Breaking Bad: Creativity and Organic Chemistry

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Abstract

Is there such a thing as a "creative person"? The literature on creativity has focused on this question for several decades now, but a clear answer has yet to be provided. On the one hand, some researchers have argued for *domain generality* within the broad umbrella of "creative activities," which posits that creative people do indeed exist: that people's creative talents (or lack thereof) are consistent across all domains of creativity (e.g., painting, problem-solving, music composition, poetry writing). On the other hand, some researchers have maintained that there is no such thing as a creative person, but that people's creative abilities are instead limited to a particular domain of creative activities (e.g., an individual may be a very creative visual artist, but this talent does not transfer to other domains, such as music composition). While there has been a longstanding debate about the nature of domain-general vs. domain-specific creative talents, whether creativity is domain-general vs. specific remains unclear. To contribute to this ongoing debate, here, I designed a domain-specific measure of creativity for organic chemistry (the *Divergent Skeletal Formula Task [DSFT])* and investigated the possible relationships among the DSFT and two widely used domain-general measures of creativity. Results demonstrated no significant relationship between the DSFT and the domain-general measures of creativity, thereby providing further support for a domain-specific view of creativity.

Keywords: creativity, divergent thinking, domain-specificity, domain-generality

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In the extant literature on creativity, while there has been support for the notion that creativity spans many different domains of human expression, there has not been a formal inquiry into creativity within the domain of organic chemistry (Amir & Biederman, 2016; Benedek et al., 2014; Liu et al., 2022; Richard et al., 2021; Simonton, 2021; Suherman & Vidákovich, 2022). Although some studies have examined creativity in a domain-specific manner in other fields of science (e.g., Diakidoy & Constantinou, 2001), the literature on creativity within STEM fields remains relatively sparse, and organic chemistry has notably been excluded from investigations. Given the considerable potential for creativity in organic chemistry, this study aims to fill this gap via a novel interdisciplinary approach.

When attempting to understand how creativity manifests in a specific field, it is important to determine the classification of the field or domain. A *domain* in this context refers to broadly defined cognitive domains, such as linguistic, mathematical, or musical domains (Baer, 1998). Proponents of a domain-specific theory of creativity postulate that an individual's creativity is dependent on the domain in which the individual is performing creatively. Previous research on domain classification has revealed that a domain-specific approach to creativity is essential for vertical/well-structured domains. Domains are determined to be vertical/well-structured if they are constrained in such a way that their critical components resist transformation. The fact that organic chemistry is defined as a vertical/well-structured domain supports the inclination that creativity within organic chemistry is domain-specific (Jeon et al., 2011; Jin Li, 1997; K. Lawless & Kulikowich, 2006).

Following the principles of domain specificity, to most accurately assess creativity in organic chemistry, investigations must be conducted in a domain-specific manner (Baer, 2015).

Given that no such measure exists, we sought to design one: The *Divergent Skeletal Formula Task* (DSFT). In this task participants were asked to draw as many constitutional isomers as possible based off the molecular formula $C_6H_{12}O$. For a more extensive discussion of the DSFT and its theoretical groundings, see Appendix A.

Creativity

What is creativity? How can wide-ranging domains like animation, music, literature, and chemistry all be "creative"? In a comprehensive review of the literature, Hennessey and Amabile (2010) concluded that, while the definition of creativity is contested, it is generally agreed that the construct of creativity constitutes novelty and appropriateness (Amabile, 1996; Baer, 1993; Hennessey & Amabile, 2010; Sternberg & Lubart, 1999). That is, creative products must be new and useful (Amabile, 1982). For instance, a painting is novel insofar as it is not a replication of a previous work, and it is useful because it allows the artist to express their emotions.

Domain-General vs. Domain-Specific Creativity

Based on the aforementioned definition of creativity, organic chemistry qualifies as creative as it focuses on producing *novel* and *useful* molecules in the form of modern drugs (Ball, 2015; Corey, 1991). Does this imply that creativity within organic chemistry relies on the same underlying cognitive mechanisms as creativity in painting or music? More formally, is creativity domain-general or domain-specific? On the one hand, proponents of a domain-specific theory of creativity postulate that an individual's creativity is dependent on the domain in which the individual is performing creatively. On the other hand, supporters of a domain-general theory of creativity argue that the cognitive processes that underlie creativity in one domain also underlie creativity in completely unrelated domains; that is, all creative activities rely on the same foundational cognitive resources and skills (Baer, 2012). Consistent with this view, an established body of work has demonstrated that the cognitive abilities and processes influencing creativity and problem solving apply across a multitude of domains (Plucker & Beghetto, 2004; Runco, 1994; Runco & Okuda, 1988).

However, at odds with the domain-general perspective, multiple studies have demonstrated that the cognitive skills that underlie creative thinking are specific to distinct domains (Baer, 1991, 1993; Runco, 1989). In such studies, researchers asked participants to produce multiple creative products (e.g., poems, stories, collages, drawings, and mathematical puzzles), which were then judged by experts. This process of expert judgment is formally known as the *Consensual Assessment Technique* (CAT) and is considered one of the gold standard measurements of creativity (Amabile, 1982). Importantly, the CAT relies on subjective judgements of creativity and its components (novelty, usefulness). Across research that features the CAT paradigm, distinctions of creativity emerge between domains.

Further evidence for domain specificity comes from creativity-training studies, which have overwhelmingly shown that training in skills relevant to a specific task will increase creative performance only on subsequent tasks that are directly related to the initial training. For instance, participants trained in poetry went on to write more-creative poetry but not more-creative short stories (Baer, 1994, 1996). The shift to a domain-specific perspective was not an isolated event, but rather, an ideological transformation during the 1980s and 1990s. A wave of researchers began to propose the centrality of the domain and its importance in creativity (Amabile, 1983; Csikszentmihalyi, 2014; Csikszentmihályi, 1990; Feldman, 1994; Gardner, 1988; Moneta, 1993).

Following this line of thought, if creativity is domain-specific (as the overwhelming majority of evidence supports), then creativity assessment ought to also be domain-specific

(Baer, 2015). Any assessment of creativity that claims to be domain-general is likely unsupported; this is evidenced not only by the domain-specific theory of creativity but also by the fact that many domain-general tests of creativity often do not correlate with each other, and thereby fail to demonstrate convergent validity (Baer, 2015; Sawyer, 2012). Accordingly, we offer a domain-specific task and assessment of creativity within organic chemistry in the following study.

Divergent Thinking

Since J.P. Guilford's 1950 American Psychological Association presidential address wherein he focused on divergent thinking as a proxy of creative thinking, divergent thinking has subsequently dominated creativity testing (Guilford, 1950; Baer, 1998; Kogan, 1983; Torrance & Presbury, 1984). Divergent thinking and its closely related sibling, convergent thinking, were initially devised as the two production factors of intellect (Guilford, 1956). While convergent thinking concerns the production of a single correct answer (e.g., multiple-choice questions), divergent thinking is "the cognitive ability to produce numerous and diverse ideas to a given stimulus or problem" (Jeon et al., 2011). As such, there are no "correct" responses in divergent-thinking tasks, as the task prompt is open-ended (e.g., the *Alternative Uses Task [AUT]*, for which participants are asked to list as many uses for a common object, like a brick). This open-endedness affords a more unrestricted expression of thought that diverges from antiquated views of "intelligence," situating creativity and divergent thinking as a distinct mode of cognition.

Early studies focusing on divergent thinking and creativity have found a mix of significant and non-significant correlations between divergent thinking and creative activity in various fields (Hocevar, 1980). To reconcile these potential discrepancies, research has since vastly expanded the implications of divergent thinking and its connection to creativity.

Subsequently, in accordance with dominating theories of creativity, contemporary forays largely approach divergent thinking within the domain-specific perspective of creativity. Not only has a strong case been made against divergent thinking as an all-purpose creative thinking skill (Baer, 1993; Brown, 1989; Crockenberg, 1972; Hallinan, 1985; Hocevar, 1981), but several studies also support the claim that divergent thinking is narrowly domain-specific (Baer, 1993, 1994, 1996).

Given its historical and theoretical groundings in measuring creativity, here we designed a domain-specific divergent thinking task to measure creativity within organic chemistry. For a more robust discussion of the DSFT and its theoretical groundings, see Appendix A.

The Present Study

Given the gap in the creativity literature that assesses divergent thinking in STEM sciences—particularly organic chemistry—this study investigated the relationships between the novel DSFT and other gold standard domain-general measures of creativity (the *Alternate Uses Task* and the *Divergent Association Task*). We hypothesized that there would be a non-significant relationship between the DSFT and the domain-general measures of creativity. If obtained, such findings would support the notion that creativity is domain-specific and not domain-general.

Method

Participants

We recruited one hundred twenty-eight participants, each of whom were enrolled in Organic Chemistry II Lab (CHEM 202L) at a private liberal arts university in the southeast, between January 2022 and January 2023. Twenty-one participants were excluded from analyses for failing to follow the directions (M_{age} = 19.3 years; range = 18-26 years; 54.2% female; 92.5% right-handed). All ethical principles and guidelines in line with the university were followed. All consent forms and study measures were approved by the university's Institutional Review Board (IRB). This study was advertised via emails sent to students enrolled in CHEM 202L, class announcements, and word of mouth. Electronic informed consent was given by all participants prior to the study and was required to participate.

Measures

Alternate Uses Task (AUT)

Two rounds of a computerized AUT were administered to participants as a measure of their domain-general divergent thinking ability. The survey was administered using Qualtrics software and participants were asked to come up with as many creative, useful, and unusual uses for a given object. They responded to two different prompts ("newspaper" and "balloon") for 3 minutes each (Guilford, 1956).

Two independent raters later scored the responses using a procedure outlined in Alhashim et al. (2020), scoring the four facets of the AUT: Originality, Flexibility, Fluency, and Elaboration. The raters then reconciled ratings to reach a consensus on responses where the level of creativity was disagreed upon (Cronbach's alpha for Originality = .87; Flexibility = .90; Elaboration = .89). Final scores were calculated as the average between the two raters as recommended by Silvia et al. (2008).

Divergent Association Task (DAT)

The DAT was administered via Qualtrics as a measure of domain-general divergent thinking. Participants were asked to name ten words as unrelated to each other as possible in four minutes. The words could only be single words and nouns, with no proper nouns or specialized vocabulary/jargon. Additionally, words had to be thought of individually (as opposed to drawing inspiration from one's surroundings).

A computational algorithm was then used to calculate average semantic distance between the first seven valid words, with related words having a shorter distance between them than unrelated words (Olson et al., 2021). The total score is the transformed average of the semantic distance between the seven words, with higher averages being deemed more creative.

Divergent Skeletal Formula Task (DSFT)

The DSFT was administered via Qualtrics as a measure of domain-specific divergent thinking in organic chemistry. For the DSFT, participants were given five minutes to draw as many constitutional isomers as possible for the molecular formula $C_6H_{12}O$. All isomers had to be drawn using a standard skeletal formula. Participants had to draw all structures on paper and were given an additional three minutes to scan and upload a copy of their work into Qualtrics (see Appendix A).

Procedure

An online Qualtrics survey was designed to address the research question. Before participation in the survey, all participants were required to give their electronic informed consent. A within subject design was used and participants completed a total of three measures/tasks: The DSFT, the AUT (Guilford, 1956), and the DAT (Olson et al., 2021). The survey ended with a brief demographics section and a debrief form.

While the survey was completed on individual participants' computers in their free time, one task, the DSFT, required participants to upload a picture of their work as a pdf into the survey. All participants were compensated with either an $15 Amazon E-Gift Card or course credit.

Results

Descriptive analyses and correlations

Descriptive statistics for the DAT, all four facets of the AUT, and all three facets of the DSFT are presented in Table 1. All measures demonstrated good psychometric properties across both samples. The Pearson product-moment correlation coefficients for the Chemical Creativity scores of the DSFT are presented in Table 2. All statistical tests were initially set to the standard $\alpha = .05$, but after correcting for multiple comparisons for all analyses investigating the potential relation of the DFST measures and the AUT and DAT (15 correlations in total), the alpha level shifted to $\alpha = .003$ (i.e., .05/15 = .003). All of the previously validated creativity measures (AUT-Originality, AUT-Flexibility, AUT-Fluency, AUT-Elaboration, and DAT) had skewness values within acceptable ranges (skew < 2; Kline, 2015). The novel Chemical Creativity (CC) scores of the DSFT also performed well, though CC-Fluency had a skewness value that required a log-transformation to place this value in an acceptable range prior to analysis (see Table 1). Participants who did not follow directions or did not complete a measure were excluded from that portion of analysis—this is why the N-Statistic differs between tasks.

As shown in previous work (Olson et al., 2021), the DAT correlated with the AUT. Specifically, the DAT positively correlated with Flexibility ($r(120) = .21$, $p = .02$) and Originality ($r(120) = .22$, $p = .02$) on the AUT, but not with Fluency. A novel finding was that the DAT also positively correlated with Elaboration ($r(120) = .25$, $p = .006$), which is a facet that was not computed in Olson et al. (2021).

Chemical creativity and domain-general creativity correlations

It was hypothesized that there would be a non-significant correlation between the DSFT and the domain-general measures of divergent thinking (e.g., the DAT and the AUT). Consistent with this hypothesis, the DAT was not significantly associated with the CC-Uniqueness, CC-Originality, or CC-Fluency scores. Neither the CC-Uniqueness nor the CC-Originality scores were correlated with any of the AUT measures. The CC-Fluency score was positively correlated with Originality ($r(107) = .25$, $p = .008$) and Flexibility on the AUT ($r(107) = .21$, $p = .03$); however, after accounting for multiple comparisons neither finding remained significant. No significant correlation was found between the CC-Fluency score and either the Fluency or Elaboration facets of the AUT.

Discussion

This study investigated the relationship between the DSFT and two domain-general measures of creativity—the AUT and the DAT (Guilford, 1956; Olson et al., 2021)—both widely used in the creativity literature. To achieve this goal, the research team administered an online survey with participants completing the DAT, AUT, and DSFT. Statistical analysis assessed the strength of the association between the DSFT and both the DAT and AUT. In line with a domain-specific theory of creativity, we hypothesized that there would be a non-significant relationship between the DSFT and the two domain-general measures of creativity.

First, replicating the work of Olson et al. (2021), results demonstrated a moderate, positive association between the DAT and both the Flexibility and Originality facets of the AUT. This replication further supports the validity of the DAT and its ability to measure domain-general creativity. The DAT was also significantly associated with the Elaboration facet of the AUT, which was not initially investigated by Olson et al. (2021). However, the DAT was not significantly associated with any of the three Creative Chemistry scores of the DSFT (Originality, Uniqueness, or Fluency). These findings supported our hypothesis and suggested that the cognitive processes that underlie general creativity do not translate to creativity within organic chemistry.

The relationship between the DSFT and the AUT provided more-interesting results: while there was no significant relationship between any facet of the AUT and the CC-Uniqueness or CC-Originality scores, the CC-Fluency score was significantly associated with two facets of the AUT (Originality and Flexibility). However, after correcting for multiple comparisons, neither finding remained significant—further supporting our hypothesis. Accounting for this correction, there were no significant correlations between the DSFT and any of the measures from the DAT or the AUT. This suggests that an individual's level of chemical creativity was in no way associated with their level of domain-general creativity. Taken together, the lack of significant associations between the domain-specific measure of creativity and the two domain-general measures provided further evidence for a domain-specific theory of creativity. This adds further evidence to a domain-specific theory of creativity and indicates that broad claims about domain-general creativity may be too strong

It is possible that a preregistered replication of the present study, which would not require corrections for multiple comparisons, may reveal some significant correlations (albeit rather small in magnitude) between the DSFT and the AUT and DAT. Even in such a case, however, it is plausible that such significant associations do not provide (weak) evidence for a domain-general view of creativity, but that these relations are instead driven by a third variable, or multiple third variables. One such third variable is fluid intelligence (Nusbaum & Silvia, 2011). It could well be the case that individuals with higher levels of fluid intelligence show superior performance on both the DSFT and the two tasks assessing domain-general creativity (i.e., the AUT and DAT), and that any significant relationship among these measures could therefore be driven by fluid intelligence, not a generalized creative ability. Similarly, motivation to perform well on research tasks could drive significant correlations between the DSFT and the AUT/DAT, not because of generalized creative abilities, but because intrinsically motivated individuals perform better on all tasks relative to extrinsically motivated individuals (Hennessey & Amabile, 2010). Thus, looking forward, we suggest that researchers preregister and attempt to replicate the present findings (without the need to correct for multiple comparisons), and that they index and statistically control for possible third variables such as fluid intelligence and motivation. If such a study were to be conducted, we would maintain our current hypothesis that creativity is domain-specific, not domain-general, as would be evidenced by the lack of a significant relationship between the DSFT and the AUT/DAT.

The debate between domain-specific and domain-general creativity has forced the creativity literature to reassess itself. The wide range of studies supporting domain-specificity and the very weak evidence supporting domain-generality make it easy to dismiss any measure that claims to be domain-general as invalid (Baer, 2008, 2015; Hennessey & Amabile, 2010). However, instead of dismissing domain-general measures of creativity as invalid, they should instead be classified in a more accurate manner, that is, domain-specific. Indeed, measures like the AUT and DAT have been validated and used in many studies, supporting their utility and popularity in research. Yet, both the DAT and AUT should be recategorized as domain-specific measures of verbal creativity. This classification would more accurately describe the measures and explain their high correlation, given that they measure creativity within the same domain.

Prior research has argued that support for a domain-general theory of creativity would come in the form of strong correlations between different creative behaviors (Ivcevic, 2007). The strong correlation between the DAT and the AUT has mistakenly been interpreted as such evidence. However, after categorizing the measures to their appropriate domain (e.g., verbal creativity), this strong evidence in favor of a domain-general theory of creativity disappears, as the creative behavior in question is now the same. Both the DAT and AUT are inherently verbal tasks that are rather different from artistic tasks, such as painting, and both tasks ask participants to manipulate the English language in similar creative ways.

Conceptual Ramifications

Theoretically, the CC-Fluency score can be thought of in terms of utility: a higher score here meant that more distinct chemical structures were drawn. These molecules are useful insofar as they achieve the purpose of the task, and organic chemistry is responsible for developing and producing modern drugs (Ball, 2015; Corey, 1991). Therefore, by drawing more molecules, one inherently increases the utility of their response.

Of note is that the CC-Originality score provides a cleaner, more error-free measure of the novelty of a response relative to the AUT. This claim is supported by the fact that the CC-Originality score used quantitative methods to measure the novelty of each structure compared to the group (indeed, in knowing exactly how many possible correct responses a given participant could provide, and in knowing exactly how many participants provided each of those correct responses, we were afforded the opportunity to perfectly quantify the novelty of each response within our sample). Importantly, equivalent methods of computing novelty are impossible to achieve with AUT, as there is a near-infinite number of possible responses and, hence, no way to perfectly quantify the novelty of a given response. Furthermore, scores derived from the AUT are reliant upon subjective qualitative coding to measure the novelty of responses. Thus, because the CC-Originality score can perfectly assess and quantify the novelty of each response, it provides a purer measure of novelty than the AUT. Of course, given that one of the defining features of creativity is novelty—in addition to utility—the ability of the CC-Originality score to allow for the perfect quantification of novelty is rather important, and suggests that the field would do well to consider not only administering the DSFT in future research, but also to consider developing new paradigms that similarly allow for the perfect quantification of novelty.

Concluding Remarks

The present study represents a first attempt to measure creativity within organic chemistry. We feel that further research examining the psychometric properties of the DSFT is necessary before the comprehensive implementation of the measure. Additionally, it must be pointed out how unrepresentative the sample employed was. All participants were attending a private liberal arts university and were enrolled in Organic Chemistry 2 Lab. Future research should employ samples from more diverse racial and socioeconomic backgrounds and expand the sample to include graduate students, professors, and industry professionals working in organic chemistry.

Despite these limitations, the DSFT has unique and exciting practical applications. Educators are now equipped with a tool to measure individuals' chemical creativity. While there are numerous ways to employ this measure in the classroom, one such way could use the DSFT to explore whether chemical creativity is associated with academic performance. Alternatively, building on pre-existing research relating to creativity-training studies, researchers could investigate the potential to increase chemical creativity through repeated iterations of the DSFT (Baer, 1994, 1996). Either way, the results of this study lend their support to a domain-specific theory of creativity and pave further insight to the creative mind in essential spheres of thinking. Future research should work to further disentangle the question of domain-specificity vs. domain-generality—realizing that a single theory is likely insufficient to describe a construct as grandiose and perplexing as creativity.

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Tables

Table 1

Descriptive statistics for all creativity measures

	N	Minimum	Maximum	Mean	Std. Deviation	Skewness (Std. Error)
Age	128	18.00	26.00	19.2969	1.10375	2.313 (.214)
Gender	128	0.00	4.00	0.4297	0.62347	2.152 (.214)
DAT	124	47.59	95.91	81.5765	6.43708	-1.290 (.217)
AUT: Originality	126	0.00	10.50	3.4921	2.00198	.832 (.216)
AUT: Flexibility	126	2.00	10.50	5.9206	2.09133	.271 (.216)
AUT: Fluency	126	2.00	19.50	8.0238	3.45882	.536 (.216)
AUT: Elaboration	126	3.00	43.00	18.0873	9.43209	.581 (.216)
CC: Originality	110	0.48	0.97	0.7547	0.13286	-.444 (.230)
CC: Uniqueness	110	0.46	0.95	0.5361	0.12759	1.835 (.230)
CC: Fluency†	110	1.00	47.00	7.9636	6.71562	2.675 (.230)

Note. AUT = Alternate Uses Task; CC = Chemical Creativity; DAT = Divergent Association Task.

†Log-transformed variable.

Table 2

Pearson product-moment correlation coefficients for the Chemical Creativity scores of the DSFT

	CC: Originality	CC: Uniqueness	CC: Fluency†
1. DAT: Creativity	.13	.02	.11
2. AUT: Originality	.17	.08	.25
3. AUT: Flexibility	.18	.04	.21
4. AUT: Fluency	.10	-.00	-.11
5. AUT: Elaboration	.14	-.01	.18

Note. After correcting for multiple comparisons (15 in total), only correlations with a p-value of .003 or less are considered significant. AUT = Alternate Uses Task; CC = Chemical Creativity; DAT = Divergent Association Task.

†Log-transformed variable. $^{*}p < 0.003$.

Appendix A

The Divergent Skeletal Formula Task (DSFT)

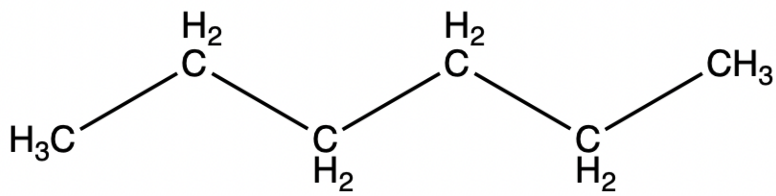
Background

As discussed in the preceding sections of this paper, divergent thinking tasks are commonly used to measure creativity. That is, divergent thinking tasks can measure fluency, novelty, usefulness, and other inherent facets of creativity. Evidence from a multitude of studies has demonstrated that creativity is likely domain-specific. Therefore, the measurement of creativity should also be domain-specific (Baer, 1993, 1996, 2012, 2015; Simonton, 1999). The Divergent Skeletal Formula Task (DSFT) was designed as a domain-specific measure of divergent thinking to accomplish this goal. In this case, the domain in question is organic chemistry. The DSFT was designed to test two out of the six production factors of divergent thinking: *originality* and *ideational fluency* (Guilford, 1956). Both are commonly emphasized within creativity research (Hocevar, 1980). To understand the DSFT, a discussion of basic chemical principles must ensue.

Organic Chemistry

Organic chemistry is the branch of science that deals with carbon-based compounds. There are approximately 15 million known organic compounds, and the number of possible organic compounds is virtually infinite. However, all of these compounds have one thing in common: they contain carbon (Loudon & Parise, 2015).

The unique aspect of organic chemistry—carbon— can also engender complexity and, of note for this paper, creative products. Carbon has the unique ability to combine with other carbon atoms to form long, complex molecules. This can prove tedious when drawing chemical structures for researchers and students alike. For example, consider the condensed formula representation below for hexane:

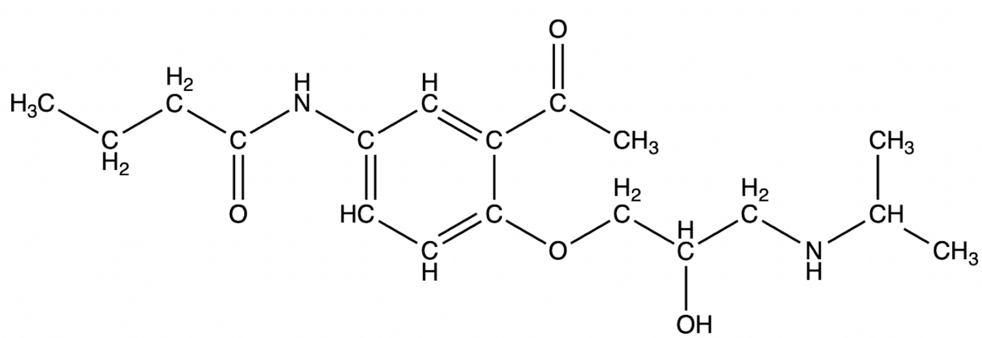


hexane

In this drawing, six carbon atoms are drawn (each denoted with a capital *C*), with each carbon attached to either two or three hydrogen atoms (each denoted with a capital *H* and a subscript for the total number of hydrogens per carbon atom). The line that connects two carbon atoms is a *chemical bond*, i.e., a strong force of attraction holding the atoms together.

Each carbon in this molecule has exactly four chemical bonds—the bonds to hydrogen atoms are not drawn; instead, they are implied. This idea of implied bonds explains why the carbons on the end of the molecule have three hydrogens while those within the molecule only have two. Note that carbon can never have more than four chemical bonds.

As molecules become larger and more complex, drawing them naturally becomes more strenuous. For example, take the blood pressure drug **Acebutolol** (a beta blocker).



N-[3-acetyl-4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl]butanamide
(Acebutolol)

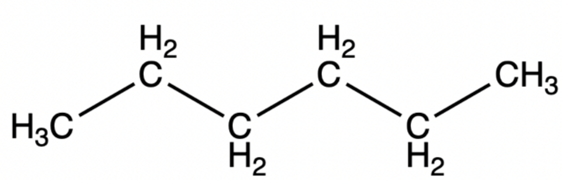
As can be seen, the molecule's structure is both elongated and elaborate. Additionally, the molecule has different connections (bonds) to atoms other than hydrogen. It also has double bonds, denoted by two lines between carbon and oxygen. To simplify the drawing of such complex carbon-based molecules, skeletal structures were invented.

Skeletal Structures

Learning organic chemistry has frequently been compared to learning a second language (Cadeddu et al., 2014). In this language, atoms are the letters and molecules are the words (Lehn, 1995). The purpose of any chemical structure diagram is to convey information—typically the identity of a molecule (Brecher, 2008). One of the most common structure-drawing conventions used in organic chemistry is the *skeletal structure.*

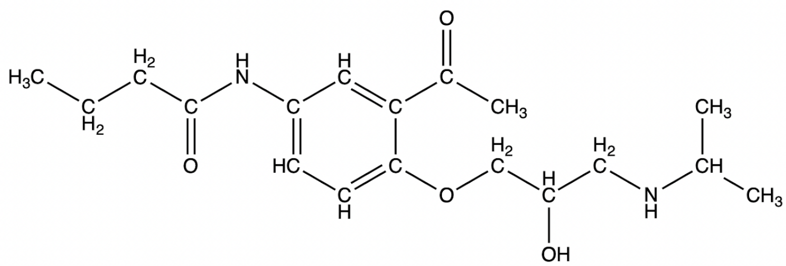
Skeletal structures are used so frequently in organic chemistry that they become second nature to organic chemists and students alike. Skeletal structures must abide by a simple set of rules: a carbon atom is located at the vertex or end of a geometric figure. It is also assumed that every carbon has four chemical bonds; if four bonds are not drawn to a vertex, then it is assumed that the remaining bonds are connected to hydrogen. Compare the skeletal structure of the six-carbon molecule above to its standard drawing:

hexane

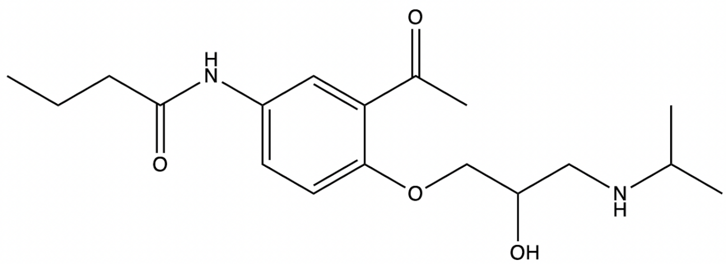


hexane

Every point on the above figure represents a carbon, and it is assumed that each carbon has four chemical bonds. This means that it is assumed that the carbons on the right and the left end of the molecule are each attached to three hydrogens, while the carbons between the two ends each are attached to two hydrogens. To see how dramatic the effects of skeletal structures are, let us return to **Acebutolol**:



N-[3-acetyl-4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl]butanamide



N-[3-acetyl-4-[2-hydroxy-3-(propan-2-ylamino)propoxy]phenyl]butanamide

It now becomes evident how beneficial skeletal structures are when drawing organic molecules. In addition to enhancing the efficiency of molecular drawings, skeletal structures also provide a unique opportunity to test divergent thinking—via constitutional isomers.

Constitutional Isomers

Constitutional isomers are molecules with the same molecular formula[1] (i.e., the same number of overall atoms) but differing connectivity (Ouellette & Rawn, 2018). To best understand the concept, an example will be given. Take the molecular formula C_2H_6O; this

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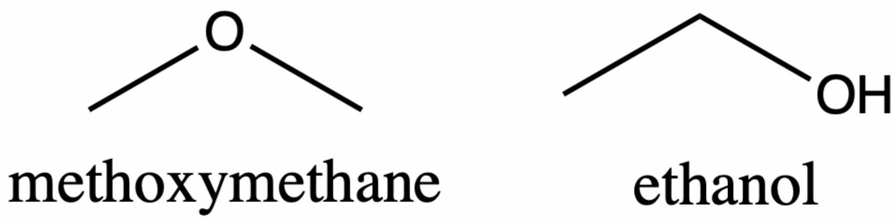
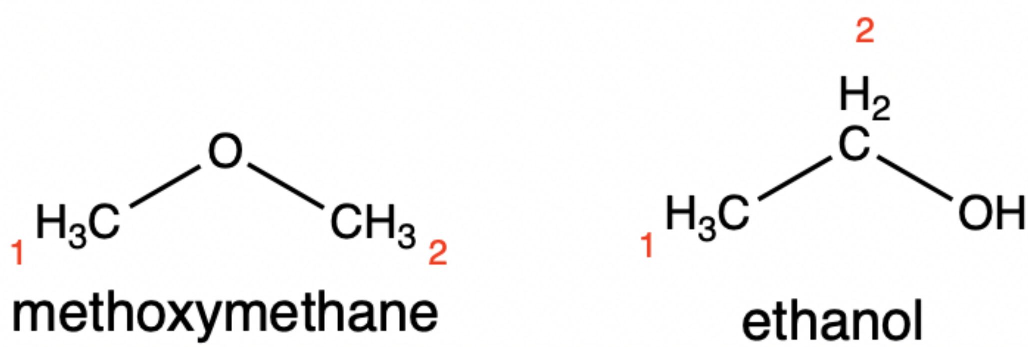
[1] A molecular formula gives the number of atoms of each of the elements present in a molecule. For example, C_4H_{10} represents any molecule that consists entirely of four carbon atoms and ten hydrogen atoms.

molecule has two constitutional isomers because there are only two ways of arranging all of the atoms in this molecular formula:



Each molecule—methoxymethane and ethanol—have exactly two carbon, six hydrogen, and one oxygen atom. To make this clearer, see the standard drawings of the two molecules:



Fundamentals of Divergent Thinking Tasks

Given the numerous outputs that can be created among carbon-based molecules, and the utility and novelty of such products, the link between organic chemistry and creativity (specifically, divergent thinking) becomes apparent. Previous research has demonstrated that divergent thinking is not only likely to be domain-specific but also heavily reliant on expertise within a domain (Baer, 2012, 2015; Baer & Kaufman, 2005; Feldhusen, 2006; Gardner, 1988, 2011; Palmiero et al., 2020; Simonton, 1999). When designing a domain-specific divergent thinking task, all participants must have adequate and equivalent levels of expertise. It is for this reason that skeletal structures were chosen as the medium.

The introduction of skeletal structures in a typical undergraduate organic chemistry course occurs within the first week of the start of the class. In a commonly used undergraduate textbook, skeletal structures are discussed almost immediately (i.e., the second chapter). Skeletal structures are then used ad nauseam for the rest of undergraduate organic chemistry courses and within the realm of chemistry academia. Due to their fundamental relevance within the subject, they were identified as an area of organic chemistry in which all students should have equal levels of expertise.

We developed a novel task, the Divergent Skeletal Formula Task (DSFT), which presented participants with a molecular formula and asked them to draw as many distinct constitutional isomers as possible using skeletal structures. Additional instructions were given to clarify the task along with specific chemical rules and paradigms that should be ignored (i.e., three-dimensional representations and molecular interactions)[2]. By having participants draw as many distinct constitutional isomers as possible, *ideational fluency* and *originality* were assessed.

Scoring the DSFT

As was previously discussed, the DSFT assessed originality and ideational fluency. Ideational fluency was assessed based on the total number of responses generated. It has previously been shown that fluency and creative achievement alone do not have a strong correlation, and thus some measure of response quality should always be used in conjunction with fluency scores (Plucker et al., 2011). Originality was assessed based on statistical probability (Reiter-Palmon et al., 2019; Sternberg, 2018). The lower the probability of a

[2] See Appendices B and C for the complete set of instructions that participants received for the DSFT.

participant drawing a structure compared to the group of participants, the more original the structure was deemed.

Each participant was given three variations of a *CC-score* (***C**hemical **C**reativity*). First, using the software ChemDraw and the website chemspider.com, it was determined that 372 unique constitutional isomers exist for the molecular formula $C_6H_{12}O$ (*Search ChemSpider*, n.d.). However, after filtering out all stereoisomers (i.e., isomers based on positioning in 3D space), 198 remained.

Every response to the DSFT was handwritten and uploaded as an image to Qualtrics. These images were re-drawn with the ChemDraw software and given computer-generated IUPAC names.[3] After naming the compounds drawn by a participant, a spreadsheet was created that kept a record of every isomer drawn by each participant. To calculate the probability of drawing any given isomer, the following formula was used:

$$P(I_x) = \frac{number\ of\ times\ isomer\ "x"\ was\ drawn}{total\ number\ of\ participants}$$

For example, if 100 participants participated in the survey and isomer #1 was drawn 12 times, the probability of drawing isomer #1 would be:

$$P(I_1) = \frac{12}{100} = 0.12$$

In other words, 12% of participants drew this isomer. This probability was calculated for all 198 isomers. These probabilities determined the *originality* of each isomer, i.e., the statistical frequency of each isomer.

The first score computed was the inverse-average of the probabilities (*CC-Originality).*

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[3] The IUPAC is the International Union for Pure and Applied Chemistry. It is the international authority on chemical nomenclature.

$$CC - Originality = \frac{1}{\frac{1}{n}\sum_{i=1}^{n} P(I_x)}$$

By inverting the average of the probabilities, the *CC-Originality* score gets larger as participants draw structures that are more statistically infrequent (i.e., original) and as they draw more structures. Thus, this score takes into account both ideational fluency and originality. If a participant did not draw any correct structures, there was no data with which to evaluate the creativity of their answer. Therefore, data from these participants was discarded from final analysis.

The second score calculated was the inverse of the single rarest probability (*CC-Uniqueness)*. The single rarest probability was the probability of the singular most statistically infrequent structure. The inverse was taken so that the *CC-Uniqueness* score increases as participants draw a structure that is more statistically infrequent (i.e., original). This score was calculated because one or two very original ideas can make a person creative, while pooling these highly creative ideas with all other ideas can weaken the effect and mask creativity (Frecska et al., 2012)

The third and final score was the fluency (*CC-Fluency)* and was the sum of the total number of structures drawn.

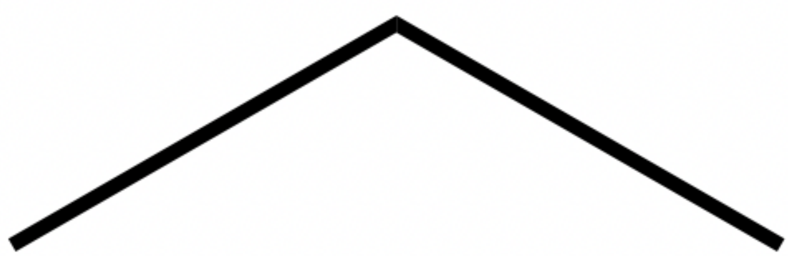
Appendix B

Instructions (introducing the task)

In this task, you will be presented a molecular formula and asked to draw as many distinct Constitutional Isomers as possible. Your molecules must be drawn in the form of skeletal structures. Keep the following information in mind:

1. Constitutional Isomers are compounds with the same molecular formula but different structural formulas.
2. All standard bonding conventions should be followed, but instability associated with sterics and bonding angles does not need to be considered
3. Pay no attention to stereochemistry, the molecules will not be scored for 3D representations (do not worry about enantiomers, diastereomers, meso compounds, S/R/E/Z configurations.)

For example, if the molecular formula was, C_3H_6, structures should be drawn in the following form:



Important: You will have 5 minutes to complete the task and 3 minutes to upload your work. After 8 minutes have elapsed you will automatically be moved to the next page of the survey. If you do not submit your work in the allotted time, your response will be marked as incomplete, and you will not receive compensation.

WARNING: **ALL RESPONSES MUST BE WRITTEN ON PAPER AND UPLOADED. NO WORK ON IPADS WILL BE ACCEPTED.**

This is to control for allowed time on the task. Before moving onto the next section, *please get a piece of paper and writing utensil read*y. If answers are not written on paper, **you will not receive compensation** for this study.

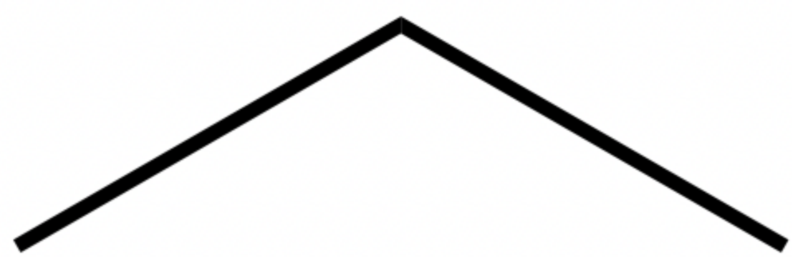
Appendix C

Instructions (as seen in survey, with specific molecular formula given)

Based on the following molecular formula, $\boldsymbol{C_6H_{12}O}$, draw as many distinct Constitutional Isomers as possible. Your molecules must be drawn in the form of skeletal structures. Keep the following information in mind:

1. Constitutional Isomers are compounds with the same molecular formula but different structural formulas (6 carbons, 12 hydrogens, and 1 oxygen must be present in every molecule you draw.)
2. All standard bonding conventions should be followed, but instability associated with sterics and bonding angles does not need to be considered.
3. Pay no attention to stereochemistry, the molecules will not be scored for 3D representations (do not worry about enantiomers, diastereomers, meso compounds, S/R/E/Z configurations.)
4. This molecule only has 1 degree of unsaturation (DoU = 1)

For example, if the molecular formula was, C_3H_6, structures should be drawn in the following form:



Important: You will have 5 minutes to complete the task and 3 minutes to upload your work. After 8 minutes have elapsed you will automatically be moved to the next page of the survey. If you do not submit your work in the allotted time, your response will be marked as incomplete, and you will not receive compensation.

***WARNING:* ALL RESPONSES MUST BE WRITTEN ON PAPER AND UPLOADED. NO WORK ON IPADS WILL BE ACCEPTED.**

This is to control for allowed time on the task. Before moving onto the next section, *please get a piece of paper and writing utensil ready*. If answers are not written on paper, **you will not receive compensation** for this study.

Appendix D

Instructions for the AUT

For this task you will be shown the name of a common object (e.g. "a brick") and your task is to come up with creative unusual uses for this object. For example if the object were “brick” you might write the following creative uses for this object:

• Use it as a paper weight
• Grind it up and use the sand to make paint
• Warm it up in the oven and put it in your bed to keep the bed warm

Your responses should be creative, useful and specific to the object. "Throw it into the ocean" is not a useful response and not specific to a brick, because you could throw anything into the ocean.

You will have 3 minutes to generate as many creative responses as possible for the object. Please separate your responses with a semicolon, colon, or comma.

There will be a total of two trials (i.e., two different items) in this experiment.

<u>Trial 1:</u>
Write down as many creative uses of a NEWSPAPER as you can

<u>Trial 2:</u>
Write down as many creative uses of a BALLOON as you can

Appendix E

Instructions for the DAT

In the following task, you will be asked to write 10 words that are as different from each other as possible, in all meanings and uses of the words. Enter the words one at a time in their designated box. There are a few rules to keep in mind:

1. Only single words.
2. Only nouns (e.g., things, objects, concepts).
3. No proper nouns (i.e., no specific people or places).
4. No specialized vocabulary (e.g., no technical terms).
5. Think of the words on your own (e.g., do not just look at objects in your surroundings).

For example, say your first word is DOG. Now for your second word you need to think of a word that is as unrelated to DOG as possible, like PAPERCLIP. Next you need to think of a third word that is as unrelated to both DOG and PAPERCLIP as possible, and so on.

Important: You will have 4 minutes to enter the 10 words for this round. Most participants finish in 1.5–2 minutes, but you may use the full time if you choose to.