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**Design, development, and evaluation of the Organic
chemistry Representational Competence Assessment
(ORCA)**

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7 Design, development, and evaluation of the Organic chemistry 8 Representational Competence Assessment (ORCA)

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14 This paper describes the design and evaluation of the Organic chemistry Representational Competence Assessment (ORCA).
15 Grounded in Kozma and Russell's representational competence framework, the ORCA measures the learner's ability
16 to *interpret, translate, and use* six commonly used representations of molecular structure (condensed structures, Lewis
17 structures, skeletal structures, wedge-dash diagrams, Newman projections, and chair conformations). Semi-structured
18 interviews with 38 first-semester organic chemistry learners informed the development of the ORCA items. The ORCA was
19 developed and refined through three pilot administrations involving a total of 3,477 first-semester organic chemistry
20 students from multiple institutions. The final version of the ORCA was completed by 1,494 students across five institutions.
21 Various analyses provided evidence for the validity and reliability of the data generated by the assessment. Both one-factor
22 and three-factor correlated structures were explored via confirmatory factor analysis. The one-factor model better captured
23 the underlying structure of the data, which suggests that representational competence is better evaluated as a unified
24 construct rather than as distinct, separate skills. The ORCA data reveal that the representational competence skills are
25 interconnected and should consistently be reinforced throughout the organic chemistry course.

23 Introduction and rationale

24 Learning and communicating with representations (e.g.,
25 chemical structures, graphs, or reaction equations) are essential
26 goals of chemistry instruction (Ainsworth, 2006; Gilbert, 2005;
27 Kozma & Russell, 2005). Correspondingly, representations are
28 integral to chemistry assessment. A historical analysis of
29 organic chemistry American Chemical Society (ACS) exams
30 revealed that more than 90% of exam items include at least one
31 representation (Raker & Holme, 2013). The ACS Exams Institute
32 includes visualizations as one of the ten anchoring concepts for
33 undergraduate chemistry (Murphy et al., 2012). Additionally,
34 the National Academies of Science emphasize the importance
35 of reasoning with representations to engage in scientific and
36 engineering practices (e.g., developing and using models,
37 analysing and interpreting data, and obtaining, evaluating, and
38 communicating information) (National Research Council,
39 2012a). It is, therefore, unsurprising that science educators and
40 discipline-based education researchers have devoted
41 considerable attention to learners' understanding of scientific
42 representations (National Research Council, 2012b).

43 Mastering the "language" of chemical representations is not

44 an easy task. Novices must learn *about* representations (e.g.,
45 how to interpret representations) and learn *with*
46 representations (e.g., use representations to make sense of
47 chemical phenomena) (Talanquer, 2022). Research shows that
48 learners rely on heuristics when making sense of
49 representations (Talanquer, 2014), primarily focus on surface
50 features of representations (Cooper et al., 2010; Popova &
51 Bretz, 2018c), and struggle to connect the external features of
52 representations to the conceptual information embedded in
53 them (Popova & Bretz, 2018a, 2018b; Rotich et al., 2024; Ward
54 et al., 2022). Despite the important role that representational
55 competence plays in learner success in chemistry (Ainsworth,
56 2006; Kozma & Russell, 2005; Schönborn & Anderson, 2008;
57 Seufert, 2003; Stieff et al., 2016), and the considerable number
58 of investigations into learners' ability to reason about symbolic
59 and submicroscopic representations (Bodner & Domin, 2000;
60 Connor et al., 2019; Cooper et al., 2010; Farheen and Lewis,
61 2021; Farheen et al., 2024; Lansangan et al., 2018; Miller & Kim,
62 2017; Padalkar & Hegarty, 2012, 2015; Popova & Bretz, 2018a,
63 2018b, 2018c; Stieff et al., 2016; Stull et al., 2016; Stull &
64 Hegarty, 2016; Ward et al., 2022; Wright & Oliver-Hoyo, 2020),
65 a limited number of assessment instruments exist that measure
66 learner competence with representations. Within this
67 manuscript, we describe the development of an assessment to
68 measure aspects of learner representational competence in the
69 context of multiple commonly used representations of
70 molecular structure.

Conceptual framework – Representational competence

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Representational competence (RC) is a "set of skills and practices that allow a person to reflectively use a variety of representations or visualizations, singly and together, to think about, communicate, and act on chemical phenomena in terms of underlying, apercceptual physical entities and processes" (Kozma and Russell, 2005, p. 131). Through an examination of expert and novice investigative chemistry practices (Kozma et al., 2000; Kozma & Russell, 1997), Kozma and Russell (2005) proposed a set of skills that comprise RC:

- use representations to describe observable chemical phenomena in terms of underlying molecular entities and processes (*use*),
- generate or select a representation and explain why it is appropriate for a particular purpose (*generate and select*),
- use words to interpret features of a particular representation (*interpret*),
- make connections across different related representations by mapping features of one representation onto those of another (*translate*),
- use representations in social situations to support claims, draw inferences, and make predictions about chemical phenomena (*use*),
- describe the limitations and affordances of different representations (*identify affordances and limitations*), and
- take the epistemological position that representations correspond to but are distinct from the phenomena that are observed (*take epistemological position*).

Most skills outlined above can be developed at a low foundational level or a higher meta-level that allows for the reflective and purposeful use of representations (diSessa, 2000; diSessa, Andrea & Sherin, 2000; Gilbert, 2005; Kozma & Russell, 2005; Ward et al., 2022). For the remainder of the article, we will use the succinct labels in parentheses to reference each skill.

RC is grounded in the cognitive theory of multimedia learning and situative theory. Together, these two theories highlight the interplay between cognitive processing and the social context of learning for understanding how students master chemical representations. The cognitive theory of multimedia learning assumes that learning occurs as a result of processing and synthesizing information across the audio and visual modes of instructional information (Kozma & Russell, 2005; Mayer, 2002). In particular, the ability to effectively process visual information is critical when it comes to learning chemical representations, as these often involve intricate visual details that convey essential information about sub-microscopic particles and processes. Situative theory suggests that the physical and social characteristics of a setting shape the processes of understanding and learning within that setting (Kozma & Russell, 2005; Lave, 1991; Lave & Wenger, 1991). As individuals become integrated into a community, they progressively develop in using its representational systems to construct new knowledge and communicate information. This integration and participation in communal practices enables learners to understand and manipulate the representations

used by that community, facilitating deeper learning and expertise in the subject matter.

Several assumptions underlie the development of RC. First, a developmental trajectory is assumed, implying that learners' ability to use chemistry representations increases as they progress in their learning. With continued learning, representations become a valuable tool for constructing and communicating understanding, resulting in the sophistication of RC over time (Kozma & Russell, 2005). Second, levels of RC are not assumed to be consistent for different types of representations. For example, a learner may be proficient with most of the RC skills for a particular representation (such as Lewis structures) and only be able to interpret the features of another (such as reaction coordinate diagrams) (Halverson & Friedrichsen, 2013; Kohl & Finkelstein, 2006; Stieff et al., 2011). Finally, RC and conceptual understanding are separate but related components of learner knowledge (Hinze et al., 2013; Maroo & Johnson, 2018). Proficiency in understanding chemical concepts is achieved in tandem with proficiency in utilizing the visualizations that represent and explain those concepts (diSessa, 2004; Kozma & Russell, 2005).

Studies investigating learner RC in chemistry have primarily relied on the use of interviews. Interviews provide nuanced and rich data on how learners engage and reason with representations that result in transferable conclusions. Many of these studies suggested a relationship between RC and conceptual understanding (Hiong & Daniel, 2015; Höst et al., 2012; Lansangan et al., 2007, 2018; Pande et al., 2015; Pande & Chandrasekharan, 2022). However, interview data do not allow for drawing robust, generalizable conclusions for various groups of learners, for example, those experiencing different learning environments (Herrington & Daubenmire, 2014). Studies that use assessments that can be easily administered and scored on a large scale have the potential to improve our understanding of RC as a construct and how to effectively develop RC through instruction. This need was highlighted by Kozma and Russell, who noted that "new assessments must be designed and used that measure investigation practices and related skills, such as visualization skills or representational competence" (Kozma & Russell, 2005, p. 142).

RC (Connor et al., 2021; Sim & Daniel, 2014), or frameworks related to RC (e.g., Visualization Competence of Matter (Chang & Tzeng, 2017) and Visual Model Comprehension (Dickmann et al., 2019)) have been the foundation of some assessments developed to elicit secondary or postsecondary chemistry learners' ability to make sense of representations. These assessments have corroborated findings from interviews stating that representational abilities are greater for learners who received more chemistry instruction (Chang & Tzeng, 2017; Vlacholia et al., 2017) or who have a higher conceptual understanding (Dickmann et al., 2019; Sim & Daniel, 2014). In addition, a few studies found that competence varies by skill or topic (Chang, 2018; Chang & Tzeng, 2017). However, these assessments are either not used to investigate learner RC explicitly (Chang, 2018; Chang & Tzeng, 2017; Dickmann et al., 2019; Vlacholia et al., 2017; Wang et al., 2017), are focused on a single aspect of RC (Connor et al., 2021), or a limited number

Journal Name	ARTICLE
1 of representations (Connor et al., 2021; Sim & Daniel, 2014)	54
2 Some of these assessments have useful but limited evidence	55
3 the validity of resulting data, primarily in the form of content	56
4 validity using expert panels (Chang, 2018; Chang & Tzen, 2017).	57
5 This contrasts with more robust evaluations of validity	58
6 and reliability, including content validity as well as a broad	59
7 array of psychometric evidence. To advance our understanding	60
8 of learner RC, quality assessments that demonstrate evidence	61
9 of valid and reliable data are needed that comprehensively	62
10 capture multiple RC skills in the context of multiple	63
11 representations (Kozma & Russell, 2005).	64
12 Purpose of this study	65
13 This work aims to develop and evaluate the Organic	67
14 chemistry Representational Competence Assessment (ORCA)	68
15 to characterize learners' RC in the context of six commonly used	69
16 representations of molecular structure in undergraduate	70
17 organic chemistry instruction: condensed structures, chair	71
18 conformations, wedge-dash diagrams, Lewis structures,	72
19 skeletal structures, and Newman projections. Chemical	73
20 representations have various dimensions (<i>i.e.</i> , iconicity,	74
21 granularity, dimensionality, and quantitateness) that impact	75
22 how learners reason about and with representations	76
23 (Talanquer, 2022). This study, in particular, centers on symbolic	77
24 representations with similar dimensions (Johnstone, 1993).	78
25 The ORCA is designed as a multiple-choice assessment	79
26 permitting testing with a large number of participants and	80
27 allowing for quick grading. The assessment captures three	81
28 skills: the ability to (a) use words to interpret features of a	82
29 particular representation – the <i>interpret</i> skill; (b) make	83
30 connections across different related representations by	84
31 mapping features of one representation onto those of another	85
32 – the <i>translate</i> skill; and (c) use representations to draw	86
33 inferences – the <i>use</i> skill. These skills are among the most	87
34 commonly taught by organic chemistry educators (Jones et al.,	88
35 2022; Linenberger & Holme, 2015; Popova & Jones, 2021) and	89
36 in organic chemistry textbooks (Gurung et al., 2022). The ORCA	90
37 does not assess the learner's ability to generate	91
38 representations, another skill typically taught in the target	92
39 course, as it is difficult to evaluate this skill properly using	93
40 multiple-choice questions. Other RC skills were not considered	94
41 for the ORCA as current instruction offers little to no support	95
42 for those skills (Gurung et al., 2022; Jones et al., 2022; Linenberger	96
43 & Holme, 2015; Popova & Jones, 2021). Two research questions	97
44 guide this study:	98
45 1. What evidence exists for the validity and reliability of	99
46 the data generated from the Organic chemistry	100
47 Representational Competence Assessment (ORCA)?	101
48 2. What do the data collected with ORCA reveal about	102
49 learner representational competence?	103
50 Methods: Data collection, analysis, and evidence	104
51 of validity and reliability of the data	105
52 Criteria for developing and evaluating the ORCA were	106
53 adopted from the Standards for Educational and Psychological	107
54	108
55	109
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Testing (American Educational Research Association, 2014) and	
guided by other primers for assessment development in	
chemistry education (Arjoon et al., 2013; Komperda et al., 2018;	
Towns, 2008, 2014). The development and evaluation processes	
are organized by the various stages and shown in Table 1 .	
Institutional Review Board guidelines were met at every	
institution where data were collected and in all stages of the	
assessment development and evaluation. All participants were	
informed that their ORCA performance would not negatively	
impact their course grades. Additionally, the participants could	
consent or decline consent for their responses to be included in	
this research study.	
We iteratively developed the ORCA by using a sequential,	
mixed-methods exploratory design (Towns, 2008) and a	
bottom-up approach that originated from analyses of learner	
reasoning about representations of molecular structure	
collected using semi-structured interviews (Bowen, 1994). At	
the time of their participation, all participants were in the first	
semester of a year-long organic chemistry course, having	
completed the two-semester general chemistry sequence. We	
wrote assessment items from the interview data collected at	
one institution (Stage I), and we refined these items through	
three pilot administrations with participants at six institutions	
(Stage II) using the Qualtrics platform. The final ORCA version	
was administered to learners at five institutions (Stage III) via	
Qualtrics. Only learners who completed the entire assessment	
received extra credit for their participation, which is why all	
participants completed ORCA in its entirety, and we did not	
have any missing data.	
Stage I – Assessment development	
We conducted semi-structured interviews; data from a	
portion of these interviews were used to design the ORCA	
items. We recruited participants (<i>N</i> = 38) from a public	
university in the southeastern US during the Fall of 2019 and	
Spring of 2020. The participants were enrolled in five different	
Organic Chemistry I course sections taught by four instructors	
using the same curriculum and textbook (Bruice, 2016). We	
purposefully sampled learners, using a stratified method	
(Patton, 2002), to ensure a range of grades (from "A" to "C") in	
General Chemistry II. Participants were compensated with a \$20	
gift card. Pseudonyms were assigned to all participants to	
protect their identities. Data were captured using an audio	
recorder, a video camera, and a Livescribe smartpen	
(http://www.livescribe.com).	
The interviews were designed to elicit learners' RC skills. To	
capture how learners <i>interpret</i> a representation, participants	
were asked to (a) describe what the representation	
communicates, (b) decode each diagrammatic feature of the	
representation (<i>e.g.</i> , dashes, wedges, lines, symbols, etc.), (c)	
explain the purpose of the representation, and (d) identify the	
atomic composition for the given representation. To elicit how	
learners <i>use</i> a representation, participants were asked to	
examine a given representation and make inferences about (a)	
chemical and physical properties, (b) bonding, and (c) energy	
and stability. To capture how learners <i>translate</i> between	
various representations of molecular structure, the participants	

were given a specific representation and asked to choose the corresponding structure(s) from four options. They were informed that each task may have more than one corresponding structure. After selecting the corresponding

structure(s), the participants were asked to explain why they believed the structure(s) corresponded and why the other options did not.

Table 1. ORCA development and evaluation.

Method	Outcome	Application
Stage I – Assessment development		
Semi-structured think-aloud interviews	Elicit learner ability to reason with representations	Generate items and distractors from participant responses to establish validity evidence based on test content
Expert evaluation	Obtain feedback from experts about the appropriateness of the items for the measurement of the target construct	Establish validity evidence based on test content and revise items accordingly
Stage II – Pilot administrations		
Item analysis	Understand item difficulty, item discrimination, and how well distractors function	Revise items accordingly to ensure item quality
Factor analysis	Investigate the number of factors, the variables that load onto each factor, and the level of correlation among factors	Establish internal structure validity and revise instrument accordingly
Cognitive interviews	Obtain insight into respondents' thought processes and feedback about items	Establish response process validity and revise items accordingly
Expert evaluation	Obtain additional feedback from experts about the appropriateness of the items for the measurement of the target construct	Establish validity evidence based on test content and revise items accordingly
Stage III – Final administration		
Item analysis	Understand item difficulty, item discrimination, and how well distractors function	Ensure item quality
Factor analysis	Confirm the factor structure of the revised ORCA instrument	Establish internal structure validity
Reliability coefficient	Understand correlations between items	Establish internal consistency/reliability

The data from the interviews were transcribed verbatim inductively coded using ATLAS.ti software (version <https://atlasti.com/>), and analyzed using constant comparative analysis (Glaser, 1965). The first and the second author coded the data and, depending on a code, obtained 84–100% agreement (Saldaña, 2013). Furthermore, they discussed each case of disagreement in their coding until a 100% negotiated agreement was reached. In addition, the first, second, and six authors met weekly to discuss the codes and analyze the data for patterns. Some of the qualitative results from these analyses have been published elsewhere (Rotich et al., 2024; Ward et al., 2022).

We then used these data to generate over 100 assessment items to capture how learners *interpret*, *translate*, and *use* representations of molecular structure. Figure 1 depicts how we used participant interview data (Figure 1A) to write an item that asks participants to *use* Newman projections to make inferences about stability (Figure 1B). Response choices, including distractors, were developed using participants' ideas from the interview and reflected the most common patterns of participant thinking. We reviewed all the items and eliminated items if: (a) there were too many items about the same representation or skill, (b) items were complex multiple-choice questions (Albanese, 1993; Towns, 2014), or (c) items were not representative of the skills learners typically learn in the course (*i.e.*, *translating* between a chair conformation and a condensed structure). This process resulted in condensing the assessment to 64 items.

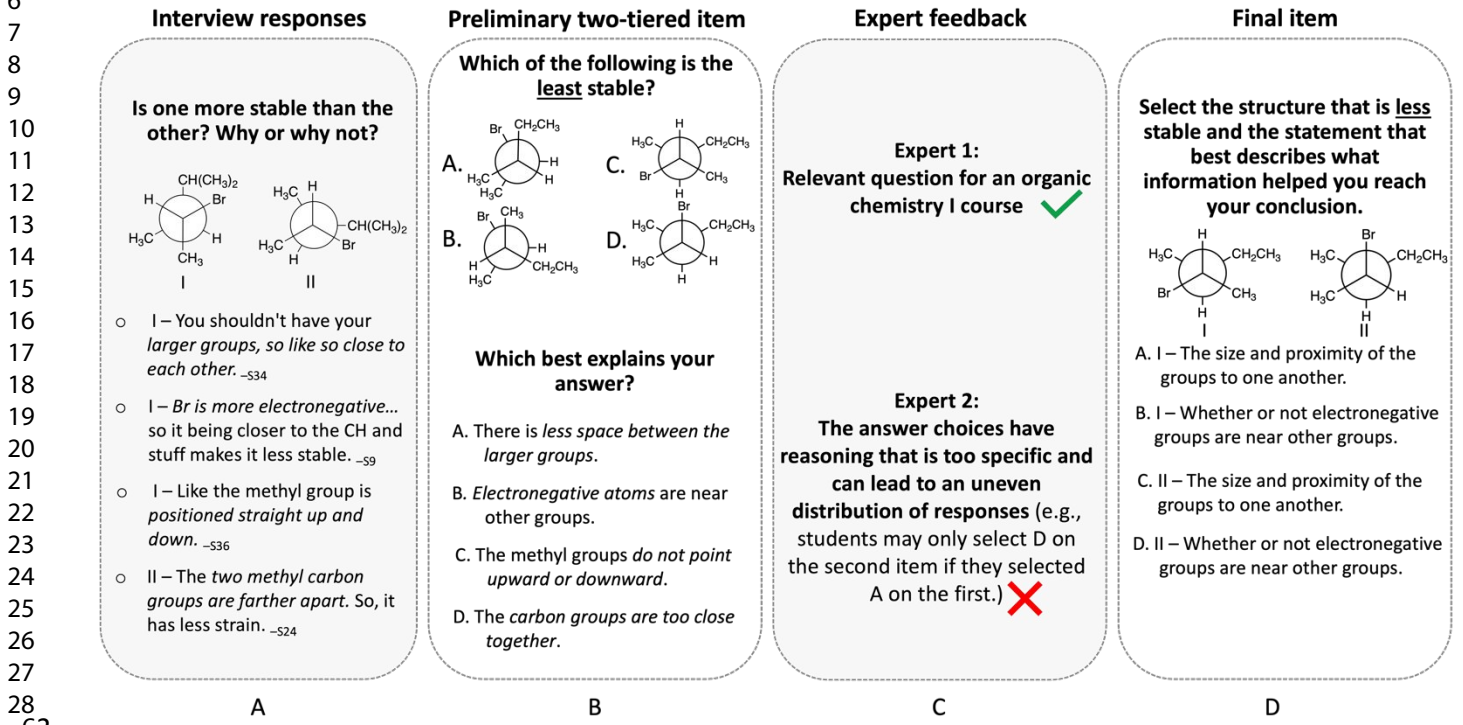
An expert panel of six organic chemistry instructors and chemistry assessment developers evaluated all 64 items for content validity. We used the feedback from the expert panel members (Figure 1C) to eliminate some items and refine other items (Figure 1D). This process resulted in 48 items for which the expert panel established that the items adequately covered the relevant content to measure the target constructs (*interpret*, *translate* between, and *use* representations of molecular structure) and were appropriate for the target population (organic chemistry learners). In addition, they provided feedback about terminology and the scoring of items.

Stage II – Pilot administrations

Following expert evaluation, we pilot-tested the 48 items. During each pilot test, participants completed the assessment at least three weeks after covering the six target representations of molecular structure in their Organic Chemistry I course. In consensus with the feedback received from the expert panel, and to minimize item priming, we administered the assessment items in a specific order, such that *translate* items appeared first, then *use* items, and lastly, *interpret* items. Within each skill, the items were randomized for each participant.

Pilot I: In Fall 2021, the 48 items were administered as a Pilot I to learners ($N = 1,120$) taught by five instructors at two (medium and large) public universities in the southeastern US. To ensure a timely assessment, we split the items into two 24-item forms that could be completed in less than 30 minutes. Each form had comparable items that featured the same

representations and targeted the same skills. For example, were to use a Newman projection to make inferences about stability. Participants randomly received one of the two Form 1 and Form 2 each contained one item where participants



Pilot III: Finally, we tested the finalized 26-item ORCA again as a Pilot III in the middle of the Fall 2022 semester with participants ($N = 1,790$) across six medium and large public universities in the southeastern, midwestern, and western US. The instrument contained seven *interpret* items, eleven *translate* items, and eight *use* items. Once again, we examined the quality of the items for distractor selection, item difficulty, and item discrimination, as well as conducted CFA to investigate the internal structure of the assessment. Only one item performed poorly on Pilot III. The terminology for this *use* item had been adjusted after the response process interviews in Pilot II and this led to poor discrimination and low difficulty. Recognizing the impact of this change, we reverted the terminology of this item to its original format from Pilot II for the final administration. Additionally, the expert panel evaluated the refined assessment instrument to confirm the content validity. Persons interested in obtaining a copy of the finalized ORCA should see the ESI.

Stage III – Final administration

The final ORCA was administered at the end of Fall 2022 to Organic Chemistry I learners from five institutions: one medium public university in the southeastern US and four large public universities in the southeastern, midwestern, and western US. Participants completed the assessment with a median time of 22 minutes, and 1,508 participants consented for their ORCA responses to be used in this study. Many participants in Pilot III were also part of the final administration. However, the timeframe between the two administrations was over six weeks to minimize the likelihood of participants recalling specific items from Pilot III. Additionally, to further reduce the possibility of recall effects, we implemented a randomization strategy for both the items and their response choices during the final administration. This means that even if students participated in both phases, the presentation of the items and response options in the final administration differed from their arrangement in Pilot III.

Next, we identified any potential data outliers. Based on the recommendations of Aguinis and colleagues (2013), we used single (*i.e.*, box plots and percentage analysis) and multiple construct techniques (*i.e.*, scatterplots, Mahalanobis distance, and studentized deleted residuals). Fourteen outliers (*i.e.*, complete response sets for a given participant) were removed through these analyses. Outlier data had *interpret* item scores of zero and often had extremely high (*e.g.*, 340 minutes) or low (*e.g.*, 94 seconds) completion times. This process resulted in a final sample of 1,494 responses for analysis.

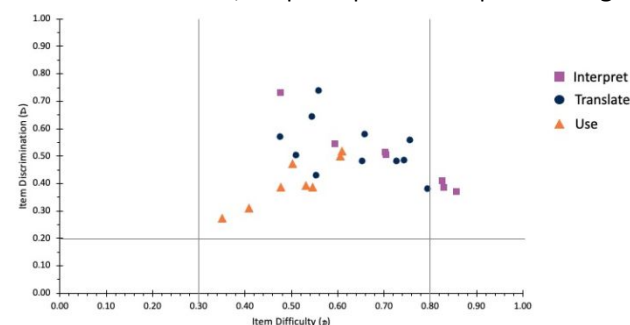
We conducted CFA using MPlus 8 (Muthén & Muthén, 2017) to investigate the internal structure of the assessment instrument. With the RC framework (specifically, the *interpret*, *translate*, and *use* skills) as a theoretical basis, we tested two hypothesized models to evaluate and confirm the number and

nature of latent factors. The Means and Variance Adjusted Weighted Least Squares (WLSMV) method was best suited for the analysis (Finney & DiStefano, 2013) as all measured variables were categorical (binary). A good model fit for these categorical data is more stringent than the criteria suggested by Hu and Bentler (Beauducel & Herzberg, 2006; Hu & Bentler, 1999; McNeish & Wolf, 2023; Xia & Yang, 2019). Though the model fit cutoffs are not absolute and the conditions for their use are still undergoing research (McNeish et al., 2018; McNeish & Wolf, 2023), we use criteria adopted by Komperda and colleagues for good fit (*i.e.*, Comparative Fit Index (CFI) $> .95$ and the Root Mean Square Error of Approximation (RMSEA) $< .05$). The proposed models were congeneric, which is why McDonald's omega (ω) was calculated as a reliability indicator to examine the internal consistency of the items within each latent factor (Hancock and An, 2018; Komperda, Pentecost, and Barbera, 2018).

Results and discussion

Gathering evidence for the internal structure validity and internal consistency of the ORCA data

Item difficulty and discrimination from the final ORCA administration with 1,494 participants are reported in **Figure 2**.



All items sufficiently discriminated ($\rho > 0.2$) between the top 27% and bottom 27% of performers (Bandalos, 2018). There was a range of difficulties for the items, with most falling in the 0.3 – 0.8 range.

Figure 2. Item difficulty and discrimination for the final ORCA administration. *Interpret* skill items are shown as purple squares, *translate* skill items as blue circles, and *use* skill items as orange triangles.

Confirmatory Factor Analysis. Based on Kozma and Russell's RC framework, we proposed two models to estimate the internal structure validity of the data. Model A is a three-factor model where each latent factor represents an RC skill (*i.e.*, the ability to *interpret*, *translate*, and *use* representations). In this model, each item was set to load onto its corresponding factor with correlations between the three factors (**Figure 3A**). Model B is a one-factor model in which all

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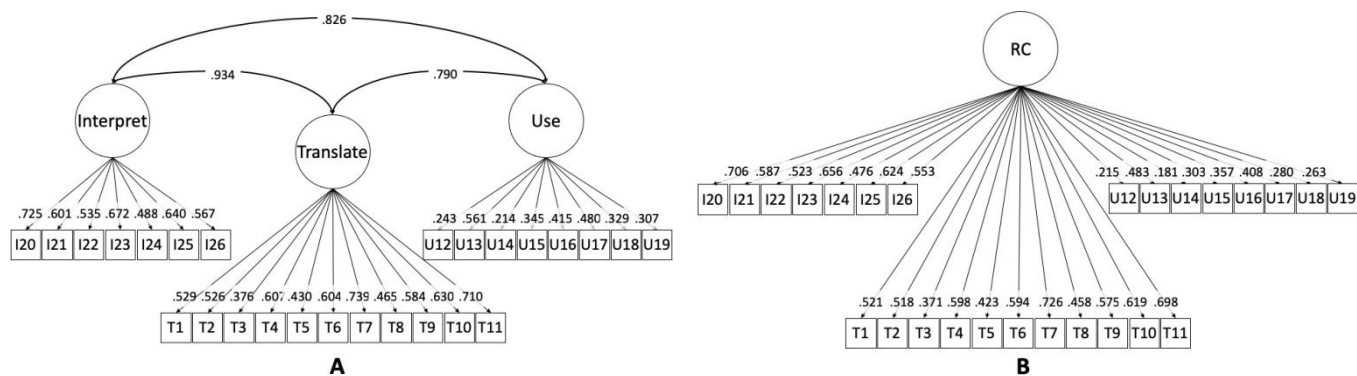


Figure 3. Standardized parameter estimates for the three-factor (A) and one-factor (B) models. Circles indicate the latent variables. Squares indicate the observed variable item scores. Double-headed arrows between circles represent correlations between factors and the arrows between circles and squares represent factor loadings. Items in model A were set to load on their assigned factors only. All factor loadings are significantly different from zero ($p < .001$).

Table 2. Fit statistics and reliability for the two proposed models.

Model	Fit Statistics					McDonald's Omega (ω)		
	χ^2	df	p	RMSEA ($\leq .05$)	CFI ($\geq .95$)	Interpret	Translate	Use
A – 3 factor	694	296	<.0001	.030	.955	.807	.843	.554
B – 1 factor	741	299	<.0001	.031	.950		.897	

items load onto a single latent factor representing RC (Figure 3B). Model fit statistics and the McDonald's omega coefficient are reported in Table 2.

The data meet the fit criteria for Model A. However, internal consistency for the factors, as measured through McDonald's omega reliability coefficient, varied by skill. The *translate* and *interpret* factors have a higher reliability, indicating that these common constructs (i.e., the ability to *translate* between representations and the ability to *interpret* features of individual representation, respectively) explain a larger amount of the observed variance to the total variance (Komperda, Pentecost, and Barbera, 2018). The *interpret* skill and *translate* skill items require learners to reason by attending to the diagrammatic features within single or multiple representations (e.g., interpreting dashes and wedges in wedge-dash diagrams, mapping dashes and wedges onto the appropriate axial and equatorial substituents in chair conformations). For this reason, the *interpret* skill and *translate* skill factors are highly correlated (Figure 3A), as students reason about the features of the representations (i.e., composition, connectivity, or spatial information, if applicable) to *interpret* and *translate* between representations.

In contrast, the *use* skill factor has a lower McDonald's omega, so a common construct (i.e., the ability to *use* representations to make inferences) explains less of the

observed variance. This is not surprising because the *use* skill items require participants to not only reason by attending to the features of representations but also by extracting the relevant domain-specific conceptual knowledge embedded in the representation. Moreover, this conceptual knowledge varies by representation (e.g., evaluating the arrangement of substituents in Newman projections to make an inference about *stability*; evaluating the functional groups in skeletal structures to make an inference about *physical properties*). In this case, not only do learners need to be able to make sense of the features of a representation, but they also need to have a conceptual understanding of stability or physical properties, and know which relevant features of the representation to attend to make inferences about these concepts. Therefore, a lower reliability for the *use* skill factor is hypothetically expected as it may not be a homogenous construct (Taber, 2018); however, this lower reliability also limits the inferences that can be made about the *use* skill from the items within this assessment. Moreover, the factor loadings (Figure 3A) for the *interpret* and *translate* factors are higher than those in the *use* factor, further indicating that the *interpret* and *translate* skill factors explain more variance within the items (Bandalos, 2018).

Komperda and colleagues (2018) suggest that when "an instrument is known to be composed of multiple scales where

scores will be reported separately, each scale should be evaluated to determine if it fits a single-factor model, and a reliability value should be provided for each scale of data." Data for each factor of Model A were evaluated with individual latent factor models; these CFA results provide support that *interpret* and *translate* scales fit the data and have factor loadings > 0.62 (see **Figure S1** and **Table S1** in the Appendix). However, while the RMSEA is appropriate, the CFI for the *use* skill is below the more stringent cut-off for categorical data. Given that the *use* scale has a weaker model fit, these analyses provide evidence that only the *interpret* and *translate* scales can function independently. In summary, although Model A has a solid theoretical basis, aligned with the stance that RC is a "set of skills and practices that allow a person to reflectively use a variety of representations" (emphasis added; Kozma and Russell, 2005, p. 131), and the data meet the thresholds for the fit statistics, the *use* scale has items that have lower factor loadings, weaker internal consistency, and, unlike the *interpret* and *translate* scales, cannot be used independently.

In comparison, Model B is a single-factor model where every item loads onto a single latent factor—RC. The data fit Model B (**Figure 3B**), suggesting that this model effectively captures the underlying structure of the data. Model B accounts for the high latent correlation between the *interpret* and *translate* scales (evidenced as 0.934 in **Figure 3A**). While it is possible that the ORCA may be limited in distinguishing these factors, it is more likely that these skills are very related and should be considered one factor, as reflected in Model B. Additionally, the internal consistency (as measured by McDonald's omega) is higher for the one-factor model B than the three-factor model A. While the increased internal consistency may be attributed to the larger number of items within a single factor (Malkever et al., 2023), the empirical data better align with the single-factor structure. This suggests that in the context of representations of molecular structure, these RC skills are better evaluated as a unified construct rather than as distinct separate skills. Below, we delve deeper into the implications of these findings and share insights into measuring student RC.

Insights gained about learner representational competence

The section below outlines two main insights from examining the data collected with the ORCA about student proficiency with six key representations of molecular structure in undergraduate organic chemistry: condensed structures, chair conformations, wedge-dash diagrams, Lewis structures, skeletal structures, and Newman projections. These representations are essential to student success in organic chemistry, and our findings provide insights into learner proficiency with these symbolic representations.

Representational competence skills are interconnected

The high correlation between each skill in Model A led to the selection of Model B as the best data-fit model (**Figure 3**). These correlations indicate that the items intended to measure separate skills may actually be assessing the same underlying construct. In practice, it is difficult to *interpret*, *translate*, or *use* representations of molecular structure independently, as these skills inherently rely on and reinforce one another. This

particularly the case with the *interpret* skill, which is requisite for the co-development of the rest of the skills. This interconnectedness suggests that RC might be better understood as an interconnected set of skills rather than distinct, separate abilities. Furthermore, many tasks and assessments in chemistry require learners to simultaneously apply multiple RC skills, reinforcing the idea that these skills are not isolated but are used in concert. This perspective highlights that the effective use of chemical representations often depends on the seamless integration of various interrelated skills.

Two examples from our item-level analysis of participant performance further illustrate the interconnectedness of RC skills. Specifically, we observed instances of students having the necessary conceptual understanding to *use* a representation to make an inference but not being able to connect this knowledge to the appropriate features of representations, which relates to the *interpret* skill.

Item U15, shown in **Figure 4A** (the same item as in **Figure 1D**), required participants to make inferences about the stability of Newman projections and justify their reasoning by relying on the concepts embedded in the diagrammatic features of the representation. With the answer choices in this item, participants could have relied on the concepts of substituent size or electronegativity. **Figure 4B** demonstrates that the likelihood of selecting the correct answer C is lower for bottom ORCA performers (bottom 27%) and higher for top performers (top 27%). Almost a quarter of participants (23%, **Figure 4C**) selected response choice A, in which they chose the wrong structure while reasoning about the appropriate concept of substituent size. These participants knew the productive conceptual information to make inferences about stability but could not connect that knowledge to the proper diagrammatic features of the Newman projection. Finally, almost a quarter of the participants relied on the wrong conceptual information (electronegativity) and selected responses D (13%) or B (11%). This quarter of participants comprise less than 9% of the top performers but over 45% of the bottom performers. For this item, the bottom performers struggled to identify the productive concept of interest.

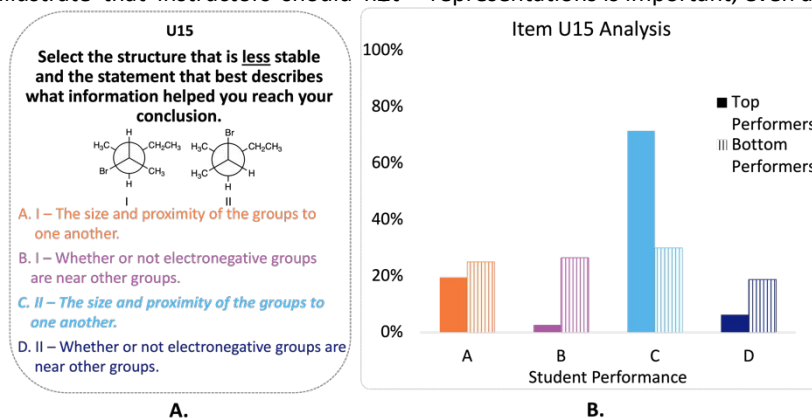
Item U14 (**Figure 5A**) demonstrated a similar pattern. The correct answer, B, was chosen by 41% of all participants. A slight majority of bottom performers (55%) relied on the productive concept reflected in choices B and D. These participants were able to identify the appropriate feature (charge) and connect it to the appropriate concept (octet). However, half of them could not connect that knowledge to the appropriate diagrammatic features to make accurate inferences about stability. Thus, they incorrectly selected the structure with an atom with an incomplete octet (D). Almost a third (30%) of all participants selected response choice D. Finally, nearly a third of the participants chose responses A (20%) or C (9%). These participants relied on features like the presence or absence of double bonds that were not as relevant to the concept of interest (stability) in this prompt.

These examples highlight the complex interplay of RC skills required to answer such questions. Successfully *using*

representations to make inferences about a concept demand a combination of knowledge and ability to (1) *interpret* diagrammatic features of a representation, (2) conceptually understand the concept of interest, (3) distinguish the relevant from irrelevant features of the representation in relation to the concept of interest, and (4) connect the relevant features of the representation to one's conceptual understanding to make an inference about the concept of interest. Each of these steps is necessary when making inferences about representations.

Representational competence should not be assumed
Instructors are not always intentional about developing learner RC (Jones et al., 2022; Linenberger & Holme, 2015; Popova & Jones, 2021). Our data illustrate that instructors should not

assume that RC has been acquired after traditional instruction. For example, instructors may assume that *interpreting* the wedge-dash diagram in **Figure 6** should be relatively simple and that learners have developed the fundamental ability to identify implicit hydrogens. However, we administered ORCA at the end of the first semester of organic chemistry, and 30% of participants selected an incorrect answer. This is problematic because the inability to identify all implicit hydrogen atoms may significantly impact learner success in the course. For example, this skill is necessary for identifying chiral centers, completing β -elimination reactions, and solving ^1H NMR spectroscopy problems. Our data show that providing learners with continuous practice interpreting implicit atoms in representations is important, even after initial instruction.



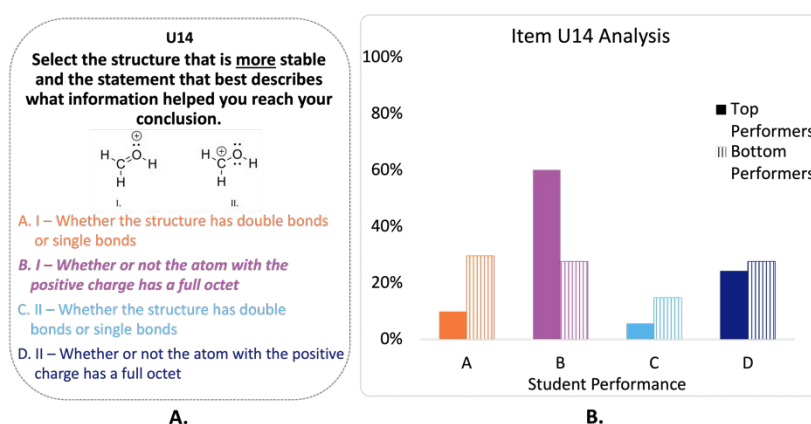
A.

B.

Option	Answer	Reasoning	Count	Percent
A	Incorrect	Appropriate	347	23%
B	Incorrect	Inappropriate	157	11%
C	Correct	Appropriate	795	53%
D	Correct	Inappropriate	195	13%

C.

Figure 4. Item U15 (A) with the correct answer in bold and italics. The chart (B) shows the response choice distribution for the top 27% and bottom 27% of participants. The count and percentage of learners selecting each answer are shown in table (C).



A.

B.

Option	Answer	Reasoning	Count	Percent
A	Correct	Inappropriate	301	20%
B	Correct	Appropriate	610	41%
C	Incorrect	Inappropriate	131	9%
D	Incorrect	Appropriate	452	30%

C.

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Figure 5. Item U14 (A) with the correct answer in bold and italics. The chart (B) shows the response choice distribution for the top 27% and bottom 27% of participants. The count and percentage of learners selecting each answer are shown in table (C).

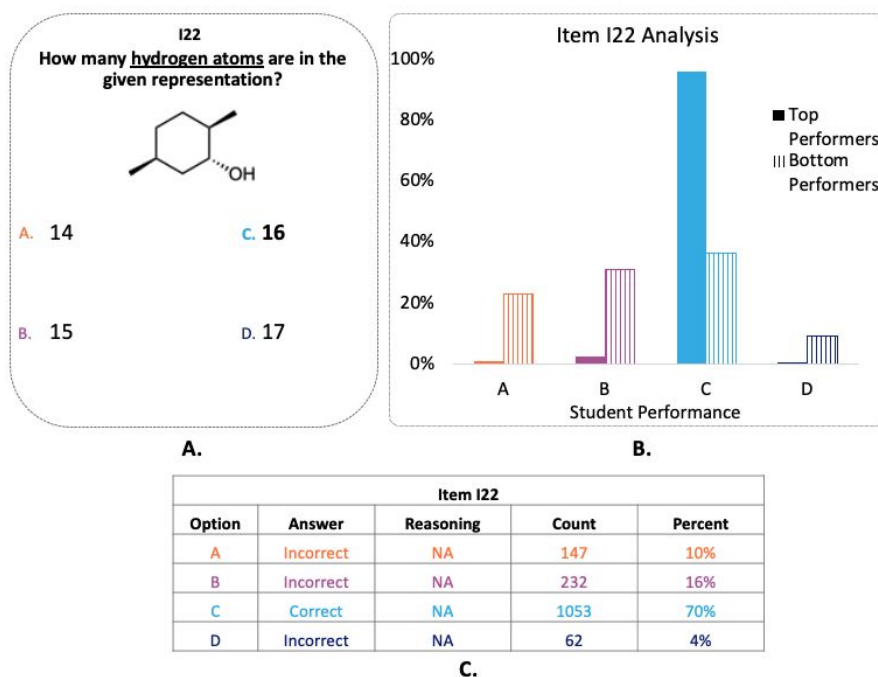


Figure 6. Item I22 (A) with the correct answer in bold. The chart (B) shows the response choice distribution for the top 27% and bottom 27% of participants. The count and percentage of learners selecting each answer are shown in table (C).

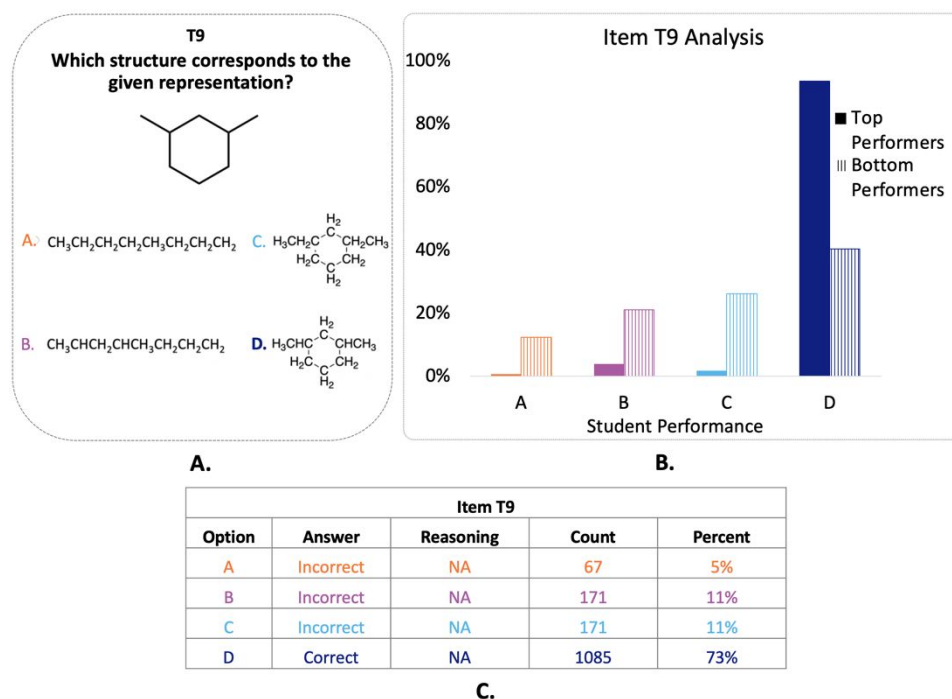


Figure 7. Item T9 (A) with the correct answer in bold. The chart (B) shows the response choice distribution for the top 27% and bottom 27% of participants. The count and percentage of learners selecting each answer are shown table (C).

Item T9 is another item that some may assume is easy but had relatively surprising responses. The item requires learners to *translate* between a cyclic skeletal structure and a condensed structure with two of the four answer choices in which the right is open (Figure 7A). Most participants selected the correct answer, but over 15% selected a non-cyclic condensed structure (Figure 7C, options A and B). Participants who select these incorrect answer options for a *translate* task do not adequately understand the representations or the chemical phenomena represented, even after a whole semester of organic chemistry. As shown, developing RC should be intentional and repeatedly reinforced throughout the curricula.

Limitations

Several limitations should be acknowledged. First, the ORCA is limited as it includes items related to only three RC skills. However, these skills are among the most commonly taught by chemistry instructors (Jones et al., 2022; Linenberger & Holme, 2015; Popova & Jones, 2021) and reinforced in organic chemistry textbooks (Gurung et al., 2022). More research is needed to investigate and develop quality assessments that will incorporate the remaining RC skills.

Second, the ORCA assesses learner RC in the context of multiple representations of molecular structure but is not exhaustive (e.g., representations such as electrostatic potential maps and ball-and-stick models are not included even though they have unique affordances to students (Farheen et al., 2024)); we selected symbolic representations only to feature representations with similar dimensions and features

(Talanquer, 2022). More assessments are needed to capture learner RC with other representations in chemistry.

Third, the *use* items capture learners' ability to make inferences about stability and boiling point only, even though there are other properties that the six target representations could convey. This narrower focus connects to what is covered in instruction and ensures the assessment can be administered in a reasonable timeframe (about 20 minutes). There is potential to consider additional items that focus on other concepts (e.g., aromaticity, acidity).

Fourth, the participants who completed the final assessment also took the assessment during the pilot III administration. There were at least six weeks between assessment administrations (depending on the institution), but this means there is a possibility of practice effects (i.e., improved performance due to familiarity with test items) (American Educational Research Association et al., 2014). Currently, there is no benchmark for when practice effects diminish. Other studies have as low as one month between test administrations (Bretz & Linenberger, 2012).

Lastly, the assessment was administered only online; however, it can be easily adapted to the classroom setting for paper-and-pencil administration. Administering the assessment online was a purposeful choice; this allowed for easy access to learners and a quick collection of data. Assessments given in different conditions (such as virtual versus in class), with differing constraints (e.g., not being able to sketch notes), and scored for correctness versus completion (including for bonus points) all likely have varying but overall consistent data (Harle & Towns, 2011).

Conclusions

Herein, we describe the development of the Organic chemistry Representational Competence Assessment (ORCA). Grounded in the RC framework (Kozma & Russell, 2005), the ORCA captures learner competence with six representations of molecular structure: condensed structures, chair conformations, wedge-dash diagrams, Lewis structures, skeletal structures, and Newman projections. ORCA items include three interconnected RC skills: the ability to *interpret* representations, *translate* between representations, and *use* representations to draw inferences. The assessment is designed to be multiple choice to permit testing (a) with a large number of learners, (b) in a short amount of time, and (c) to allow for quick and easy scoring. Evidence of the validity and reliability of the ORCA data were established through multiple administrations at several institutions in the US and captured via a variety of methods such as response-process interviews, expert panel feedback, CFA, and McDonald's omega (Table 1).

Two models were proposed to evaluate the internal structure validity of the data generated: a three-factor Model A and a one-factor Model B. While Model A has a solid theoretical basis, our data showed a better fit with Model B. This single-factor model consolidates the skills into a unified latent RC construct, accounting for the high correlation between the *interpret* and *translate* skill factors in Model A. This model can be readily used to assess organic chemistry learner RC in the context of representations of molecular structure. Our study is an important step toward advancing and reconceptualizing our understanding of RC as a *network of interconnected* skills.

Implications

The ORCA can be used as a formative assessment in instruction or as an assessment instrument in research. The ORCA takes about 20 minutes to complete and can be used by instructors to make the necessary adjustments to their instruction and provide feedback to their students about their competence with representations of molecular structure. A single score from the ORCA can provide a measure of learner RC, as reflected by Model B. Given that formative assessments are regarded as a high-impact instructional practice (National Research Council, 2012; Offerdahl & Arneson, 2019), the use of ORCA to receive and implement formative feedback has the potential to improve learner RC and conceptual understanding.

For example, ORCA can be used as a diagnostic tool early in the course to identify areas where students may need additional support, such as with more complex skills like *use* of representations. Based on students' performance, instructors can implement progressive scaffolding, offering explicit guidance early in the semester on how to *use* different representations. As students build confidence, the level of support can be gradually reduced to encourage independent *use* of representations.

At the same time, instructors should not assume that it is sufficient to discuss a given representation once, early in the semester. Our findings show that even by the end of the

semester, many students struggled with basic tasks, such as identifying implicit hydrogen atoms in wedge-dash diagrams or distinguishing between cyclic and acyclic molecules. It is, therefore, imperative that instructors periodically incorporate explicit explanations of the features of representations that they use in their instruction without assuming that students mastered these representations at the beginning of the course.

Additionally, it's crucial for students to articulate their reasoning, especially when tackling more complex tasks that require *using* representations to make inferences. Our item analysis revealed that for students to effectively *use* molecular representations to make inferences, they must be able to do four essential steps: (1) interpret the diagrammatic features, (2) understand the underlying concept, (3) identify relevant versus irrelevant features, and (4) connect those relevant features to their conceptual understanding to draw inferences. Without eliciting students' reasoning, an instructor or researcher will not be able to understand which of these steps present the challenge for students when *using* representations to make inferences. This complexity should be taken into consideration when designing assessment tasks or interview prompts.

The ORCA can also be used or adapted as an assessment instrument in studies that aim to advance our understanding of RC as a construct or how to best support learners in developing RC. Prior to using the ORCA, it is imperative that researchers evaluate their data for evidence of validity and reliability (American Educational Research Association et al., 2014; Lazenby et al., 2023). For example, the ORCA can provide evidence of how instructional practices impact learner RC and can be used in longitudinal studies to show how learner RC changes throughout instruction (Kozma et al., 2000). These investigations could help elucidate a learning progression for the development of RC or identify an optimal organic chemistry curriculum for developing RC with representations of molecular structure. While there are existing interventions that support individual RC skills in organic chemistry (Stieff et al., 2016; Stull et al., 2016; Stull & Hegarty, 2016), more research needs to be done to develop interventions that support RC more broadly. In this way, the ORCA can be used as a pre-post measure to provide empirical evidence of approaches that may be useful to support organic chemistry learners.

Future research could also use the ORCA data to conduct Structural Equation Modelling (SEM) to evaluate the relationship between learner RC and other relevant constructs such as their visuospatial ability, conceptual understanding, or success in the organic chemistry course (Nitz et al., 2012; Sim & Daniel, 2014; Stieff et al., 2014, 2018; Stieff & DeSutter, 2020).

While this work focuses on symbolic representations of molecular structure, organic chemistry and other chemistry disciplines also rely on a variety of other representations (e.g., ball-and-stick models, spectra, reaction coordinate diagrams, phase diagrams, and molecular orbital diagrams) that require RC. The process we used to develop the ORCA can be adapted to assess RC skills in these other contexts. Expanding this approach across different contexts will deepen our understanding of how learners develop RC. We encourage the community to build on this work to refine our collective

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understanding of RC and explore the most effective strategies for supporting learners in developing these important skills.

Ethical Considerations

This study has been approved by the University of North Carolina's Institutional Review Board (IRB #20-0511). IRB guidelines were met at every institution where data were collected and in all stages of the assessment development and evaluation. All participants were informed that their ORCA performance would not negatively impact their course grades. Additionally, the participants could consent or decline consent for their responses to be included in this research study. In accordance with the approved IRB protocol, the findings are presented only in aggregate, and the original data sets cannot be shared due to confidentiality considerations.

Author Contributions

All authors participated in data collection and/or analysis. Author M.P. conceptualized and led the project and obtained funding for the work. F.R. conducted the interviews and assisted in analyzing data. L.W.W. led the qualitative and psychometric analyses. J.R., S.N., and R.K. provided guidance on the psychometric analyses. L.W.W., M.P., and F.R., wrote the manuscript with input from the rest of the authors.

Conflicts of interest

There are no conflicts to declare.

Acknowledgments

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Appendix

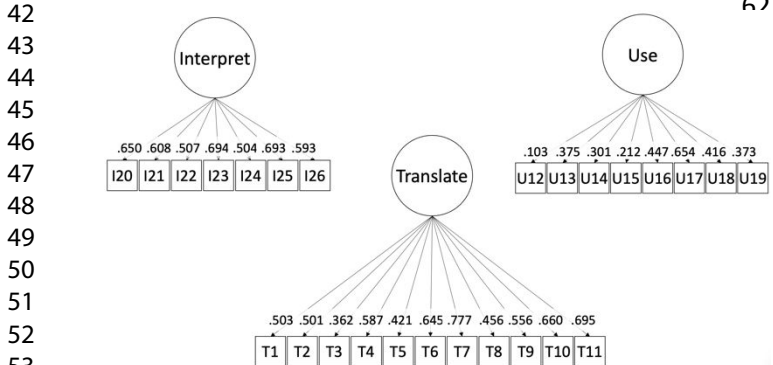


Figure S1. Item loadings of the one-factor models for the *interpret*, *translate*, and *use* scales.

Table S1. Fit statistics and reliability for each latent factor in Model A as a single-factor model.

Factor	Fit Statistics					Reliability
	χ^2	df	p	RMSEA	CFI	McDonald's Omega (ω)
Interpret	7.709	14	.9039	<.0001	>.999	.807
Translate	200.343	44	<.0001	.049	.950	.843
Use	52.015	20	<.0002	.033	.915	.554

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Electronic Supplemental Information
Design, development, and evaluation of the Organic chemistry Representational
Competence Assessment (ORCA)

Lyniesha Ward,^a Fridah Rotich,^a Jeffrey R. Raker,^b Regis Komperda,^c Sachin Nedungadi,^d and Maia Popova^{*a}

^aUniversity of North Carolina at Greensboro, Greensboro, North Carolina, USA

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^cSan Diego State University, San Diego, California, USA

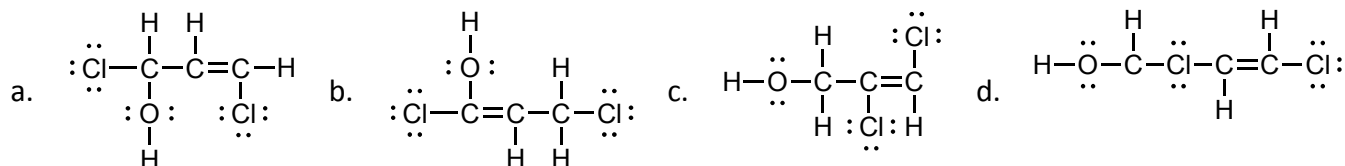
^dUniversity of Nebraska at Omaha, Omaha, Nebraska, USA

*E-mail: m_popova@uncg.edu

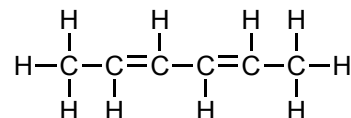
NOTE: If you are interested in using ORCA, please contact the corresponding author.

Directions: Identify the choice that best completes the statement or answers the question.

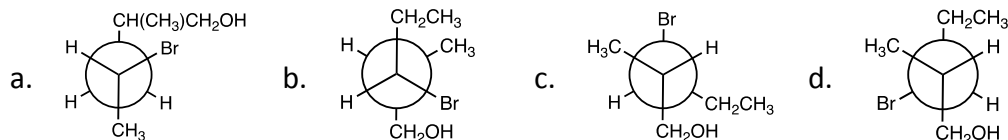
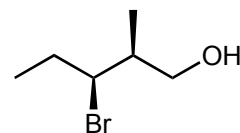
1. Which structure corresponds to the given representation?



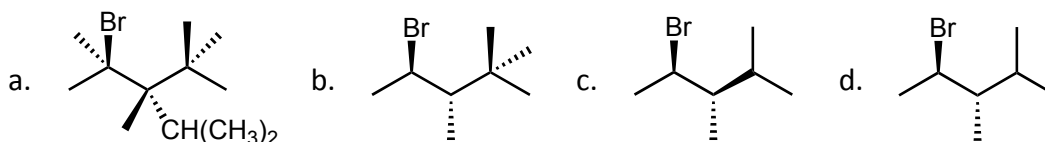
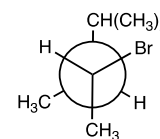
2. Which structure corresponds to the given representation?



3. Which structure is different from the given representation?



4. Which structure corresponds to the given representation?



5. Use the given representation below to answer this question.

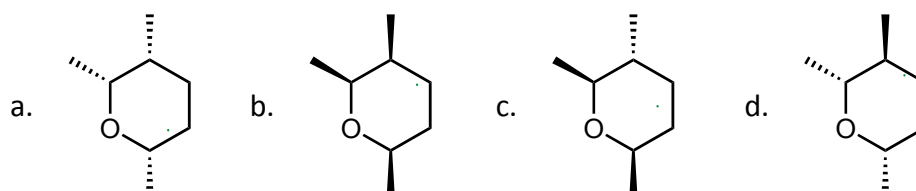
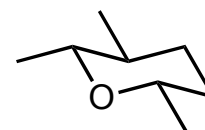


Select the structure that is the same molecule as the given representation and the statement that best describes what information you focused on to reach your conclusion.

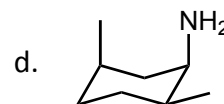
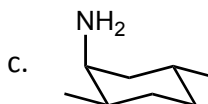
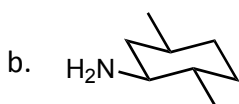
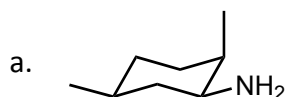
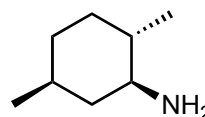


- a. I – Whether the groups are on the left side in relation to the ring
- b. I – Whether the groups are up versus down in relation to the ring
- c. II – Whether the groups are axial versus equatorial in the ring
- d. II – Whether the groups are on the outer edges of the ring

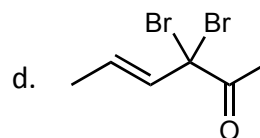
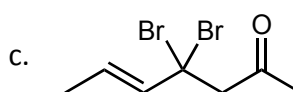
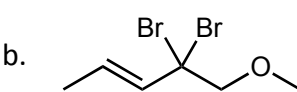
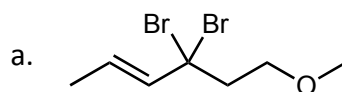
6. Which structure corresponds to the given representation?



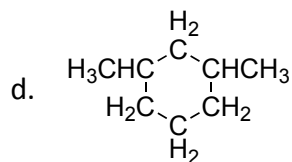
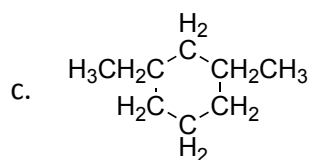
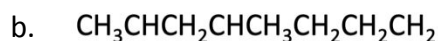
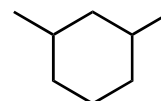
7. Which structure corresponds to the given representation?



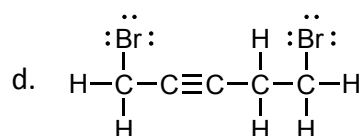
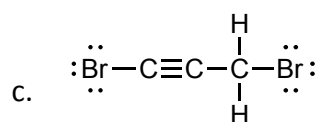
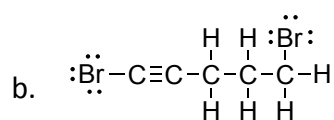
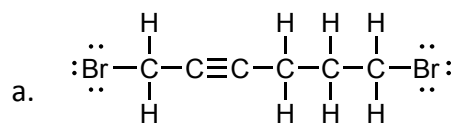
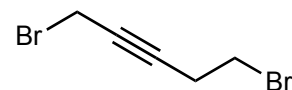
8. Which structure corresponds to the given representation?



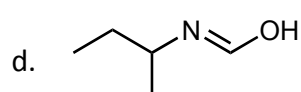
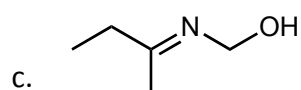
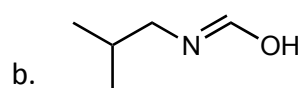
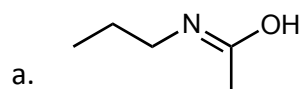
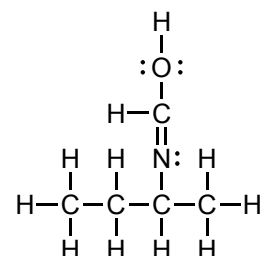
9. Which structure corresponds to the given representation?



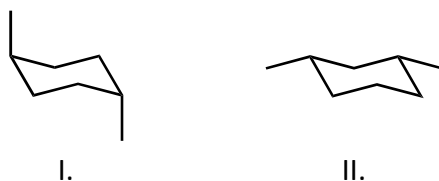
10. Which structure corresponds to the given representation?



11. Which structure corresponds to the given representation?



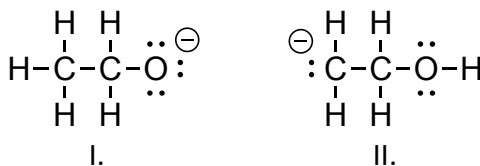
12. Select the structure that is the more stable and the statement that best describes what information you focused on to reach your conclusion.



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- a. I – The amount of space between the groups
 - b. I – Whether the groups are pointing up or down
 - c. II – The amount of space between the groups
 - d. II – Whether the groups are pointing up or down

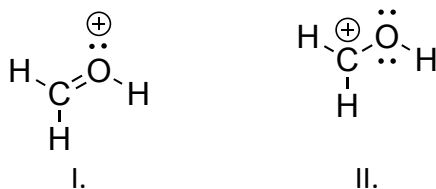
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13. Select the structure that is the less stable and the statement that best describes what information you focused on to reach your conclusion.



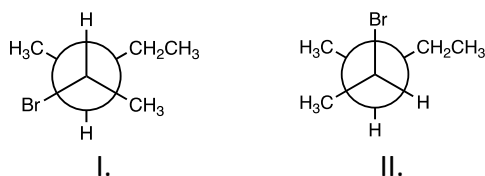
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- a. I – The electronegativity of the atom with the negative charge
 - b. I – The absence of a full octet on the atom with the negative charge
 - c. II – The electronegativity of the atom with the negative charge
 - d. II – The absence of a full octet on the atom with the negative charge

14. Select the structure that is the more stable and the statement that best describes what information you focused on to reach your conclusion.



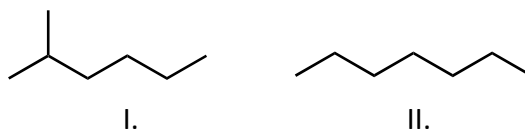
- a. I – Whether the structure has double bonds or single bonds
- b. I – Whether or not the atom with the positive charge has a full octet
- c. II – Whether the structure has double bonds or single bonds
- d. II – Whether or not the atom with the positive charge has a full octet

15. Select the structure that is the less stable and the statement that best describes what information you focused on to reach your conclusion.



- a. I – The size and proximity of the groups to one another
- b. I – Whether or not electronegative groups are near other groups
- c. II – The size and proximity of the groups to one another
- d. II – Whether or not electronegative groups are near other groups

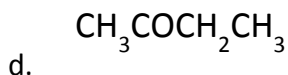
16. Select the structure with a lower boiling point and the statement that best describes the information you focused on to reach your conclusion.



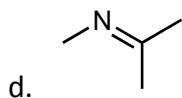
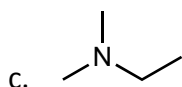
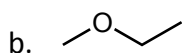
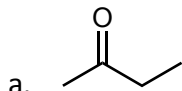
- a. I – Whether the molecule has branching
- b. I – Whether the molecule is symmetrical or asymmetrical
- c. II – Whether the molecule has branching
- d. II – Whether the molecule is symmetrical or asymmetrical

17. Which of the following compounds has the highest boiling point?

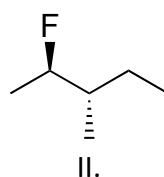
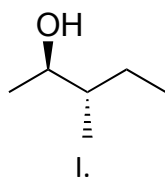
- a. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$
- b. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$
- c. $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$



18. Which of the following compounds has the highest boiling point?

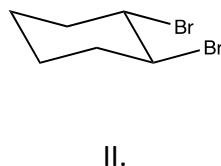
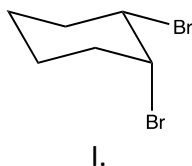


19. Select the structure with a higher boiling point and the statement that best describes the information you focused on to reach your conclusion.



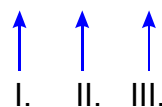
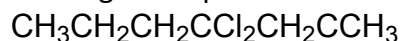
- a. I – How strong the bonds are between atoms
- b. I – How strong the interactions are between molecules
- c. II – How strong the bonds are between atoms
- d. II – How strong the interactions are between molecules

20. Select the structure that has bromine atoms on opposite sides in relation to the ring and the statement that best describes what information you focused on to reach your conclusion.



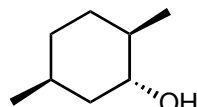
- a. I – Whether the bromine atoms are axial versus equatorial in relation to the ring
- b. I – Whether the bromine atoms are up versus down in relation to the ring
- c. II - Whether the bromine atoms are axial versus equatorial in relation to the ring
- d. II - Whether the bromine atoms are up versus down in relation to the ring

21. To which labeled atom(s) is/are the chlorine atoms connected in the given representation?



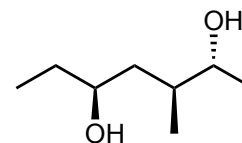
- a. Carbon I
- b. Carbon II
- c. Carbon III
- d. Carbons II, III

22. How many hydrogen atoms are in the given representation?



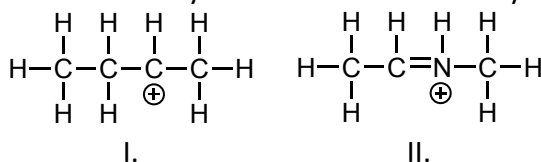
- a. 14
- b. 15
- c. 16
- d. 17

23. Which best describes the given representation?



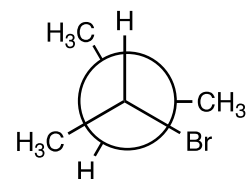
- a. The broken dash line is directed out of the page.
- b. The bold wedge lines are directed into the page.
- c. The thin lines are flat in the plane of the page. The bold wedge and broken dash lines are not.
- d. Neither the thin lines, the bold wedge lines, nor the broken dash lines are flat on the plane of the page.

24. Select the structure(s) that has/have an atom with an incomplete octet and the statement that best describes what information you focused on to reach your conclusion.



- a. I – It is missing a pair of electrons.
- b. II – It is missing a pair of electrons.
- c. I, II – They have a positive formal charge.
- d. I, II – Their outer shells are not filled.

25. How many carbon atoms are in the given representation?

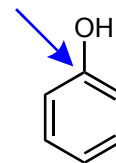


- a. 3
- b. 4
- c. 5
- d. 6

26. Which best describes the atom indicated with an arrow in the given representation?

It is connected to...

- a. Two carbons and one oxygen.
- b. Three carbons and one oxygen.
- c. Two carbons, one oxygen, and one hydrogen.
- d. Three carbons, one oxygen, and one hydrogen.



Data Availability Statement

Design, development, and evaluation of the Organic chemistry Representational Competence Assessment (ORCA)

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In agreement with the confidentiality measures and procedures approved by the University of North Carolina's Institutional Review Board (IRB # 20-0511), the data cannot be made available.