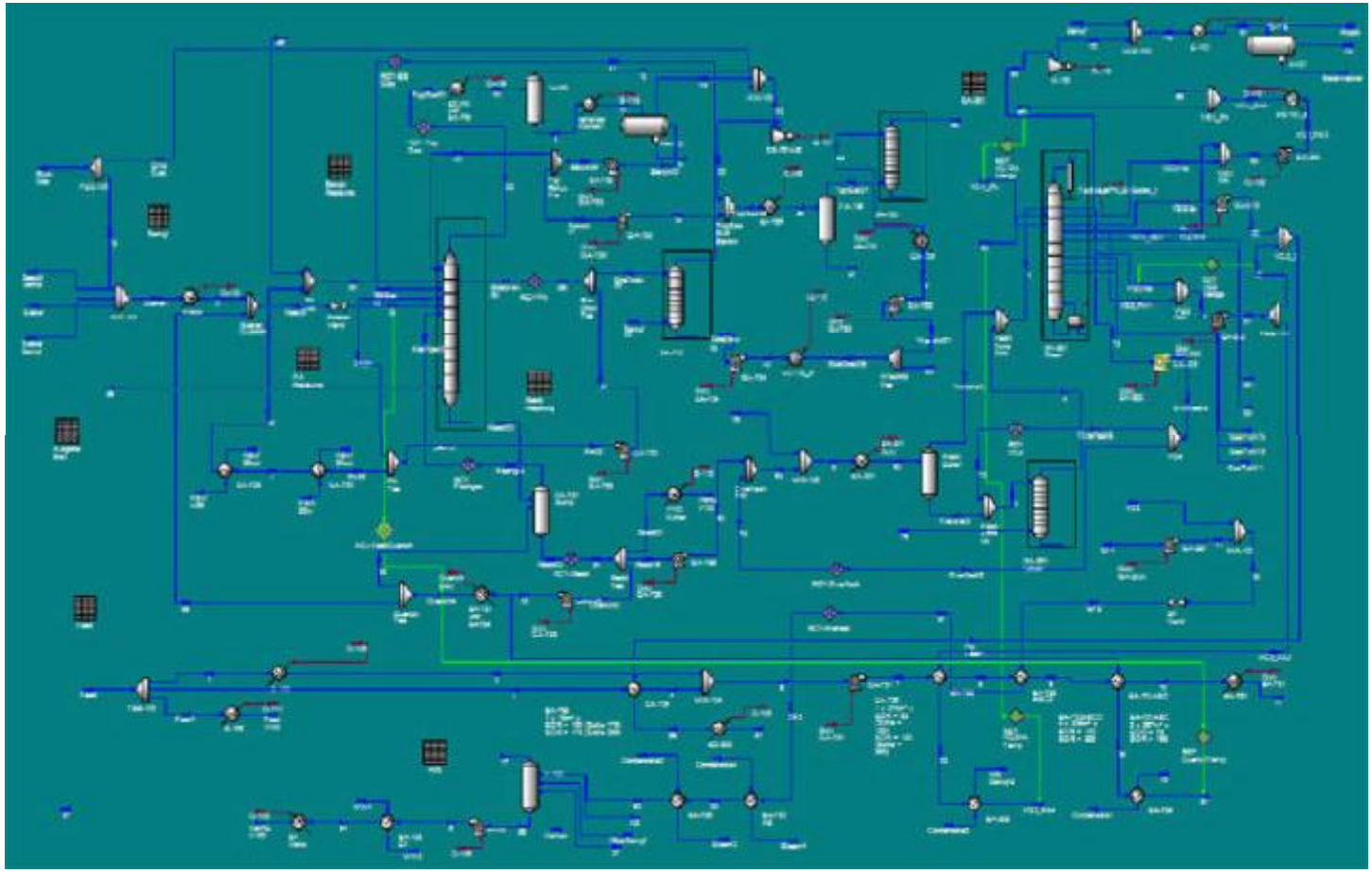


2. 示意图

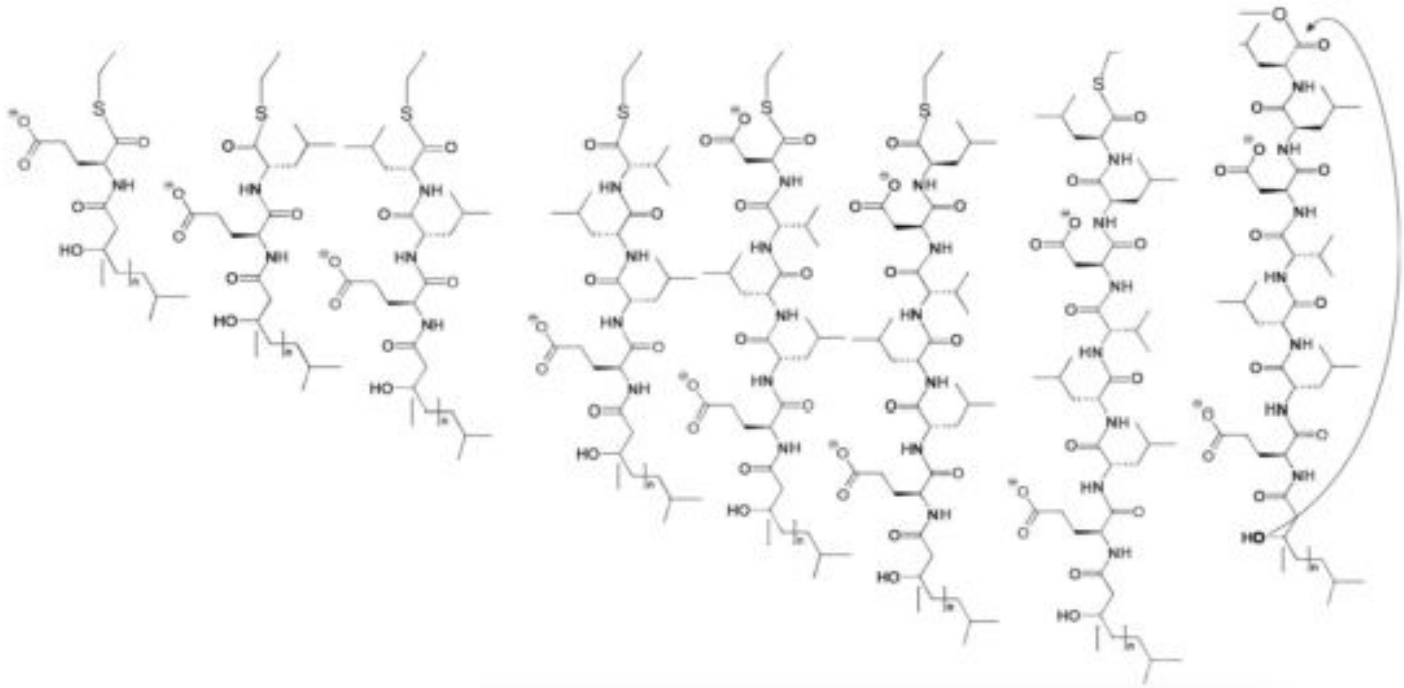


细胞作用示意图

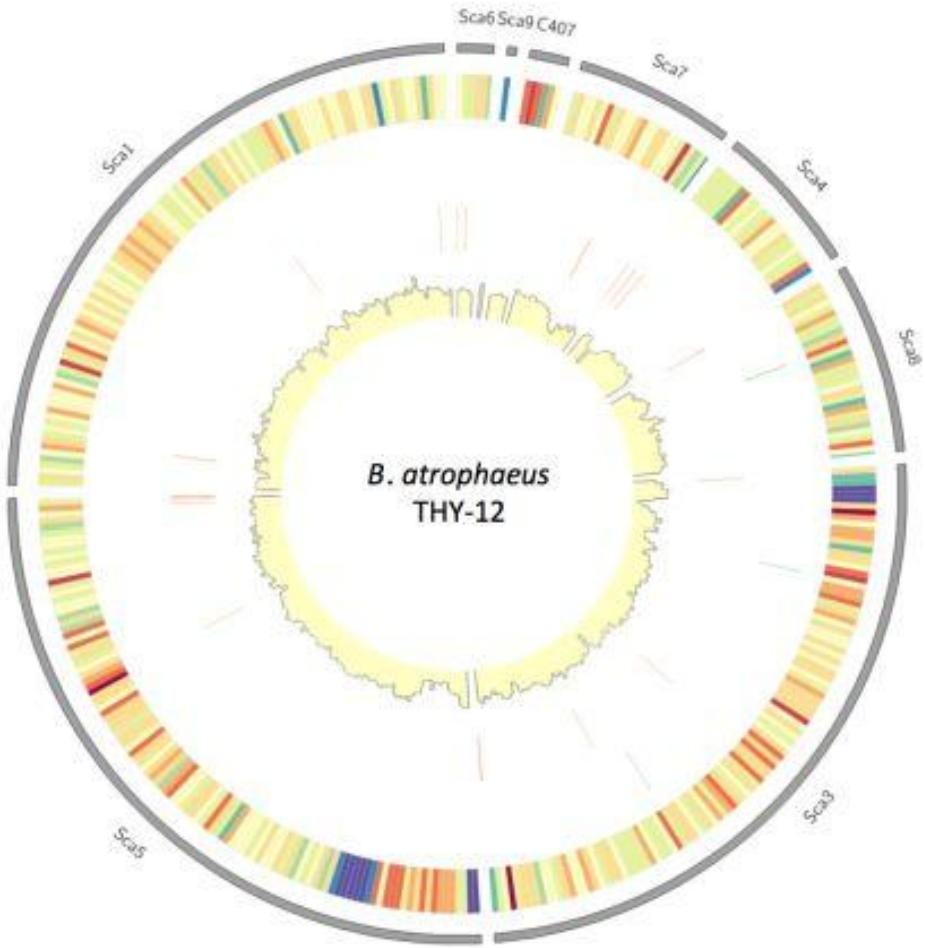
简单的PPT
精致的PS+AI



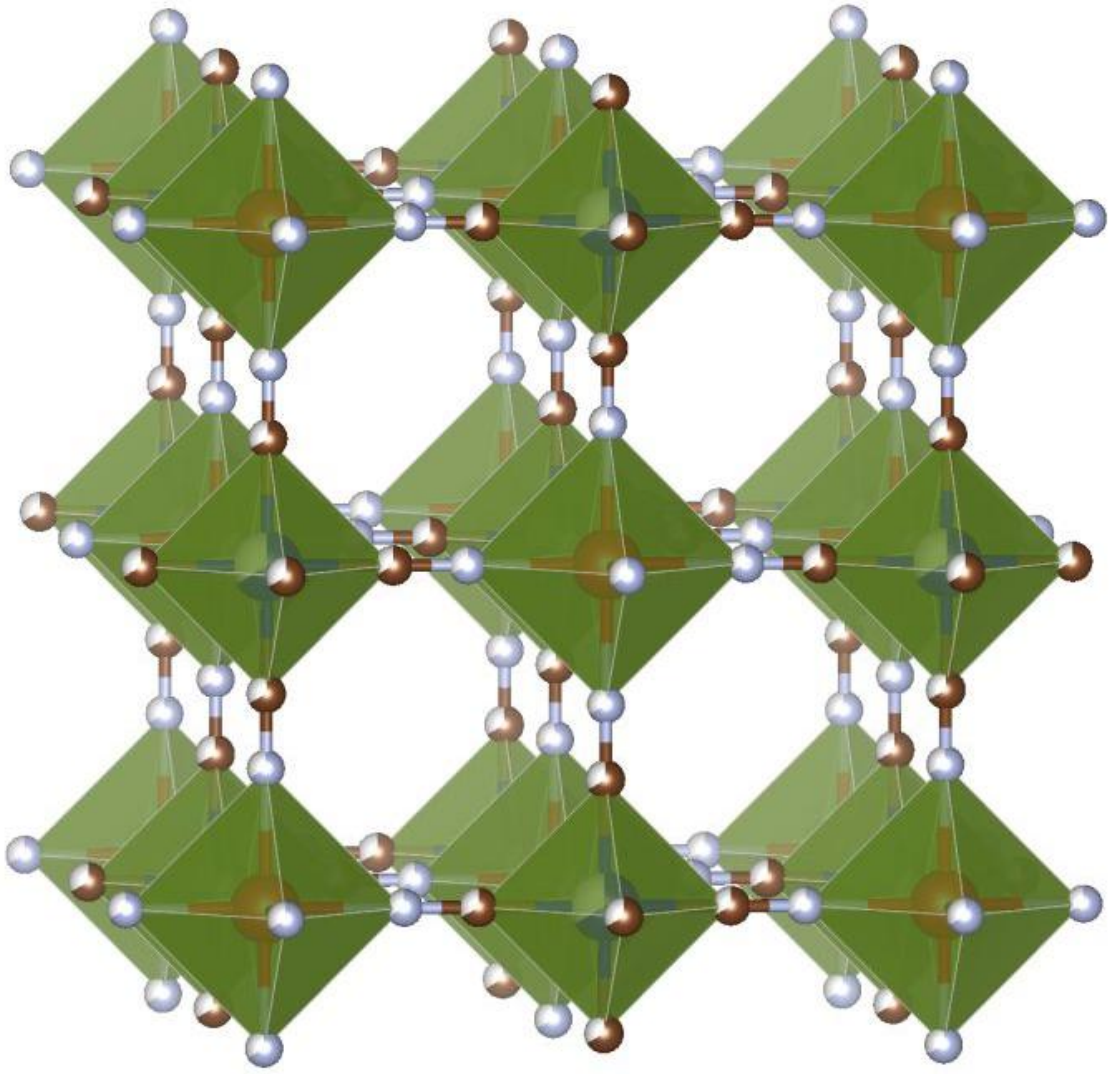
Aspen Plus 流程图



ChemDraw化学式绘图软件

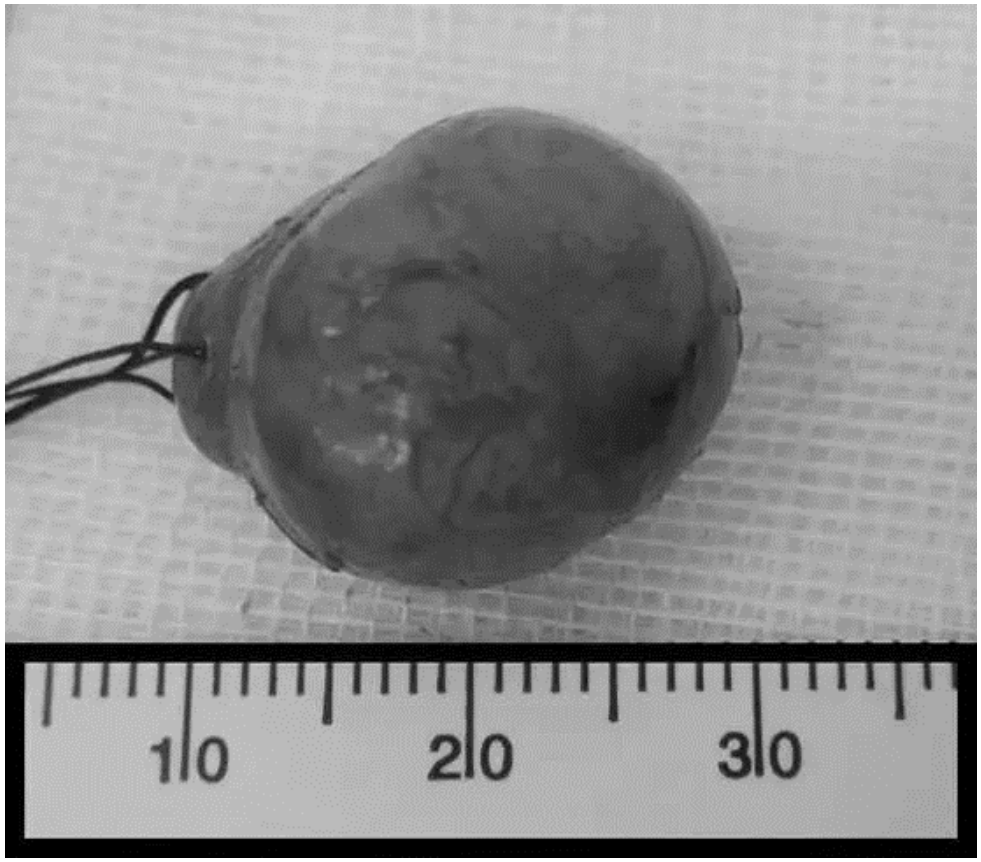


Circos圈状信息图



Vesta晶体结构绘图软件

3. 照片图



亮度、对比度、比例尺

科学论文图表的制作原则

① **规范：** 符合期刊要求，如单位、字体、坐标、图例、标题。

② **简洁：** 科学论文图表尽量简单简洁，清楚地表达数据信息。

③ **美观：** 图表要简单且具有美感，关注配色、构图和比例。

④ **专业：** 图表类型的选择，能全面地反应数据的相关信息。

插图整体要求

论文插图制作流程及注意事项

照片的拼接

条带图片的拼接

表格的拼接

综合案例

Nature 杂志对图片要求

For publication, we prefer to use **TIFF** and **EPS** files in PC format, preferably from Photoshop or Illustrator software. We can also accept Freehand 8, Canvas and CorelDraw (version 8 and above), but these files must be converted to postscript (EPS) format. For any figures submitted in Photoshop or TIFF format we require layered files to be sent whereby all text, arrows or additional attributes are placed on individual layers within the file. We can also accept Adobe PDF (output to print or press settings), native PowerPoint, Word and Excel* files, provided that each figure element is editable (in these programs the elements should be 'ungrouped'). Please note however that these software packages only allow RGB colour file creation (not suitable for print production), and colour conversions from RGB to CMYK may have unpredictable results.

Ensure all placed or linked pictures are correctly embedded into your final figure files.

For **photographic type images**, Adobe Photoshop 6 is the minimum preferred form layers, please save your image in the native Photoshop format (**PSD**). If not, please also accept **JPEG** and **EPS**. The minimum acceptable resolution is 300 DPI.

File size and specifications

File sizes must be as small as possible, so that they can be downloaded quickly. The number of files should be limited to eight, and the total file size should not exceed 8MB. Individual files should not exceed 1MB. Please seek advice from the editorial office before sending files larger than our maximum size to avoid delays in publication.

Images should not exceed **640 x 480 pixels** (9 x 6.8 inches at 72 pixels per inch) but we would recommend **480 x 360 pixels** as the maximum frame size for movies. We would also recommend a frame rate of **15 frames per second**. All supplementary information must have its own legend and must be referred to in the manuscript.

For **line art/charts/graphs** we prefer to work with Adobe Illus also accept Freehand 8, PDF, PostScript (up to Level 3), ChemI sheet) and TeX/LaTeX.

Avoid outputting JPEGs from SPSS/PASW Statistics (any versio DPI. Other **unacceptable** formats include: CorelDraw (prior to

Colour images

For printing purposes, all RGB colours need to be converted to should be aware that this can make colours less vibrant and s

Tables

Please submit tables in (editable) Word or Excel* format at th setting Table rows in picture format and then saving the docu

*Please ensure any MS Office 2007 files are set to 'compatibil

Science 杂志对图片要求

To expedite publication of your paper, please follow these style guidelines in preparing your figures for your revised manuscript. Note that some of these instructions (with respect to format and resolution) differ from the instructions for figures with initial manuscript submission. You can download a copy of these files in Word or PDF format for printing using the links to the right.

[Important note: We cannot accept figures in prepared in Microsoft PowerPoint or Word format at the revision stage! Please adhere to the formatting guidelines in this document.]

Resolution. For manuscripts in the revision stage, adequate figure resolution is essential to a high-quality print and online rendering of your paper. Raster line art should carry an absolute minimum resolution of 600 dots per inch (dpi) and, preferably, should have a resolution of 1200 dpi. Grayscale and color artwork should have a minimum resolution of 400 dpi, and a higher resolution if possible.

Please note that these resolutions apply to figures sized at dimensions comparable to those of figures in the print journal. Reducing or enlarging the dimensions of a digital raster image will also change its resolution. For example, reducing the dimensions of an image by 50%, with no change in file size, will double its dpi resolution; doubling the dimensions of the image will cut resolution by 50%. Authors are encouraged to review past issues to gauge the approximate size their figures will take in the print publication, and set the resolution of their figures accordingly.

Cell 杂志对图片要求

Cell Press Figure Guidelines

On this page we provide tools and guidelines for creating high-quality figure files that are optimized for submission via EES and production in the journal. Please review these guidelines and make sure that your figures meet our requirements. To optimize your figure files for production, we provide a link to an Adobe Acrobat Job Options file (see below) that you can use to create production-quality PDF files from many file types.

- We prefer TIFF, PDF, EPS, or JPEG formats for electronic artwork.
- Our maximum file size is 20 MB per file.
- Don't send figure panels as individual files.
- Each figure should be able to fit on a single 8.5 x 11 inch page.
- For color figures, the resolution should be 300 dpi.
- For black and white figures, the resolution should be 500 dpi.
- For line-art figures, the resolution should be 1000 dpi.

FILES SIZES FOR ARTICLES UNDER REVIEW

For newly submitted articles or revisions still under review, please try to keep your figure files as small as possible (1-2 MB) so that editors and reviewers can more easily work with the files. If your article is accepted for publication, we will ask for higher quality production figure files.

插图整体要求

图片尺寸要符合规范	
只接受指定格式的图片	tiff
插图上元素要求对位整齐	
图片清晰度要求符合印刷要求	400dpi、500dpi
插图中相同类型的文字大小应统一	7-12号字
文字字体符合要求并保持一致	Arial 、TNR
线条粗细应统一	坐标轴0.1mm-0.4mm

插图尺寸

- 期刊多为左右两栏

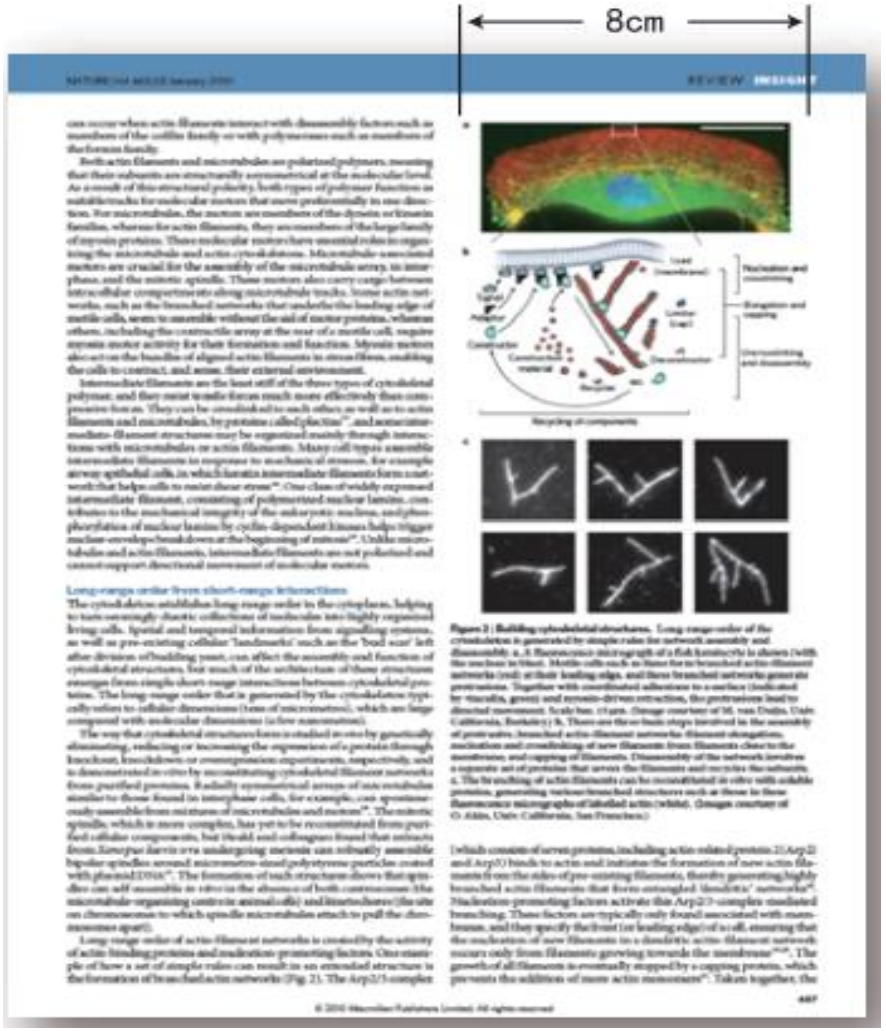
  插图排版：

  ① 半版图

  ② 2/3版图

  ③ 整版图

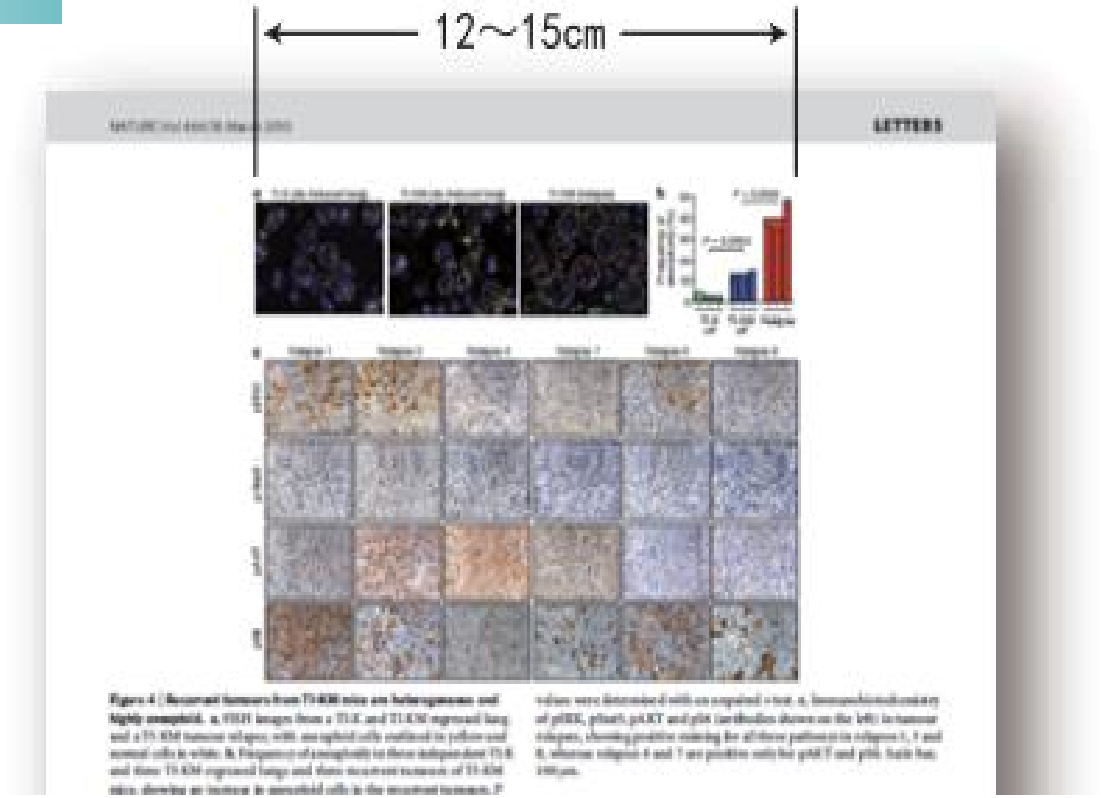
半版图



建议半版图尺寸为8cm

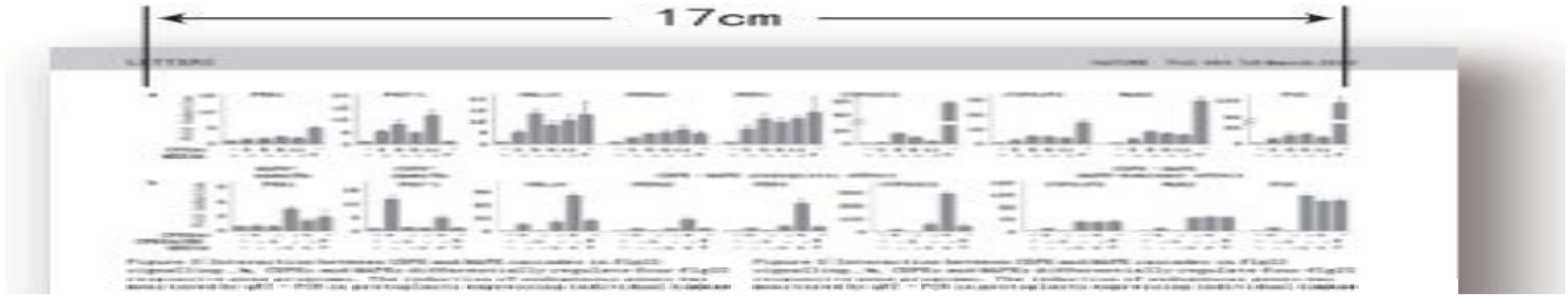
即使是单张图片也最好是8cm的半版图

2/3版图



几个部分算作一张figure
总宽度12-15cm　高度<20cm
缝隙0.5mm-0.8mm
小图片用a、b、c、d等标注（或A，B，C,D ）

整版图



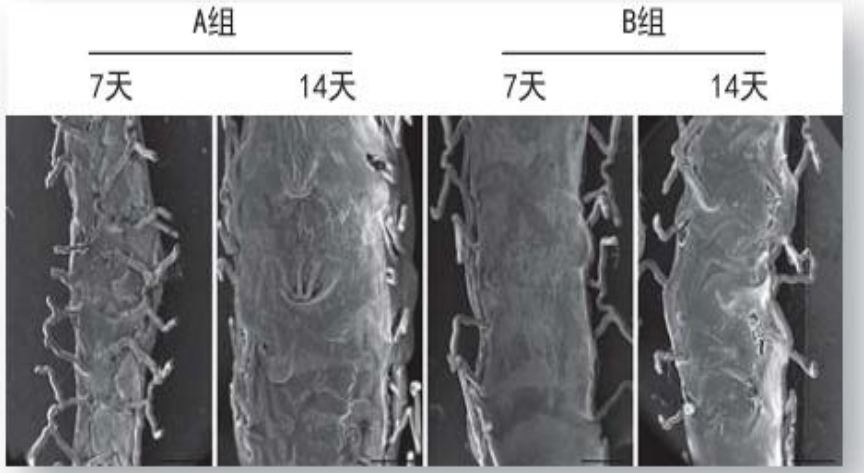
几个部分算作一张figure
总宽度17cm　高度＜20cm
缝隙0.5mm-0.8mm
小图片用a、b、c、d等标注（或A，B，C,D ）
如果文字7pt字号无法排满建议用2/3版图

Photoshop 和Illustrator结合

- PS：裁切、校色、上色、测量、修补、抠图
  格式：psd、jpeg、tiff、png等位图格式

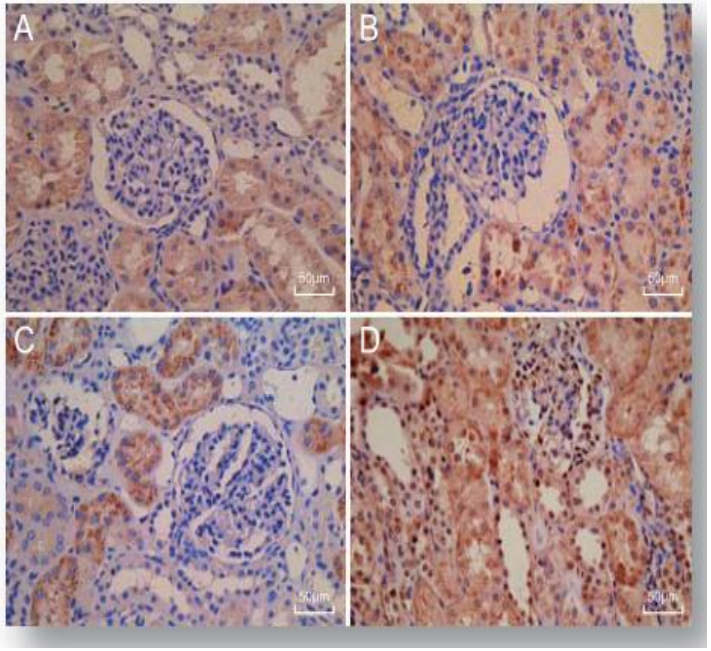
- AI：拼排、写字、画线、标注、绘图
  格式：AI、pdf、eps、emf等矢量格式
  作图结束最后可导出成tiff格式供稿
  不要用AI打开psd，tiff，JPEG、png等位图格式

灰度图



黑白照片，如电镜照片，电泳条带等
Tiff格式，分辨率300dpi，采用LZW无损压缩
Eps格式，辨率300dpi，文字等保持矢量特性

彩色图



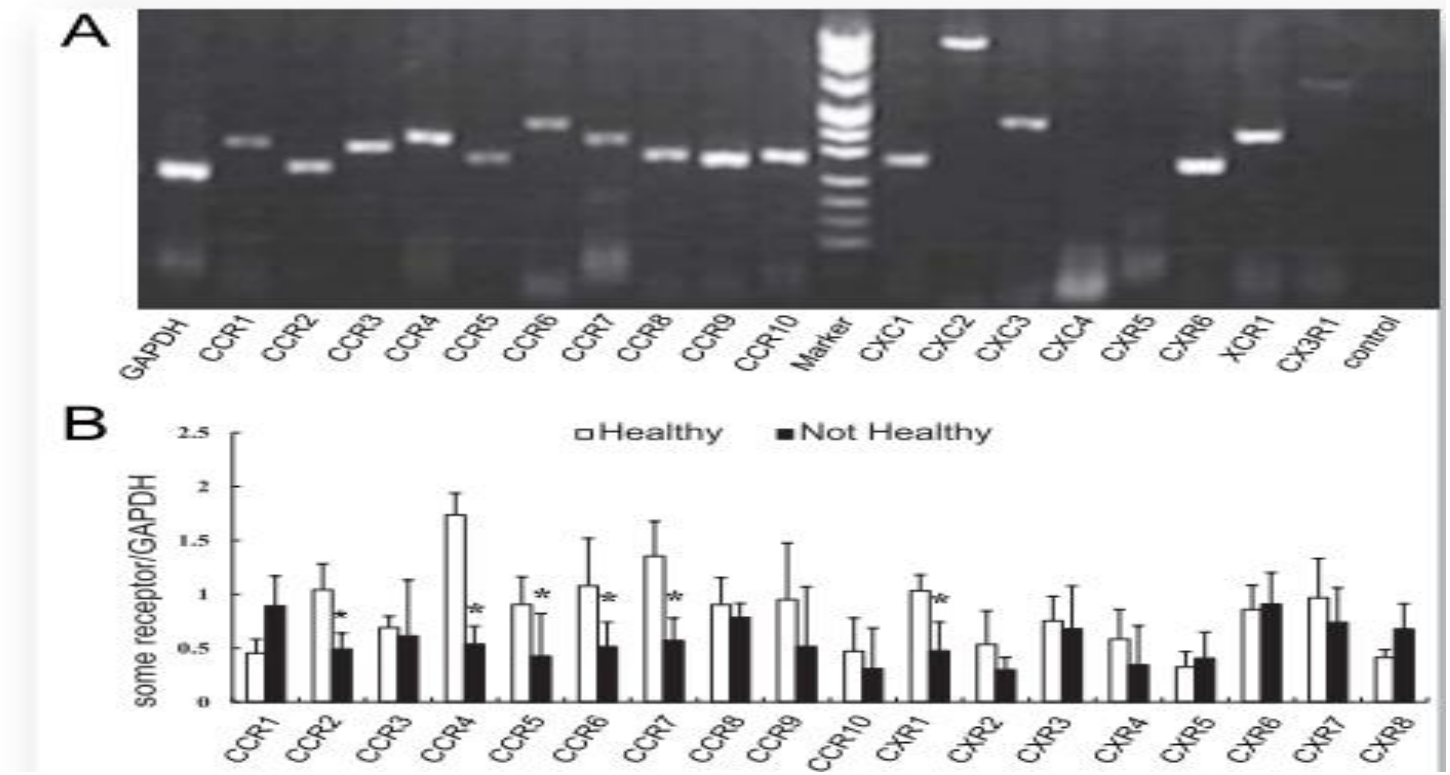
彩色照片，包括电镜照片、病理切片、荧光显微镜照片等

专指彩色照片，不包括以彩色印刷的图表类线条图

Tiff格式，分辨率300dpi，采用LZW无损压缩

Eps格式，分辨率300dpi，文字等保持矢量特性

复合类型图

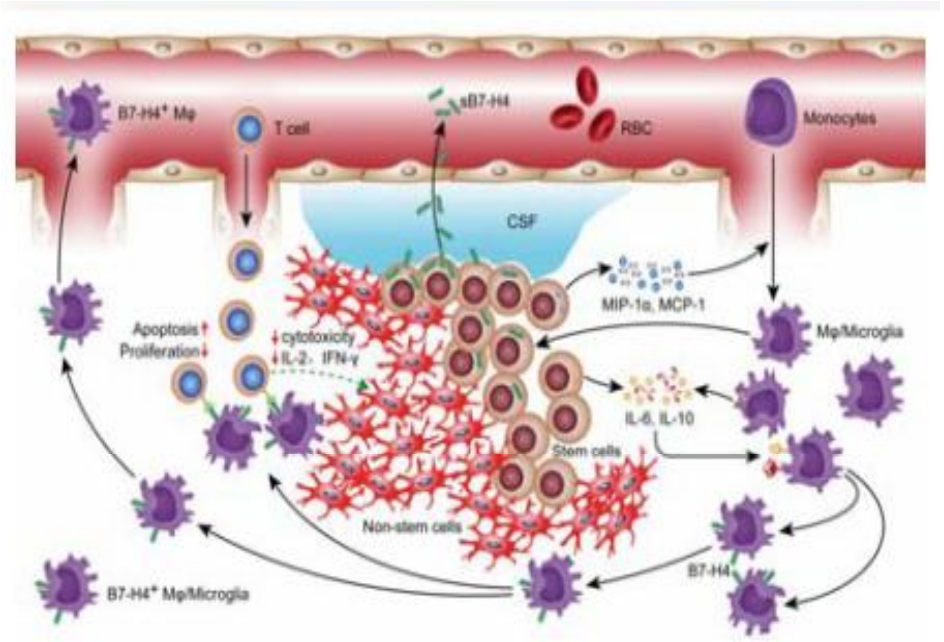


包括彩色图片，黑白图片，柱状图等

Tiff格式，灰度图和彩色图片分辨率500dpi，采用LZW无损压缩

Eps格式，灰度图和彩色图分辨率500dpi，保持矢量特性

示意图



用电脑软件人工绘制的用以辅助反应课题设计、研究机制、实验通路等机理或者机制的彩图，多出现在高影响因子论文之中

Tiff格式，分辨率500dpi，采用LZW无损压缩

Eps格式，分辨率500dpi，文字等保持矢量特性

图片色彩模式和字体

- 印刷要求使用CMYK格式，电子期刊要求使用RGB模式，具体查看投稿期刊的要求，灰度图请使用灰度模式，另外请使用8位图通道
- 字体类型Arial 或者Time News Roman字体
- 字体大小没有严格要求，但整篇论文中多幅插图中同类型的文字部分的字体大小应保持一致，原则上不超过14号字，尽量使用7-12号字，尽量少使用小于6号以下的字体，最多见的文字大小推荐使用7号字

图片压缩及文件大小

- 为了便于投稿时插图文件尽量快速的网络传输，建议对于tiff格式图片统一采用LZW格式的无损压缩，否则高分辨率（如1000bpi）的tiff格式线图大小甚至可以达到50MB，线条图使用LZW格式压缩后大小改变十分明显，彩色照片类图片进行LZW压缩后大小改变相对较小
- 单个图片大小最好不要超过10MB，如果经过LZW处理后的图片大小仍超过10MB，意味着图片版面过大，需要从新制作或者分成几个图片

插图文件格式

- TIFF格式：位图。如使用photoshop编辑的插图，导出tiff格式图片时请拼合图层。
- EPS格式：矢量图。其中可嵌入位图，嵌入的位图需要保证足够的分辨率（以400dpi为佳，最低不低于300dpi）。
- 只接受这两种类型的插图文件格式。鼓励使用EPS矢量图格式，因为矢量图印刷出来的文字和线条最清晰。Tiff格式需要达到相应的分辨率。
- 不接受JPG格式的插图，不接受doc、ppt文档中的插图。

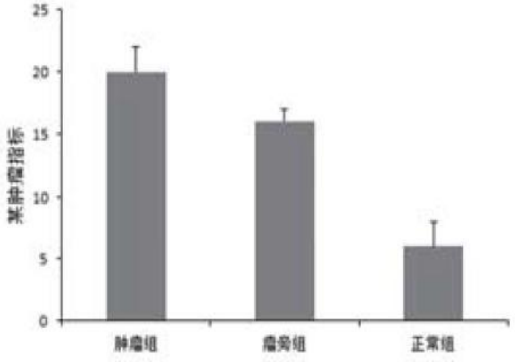
文件名

提交的文件名应使用相应的规范

- Fig1.tiff、 Fig2.tiff、 Fig3.tiff…..
- Fig1.eps、 Fig2.eps、 Fig3.eps
- 如果一张图由几个部分组成，算作一张图，应在PS、AI等软件中拼合成后提交，而不是提交诸如Fig1A.tiff、Fig1B.tiff

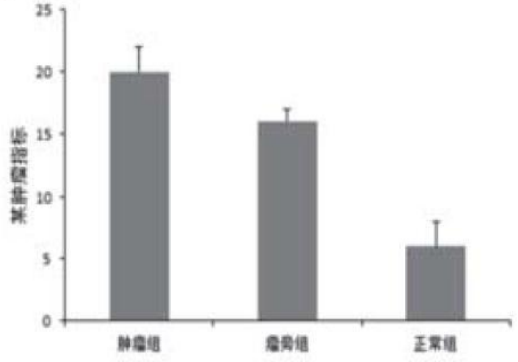
严禁出现的做法

A



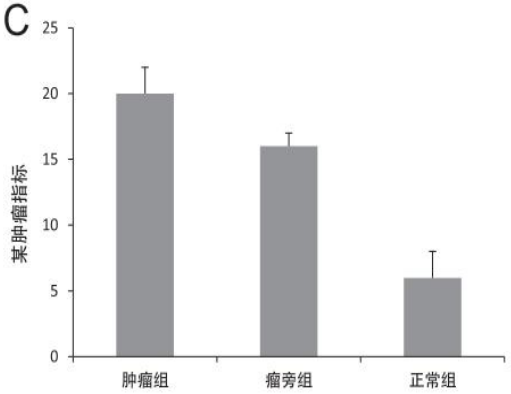
截屏图片电脑上显示合格

B



截屏图片印刷后模糊不堪

C



符合要求的印刷显示效果

如果您现在查看的此文档是pdf格式，您可在pdf阅读软件中放大阅读视图比例到300%以上，然后对比ABC三图的显示效果。可见到C图是最清晰的

为达到指定分辨率而使用图片编辑软件强行放大

直接将软件输出的线条或者图表使用截屏后制作的插图

对图像做局部修改，属于伪造数据

何时编辑部要求提供原始照片和数据

- 审稿专家认为根据你论文的数据不至于得到你论文中的结果
- 审稿专家认为你的结果非常令人吃惊，可能意义重大，因而希望查看一下你的原始照片或者数据以肯定这种结果，满足好其心
- 制作插图的过程中都应该对原始图片做保留，在编辑突变时应该复制一份作为修改，而不能替换掉原始图片。

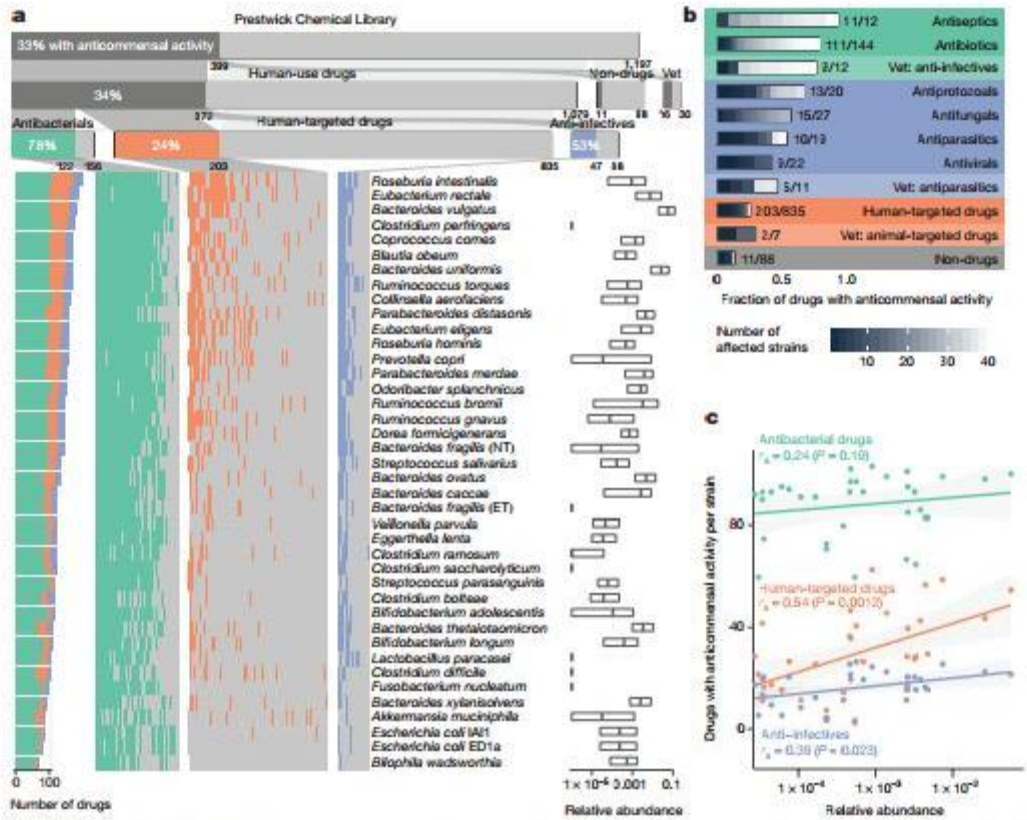


Figure 1 | Systematic profiling of marketed drugs on a representative panel of human gut microbial species. a, Broad impact of pharmaceuticals on the human gut microbiota. Compounds from the Prestwick Chemical Library are divided into drugs used in humans, drugs used exclusively in animals (vet) and compounds without medical or veterinary use (non-drugs). Human-use drugs are further categorized according to targeted organism. Strain–drug pairs (that is, instances in which a drug significantly reduced the growth of a specific strain; see Methods) are highlighted with a vertical coloured bar in the matrix. the right (boxes correspond to interquartile range (IQR) and central line to median relative abundance). **b**, Fractions of drugs with anticommensal activity by sub-category. Grey scale within bars denotes inhibition spectrum (the number of affected strains per drug). **c**, Correlation between species abundance in the human microbiome and drug sensitivity. For each strain ($n = 40$), the number of drugs that affect its growth is plotted against its median relative abundance in the human gut microbiome. Lines depict the best linear fit, r_S the Spearman correlation and grey shading the 95% confidence interval of the linear fit. All drugs, and in particular

Maier L, Pruteanu M, Kuhn M, et al. Extensive impact of non-antibiotic drugs on human gut bacteria[J]. Nature, 2018, 555(7698):623-628.

this disruption, and how it might promote disease, is poorly understood. Writing in *Cell*, Guo *et al.*[5] precisely map the organizational and structural features of poly(GA) aggregates and associated macromolecular complexes in neurons using a technique called 3D cryo-electron tomography (cryo-ET), to provide direct visualization of how proteasomes are disrupted by poly(GA) proteins.

Cryo-ET in 3D uses electron microscopy to view very thin, frozen but hydrated sections of a cell from various angles. The resulting images are combined to produce a 3D image called a tomogram. Guo *et al.* used 3D cryo-ET to visualize neurons that had been genetically engineered to express a poly(GA) tract that contained either 175 or 73 repeats. The tracts were fused with a green fluorescent protein that enabled their precise position to be determined using correlative light microscopy. The engineered protein mimics poly(GA) tracts that are produced from *C9orf72* expansion, which take a long time to form *in vivo*. The authors found that poly(GA) proteins form highly clustered and often bifurcated twisted ribbon structures that are of relatively uniform thickness, but of variable length and width, similar to poly(GA) structures previously observed by conventional electron microscopy *in vitro*[6].

computational approaches to search for known macromolecular complexes in each aggregate,

a reaction cycle that involves ground, committed and substrate-engaged states. Guo

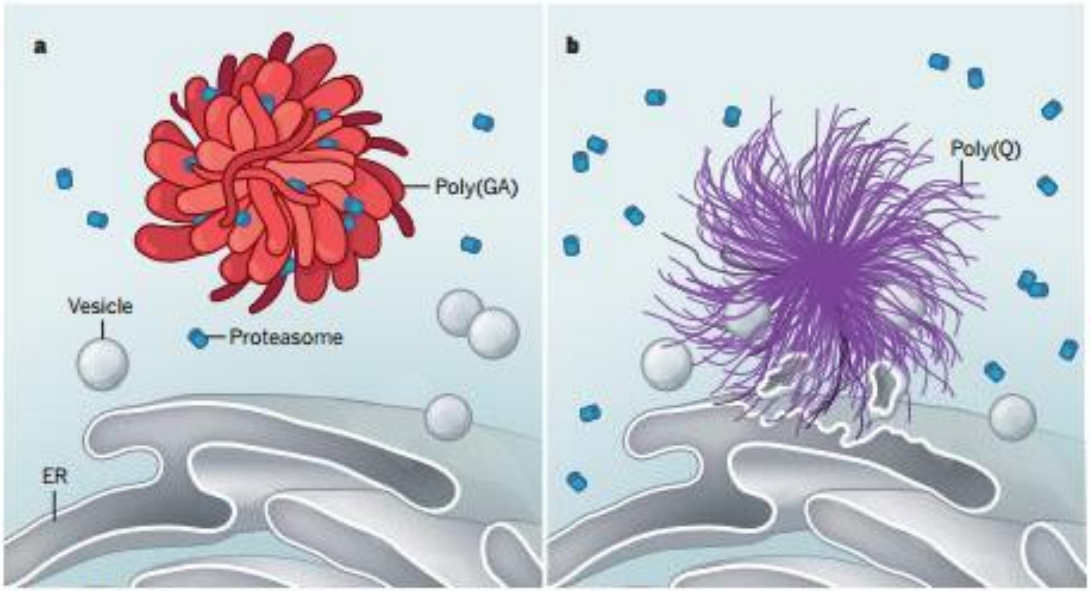


Figure 1 | Contrasting mechanisms of aggregate toxicity. **a**, In some cases of the neurodegenerative disorder amyotrophic lateral sclerosis, long chains of glycine and alanine amino-acid residues (dubbed poly(GA) tracts) aggregate in neurons. Guo *et al.*[5] show, through high-resolution structures in cells, that poly(GA) tracts form ribbon-like aggregates that capture protein complexes called proteasomes, which normally process other proteins for degradation. Such capture causes proteasome stalling, providing an explanation for the toxicity of this aggregate. Poly(GA) aggregates do not bind membrane-bound organelles such as vesicles and the endoplasmic reticulum (ER). **b**, By contrast, repetitive tracts of the amino acid glutamine (poly(Q) tracts), which are associated with Huntington's disease, form fibril-like aggregates[7]. These aggregates deform the membranes of vesicles and the ER, suggesting that different aggregates cause neurodegeneration through different mechanisms.

L Vaites Pontano, JW Harper. Protein aggregates caught stalling.[J]. Nature, 2018, 555(7697):449-451.

Advances in Tetrazine Bioorthogonal Chemistry Driven by the Synthesis of Novel Tetrazines and Dienophiles

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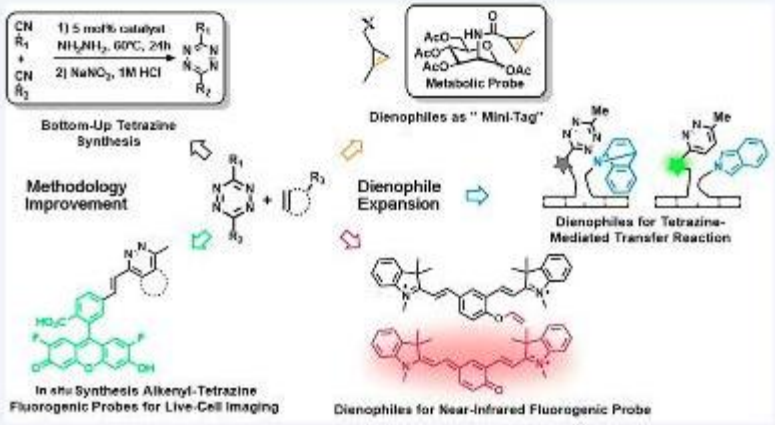
‡Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, California 92093, United States

CONSPECTUS: Bioorthogonal chemistry has found increased application in living systems over the past decade. In particular, tetrazine bioorthogonal chemistry has become a powerful tool for imaging, detection, and diagnostic purposes, as reflected in the increased number of examples reported in the literature. The popularity of tetrazine ligations are likely due to rapid and tunable kinetics, the existence of high quality fluorogenic probes, and the selectivity of reaction. In this Account, we summarize our recent efforts to advance tetrazine bioorthogonal chemistry through improvements in synthetic methodology, with an emphasis on developing new routes to tetrazines and expanding the range of useful dienophiles. These efforts have removed specific barriers that previously limited tetrazine ligations and have broadened their potential applications.



Among other advances, this Account describes how our group discovered new methodology for tetrazine synthesis by developing a Lewis acid-promoted, one-pot method for generating diverse symmetric and asymmetric alkyl tetrazines with functional

Wu H, Devaraj N K. Advances in Tetrazine Bioorthogonal Chemistry Driven by the Synthesis of Novel Tetrazines and Dienophiles[J]. Acc Chem Res, 2018.

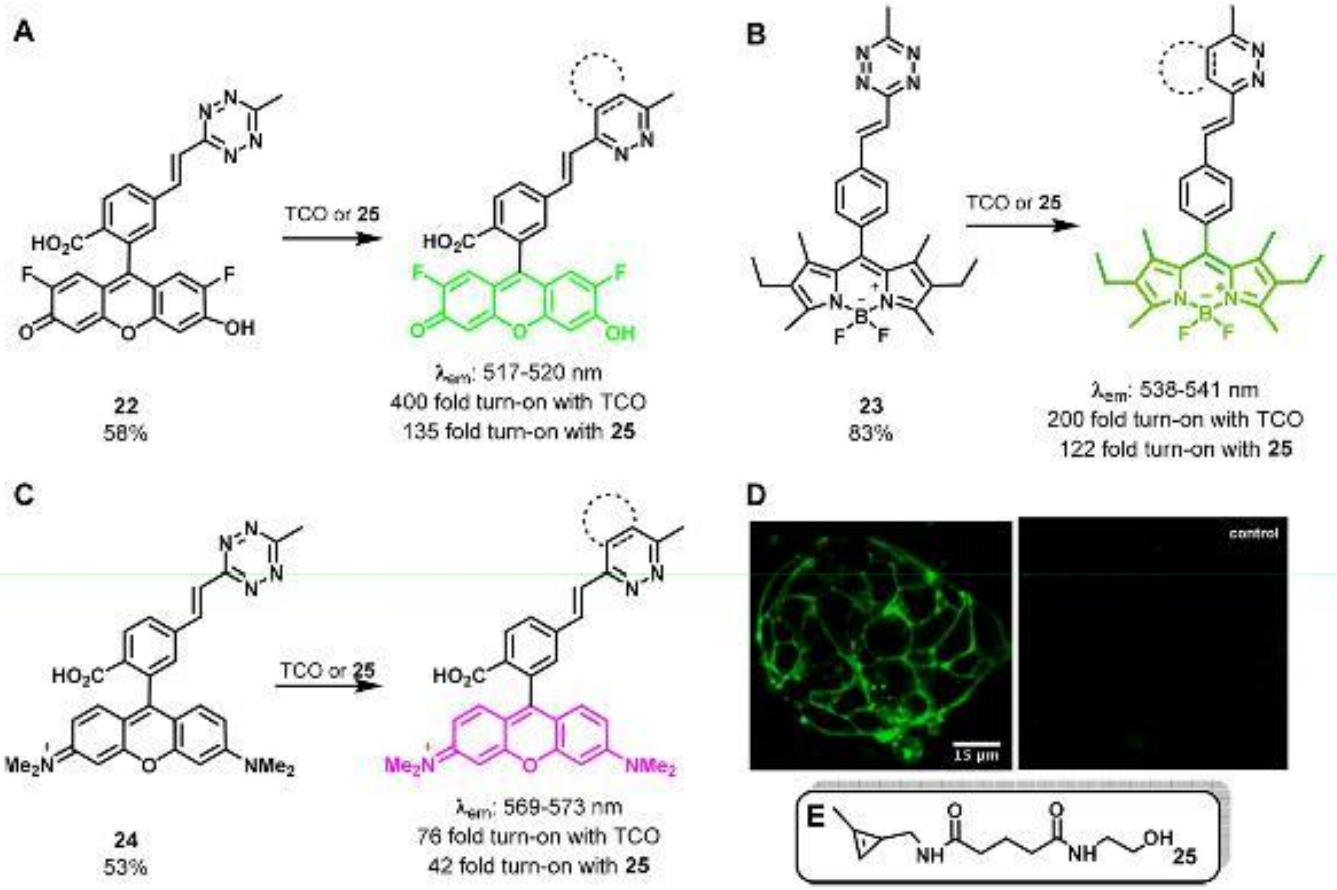


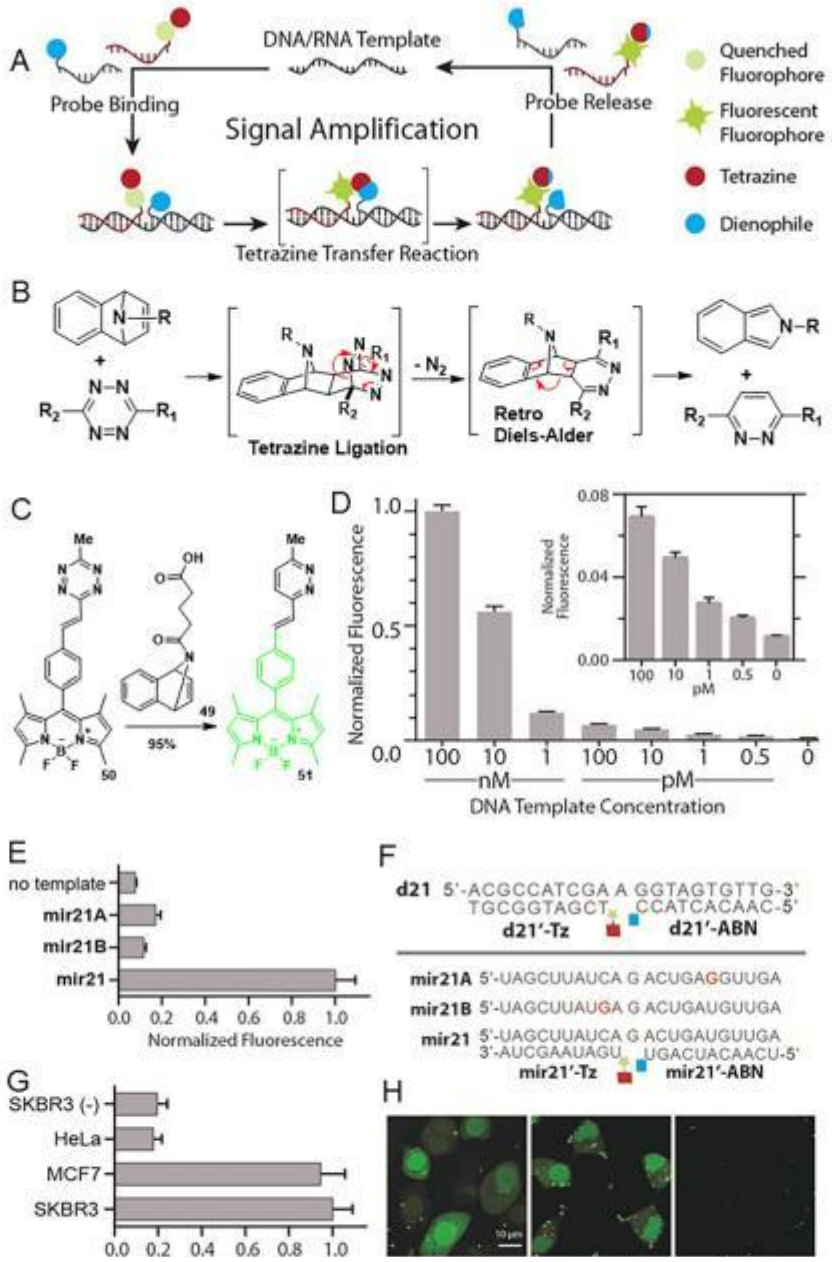
Figure 3. (A–C) Fluorogenic reaction of **22**–**24** with dienophiles. (D) Live-cell imaging of LS174T cells using fluorogenic probe **22**. Left: cells were pretargeted with TCO-decorated A33 antibodies. Right: cells were treated with unmodified antibodies. (E) Structure of cyclopropene **25**.

our tetrazine synthetic methodology in hand, we aimed to design a new generation of tetrazine fluorogenic probes.[25]

Since the double bond generated by the Heck reaction is the ideal bridge for energy transfer, we hypothesized that a

have an inherent absorbance around 500–550 nm. Thus, far-red and NIR fluorophores with relatively longer emission wavelengths are challenging to quench. Therefore, we decided to design a tetrazine near-infrared fluorogenic probe through a

Wu H, Devaraj N K. Advances in Tetrazine Bioorthogonal Chemistry Driven by the Synthesis of Novel Tetrazines and Dienophiles[J]. Acc Chem Res, 2018.



Wu H, Devaraj N K. Advances in Tetrazine Bioorthogonal Chemistry Driven by the Synthesis of Novel Tetrazines and Dienophiles[J]. Acc Chem Res, 2018.

谢 谢

THANKS FOR YOUR ATTENTION