OBSERVATION OF CHROMATOGRAPHIC DIFFERENCES BY NON-SPECIALIST VIEWERS FOR 1D GC AND GC×GC OUTPUT

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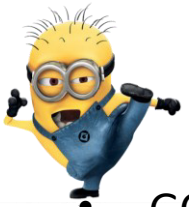
GC×GC-MS for Communication

- Comprehensive two-dimensional gas chromatography has been proposed in research for many purposes:
  - Death investigation
  - Drug analysis
  - Toxicology
  - Arson investigation
  - Chemical agent detection
  - Oil spill investigations

Reporting/communication of results is an **essential component** of scientific research and routine analysis.



The Debate

- GC×GC-MS is “too complex” and will *never* be suitable for routine forensic analysis
- Expert witnesses will *never* be able to explain GC×GC-MS data in a courtroom
- GC-MS has always worked just fine…

- GC×GC-MS provides substantial benefits for nontargeted profiling
- GC×GC-MS provides “images” as output that could help laypersons understand data better
- Expert witness testimony would be more effective with GC×GC output


FIND 10 DIFFERENCES
Find 10 differences


Kathy Garst Sales Team - The Real Estate Group
Suggested for you · 3d ·
Subtle changes can make such a big impact on your home's curb appeal. 😍
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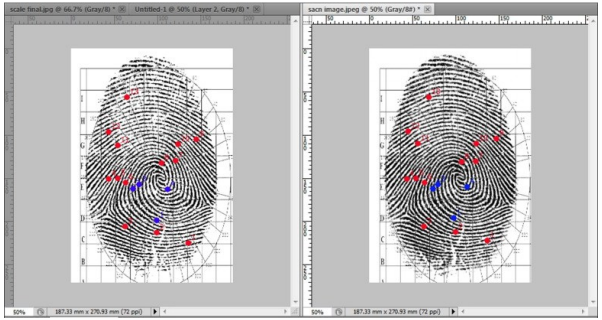
Forensic Expert Witness Testimony

- Often involves comparative analysis
  - Known vs. reference
- Can involve visual aids
  - Some studies have shown improved jury understanding when 3D models were used instead of photographs[1]
- There exists a general lack of information on how jurors process scientific data
  - More exists on fingerprint comparison and DNA analysis
  - Very little on chemical analysis



[1]Blau, S., Phillips, E., O'Donnell, C., & Markowsky, G. (2019). Evaluating the impact of different formats in the presentation of trauma evidence in court: a pilot study. Australian Journal of Forensic Sciences, 51(6), 695–704.

Study Objective

- **To provide the first empirical study[1] of the observation of chromatographic differences by non-specialists**
  - Are individuals effective at identifying if two chromatographic profiles are distinguishable vs. indistinguishable?
  - Are individuals effective at identifying the degree of similarity between pairs of chemical output?
  - Do individuals feel that chromatographic data is challenging to compare based on output?

- Subjects were asked to play a virtual “spot-the-difference” game without any case details or explanation from an expert

[1]Clarissa Camara, Cynthia Cheung, and Katelynn A. Perrault Uptmor. "Observation of chromatographic differences by non-specialist viewers for one-dimensional gas chromatography and comprehensive two-dimensional gas chromatography output." *Forensic Chemistry* 41 (2024): 100620.

Human Subjects Research

- IRB Protocol CUH 0070-2018
- Recruited participants via
  - department emails
  - poster advertisements
  - within online learning management systems
  - email lists
- Chaminade University of Honolulu & wider University of Hawaii School System
- Participants had to meet criteria for jury eligibility and not currently hold a degree in a natural science
- 70 eligible participants responded

Image Comparison Survey

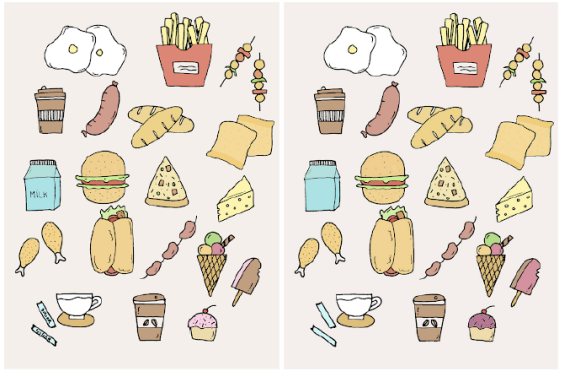
Thank you for your interest in participating in this research study. We greatly appreciate your time to help us collect valuable data.

The first step is to read the informed consent form for the study to understand the purpose, benefits, and risks of the study. You will then be prompted with questions to determine if you meet eligibility to participate in this study. If you are ineligible to participate, you will be able to leave the survey and we thank you for your time anyway! If you are eligible to participate, allow yourself 30-60 minutes to complete the study.

This process is designed to be completed on a computer. Please do not use a phone, tablet, or other such devices.

Please click “Fill out form” to start the survey, and then "next" to continue.

Step 1: Assess the two images. Are there any differences?



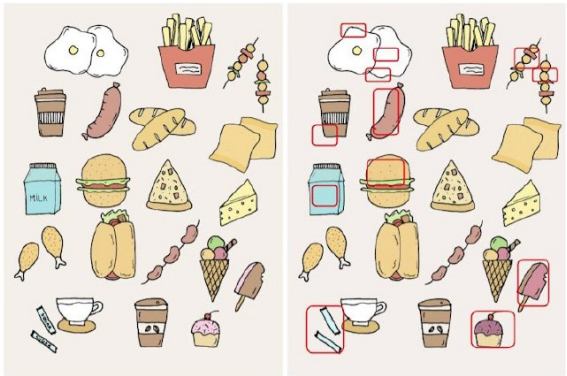
Example Question #1

"These two images are the same."

- ○ Yes, they are identical images.
- ◉ No. Only a few differences exist.
- ○ No. Several differences exist.
- ○ No. Many differences exist.
- ○ No. They are completely different images.

INDISTINGUISHABLE/ Match

DISTINGUISHABLE/ Non-Match



Example Question #2

How difficult was it to perceive the differences between the images above? *

- ○ Easy
- ◉ Moderate
- ○ Hard

Table 1
Image difference levels for all three image categories.

Level	Description of Image Comparison
0 %	Two identical images were presented to the viewer.
10 %	10 % of the grids within the image had alteration between the two images presented to the viewer.
25 %	25 % of the grids within the image had alteration between the two images presented to the viewer.
50 %	50 % of the grids within the image had alteration between the two images presented to the viewer.
100 %	Two completely different images were presented to the viewer.

Table 2
Responses to the prompt "These two images are the same".

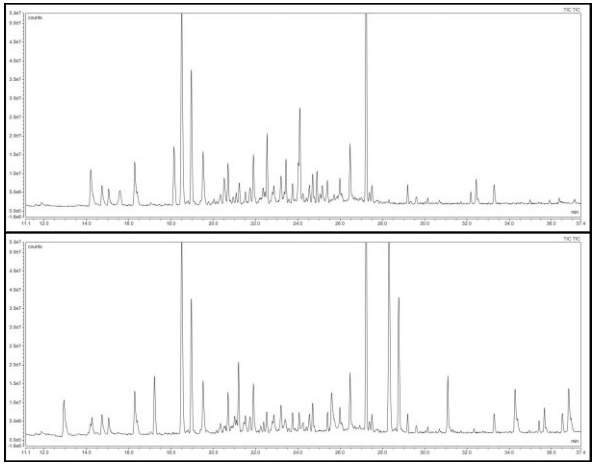
Difference Level	Statement	Assigned Code
0 %	"Yes, they are identical images"	1
10 %	"No, only a few differences exist"	2
25 %	"No, several differences exist."	3
50 %	"No. Many differences exist."	4
100 %	"No. They are completely different images."	5

Table 3
Responses to the prompt "How difficult was it to perceive the differences between the images above?".

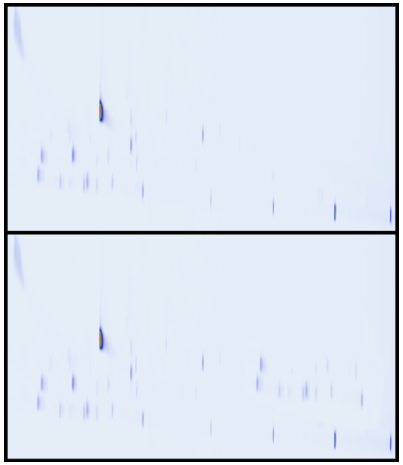
Difficulty Level	Code
Easy	1
Moderate	2
Hard	3

Examples

Non-Chromatographic Image (Photograph)
25% Difference



GC-MS Data
50% Difference



GC×GC-MS Data
10% Difference

Difficulty

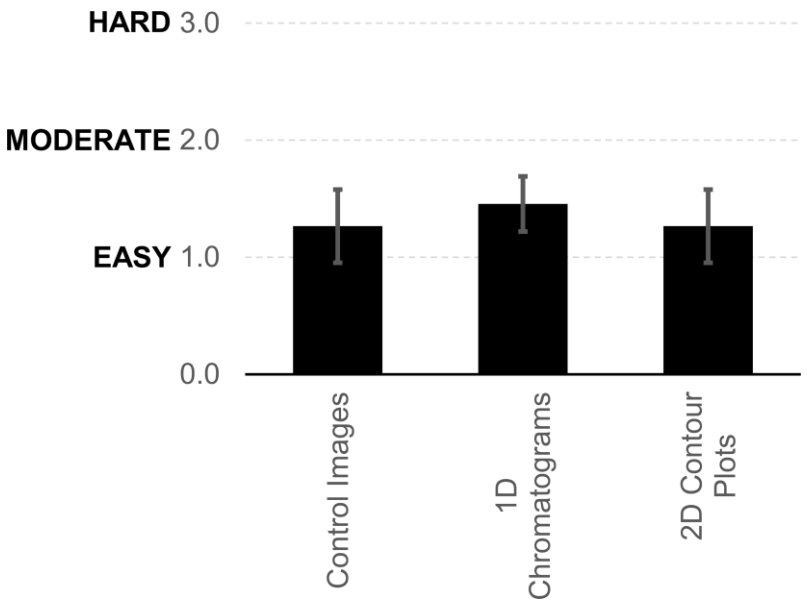
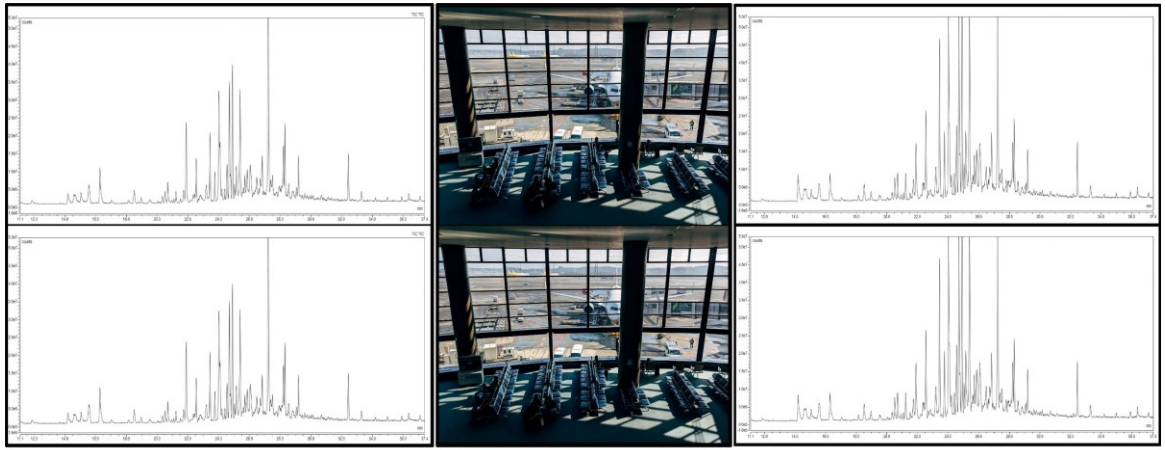


Fig. 1. Average difficulty score for image comparisons across different categories. Each category represented 15 comparisons performed by n= 70 individuals. Error bars represent standard deviation.

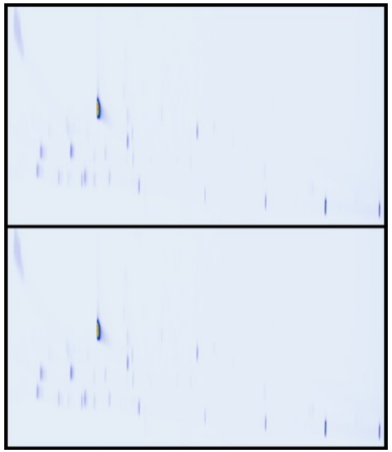


Question 32 (0% difference)
Average Difficulty = 1.8/3.0

Question 37 – 0% difference
Average Difficulty = 1.9/3.0

Question 44 (0% difference)
Average Difficulty = 1.8/3.0

Fig. 2. The three comparisons that presented the highest difficulty level to participants. Question number within the survey, level of different, and average difficulty across 70 participants are shown beneath each comparison.



Question 42 (0% difference)
Average Difficulty = 1.6/3.0

Fig. 3. Example of comprehensive two-dimensional gas chromatography (GC×GC) identical contour plot comparison with highest difficulty score within the GC×GC-MS category.

NOTE: Out of 45 comparisons, only one question was scored correctly by every single participant (n=70). It was a GC×GC contour plot.

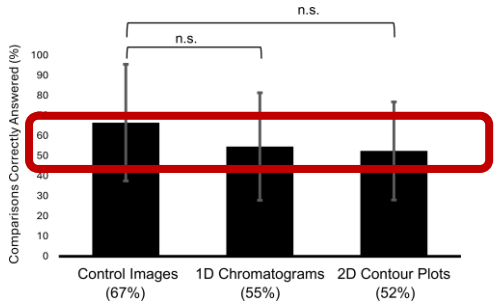


Fig. 4. The percentage of correctly answered comparisons across all 45 comparisons performed by 70 study participants. Participants conducted 15 comparisons in each category across a variety of 0–100% difference in images. A two-tailed student's t-test demonstrated no significant difference (n.s.) between each of the groups and the control group. Error bars represent standard deviation.

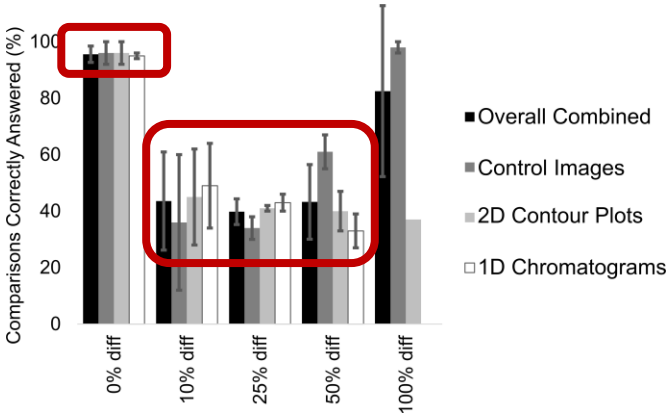


Fig. 5. Success rate of participants to correctly distinguish the difference level of the comparison based on phrase options based on both difference level and image comparison type. Error bars represent standard deviation.

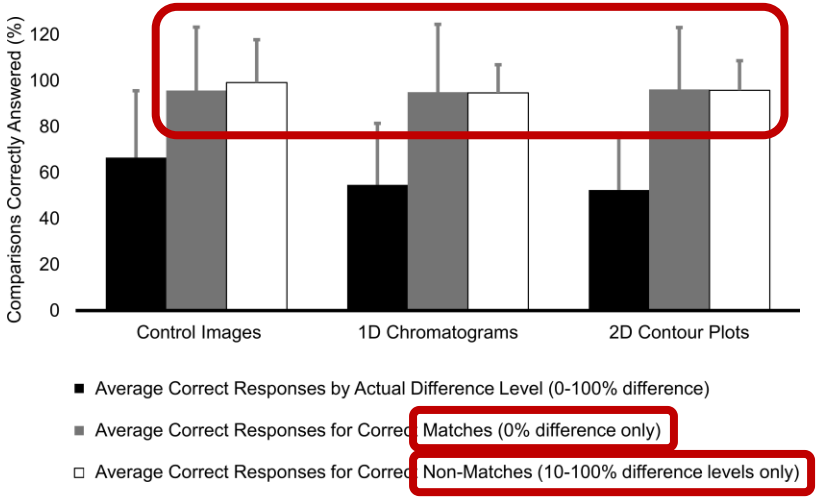
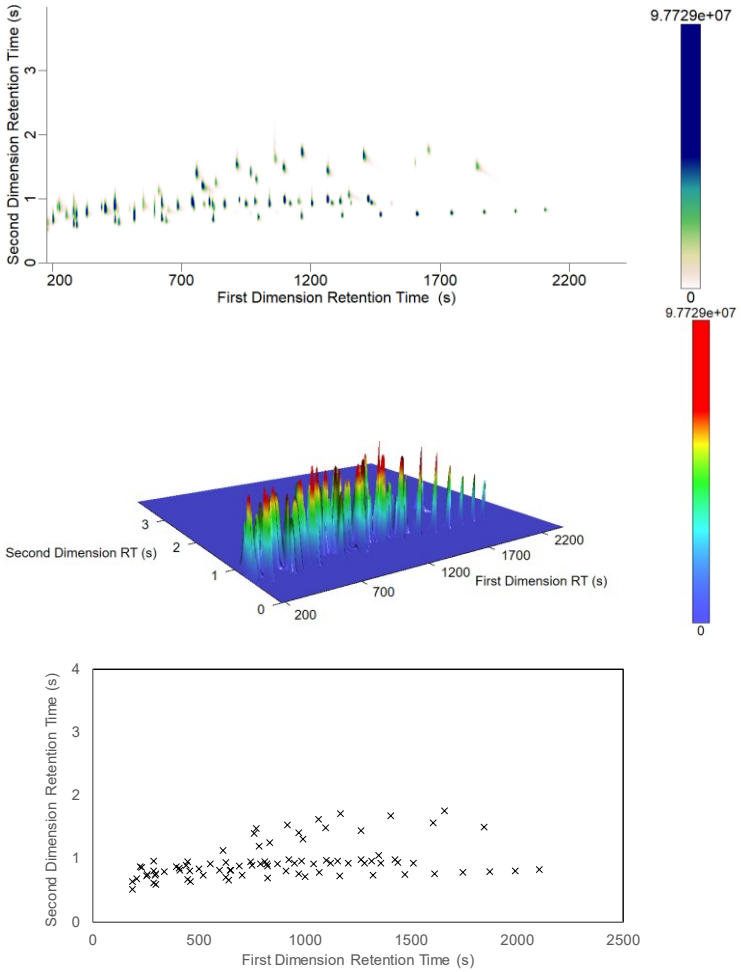


Fig. 6. Assessment of correct responses by original scoring system (black) accounting for allocation to correct category of image, compared to Correct Match (grey) and Correct Non-match (white) system. Correct Match/Non-match scoring of correct answers was performed to assess the ability of participants to determine whether the two images were simply distinguishable or indistinguishable without requiring the difference level assessment. Error bars represent standard deviation.

Future Directions

- Increase participation rate
- Accompanying explanation
  - Different evidence types
  - Mock case scenarios
- Plot types
  - Contour plot, surface plot, apex plot…
- Color scheme and color scale
- Deep learning strategies



Conclusions

Participants were:

- Generally confident in their ability to compare images
- Most challenged by comparison of identical images
  - Possibly due to large/time effort devoted to comparison
  - But…successful at this task despite difficulty
- Not very successful at quantifying the amount of difference between distinguishable plots (all categories)
- Very successful at determining whether two plots were distinguishable or indistinguishable (match/non-match)

No significant difference was observed between performance across photographs, GC-MS chromatograms, or GC×GC-MS contour plots

Current data supports that GC×GC-MS data is no more or less challenging to understand than GC-MS data for laypersons.

Acknowledgements

National Science Foundation CAREER Award
This material is based upon work supported by the National Science Foundation under Grant Number 1752607. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

Camille & Henry Dreyfus Foundation – Henry Dreyfus Teacher Scholar Award
Restek Academic Support Program
W&M SEED Funding
W&M Faculty Research Grant
4-VA Research Funding

Camara, Clarissa, Cynthia Cheung, and Katelynn A. Perrault Uptmor. "Observation of chromatographic differences by non-specialist viewers for one-dimensional gas chromatography and comprehensive two-dimensional gas chromatography output." *Forensic Chemistry* 41 (2024): 100620.

https://doi.org/10.1016/j.forc.2024.100620

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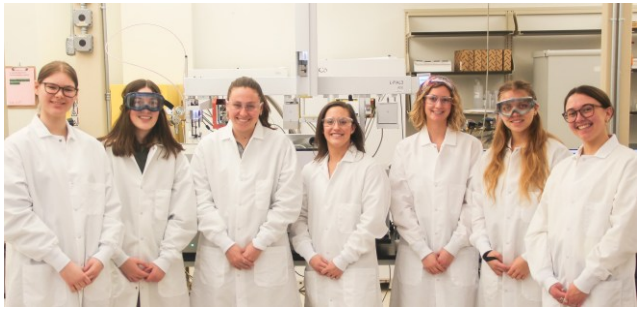
Industry Partners
SepSolve Analytical
Thermo Scientific
LECO Corporation
Restek Corporation



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