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To be or not to be a model? Exploring chemistry students' ideas about general and specific meta-modeling knowledge regarding reaction mechanisms in organic chemistry

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Developing and using models is recognized as a core scientific practice. This includes, among other things, the reflection on models at the epistemic level, referred to as meta-modeling knowledge (MMK), which encompasses both media-oriented and methodological perspectives regarding models. In organic chemistry, reaction mechanisms function as central models to describe, explain, and predict chemical reactions. Given the discipline- and context-dependent character of MMK, we distinguish between general MMK and specific meta-modeling knowledge (SMMK) related to organic reaction mechanisms. While prior work has examined students' challenges with models and modeling as well as mechanisms in organic chemistry, little is known about how students' general MMK and their discipline-specific epistemic perspective on reaction mechanisms interact in shaping students' reasoning. To address this, we conducted a qualitative interview study with 22 chemistry students. The study explored how students perceive the modeling character of reaction mechanisms and patterns across students' ideas within the SMMK and MMK dimensions. The findings show that students expressed a diverse range of ideas, from viewing reaction mechanisms as pictorial representations of reaction pathways to understanding them as epistemic tools used in inquiry processes or for practical purposes. Students' ideas varied not only within the SMMK dimension but also in how these were related to ideas within the MMK dimension, indicating multiple, coexisting epistemic ideas. Different patterns emerged across the identified student groups: some students demonstrated comparable ideas across both dimensions, whereas others showed rather varying ideas within and across the two dimensions.

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Introduction

In recent years, science education has experienced a shift from the mere teaching of scientific ideas by authorities to students' engagement in more authentic scientific practices (Duschl, 2008; Osborne, 2014; Forman, 2018). Hodson (2014) emphasizes that learning goals should no longer focus solely on *learning science* but should also address the dimensions *learning about science* and *doing science*. The ambition is to enable students to become epistemic agents who actively engage in knowledge construction (Berland *et al.*, 2016; Miller *et al.*, 2018). Within this practice turn, the National Research Council (2012) identified eight core scientific practices that foster meaningful learning among students, one of which is *developing and using models*.

Models are central tools in scientific practices (Giere, 1999) that enable access to explanations of the empirical world (Bailer-Jones, 2003). Accordingly, modeling includes the construction and refinement of models to describe, explain, and predict phenomena (Gilbert and Osborne, 1980; Gilbert *et al.*, 1998; Schwarz *et al.*, 2009; Oh and Oh, 2011). Through modeling, scientists are provided with frameworks that allow them to formulate hypotheses, manipulate variables, and establish connections between observations and explanations in the empirical world (Gilbert, 1991; Odenbaugh, 2005). In doing so, all models are based on assumptions that inherently involve idealizations (Winkelmann, 2023), which results in models having distinct contexts of application, limitations, and being dependent on the modeler's perspective (Grosslight *et al.*, 1991; Bailer-Jones, 2003). Awareness of this nature of models and active engagement in the practice of modeling can contribute to a deeper understanding of the Nature of Science (Harrison and Treagust, 2000; Schwartz, 2019). In turn, this can foster scientific literacy (Lederman and Lederman, 2014; Justi and Gilbert, 2016), which, in the sense of a "functional understanding of science" (Ke *et al.*, 2021, p. 590), may be seen as an overarching goal of science education – both within scientific disciplines and for everyday life.

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To develop such an understanding, students at all levels need to engage with models and in modeling processes. There are two ways in which models are used in science that are relevant in this regard: thinking *with* models and thinking *about* models (Passmore *et al.*, 2017). Thinking *with* models involves using previously established models to explain or predict phenomena within a specific context, as well as constructing, evaluating, and refining individual models to address diverse questions (Passmore *et al.*, 2017). In contrast, thinking *about* models refers to active reflection on an epistemic level – considering, for instance, what is incorporated into a model, which boundaries, limitations, or domains of application it has, and how it can be used within the modeling process (Grosslight *et al.*, 1991; Passmore *et al.*, 2017; Upmeier zu Belzen *et al.*, 2019). Thinking *about* models is also referred to in the literature as meta-modeling knowledge (*e.g.*, Schwarz and White, 2005; Krell, 2019; Lazenby *et al.*, 2020) or, less frequently, as epistemic modeling knowledge (Lateef *et al.*, 2025).

While models and modeling practices are relevant across all sciences, they are particularly prominent in chemistry. The discipline is inherently model-based (Justi and Gilbert, 2003a Closing parenthesis appears in the next line; please adjust formatting. (p. 2, left column, l. 24-25)), as chemists model phenomena at the macroscopic, the submicroscopic, and the symbolic level (Johnstone, 1993). At the macroscopic level, relevant entities are first identified, idealized, and represented through macroscopic models. At the submicroscopic or symbolic level, the underlying processes and interactions are then explained through models and representations (Talanquer, 2022; Talanquer, 2025). The content in chemistry is therefore mostly embedded in models (Justi and Gilbert, 2002; Lazenby *et al.*, 2019b), and the forms of representation as well as the types of information contained in these models can vary considerably, for instance, mathematical equations, structural formulas, or three-dimensional physical orbitals (Justi and Gilbert, 2003b; Downes, 2020).

In organic chemistry, models of chemical transformation are foundational tools for the analysis, construction, and synthesis of organic compounds, making reaction mechanisms central models of the discipline (*e.g.*, Carpenter, 2000; Goodwin, 2003; Goodwin, 2012; Hendry, 2023). They allow scientists to explain reaction pathways, enable them to make mechanistic predictions, and to design novel products (Machamer *et al.*, 2000; Lazenby *et al.*, 2020). Typically, students in instructional settings are encouraged to think *with* reaction mechanisms by working on a wide variety of tasks. These commonly include, for example, completing missing steps, reactants, or products of a reaction mechanism, or drawing a reaction mechanism for given reactants and products (Bhattacharyya, 2022). Depending on the type of task, students may encounter different kinds of difficulties when thinking *with* reaction mechanisms. Such difficulties may, for instance, relate to identifying explicit and implicit information in representations, applying the electron-pushing formalism, or employing productive reasoning strategies (Graulich, 2015; Dood and Watts, 2022a; Dood and Watts, 2022b). However, a more holistic perspective on reaction mechanisms requires both thinking *with* but also thinking *about* reaction mechanisms as models.

This raises the question of the relationship between thinking *about* reaction mechanisms and thinking *with* reaction mechanisms, and how these two might affect each other. It remains unclear to what extent students even recognize the modeling character of reaction mechanisms, such as their provisional nature or their plurality (Schummer, 2015), and how this relates to students understanding of models in general. If students are unaware of the modeling character of reaction mechanisms, it may be challenging to use these mechanisms as hypotheses or epistemic tools that serve specific purposes rather than being mere representations. Connecting the thinking *about* reaction mechanisms and thinking *about* models in general provides an opportunity to contribute to a more coherent scientific meta-knowledge (White *et al.*, 2011). Against this background, the present study aims to explore undergraduate chemistry students' ideas that reflect their specific meta-modeling knowledge regarding reaction mechanisms (*i.e.*, thinking *about* reaction mechanisms) and to examine how these ideas co-occur with their ideas related to their general meta-modeling knowledge (*i.e.*, thinking *about* models).

Theoretical background

Building on these considerations, a theoretical foundation is needed that clarifies how students engage in thinking *about* models and thinking *about* reaction mechanisms. The former concerns students' general meta-modeling knowledge, whereas the latter captures their specific meta-modeling knowledge related to reaction mechanisms. A contextualized perspective on reaction mechanisms as models is therefore essential for identifying students' ideas in this domain and for examining how these relate to their more general, decontextualized ideas.

Conceptualizing meta-modeling knowledge (MMK)

Meta-modeling knowledge (MMK) is considered a component of scientific meta-knowledge (White *et al.*, 2011). It encompasses the epistemic understanding about the nature and purpose of models and modeling, their limitations, and how they can be used in specific contexts (Schwarz and White, 2005; Schwarz *et al.*, 2009). It is a necessary component of modeling competence (*e.g.*, Nicolaou and Constantinou, 2014; Chiu and Lin, 2019; Nielsen and Nielsen, 2021; Göhner *et al.*, 2022; Xue *et al.*, 2024).

For developing MMK, it is essential to understand that models serve a dual purpose in science: on the one hand, they are products of scientific inquiry used to communicate established knowledge to others within or beyond the scientific community. On the other hand, they serve as tools for generating new hypotheses and insights (*e.g.*, Van der Valk *et al.*, 2007; Passmore *et al.*, 2014; Justi and Gilbert, 2016). Gouvea and Passmore (2017) introduced a heuristic distinction between "models of" and "models for" to describe how models can be used. Their approach is grounded in philosophical considerations that a model is always *of* something and *for* a particular purpose (Halloun, 2007; Giere, 2010). However, they note that "too often models make their way into science classrooms in ways that focus entirely on their representational nature (what they are of) and exclude any reference to their epistemic function (what they are for)" (Gouvea and Passmore, 2017, *p. 51*). Accordingly, the concrete purpose that models serve (models *for*) depends on the cognitive agents who define the scope and limitations of the model. A model is therefore no longer judged solely by the accuracy of its representation of an original (Gouvea and Passmore, 2017). The representation of a phenomenon may be physical, symbolic, or theoretical (Upmeier zu Belzen *et al.*, 2019). Understanding both facets of the models *of* and models *for* heuristic lies at the core of what constitutes MMK.

Building on this, several conceptualizations have been developed in science education to capture and describe MMK (*e.g.*, Grosslight *et al.*, 1991; Crawford and Cullin, 2005; Schwarz and White, 2005; Van der Valk *et al.*, 2007; Oh and Oh, 2011; Upmeier zu Belzen *et al.*, 2019; Lazenby *et al.*, 2020; Upmeier zu Belzen *et al.*, 2021). The present study draws on the framework by Krüger and Upmeier zu Belzen (2021), shown in Fig. 1, which is a further development of the earlier framework by Upmeier zu Belzen and Krüger (2010) and was originally established in the context of biology education. This evidence-based, normatively developed framework comprises five central aspects: *nature of models*, *multiple models*, *purpose of modeling*, *testing models*, and *changing models*. While the first two aspects address ontological and epistemological considerations about models, the remaining three aspects focus on reflection on the modeling process (Grünkorn *et al.*, 2014b). The framework should be interpreted as aspect-dependent, meaning that the aspects of the MMK may develop independently of one another and should not be interpreted as a single holistic level of understanding (Krell *et al.*, 2014). Nevertheless, individual aspects are not necessarily isolated and may be interconnected by mutually influencing one another or developing simultaneously.

Each of the five aspects comprises four levels that capture students' ideas within each respective aspect. The detailed descriptions of all levels are presented in Fig. 1. The four levels within each aspect can be grouped into two overarching perspectives. Level 1 and level 2 represent the **media-oriented perspective** on models and modeling, in which models are understood as models *of* something (Passmore *et al.*, 2014; Gouvea and Passmore, 2017). For instance, as products of scientific inquiry used to communicate content across different contexts. Level 1 refers to reflections focused on the model object itself, whereas level 2 involves reflections related to developing an understanding of phenomena (Mahr, 2011; Upmeier zu Belzen *et al.*, 2021).

Level 3a and level 3b represent the **methodological perspective**, aligning with the model *for* something approach. In this perspective, models and modeling serve as methods within inquiry processes, used to generate new explanatory insights about phenomena and to derive hypotheses from those phenomena (Mahr, 2011; Gouvea and Passmore, 2017; Upmeier zu Belzen *et al.*, 2021). Level 3a, in this extended version of the framework, incorporates abductive reasoning as a form of explaining unfamiliar phenomena and constitutes an elaboration of level 3 in the original framework (see: Upmeier zu Belzen *et al.*, 2019). Abductive reasoning involves providing the most plausible explanation for a hypothesis based on available data and is therefore not truth-preserving (Walton, 2014). Accordingly, level 3a captures reflection at the level of abductive reasoning to explain phenomena, while level 3b refers to reflection at the level of deductive reasoning to predict phenomena (Mahr, 2011; Upmeier zu Belzen *et al.*, 2021).

media-oriented perspective		methodological perspective	
Level 1 Models as aesthetic resources	**Level 2** Understanding a phenomenon	**Level 3a** Abductive reasoning to explain a phenomenon	**Level 3b** Deductive reasoning to predict about a phenomenon
Nature of models			
Copies of a phenomenon	Idealized representations of a phenomenon	Best explanation of a phenomenon	Theoretical reconstruction of a phenomenon
Multiple models			
Different model objects	Different foci on a phenomenon	Different theoretical explanation	Different hypotheses about a phenomenon
Purpose of modeling			
Describing a phenomenon	Explanation to understand a phenomenon	Creating the best explanation	Predict about a phenomenon
Testing models			
Testing the model object	Comparing the model and a phenomenon	Testing the explanation for consistency	Testing hypotheses about a phenomenon
Changing models			
Enhancing correctness and beauty	Revising due to new insights	Revising the explanation	Revising due to falsification of hypotheses

Fig. 1 Framework for decontextualized meta-modeling knowledge, including abductive reasoning (Upmeier zu Belzen *et al.*, 2021). The media-oriented perspective is reflected in levels 1 and 2 (light orange), while the methodological perspective is represented in levels 3a and 3b (dark orange).

Since chemistry investigates interactions at the submicroscopic level, which are not directly accessible through empirical observation (Johnstone, 1993), modeling and explaining in this discipline rely primarily on abductive reasoning (Wackerly, 2021). Building on such abductive inferences and the insights they generate, hypothetico-deductive hypotheses can be derived and subsequently tested (level 3b). With respect to reaction mechanisms, reaction pathways can be explained by abductive reasoning, and these explanations can serve as a foundation for formulating hypotheses about the behavior of similar, yet unknown, syntheses. Since the presented study is situated in the field of organic chemistry, where an understanding of abductive reasoning is a part of the reasoning styles (Wackerly, 2021), we adopted the extended framework that explicitly includes abductive reasoning (level 3a).

The different levels of the framework are ordinally scaled, meaning that the distances between levels cannot be considered equidistant, as progressing from one level to the next may vary in complexity (Krell *et al.*, 2014; Krüger and Krell, 2020). In the original framework, the highest level, level 3, is viewed as the desired target state that reflects a scientific understanding (Upmeier zu Belzen and Krüger, 2010; Upmeier zu Belzen *et al.*, 2019). However, in our interpretation, this hierarchical structure is not understood in a strictly normative way. A higher level does not necessarily indicate a better or more advanced understanding in *all* respects. Rather, a scientific understanding also includes the ability to communicate and apply models appropriately within their intended scope while recognizing their specific affordances. From this perspective, a media-oriented view of models can likewise represent a sophisticated form of MMK. In addition, advanced methodological perspectives include an understanding of knowledge generation and may integrate media-oriented views. Consequently, well-developed methodological perspectives can be considered comparatively more holistic regarding a broader scientific understanding.

Prior research on meta-modeling knowledge

Several studies have examined the ideas that students and teachers express regarding the MMK (*e.g.*, Grosslight *et al.*, 1991; Treagust *et al.*, 2002; Crawford and Cullin, 2005; Schwarz and White, 2005; Van der Valk *et al.*, 2007; Gobert *et al.*, 2011; Krell *et al.*, 2015b; Lazenby *et al.*, 2020). Grosslight *et al.* (1991) were the first to analyze the understanding of models among seventh- and eleventh-grade students and derived different levels of generalized model understanding. Their findings showed that students had limited experience with scientific models and largely reduced the purpose of models to the transmission of information, which corresponds to a media-oriented perspective.

Building on this initial study, numerous subsequent investigations emerged. These studies mainly showed that MMK should not be viewed as a holistic construct with general levels of understanding but rather as aspect-dependent, allowing for more detailed analyses of individual aspects and their interrelations (*e.g.*, Crawford and Cullin, 2005; Upmeier zu Belzen and Krüger, 2010; Grünkorn *et al.*, 2014b; Krell *et al.*, 2014). In an aspect-dependent view, the aspects of MMK do not necessarily develop simultaneously; rather, they may emerge to varying degrees and independently of one another. For example, students may already describe model testing as hypothesis evaluation in research contexts (methodological perspective), while still holding the view that the primary purpose of models is to describe phenomena (media-oriented perspective). Within such an aspect-dependent perspective, Krell *et al.* (2014) identified, for example, seemingly contradictory patterns among secondary school students: some described models as idealized representations of an original (corresponds to level 2 in the aspect *nature of models*), while simultaneously allowing multiple models only when they referred to different model objects (level 1 in *multiple models*), rather than acknowledging that multiple models may arise from different idealizations. Comparable findings also emerged with the Students Understanding of Models in Science (SUMS) instrument, both in its original version (Treagust *et al.*, 2002) and in a German adaptation (Rost *et al.*, 2025).

Despite the inconsistencies observed across individual aspects in various studies, the overall pattern indicates that media-oriented perspectives predominate across different groups (*i.e.*, secondary school students, university students, teachers). In contrast, the role of models and modeling within inquiry processes was expressed far less frequently (Justi and Gilbert, 2003b; Justi and Gilbert, 2003a; Grünkorn *et al.*, 2014b; Krell and Krüger, 2016; Krell and Krüger, 2017). Within each status group, however, further differences were identified. An important differentiation concerns MMK in relation to the disciplinary background of the individuals studied (Gobert *et al.*, 2011; Krell *et al.*, 2015b; Krell and Krüger, 2017). For secondary school students, for example, research has shown that learners in chemistry and physics express more methodological ideas than learners in biology (Gobert *et al.*, 2011; Krell *et al.*, 2015b). Disciplinary differences were also found among university students, as those from STEM fields expressed more differentiated methodological ideas than students from non-scientific disciplines (Krell and Krüger, 2017). This discipline dependence thus appears to be independent of status group and may be related to the nature and instructional practices characteristic of each discipline.

Even within a single discipline, differences in students' MMK have been observed across various contexts (Grünkorn *et al.*, 2014b). Further, findings indicate that MMK can vary not only between different specific contexts within a discipline but also between a specific contextualized setting (*e.g.*, organisms, predator and preys, or atomic models) and students' decontextualized conceptions of models and modeling in general (Krell *et al.*, 2013; Lateef *et al.*, 2025). In the study by Krell *et al.* (2013), it was found that, in the decontextualized case, students predominantly expressed the idea that models serve as tools for describing phenomena. In specific contexts, however, students expressed ideas that extended beyond description, depending on the type of model presented (*e.g.*, diagrammatic models, functional models). For example, in the context of a functional model of a palm leaf made of paper, students more frequently expressed methodological perspectives regarding its purpose (Krell *et al.*, 2013).

Overall, various findings suggest that MMK should be understood from an aspect- and context-dependent perspective. Moreover, empirical studies have shown that across status groups, media-oriented and fragmented ideas predominated (*e.g.*, Grosslight *et al.*, 1991; Justi and Gilbert, 2003b; Grünkorn *et al.*, 2014b; Krell and Krüger, 2016; Krell and Krüger, 2017). However, various researchers have also emphasized the diverse potential of a well-developed MMK. For instance, it can positively influence mechanistic reasoning abilities (Baek and Schwarz, 2015), enhance conceptual learning (Schuchardt and Schunn, 2016), and support learning about scientific practices and the Nature of Science (Harrison and Treagust, 2000; Gilbert, 2004; Passmore *et al.*, 2014). Therefore, the development of MMK should be fostered at all educational levels: in school, at the university level, and among instructors (Grünkorn *et al.*, 2014b; Hartmann *et al.*, 2015; Krell *et al.*, 2015a; Krell and Krüger, 2017). To achieve this, it is important to conceptualize MMK not only as content-free but also in ways that account for specific contexts. We therefore propose distinguishing between general and specific meta-modeling knowledge.

Specific meta-modeling knowledge regarding reaction mechanisms

In the context of reaction mechanisms, the specific meta-modeling knowledge (SMMK) regarding reaction mechanisms includes ontological and epistemic ideas about what reaction mechanisms are, as well as ideas about how they are used both as communicative media (media-oriented perspective) and within processes of knowledge generation (methodological perspective). This definition of SMMK is aligned with the framework for the decontextualized version of MMK (Upmeier zu Belzen *et al.*, 2021). Since the framework, similar to the earlier version without abductive reasoning (Upmeier zu Belzen *et al.*, 2019) is content-independent, it needs to be adapted for specific contexts and domains. An example of such an adaptation is provided by Kirchhoff (2025), who adapted the original framework from Upmeier zu Belzen and Krüger (2010) to the context of computer simulations. Following a similar approach, we adapted the original framework for reaction mechanisms in organic chemistry to capture students' understanding of reaction mechanisms as models (Fig. 2). The framework is intended as an overarching structure for the context of reaction mechanisms in general rather than being tied to one particular course or instructional setting.

media-oriented perspective		methodological perspective	
Level 1 Exclusive view on the representation of chemical reactions	**Level 2** Understanding chemical reactions	**Level 3a** Abductive reasoning to explain chemical reactions	**Level 3b** Deductive reasoning to predict about chemical reactions
Nature of reaction mechanisms			
Reaction mechanisms (=RM) as copies of reaction pathways	RM as idealized representations of reaction pathways	RM as best explanations of reaction pathways	RM as epistemic artifacts to achieve specific goals related to the purpose of RM
Multiple reaction mechanisms			
Only one plausible RM for a reaction pathway from reactants to products with only one representation	Only one plausible RM for a reaction pathway from reactants to products, which can be presented through different representations	Multiple RM and reaction pathways for a chemical reaction due to varying conditions	Multiple competing RM for one reaction pathway of a chemical reaction none of which has been disproven yet
Purpose of reaction mechanisms			
Description of **how** chemical reactions proceed	Explanation to understand **why** chemical reactions proceed (including instructions for known syntheses)	Creating the best explanation based on chemical concepts to understand **why** unknown chemical reactions proceed (including optimizations of synthesis instructions)	Creating best explanations to predict about unknown chemical reactions (including development of new syntheses)
Testing reaction mechanisms			
Testing the representation in terms of coherence, correctness and formalisms (*e.g.*, EPF)	Testing RM in terms of conceptual plausibility (application of concepts; *e.g.*, nucleophilicity/electrophilicity) and verifying the RM with experimental evidence	Testing if a RM is the most plausible possible reaction pathway in terms of chemical concepts and experimental evidence	Testing new RM by empirical investigation of derived hypotheses (*e.g.*, product distributions of unknown syntheses, transition states)
Changing reaction mechanisms			
Enhancing the representation of a RM in terms of coherence, correctness, and formalisms (*e.g.*, EPF)	Changing RM to align them with chemical concepts and known evidence	Changing RM because alternative reaction pathways are more plausible by considering chemical concepts and new experimental evidence	Revising new RM due to the falsification of derived hypotheses or new experimental evidence

Fig. 2 Framework for specific meta-modeling knowledge (SMMK) regarding reaction mechanisms in organic chemistry (adopted from Upmeier zu Belzen *et al.*, 2021). The media-oriented perspective is reflected in levels 1 and 2 (light pink), while the methodological perspective is represented in levels 3a and 3b (purple). In cases where ideas related to level 1 are not demonstrated, a level 0 (basal level) can be added.

Therefore, it is intended to remain closely aligned with the original version, since the same ontological and epistemic considerations apply to reaction mechanisms as models as they do in the content-independent case (Carpenter, 2000; Upmeier zu Belzen *et al.*, 2019). Accordingly, the structure likewise comprises five aspects with four levels each. The five aspects are *nature of reaction mechanisms*, *multiple reaction mechanisms*, *purpose of reaction mechanisms*, *testing reaction mechanisms*, and *changing reaction mechanisms*.

In this specific context, the two overarching perspectives also emerge. The media-oriented perspective follows from the fact that reaction mechanisms represent central content in organic chemistry instruction at the university level and in curricular materials (Dood and Watts, 2022a), as well as in industry for synthesis instructions. Level 1 focuses on the representation of the mechanism itself, whereas level 2 addresses the understanding of reactions through reaction mechanisms. The methodological perspective derives from their role as essential tools in research, where reaction mechanisms serve both as products of scientific inquiry about reaction pathways and as starting points for predicting unknown or yet uncharacterized reaction courses (Goodwin, 2017). Level 3a refers to abductive reasoning to explain chemical reactions based on the best available evidence, whereas level 3b comprises hypothetico-deductive reasoning to predict unknown chemical reactions by formulating and testing hypotheses. The following section provides a more detailed explanation of each of the five aspects.

In the aspects *nature of reaction mechanisms* and *multiple reaction mechanisms*, the media-oriented perspective reflects the idea that reaction mechanisms are highly accurate pictures (level 1) or idealized (level 2) representations of the submicroscopic level, like "zooming in" on submicroscopic processes. This zooming-in perspective at level 1 has also been reported in other contexts: Adbo and Taber (2009) found that, in the context of atomic models, students often attribute macroscopic properties to submicroscopic entities. This may result from the way such entities are treated in instructional settings (Taber, 2003). Similar perspectives can be attributed to reaction mechanisms, when they are interpreted as submicroscopic copies of reality at level 1, which is why it is included in the framework. Level 2 further acknowledges that the representation of a reaction mechanism may vary, while it is still based on the assumption that a reaction pathway is predetermined. Because reaction mechanisms represent dynamic processes rather than a single snapshot or substance, different ways of representing mechanisms may combine mechanistic steps, separate them, or omit side reactions. At the higher levels, abductive reasoning is incorporated (level 3a), which accounts for how reaction mechanisms are constructed and emphasizes their inherently provisional nature (Schummer, 2015; Wackerly, 2021). At these levels, there is no longer an expectation that the representation mirrors reality; instead, reaction mechanisms are understood as epistemic artifacts, which are constructs developed to serve specific purposes (level 3b) (Rost and Knuuttila, 2022). This creates a direct link to the *purpose of reaction mechanisms*. Within this perspective, multiple reaction mechanisms may exist because multiple reaction pathways can occur in parallel or in competition (level 3a), or because several hypotheses about a reaction pathway are possible (level 3b).

The aspects *purpose of reaction mechanisms*, *testing reaction mechanisms*, and *changing reaction mechanisms* concern the reflection on how reaction mechanisms are used. Beginning with the *purpose of reaction mechanisms*, the media-oriented perspective includes ideas, such as that reaction mechanisms serve solely to describe chemical processes (level 1) or are used in instructional settings to explain (known) reaction pathways (level 2). Reaction mechanisms also play an important role in the synthesis of known chemical compounds in established procedures (Bruckner, 2010). In this context, a reaction mechanism can be understood as a kind of "recipe" that specifies the sequence of steps in a synthesis. Since this type of use is primarily communicative, it is likewise included in level 2 (see Fig. 2).

The methodological perspective, in contrast, emphasizes that the *purpose of reaction mechanisms* lies in explaining new reaction pathways through abductive reasoning (level 3a), which can then serve as the basis for predicting related, yet unknown, reaction mechanisms (level 3b). With regard to synthesis and laboratory work, level 3a includes optimizing existing syntheses, whereas level 3b encompasses planning new, yet uncharacterized syntheses guided by mechanistic hypotheses.

For *testing* and *changing reaction mechanisms*, the media-oriented perspective refers to checking and adjusting either the representation itself (level 1) or its conceptual consistency and correctness at an explicit level (level 2). The methodological perspective regarding *testing reaction mechanisms* includes evaluating alternative mechanistic pathways by drawing on conceptual knowledge and (new) empirical evidence, such as measured data or spectra (level 3a), as well as testing derived hypotheses through systematically planned and controlled experiments (level 3b). Regarding *changing reaction mechanisms*, the methodological perspective includes abductive reasoning in level 3a, where reaction mechanisms are revised to arrive at a more plausible explanation and may be adjusted when new evidence suggests a better account. In contrast, level 3b reflects the hypothetico-deductive approach, in which known reaction mechanisms are used to derive and test hypotheses about previously unknown mechanisms. These hypotheses are revised when they are falsified by new evidence, while the known mechanism is treated as given.

Taken together, the original framework by Upmeier zu Belzen *et al.* (2021) (see Fig. 1) has been adapted to the context of reaction mechanisms (see Fig. 2). As a result, two complementary frameworks now exist that allow to characterize students' expressions regarding the two dimensions of meta-modeling knowledge (*i.e.*, MMK and SMMK). It is already known that, in both school and university chemistry courses, little emphasis is typically placed on fostering epistemic modeling knowledge (Lazenby *et al.*, 2020), even though such knowledge would help students more deeply reflect on the content they encounter. Research from general chemistry courses further suggests that while students often learn conceptual content through models, a discrepancy tends to arise between their conceptual understanding and their MMK (Becker *et al.*, 2017; Lazenby *et al.*, 2019a; Lazenby *et al.*, 2019b; Lazenby *et al.*, 2020). Similar trends can be assumed for organic chemistry, and for reaction mechanisms in particular. This raises the question of whether students actually perceive reaction mechanisms as models and how this is reflected in the aspects of their (specific) meta-modeling knowledge.

Interplay of general and specific meta-modeling knowledge

Because SMMK may vary across disciplinary contexts, the situational character of epistemic ideas about models becomes more apparent. Nevertheless, general (uncontextualized) MMK and SMMK can be closely interconnected and potentially shape each other (see for illustration Fig. 3). While SMMK is particularly relevant within a specific context (here, reaction mechanisms in organic chemistry), MMK can be understood as an overarching dimension that may allow for the transfer of understanding between disciplines and represents an abstract, general understanding of science. Empirical investigations are needed to determine how MMK and SMMK can shape each other.

The relationship of the two dimensions can be viewed as a continuum of increasing contextualization, with ideas in both dimensions referring to forms of meta-knowledge rather than to modeling practices. From this perspective, SMMK can be conceptualized as an enacted version of MMK, representing a shift from thinking *about* models to thinking *about* reaction mechanisms. Following this perspective, SMMK regarding reaction mechanisms can be further contextualized by being enacted in concrete practices involving specific reaction mechanisms (see Fig. 3). Here, we refer to this third dimension as specific modeling practices (SMP), which comprises contextualized modeling practices related to reaction mechanisms. Accordingly, SMP can be further thought as moving from thinking *about* reaction mechanisms to thinking *with* reaction mechanisms. The practices, constituting SMP, were adapted from Nielsen and Nielsen (2021) and include, for example, evaluating the plausibility of given reaction pathways for a specific reaction or using reaction mechanisms to explain reactions or resulting products. SMP and SMMK may also shape each other. Fig. 3 illustrates the relationship between the three dimensions with increasing contextualization. Since we initially focus on thinking *about* models and reaction mechanisms as models, the SMP dimension is shown greyed out in Fig. 3.

Research questions

While MMK has been examined in various studies, both in general and within other disciplines, its role in the context of reaction mechanisms in undergraduate organic chemistry remains unexplored. However, exploring students' ideas about reaction mechanisms could help gain a more holistic impression, as it is unclear to what extent reaction mechanisms are perceived as models and what epistemic ideas students hold regarding them. Moreover, the question arises as to which patterns can be observed in students' ideas regarding SMMK and MMK. Investigating these aspects could provide insights into students' ideas related to reaction mechanisms and help refine instructional approaches. Specifically, the study addressed the following two research questions:

(1) What ideas about reaction mechanisms do students express that reflect their SMMK?

(2) What patterns can be identified between students' ideas about reaction mechanisms (SMMK) and their ideas about models and modeling in general (MMK)?

To address these research questions, we conducted qualitative interviews with chemistry students, encouraging them to

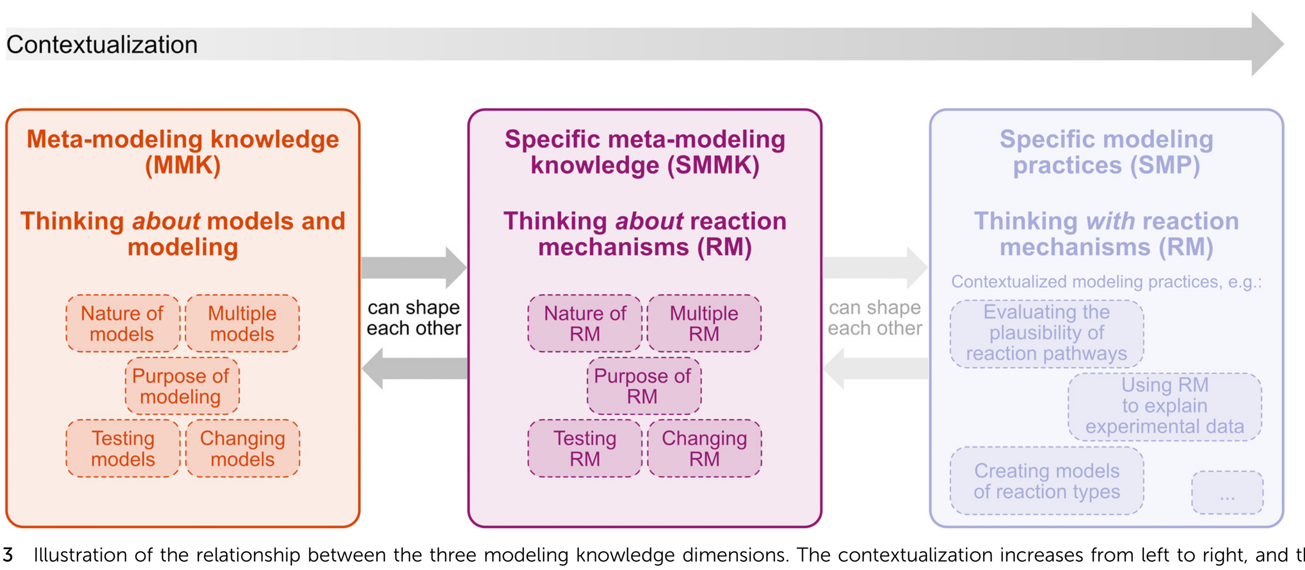

Fig. 3 Illustration of the relationship between the three modeling knowledge dimensions. The contextualization increases from left to right, and the dimensions may mutually shape each other.

elaborate on questions related to the aspects within both the SMMK and MMK dimensions.

Since students have so far received only introductory instruction on basic reaction mechanisms, we expect media-oriented ideas to be predominant in the SMMK dimension. In the MMK dimension, we also anticipate the presence of methodological ideas, as students are likely to have learnt about scientific inquiry processes and models during school.

Methods

Context and study setting

The study was conducted at a German university in October and November 2024. 22 participants were recruited from a chemistry education course, which is a mandatory component of the chemistry teacher education program at this university. In this course, students engage with topics such as lesson planning based on the German curriculum and the use of experiments in chemistry teaching. Although they were enrolled in this course, the participants can be considered typical chemistry students at this stage, as they were attending the same courses as the chemistry bachelor students and had not yet completed any specialized chemistry education course. Models and modeling are addressed in a subsequent chemistry education course that the students had not attended at the time of the study.

We selected students in their second year of studying chemistry before entering organic chemistry. While they had not yet attended this lecture, they had prior experiences from school and previous courses at the university: In German secondary schools, students already encounter basic topics in organic chemistry, such as functional groups, and have been introduced to basic reaction mechanisms (*i.e.*, addition reactions, radical and nucleophilic substitutions). In addition, models and modeling are explicitly addressed in school curricula in Germany, particularly in biology but also in chemistry, as part of scientific inquiry processes.

At the university level, all participants had completed the general and inorganic chemistry course and a general chemistry laboratory course. The laboratory course covered basic laboratory techniques (*e.g.*, distillation and titration) and included introductory organic experiments illustrating basic reaction mechanisms, such as esterification and saponification.

As basic ideas may already have emerged from their prior school and first-year chemistry courses, we were interested in their developmental ideas in both meta-modeling dimensions (*i.e.*, SMMK and MMK). Focusing on students' ideas prior to the organic chemistry lecture allows for a more differentiated understanding of their individual starting points, which provides opportunities for informing instructional design. In contrast, examining students only after completing the organic chemistry lecture would not allow for evaluating the alignment of instruction with their initial ideas.

Participants

All students participated voluntarily and consented to the recording and analysis of their data. 15 of the 22 participants identified as female and seven as male; their ages ranged from 20 to 41 years, with a median age of 21. Eleven students had taken chemistry at an advanced level in upper secondary school, ten at a basic level, and one student had not taken chemistry in the final years of secondary school. This refers to prior school-level exposure and is independent of their shared university-level chemistry instruction. 15 students were in their third semester, while seven were in their fifth semester. In German teacher education programs, students study a second subject (*e.g.*, mathematics, physics, or French), which was recorded as part of the demographic data. Variations in semester status mainly reflect differences in the sequencing of this second subject within the teacher education program. Although students were in different semesters, all participants received the same instruction in inorganic chemistry and the general chemistry laboratory course. The Organic Chemistry 1 course is a compulsory component of the chemistry teacher education program, which participants had not yet taken at the time of data collection. Participants' prior professional experiences in chemistry were also assessed; however, none of the participants reported any such experience beyond their current study program.

Although Institutional Review Board (IRB) approval is not required for chemistry education research at German universities, we adhered to a strict internal protocol to ensure full compliance with ethical guidelines. Before data collection started, students were informed about the interview topic, their rights, and the data processing procedures. They were also explicitly assured that they could withdraw from the interview at any time without providing a reason. Written consent for (1) the collection of audio and video recordings, (2) the transcription of the interviews, (3) the use of recordings, transcripts, and drawings by the research team, and (4) the analysis and publication of the collected data was obtained. Pseudonyms were assigned to all students, and only their voices and any drawings or materials used were recorded. The interviews and the data analysis were conducted in German. All direct quotes in this manuscript were translated into English and reviewed by the research team to ensure the validity of the translations.

Data collection

Before the interview, all participants completed a demographic questionnaire. The interviews were audio- and video-recorded and lasted between 74 and 102 minutes, including a brief warm-up part. The video recording captured students' interactions with objects on the table and was used to classify references to, *e.g.*, "here" or "this", in the transcripts. If students took notes, these were anonymized and scanned. After completing the interview, they were asked not to discuss its content with their colleagues. A semi-structured interview protocol based on the (adapted) framework for meta-modeling knowledge (see Fig. 1 and 2) guided the data collection. The interview consisted of three parts, two of which (*i.e.*, MMK and SMMK) are relevant for this manuscript. The third part, which involved working with a specific reaction, is not analyzed here.

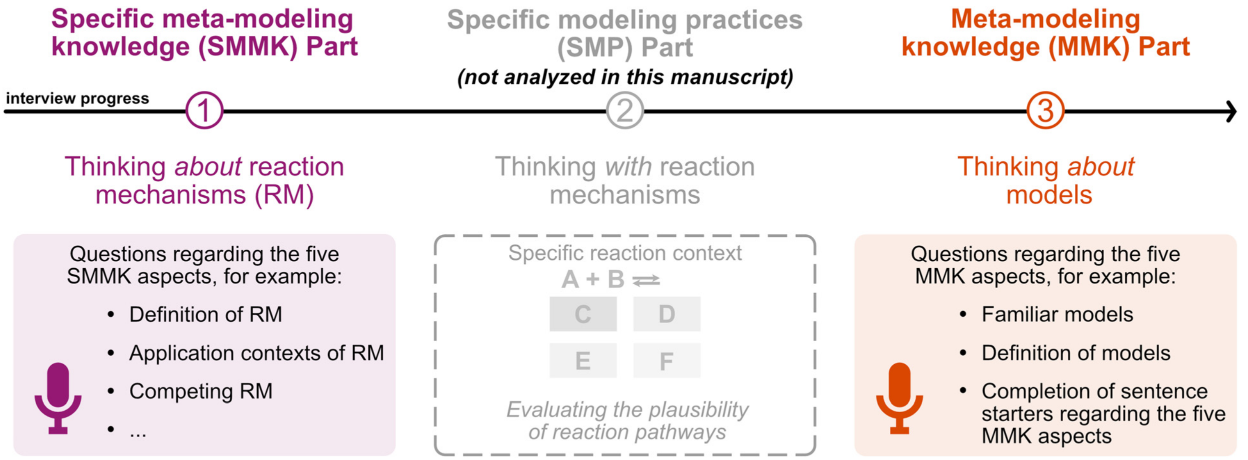

Fig. 4 Illustration of the study design, the second interview part is not part of this manuscript.

To minimize potential cross-influences between the two relevant parts, the SMMK section was placed at the beginning and the MMK section at the end of the interview. The study design is illustrated in Fig. 4.

In the SMMK part, students were asked questions addressing all five aspects, including definitions and purposes of reaction mechanisms, how they are developed and evaluated, and how competing reaction mechanisms can be explained. Follow-up questions were used to further explore their ideas. In the MMK part, students were first asked to name familiar models and to define what a model is from their perspective. They were then presented with pre-formulated sentence starters on a card, which they were asked to complete and elaborate on verbally. They consisted of the following prompts: (1) The relationship between the model and the original is... (2) Multiple models are used because... (3) Models serve the purpose of... (4) Models are tested by... (5) Models are changed because... These sentence starters were taken from the literature (Grünkorn *et al.*, 2014a) and were specifically designed to address the five aspects of MMK. Accordingly, they aim to address both ontological and epistemological considerations about models (sentence starters 1 and 2) as well as reflection on the modeling process (sentence starters 3 to 5) (Grünkorn *et al.*, 2014b).

Data analysis

The interviews were transcribed verbatim and uploaded to *MAXQDA* for qualitative analysis (Saldaña, 2016). The analysis followed several consecutive steps, all of which were discussed multiple times among the three authors to ensure consistency. An overview of the data analysis process is illustrated in Fig. 5.

Step 1: coding and assignment of students' ideas within the MMK and SMMK dimensions. We started the data analysis with the MMK part of the interview. Students' responses to the sentence starter were coded deductively according to the MMK framework by Upmeier zu Belzen *et al.* (2021), which assigns statements to levels 0 to 3b within each aspect. Compared with the original framework (see Fig. 1), we added level 0 for cases in which students' statements did not sufficiently meet the criteria for level 1. For example, this applied when students suggested that reaction mechanisms do not need to be tested (*testing reaction mechanisms*). After the initial coding, a second cycle was conducted by two of the authors to refine the codes and resolve discrepancies. Based on the coded segments, each student received an overall level for every aspect within their MMK. In cases where multiple levels occurred within one aspect, the highest level was generally assigned. However, isolated statements at a higher level were not sufficient on their own if they relied solely on certain keywords (*e.g.*, "hypothesis" for level 3b) without reflecting a genuine understanding. In such cases, the student's predominant ideas determined the overall classification. Classification decisions were discussed and agreed upon by the authors.

For the SMMK part, the adapted framework for SMMK was applied in the same way for deductive coding. An exemplary excerpt of the coding manual for the *purpose of reaction mechanisms* is provided in Table 1. The coding manual for the remaining four aspects of SMMK is presented in Appendix C (see Tables 4–7). After coding the students' statements, they were assigned to an overall level for each aspect within the SMMK dimension.

Step 2: determining the overall distribution of levels. To obtain an impression of patterns at the overall level of the cohort, this step of the data analysis involved counting the assigned levels of all students for both the MMK and SMMK dimensions. For each of the five aspects in both dimensions, we recorded how often a level was assigned as the overall level based on the individual coding results.

Step 3: classifying students' ideas and building groups of students. To identify patterns across the two dimensions, we examined the assigned overall levels based on students' ideas expressed within the MMK and SMMK dimensions (see Fig. 6, left side). Although the levels are ordinally scaled, it cannot be assumed that the distance between each level is equal or that the order is strictly hierarchical. Elaborated media-oriented perspectives are as valuable as methodological ones and can

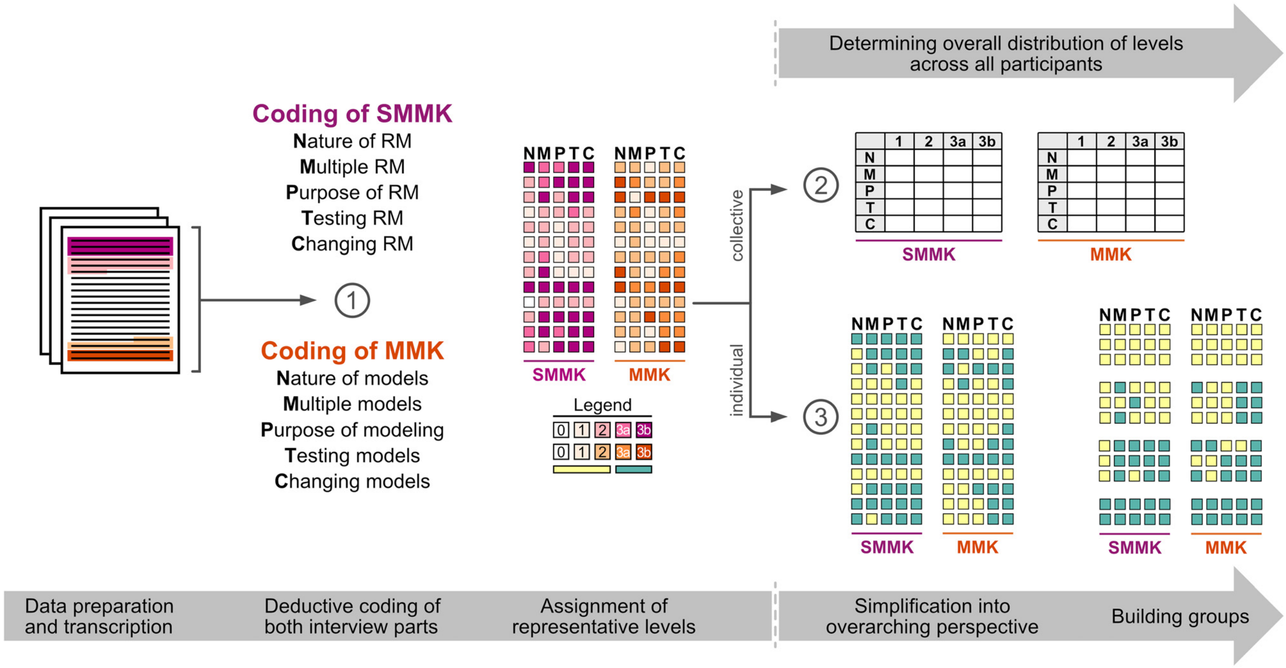

Fig. 5 Illustration of the data analysis process.

Table 1 Coding manual for the purpose of reaction mechanisms within the SMMK dimension

Level	Code	Description	Example
0	No description of the purpose of reaction mechanisms	Even when prompted directly, students did not provide any statements about the purpose of reaction mechanisms, or they explicitly stated that they did not know what RM are used for.	Not present in the data.
1	Description of *how* chemical reactions proceed	Students describe reaction mechanisms (RM) as representations that help them follow and visualize *how* a reaction proceeds. RM are understood as detailed depictions of reaction pathways that support a clearer and more precise comprehension of the reaction pathway.	*"So that you can really see the individual steps, what is actually reacting, what happens, and then be sure that, okay, when I'm in the lab, I know what is happening, [...] even if I can't see it." (Judy)*
2	Explanation to understand *why* chemical reactions proceed (including instructions for known syntheses)	Students describe RM as tools that support individual understanding of *why* a reaction proceeds in a particular way and how products emerge from specific starting materials. RM are also viewed as practical guides that can be used to synthesize known products or to provide procedural orientation in laboratory settings.	*"A reaction mechanism shows the intermediate steps from the beginning to the final products. For example, water may split off in the process, and that part of the substance reacts with it. And that is basically the explanation for why the reaction ends up the way it does." (Janet)*
3a	Creating the best explanation based on chemical concepts to understand *why* unknown chemical reactions proceed (including optimizations of syntheses instructions)	Students describe RM as tools for generating new insights by using chemical concepts to explain unknown reaction pathways. RM provide explanatory accounts of *why* reactions occur. They are also seen as means for optimizing syntheses by evaluating alternatives and considering *e.g.*, intermediate steps.	*"Well, I think that [...] they're used in industry [...]. If you want to produce something, [...] like Styrofoam, then it makes sense to understand how to get there, and where [...] a lot of energy might be needed, [...] or where you might need more of one substance than another because it reacts better that way." (Naomi)*
3b	Creating best explanations to predict about unknown chemical reactions (including development of new syntheses)	Students describe RM as purpose-driven hypotheses that guide scientific inquiry. They are used to plan unknown syntheses and to design pathways for obtaining novel products from chemical concepts and evidence. RM serve as analytical tools for generating and testing predictions about new reaction outcomes.	*"[Reaction mechanisms] also help in research to [...] figure out that if I take a certain substance, then based on how it reacted with similar substances [...], something similar should happen when I combine this new substance with it, because it is all chemically connected." (Ted)*

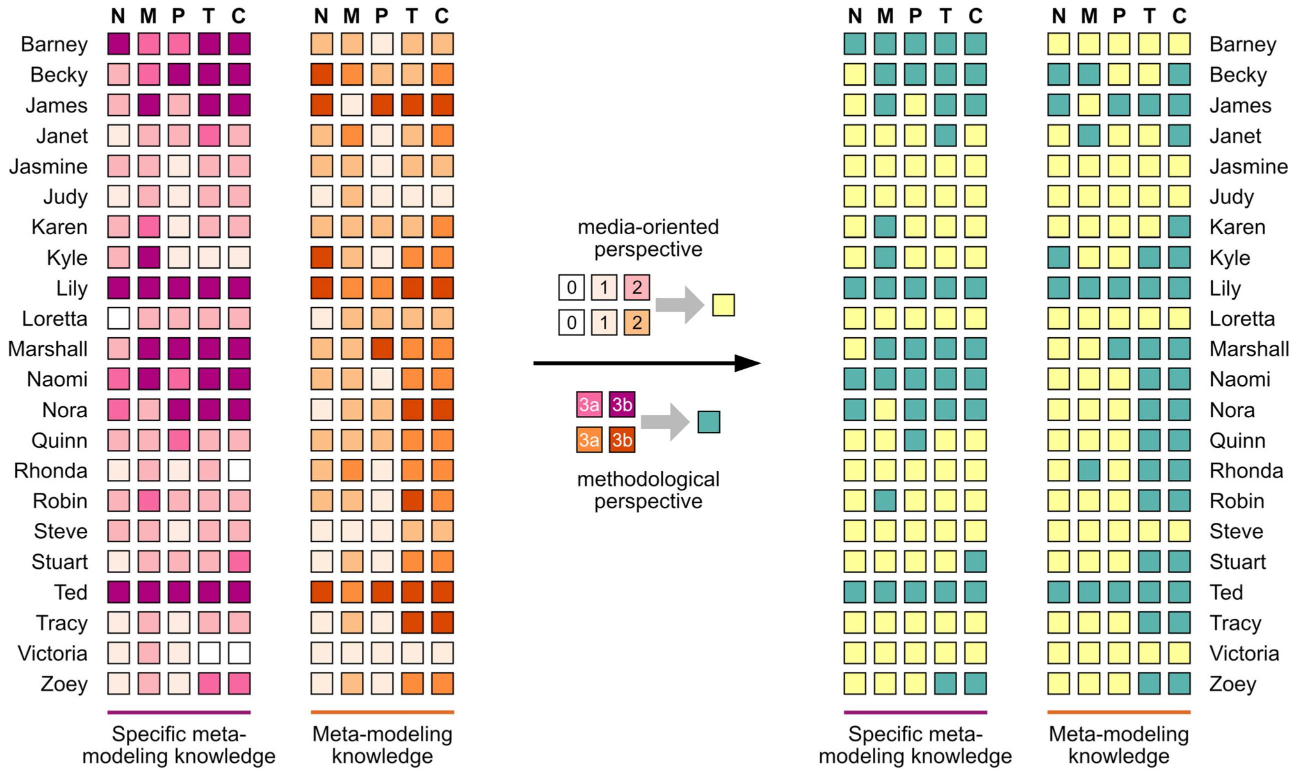

Fig. 6 Assigned levels of students' ideas within the SMMK and MMK dimensions (left) and their summative overview into media-oriented and methodological perspectives (right).

also express a scientific understanding of models (Krell *et al.*, 2014). Therefore, we grouped the levels according to their overarching perspective (see Fig. 6, right side). Levels 0 to 2 were categorized as media-oriented, and levels 3a and 3b as methodological. Based on our qualitative analysis of students' ideas expressed across the aspects of the MMK and the SMMK, we formed four groups of students that showed similar patterns in their expressed ideas (see Fig. 7).

Results and discussion

RQ1: What ideas about reaction mechanisms do students express that reflect their SMMK?

To address this question, we examined the collective distribution of assigned levels within the SMMK dimension to provide an overview of students' ideas related to SMMK. The distribution is presented in Table 2. It is important to emphasize that the data analysis could only be based solely on the ideas explicitly made by the students in their statements. These do not necessarily capture the full range of resources the students possess within the dimensions, but rather only those that were activated in this specific context (Hammer *et al.*, 2005).

As outlined earlier, levels 0 to 2 reflect a media-oriented perspective on reaction mechanisms, whereas levels 3a and 3b represent a methodological perspective in which reaction mechanisms are understood as tools for scientific inquiry.

Overall, the distribution revealed a broad range of ideas across all five aspects. At the collective level, students already showed emerging methodological perspectives by recognizing and expressing the role of reaction mechanisms in knowledge generation in various ways. However, the relative prevalence of media-oriented *versus* methodological perspectives differed across aspects. While the aspects *multiple reaction mechanisms*, *testing reaction mechanisms*, and *changing reaction mechanisms* showed a relatively balanced distribution, students' ideas regarding the *nature* and *purpose of reaction mechanisms* more often aligned with media-oriented perspectives (see Table 2).

To further explore these differences, we conducted an exploratory, descriptive comparison of students' SMMK perspectives and demographic background characteristics (gender, second subject in teacher education, age, and prior school chemistry experience). In this process, we looked for noticeable patterns or tendencies in the data, and no statistical tests were applied. Within our sample, no consistent patterns could be identified between participants' background information and, for example, more methodological perspectives. The observed variation may instead be more strongly related to individual prior learning experiences in school, where the treatment of reaction mechanisms can vary considerably due to curricular flexibility. This variation may even exceed differences between basic and advanced level of chemistry in high school. Depending on the teacher, instruction may explicitly address the modeling character of reaction mechanisms and thereby introducing methodological perspectives, whereas other instruction

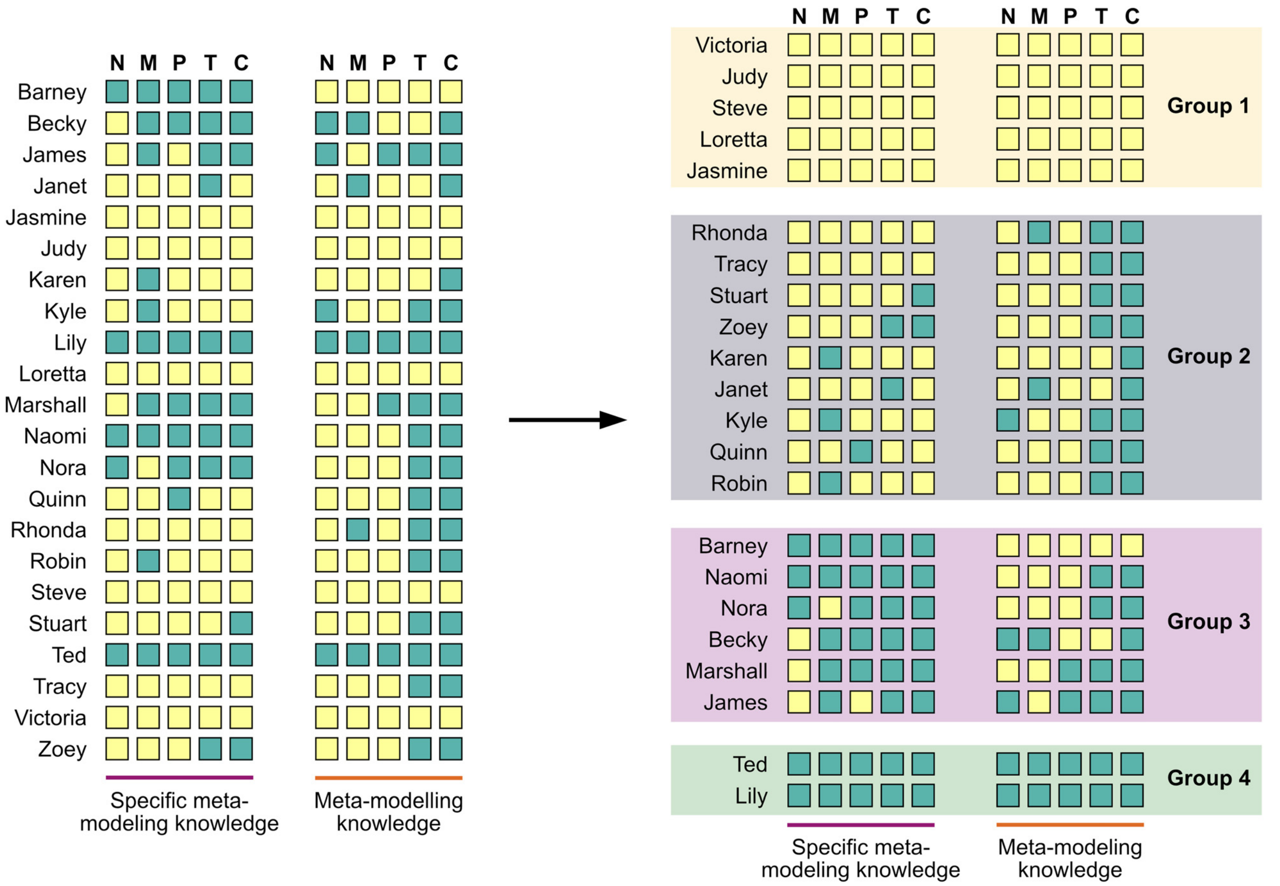

Fig. 7 Distribution into overarching perspectives (left) and grouping based on similar patterns in their expressed ideas (right).

Table 2 Group distribution of assigned levels based on students' ideas within the five aspects of specific meta-modeling knowledge (SMMK) regarding reaction mechanisms

	Media-oriented perspective			Methodological perspective	
Aspect	Level 0	Level 1	Level 2	Level 3a	Level 3b
Nature of reaction mechanisms	1	7	9	2	3
Multiple reaction mechanisms	0	0	12	4	6
Purpose of reaction mechanisms	0	9	5	3	5
Testing reaction mechanisms	1	1	10	2	8
Changing reaction mechanisms	2	1	9	2	8

may focus primarily on content transmission. This interpretation is supported by Vo *et al.* (2015), who argue that teachers' epistemic considerations about models (*i.e.*, meta-modeling knowledge) can shape their classroom practice with models. However, without further data on students' prior school experiences, this explanation remains speculative.

To gain a more detailed understanding of the variation in students' ideas, we examined each aspect qualitatively.

Nature of reaction mechanisms

In the aspect *nature of reaction mechanisms*, most students expressed ideas that reaction mechanisms are (idealized) representations of chemical reactions. Whether understood as direct depictions of reaction pathways or as simplified illustrations, these ideas align with the media-oriented perspective. Overall, ideas expressed by 17 of the 22 students were assigned to this perspective (see Table 2). As a typical example, Victoria's idea can be considered:

Victoria: "*With reaction mechanisms, it's more, I would almost say, a graphical or visual kind of representation, in a pictorial way. [...]*" (SMMK, nature of RM, level 1)

Her description emphasizes the depictive character of reaction mechanisms and was therefore assigned to level 1. Only a few students expressed a methodological perspective. Lily, for instance, expanded this notion of visual representation by emphasizing that reaction mechanisms are always simplifications that depict only what is related to a specific purpose:

Lily: "*It's obviously not a direct depiction of reality, but a simplification. I don't have weird orbitals or anything like that [...] but rather what's relevant to me first. [...] If I want to produce a substance, I'm primarily interested in the path that leads to it.*" (SMMK, nature of RM, level 3b)

By highlighting both simplification and purpose-dependence, her ideas correspond to level 3b. These contrasting statements illustrate the broad range of ideas in this aspect. While most students expressed to perceive reaction mechanisms as visual representations, some already demonstrated more advanced ideas, emphasizing their provisional and purpose-dependent character.

The fact that most students expressed ideas that focused on the representational character of reaction mechanisms may be related to the way reaction mechanisms are treated in instructional settings. The focus while teaching reaction mechanisms in instruction often lies on the isolated presentation of the mechanism as the product of scientific inquiry rather than on the process of how such knowledge is developed (Graulich, 2015; Dood and Watts, 2022a).

In an authentic setting, reaction mechanisms should be treated as hypotheses that are formulated through a combination of energetic considerations, the interpretation of experimental data, and structure–property relationships (Esselman *et al.*, 2023). However, in schools and universities, reaction mechanisms are often taught detached from the actual scientific inquiry process. In particular, laboratory courses could have the potential to convey authentic inquiry processes (*e.g.*, Carnduff and Reid, 2003; Hofstein and Lunetta, 2004; Reid and Shah, 2007). But they are often organizationally separated from lecture-based instruction and offered as independent courses, and they tend to follow predetermined verification-practices rather than genuine exploration of hypotheses (Hofstein and Lunetta, 2004; Galloway and Bretz, 2015). As a result, opportunities for practicing authentic communication using reaction mechanisms rather than simply applying conceptual skills are frequently neglected (Esselman *et al.*, 2023). This way of instruction may contribute to the manifestation of media-oriented perspectives. As Schwarz *et al.* (2025) claim, there is a need to shift from focusing solely on conceptual understanding to explicitly addressing epistemic aspects in teaching, such as the nature of specific models, such as reaction mechanisms. Lily's ideas, for instance, indicate such an epistemic understanding, which is reflected in methodological perspectives.

Purpose of reaction mechanisms

While Lily already considered the *purpose* in relation to the *nature of reaction mechanisms*, other students expressed ideas regarding the *purpose of reaction mechanisms* when explicitly asked what reaction mechanisms are used for. In this aspect, students expressed a wide range of ideas, reflected in a broad distribution of levels, with, again, a predominance of media-oriented ideas. Many students described reaction mechanisms primarily as tools for illustrating or clarifying how a reaction proceeds. For instance, nine students expressed ideas that were assigned to level 1 (see Table 2). When students described the *purpose of reaction mechanisms* solely as a means of communicating information, this was often expressed, as in the case of Judy:

Judy: "*So that you can really see the individual steps, what is actually reacting, what happens, and then be sure that, okay, when I'm in the lab, I know what is happening, [...] even if I can't see it.*" (SMMK, purpose of RM, level 1)

In Judy's statement, it became clear that she simultaneously assumed that reaction mechanisms are representations of reality and that the mechanism acts like a magnifying lens on the submicroscopic level, "that you can really see the individual steps," without losing information. This indicates a predominantly descriptive function of reaction mechanisms, that is, *how* a reaction proceeds (level 1), without considering the explanatory function (*why* a reaction occurs). Ideas like Judy's align with existing literature. Early findings by Kraft *et al.* (2010) have shown that even graduate students often do not use reaction mechanisms in a model-based way. Instead, students in their study relied on case-based or rule-based reasoning without drawing on the explanatory or predictive potential of reaction mechanisms – indicating that students viewed the *purpose of reaction mechanisms* mainly in terms of representing reaction pathways, consistent with a media-oriented perspective. Moreover, Anderson and Bodner (2008) early on demonstrated that acknowledging reaction mechanism as a model and practicing modeling purposefully with students is often sacrificed for covering content in organic chemistry. When instructors do not emphasize the *purpose of reaction mechanisms*, it can be particularly challenging for students to develop those ideas independently.

Some students articulated more advanced, application-oriented purposes. Naomi, for example, related reaction mechanisms to practical contexts such as using them in industrial syntheses:

Naomi: "*[Reaction mechanisms] are used in industry [...]. If you want to produce something, [...] like Styrofoam, then it makes sense to understand how to get there, and where [...] a lot of energy might be needed, [...] or where you might need more of one substance than another because it reacts better that way.*" (SMMK, purpose of RM, level 3a)

Her statement reflected a very practical idea of the *purpose of reaction mechanisms*. In this case, she referred to how steps in the synthesis of products could be made more efficient, based on the structure–property relationships of the substances involved. Her idea indicated that some students link reaction mechanisms to the usefulness in chemical synthesis to derive new syntheses or, more generally, new knowledge, comparable to how practicing chemists actually use them (Jackson, 2004). Here again, it is important to emphasize that the explicit communication of epistemic aims in instructional settings is essential for students to have the opportunity to understand how organic chemists authentically work with reaction mechanisms (Schwarz *et al.*, 2025; Heinrich *et al.*, 2026).

Multiple reaction mechanisms

In the aspect *multiple reaction mechanisms*, the distribution of assigned levels among students' ideas was roughly balanced between the media-oriented and methodological perspectives (ideas of 12 students in the media-oriented perspective and 10 in the methodological perspective; see Table 2). In this aspect, the media-oriented perspective relates to the idea that there is exactly one predetermined reaction mechanism for a given reaction. At level 1, the underlying idea is that this single reaction mechanism also has a single, fixed representation. At level 2, by contrast, the same predetermined reaction pathway can be depicted through different representations. If it was not explicitly stated that the representation had to be fixed, students' statements were assigned to level 2. The media-oriented perspective was expressed, for example, by Zoey:

Zoey: "*Well, ultimately, all molecules that react go through the same mechanism.*"

Interviewer: "*Could you elaborate on that?*"

Zoey: "*All molecules from the reactants that take part in the reaction follow the same pattern. So that, in the end, the product we observe is formed.*" (SMMK, multiple RM, level 2)

The idea that reaction mechanisms are predetermined and irrespective of the reaction condition (non-changeable) may be related to viewing them as direct representations of reality (*nature of reaction mechanisms*). The latter idea is also supported by previous research, which shows that students tend to focus solely on major products and omit other reaction species (Popova and Bretz, 2018), thereby reflecting the perception of a single, definite reaction pathway.

About half of the students, however, expressed ideas that reaction pathways depend on reaction conditions (level 3a). Overall, students tended to assume that reactions proceed along a single route under constant conditions, a difficulty also noted in previous research on students' mechanistic reasoning (Grove and Bretz, 2010). In this study, they found that students show conceptual challenges whenever reactions proceed *via* competing mechanisms, such as in eliminations or substitutions. In mechanism tasks, students were found to interpret the task in ways that align with their existing ideas rather than engage in forms of multivariate reasoning (Kraft *et al.*, 2010). The latter requires recognizing different chemical variables that may influence a reaction pathway and evaluating their relative importance (Watts *et al.*, 2021). Moreover, Bhattacharyya (2022) showed that assessment formats in organic chemistry frequently emphasize tasks that do not address chemical reasoning and therefore do not require multivariate reasoning. As a result, students can perform successfully without understanding the multivariate nature of reaction mechanisms. Since assessment formats send messages to students about what might constitute central learning outcomes, students may not focus on chemical reasoning in their exam preparation either (Stowe *et al.*, 2021; Esselman *et al.*, 2023). These findings from previous literature align with the ideas expressed here regarding multiple reaction pathways and suggest how SMMK and SMP, as well as conceptual knowledge, may influence each other.

However, in our sample, six students expressed ideas at level 3b, acknowledging that reactions may proceed through different pathways even under identical conditions, or that the exact pathway cannot always be determined. Ted's explanation exemplifies this form of reasoning:

Ted: "*In organic chemistry, there are also some reactions where we talk about these resonance structures, where we don't exactly know the precise position of the charge or the functional group. And depending on where that group happens to be during a reaction, it might actually lead to two different reactions. And because of that, theoretically – like I said – if one scientist, for example, says the group is located here, and another says it's over there [...] and the groups are shifting back and forth, then of course both mechanisms could theoretically be correct in a reaction.*" (SMMK, multiple RM, level 3b)

Although his use of resonance was conceptually inaccurate because he explained resonance with delocalized functional groups instead of electrons, Ted's statement shows how his existing conceptual ideas shaped his perspective on mechanisms as theoretical models. This highlights that SMMK and conceptual knowledge are intertwined and may influence each other, which is in line with findings suggesting that MMK can positively affect the ability to provide mechanistic explanations (Baek and Schwarz, 2015).

Overall, the SMMK in the aspect *multiple reaction mechanisms* and the concrete practice of handling such competing reaction mechanisms may mutually influence each other, both positively and negatively. This indicates a connection between the SMMK and SMP dimensions that should be explored explicitly. It became clear that, in our sample, a wide range of levels were present and that there was no single predominant trend regarding the aspect *multiple reaction mechanisms*. To address this aspect, tasks that prompt engagement with different, potentially plausible reaction pathways may foster multivariate reasoning and an understanding of multiple possible reaction pathways and products (Lieber and Graulich, 2020).

Testing and changing reaction mechanisms

The two aspects *testing* and *changing reaction mechanisms*, were closely connected in students' expressed ideas. With only three exceptions, students' ideas were assigned to the same level in both aspects, suggesting that they drew on similar underlying ideas. Overall, the distribution between media-oriented (12 students) and methodological perspectives (10 students) was relatively balanced (see Table 2).

Many students described *testing reaction mechanisms* as comparing a proposed mechanism with experimental outcomes or with established chemical principles. For example, Tracy described that a reaction mechanism is established based on chemical concepts and then needs to be experimentally verified:

Tracy: "*You look at the chemical principles to see which individual steps must be carried out in order to obtain this product, which you should then verify again.*"

Interviewer: "*What do you mean by verify?*"

Tracy: "*The product. That you verify it again at the end [in the laboratory].*" (SMMK, testing RM, level 2)

In her description, Tracy did not further elaborate on how the verification of products might proceed in detail. It was observed in several participants that, while they described a verification or comparison with the experiment, they did not have a concrete idea of how this process could actually take place when being prompted. In these cases, the testing and changing of reaction mechanisms was described through a confirmatory approach, applying known ideas and verifying them retrospectively, rather than in a hypothesis-driven manner.

In line with her ideas on *testing reaction mechanisms*, Tracy mentioned that reaction mechanisms can be changed by applying chemical conceptual knowledge to correct the steps if they are no longer chemically accurate, for example, if a different product is obtained during verification:

Tracy: "*I would say it depends on the step where the error might occur [...]. That you might be able to fix this error using chemical knowledge, or conceptual knowledge, if that is actually the case.*" (SMMK, changing RM, level 2)

Tracy's statement on fixing errors through conceptual knowledge could likely stem from her familiarity with this type of verification from other task contexts. In various settings, particularly in organic chemistry, typical tasks (see *e.g.*, Bodé *et al.*, 2019; Lieber and Graulich, 2022; Weinrich and Britt, 2022) often focus solely on establishing the correctness of the mechanism, such as when students are asked to propose a reaction mechanism. In her expressed idea, Tracy focuses on the conceptual correctness without referring to the macroscopic level in the form of experimental evidence or data, closely resembling common task formats that likewise emphasize conceptual components.

While Tracy primarily related *testing reaction mechanisms* to verifying the representation of the individual steps of a known mechanism and modifying this representation, if necessary, Lily went a step further by describing how new reaction mechanisms can be proposed in a hypothesis-driven manner:

Lily: "*You can probably formulate a lot of hypotheses and make assumptions about what should or might happen. [...]. And I start by forming well-founded assumptions. [...] I test them in small series by thinking, okay, this part here is strongly positive, that one strongly negative, I don't know, maybe I have a carboxylic acid group that is relatively electron-rich. And with that, I try to interact somehow, and then I look to see whether something different happens when I use a stronger substituent. And of course, the question is always at which position on the molecule this takes place. And then I believe all those methods like spectroscopy, crystallography, and so on, become relevant*." (SMMK, testing RM, level 3b)

In her descriptions, she already addressed specific chemical aspects, such as electron interactions, and mentioned experimental and analytical methods for testing. This indicates that she already engages with core elements of inquiry in organic chemistry, such as making assumptions, probing them systematically, and using experimental evidence to refine the hypothesis. Lily's ideas, therefore, may be particularly valuable, as they already reflect how reaction mechanisms can serve as tools for sensemaking to predict and control reactions. This way of engaging with reaction mechanisms aligns closely with how models are used by experts in authentic scientific practice in organic chemistry (Stowe and Esselman, 2023).

Overall, approximately half of the students, including Tracy, related *testing* and *changing reaction mechanisms* to verification, that is, checking an existing known reaction mechanism. This finding may not be surprising as chemistry courses often place less emphasis on engaging students in inquiry processes and instead focus on conveying declarative knowledge as end products of the inquiry process (Freire *et al.*, 2019). The students in our sample had completed a laboratory course in general chemistry before. Although laboratory courses are commonly described as a bridge between theory and practice (*e.g.*, Carnduff and Reid, 2003; Hofstein and Lunetta, 2004; Reid and Shah, 2007), they rarely involve genuine hypothesis-driven explorations (Carnduff and Reid, 2003). Rather, students typically follow predetermined procedures aimed at verification processes (Hofstein and Lunetta, 2004; Buck *et al.*, 2008; Galloway and Bretz, 2015). In chemistry labs in particular, factors that would support an emphasis on inquiry processes, such as communication or error analysis, receive little emphasis (Bruck and Towns, 2013). This may help explain why half of the students in our sample also described *testing* and *changing reaction mechanisms* as verification of known mechanisms.

The other half focused on deriving possible reaction mechanisms for unknown reactions. They described building hypotheses for unknown reactions either from known reaction mechanisms of similar substances or from relevant chemical concepts. These constructed hypotheses then get examined. In most cases, *changing* was closely intertwined with *testing*, as mechanisms are changed when unexpected results are identified during testing.

Taken together, the 22 students expressed a broad range of SMMK across all five aspects. Media-oriented perspectives predominated regarding the *nature of reaction mechanisms* and *purpose of reaction mechanisms*, where students mainly viewed them as (idealized) representations used to illustrate reaction pathways. This pattern has also been reported in other studies (Krell *et al.*, 2015b; Krell and Krüger, 2017; Krell, 2019), which included different sample groups (*i.e.*, secondary school students), investigated MMK rather than SMMK, and had different study foci. Possible explanations for the predominance of media-oriented ideas discussed in these studies include the respective disciplinary context or the way students experienced models through instruction. In particular, the *nature of models* and the *purpose of modeling* may reflect how models were used as media in instructional settings. The aspects *multiple reaction mechanisms*, *testing*, and *changing reaction mechanisms* showed a more balanced distribution of ideas in our study, with a higher number of methodological perspectives. Here, students referred not only to representational functions but also to how mechanisms relate to the macroscopic level (Johnstone, 1993).

The close connection between the *testing* and *changing reaction mechanisms* is also supported theoretically. Windschitl *et al.* (2008) identified testability and revisability as core epistemic features of scientific knowledge, grounded in hypothesis formulation and rejection. It is therefore encouraging that students have already expressed the connection between these ideas across the two aspects. Also, they argue that scientific knowledge is conjectural. In the context of reaction mechanisms, recognizing the existence of alternative reaction pathways (*multiple reaction mechanisms*) relates directly to understanding the provisional nature (*testing reaction mechanisms*) and modifiability (*changing reaction mechanisms*) of reaction mechanisms (Windschitl *et al.*, 2008). Taken together, these perspectives highlight that a well-developed SMMK is valuable for engaging with organic chemistry because it aligns closely with how reaction mechanisms are constructed, tested, and refined in the discipline.

Building on this, the goal should be to support students in developing an integrated understanding that connects reaction mechanisms to broader scientific activities, like, for example, evaluating information or constructing explanations in contexts beyond reaction mechanisms (National Research Council, 2012; Osborne, 2014). Students should have opportunities to link core epistemic features of science with their work on reaction mechanisms and to transfer this understanding across contexts. However, since prior research has shown that MMK is context- and discipline-dependent (Krell *et al.*, 2015b), the extent to which a well-developed SMMK regarding reaction mechanisms contributes to other contexts and to a broader understanding of science (Ke and Schwarz, 2021) requires further investigations. At the collective level, students in our study already demonstrated resources that can support such an understanding of science. However, questions remain about how these resources are distributed individually and how they appear in relation to general MMK.

RQ2: What patterns can be identified between students' ideas about reaction mechanisms (SMMK) and their ideas about models and modeling in general (MMK)?

Since the modeling character of reaction mechanisms may not be obvious, compared to models, such as atomic models in chemistry, it remains unclear what patterns exist between ideas in the SMMK and students' ideas within the MMK in general. While the group-level distribution within the SMMK dimension was presented in the first research question, the group-level distribution of the MMK dimension can be found in Appendix B. The distribution of the assigned representative levels for each student's ideas at the individual level within the SMMK and MMK dimensions is shown on the left side of Fig. 6.

To analyze the patterns between the MMK and SMMK dimensions, we first considered the overarching perspectives (*i.e.*, media-oriented, methodological) on models and reaction mechanisms expressed in students' ideas (see Methods section), which are shown on the right side of Fig. 6 and, identically, on the left side of Fig. 7. Based on these overarching perspectives and qualitative analyses, we formed four groups of students. The illustration of these groups derived from the overarching perspectives is presented on the right side in Fig. 7.

Groups 1 and 4 showed consistent perspectives across both dimensions: predominantly media-oriented in Group 1 and predominantly methodological in Group 4. Group 2 included students whose ideas were largely media-oriented but already showed emerging methodological elements. Interestingly, these students tended to express more methodological ideas about models than about reaction mechanisms. Group 3 showed the opposite pattern: students demonstrated mostly methodological perspectives regarding reaction mechanisms, while their ideas in the MMK still reflected mainly media-oriented perspectives. These group characteristics become clearer when examining exemplary ideas expressed by individual students, which will be presented in the following.

Group 1: exclusively media-oriented perspectives in the MMK and SMMK. Group 1 consisted of five students who expressed media-oriented ideas (*i.e.*, level 0, 1, or 2) across all aspects of both dimensions (see Fig. 7). They viewed models and reaction mechanisms throughout the interview primarily as representations of an original, used to illustrate or describe phenomena. Jasmine, for instance, explicitly connected her views on the *nature of reaction mechanisms* with those on the *nature of models* by describing reaction mechanisms as "kind of a model" (see Fig. 8).

As shown in the upper part of Fig. 8, she described reaction mechanisms as focused representations of certain properties of an original. She further explained that this representation helps to better understand the pathway of a reaction. Overall, her idea was assigned to level 2. Later, when asked about the *nature of models*, she again emphasized their representational role. As shown in the lower part of Fig. 8, she again focused on the idea of "making things understandable." Although her explanation was less detailed at this point, the similarity to her statements about the *nature of reaction mechanisms* is clearly recognizable.

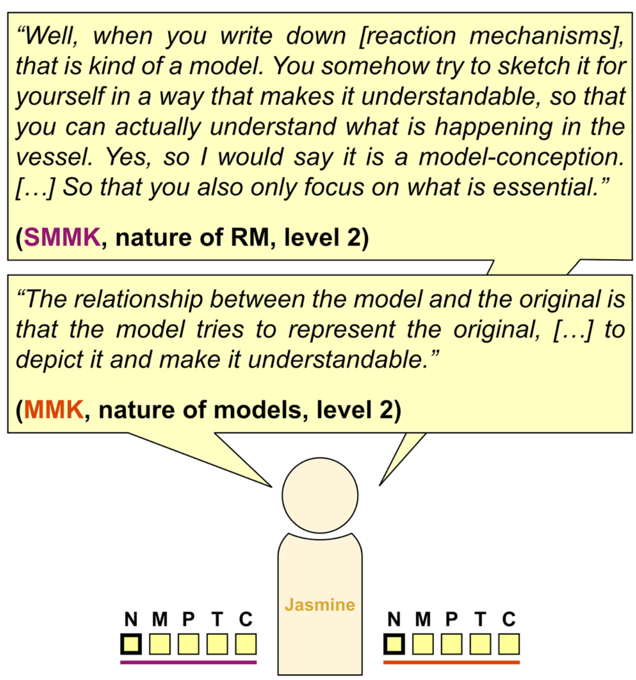

Fig. 8 Jasmine's media-oriented ideas regarding the nature of reaction mechanisms (above) and the nature of models (below).

The parallels between the ideas in the SMMK and MMK suggest that she activates similar ideas across both contexts. Comparable patterns appeared across other aspects: for example, Jasmine described *testing reaction mechanisms* and *testing models* in almost identical ways, by comparing representations with experimental results. This comparability indicates that she activated the same media-oriented perspective, focusing on the representational character of models, when thinking about models in general and reaction mechanisms in particular.

These media-oriented ideas within different aspects align with findings from previous research showing that many learners initially understand models mainly as illustrative tools, while methodological perspectives like seeing models as instruments for inquiry are more difficult to develop (*e.g.*, Grosslight *et al.*, 1991; Crawford and Cullin, 2005). Similar findings regarding the predominance of media-oriented ideas within the MMK have been reported across various sample groups: for instance, for pre-service biology teachers (Göhner *et al.*, 2022), for in-service biology teachers (Krell and Krüger, 2016), for university students from different disciplines (Krell and Krüger, 2017), and for secondary school students (Krell *et al.*, 2015b). A similar predominance of media-oriented ideas was also observed for reaction mechanisms as models among students in Group 1. One plausible explanation for this predominance of media-oriented perspectives is that students have so far encountered both models and reaction mechanisms mainly in instructional contexts, where their representational functions are emphasized. Reaction mechanisms, in particular, are typically introduced only briefly in secondary school. As suggested by Lazenby *et al.* (2020), limited opportunities to engage in authentic modeling practices may make it difficult for students to develop methodological perspectives. Furthermore, research has shown that chemistry students, especially in the case of particle-level models, emphasize the representative character of models for illustrating non-observable phenomena (Lazenby *et al.*, 2019a). Since reaction mechanisms operate at the particle level, this is consistent with our results for Group 1.

Taken together, students in Group 1 demonstrated foundational ideas in both their SMMK and MMK. They clearly recognized the representational function of reaction mechanisms and models, which provides an important basis for further conceptual development. At the same time, their ideas did not yet indicate an awareness of the epistemic role that both models in general and reaction mechanisms can play within inquiry processes.

Group 2: emerging methodological perspectives in the MMK and SMMK. Group 2 consisted of nine of the 22 students who showed an emerging methodological perspective in at least one of the two dimensions, either MMK or SMMK. Students were assigned to this group if they demonstrated a methodological perspective in at least one aspect (see Fig. 7). However, most of their ideas still reflected a media-oriented view across both dimensions, meaning that at least six out of ten aspects (MMK and SMMK combined) were assigned to the media-oriented perspective overall. For building this group, no distinction was made regarding which of the two dimensions the students expressed emerging methodological views. Group 2, therefore, included students who have already expressed methodological ideas in some aspects of MMK or SMMK. A characteristic pattern emerged: these students often described *testing* and *changing models* from a methodological perspective, while *testing* and *changing reaction mechanisms* were still described from a more media-oriented, verification-focused perspective. In the remaining aspects, methodological ideas appeared only sporadically.

Robin illustrates this trend. Her views on the *nature of models* and *reaction mechanisms* resembled the media-oriented perspectives found in Group 1, but clearer differences appeared in the aspects of *testing* and *changing*. As shown in the upper part of Fig. 9, she described for *testing reaction mechanisms* that established reaction mechanisms are, in her view, correct. This suggests that the provisional character of reaction mechanisms when thinking about the testing process is missing. At the same time, she differentiated between herself and experimental chemists, who, in her opinion, are the ones actually conducting the testing of reaction mechanisms. Accordingly, testing primarily refers to verification in the laboratory, specifically the verification of previously made deductive claims. This perspective was also reflected in her assumption that once a mechanism has been established, it can generally be seen as reliable.

Her ideas about the *testing models*, shown in the lower part of Fig. 9, reflected a more hypothesis-driven perspective. She perceived models as a starting point from which hypotheses can be derived and experimentally tested, or as a tool for purposefully observing natural phenomena. This illustrates

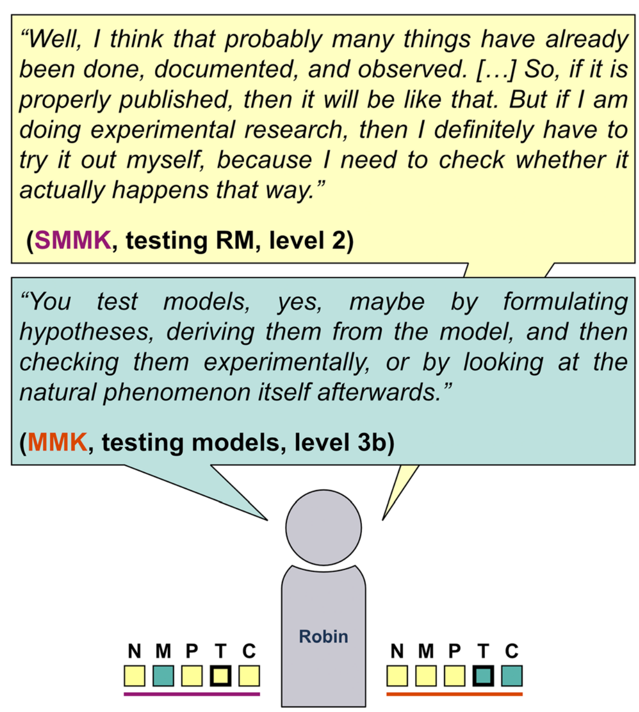

Fig. 9 Robins ideas regarding the testing reaction mechanisms (above; media-oriented) and testing models (below; methodological).

the dynamic, research-oriented role of models. In contrast to her ideas about reaction mechanisms, her description here also reflected elements of abductive reasoning: models, based on data such as experiments and observations, serve to provide the most plausible explanations (Johnson and Krems, 2001).

Most students in Group 2 demonstrated a similar pattern: they approached *testing* and *changing models* in a hypothesis-driven manner and included elements of abductive reasoning, but described *testing* and *changing reaction mechanisms* primarily as verification of known information.

Previous research on students' MMK similarly indicates that *testing* and *changing models* can be more methodologically oriented than other aspects, aligning with our findings in Group 2 (*e.g.*, Krell *et al.*, 2015b; Lazenby *et al.*, 2020). However, we only observed this pattern in the MMK dimension and not in the SMMK dimension in this group. This difference may reflect that students often perceive reaction mechanisms as certain and established elements of knowledge shaped by how chemistry is typically taught in school (Freire *et al.*, 2019).

Yet, the epistemic underpinnings become particularly visible when focusing on the development, testing, and changing of models or reaction mechanisms in particular.

In turn, when thinking about models in general, students might have found it easier to consider the testing as an abstract, hypothesis-driven process. Considering the work of Grove and Bretz (2010) on student difficulties in learning organic chemistry, the ideas of students in Group 2 may be interpreted through the lens of dualistic thinking. This perspective is characterized by a linear view of problems and answers and can be expressed by an emphasis on verification rather than exploratory approaches to *testing of reaction mechanisms*. Overall, students in Group 2 shared predominantly media-oriented ideas but showed emerging methodological reasoning, particularly in the MMK dimension. The variation in ideas between MMK and SMMK is noteworthy: while methodological perspectives appeared in students' ideas with their MMK, their ideas on reaction mechanisms were largely verification-oriented. Interestingly, Group 3 displayed the opposite trend.

Group 3: predominantly methodological perspectives in the SMMK. Group 3 comprised six students who already demonstrated predominantly methodological ideas overall. This means their ideas were assigned to the methodological perspective in at least five out of ten aspects across both dimensions. Remarkably, students in this group showed predominantly methodological ideas across all aspects within the SMMK dimension, while their ideas within the MMK dimension were comparatively more media-oriented (see Fig. 7).

Barney illustrated this pattern. Throughout the SMMK part, he consistently emphasized the role of reaction mechanisms in inquiry-oriented processes. As shown in Fig. 10, he highlighted their function in optimizing industrial syntheses, such as drug production, by analyzing mechanistic steps to identify how to increase the product yield. These ideas corresponded to level 3a and were associated with a methodological perspective. However, when discussing models in general and their purpose,

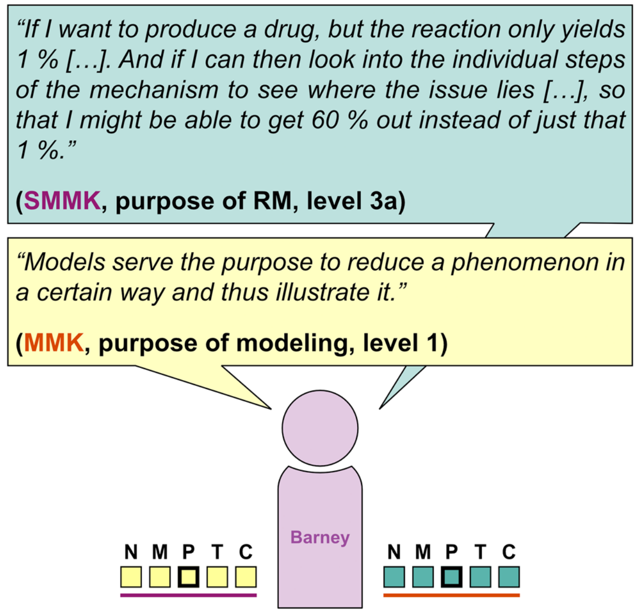

Fig. 10 Barney's ideas regarding the purpose of reaction mechanisms (above; methodological) and the purpose of modeling (below; media-oriented).

Barney did not express similar methodological ideas. As shown in the lower part of Fig. 10, he described models as simplified representations used to illustrate phenomena (MMK, purpose of modeling, level 1), reflecting a more media-oriented idea without reference to any application contexts. His MMK statements, therefore, did not mirror the methodological reasoning he expressed about reaction mechanisms. This difference in ideas may stem from the higher level of abstraction when discussing models in general or from activating different examples as reference points. This deviation between his ideas in the MMK and SMMK was also evident across the other aspects for him and was also observed among the other students in this group (see Fig. 7).

They showed well-developed methodological ideas within the SMMK dimension, contrasted with more media-oriented ideas within the MMK dimension. The overall consistency and methodological level within students' ideas in the SMMK dimension suggested an already elaborated epistemic understanding of reaction mechanisms. When looking at students' ideas within the MMK dimension, there were isolated indications that models can be used in inquiry processes, but students nevertheless showed similar patterns to those in Group 2: *testing* and *changing* stood out from the other three aspects, while *nature of models*, *multiple models*, and *purpose of modeling* were often addressed from a media-oriented perspective to describe or understand phenomena.

Taken together, these findings indicate that the students in this group did not consistently connect their ideas regarding reaction mechanisms with their ideas about models in general. This supports the context-dependence of MMK (*e.g.*, Krell *et al.*, 2015b; Krell, 2019; Ke and Schwarz, 2021), meaning that students activated different resources depending on the context without linking them to each other. Since the students in this group already demonstrated well-developed methodological ideas regarding reaction mechanisms, explicitly emphasizing their modeling character may help students to develop similar methodological ideas within the MMK dimension regarding models in general.

Group 4: methodological perspectives across all aspects within MMK and SMMK. Finally, Group 4 included two students who expressed methodological perspectives in almost all aspects of both dimensions. This referred to students who showed methodological ideas both on models and reaction mechanisms in at least four out of five aspects in each dimension (see Fig. 7). This group, therefore, demonstrated coherent and advanced ideas of models and reaction mechanisms as research tools in scientific inquiry processes. Lily serves as an illustrative example. She explicitly referred to the modeling character of reaction mechanisms and integrated ideas across both SMMK and MMK.

As shown in Fig. 11, she began by stating that reaction mechanisms have a modeling character. She immediately linked this modeling character to the notion that reaction mechanisms are provisional and cannot be conclusively proven. In addition to connecting the SMMK and MMK ideas, she also demonstrated links between the individual aspects within the SMMK dimension. This became evident as she described how reaction mechanisms get developed and, in doing so, also tested or verified. She explicitly characterized reaction mechanisms as model-based and not fully verifiable, describing them as "a theoretical construct" that "represents what probably happens", which suggests an understanding of their provisional nature.

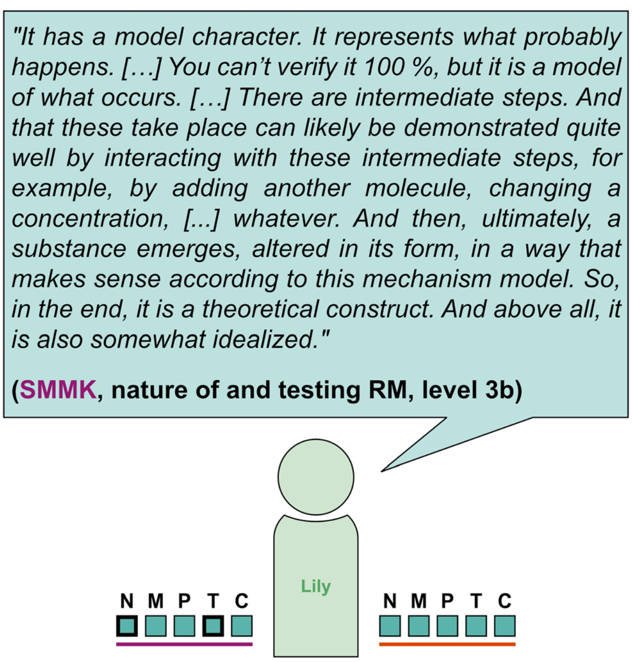

Fig. 11 Lily's methodological ideas regarding the nature of and testing reaction mechanisms.

Lily can be seen as an example of a meaningful integration of her ideas within the SMMK regarding reaction mechanisms and MMK. She combined ideas from both dimensions and demonstrated a consistent connection of her SMMK and MMK. This reflects the coherent transfer of her resources across contexts (Hammer *et al.*, 2005). Lily's understanding allowed her to view reaction mechanisms simultaneously as theoretical constructs, explanatory models, and predictive tools within inquiry processes. Her statements illustrate what an advanced integration of SMMK and MMK can look like and thus provide a purposeful reference for potential support in fostering the connection between both dimensions. Furthermore, such well-connected resources across contexts can contribute to a broader understanding of scientific ideas and of the nature of scientific disciplines (Taber, 2017). At the same time, a coherent connection between SMMK and MMK may help students develop epistemic ideas related to the specific discipline within a given context. In the case of chemistry, this may promote chemical thinking (Talanquer, 2021; Talanquer, 2025).

All in all, we identified four groups of students who showed similar patterns in their ideas. While some students expressed consistently media-oriented perspectives (Group 1) or consistently methodological perspectives (Group 4), Groups 2 and 3 displayed varying patterns. In Group 2, students often described the *testing* and *changing models* from a methodological, inquiry-related perspective, yet framed the *testing* and *changing reaction mechanisms* mainly as the verification of representations or known rules and reactions. Students in Group 3 described reaction mechanisms predominantly from a methodological perspective, whereas their general ideas within the MMK dimension remained more media-oriented.

Taken together, no uniform pattern emerged regarding how the ideas within the aspects of MMK and SMMK co-occurred across the four groups. Instead, different forms of alignment appeared within and across both dimensions. Across the dataset, *testing and changing* were closely connected in both MMK and SMMK, and the aspects *nature* and *purpose of models* and *reaction mechanisms* were likewise often described from similar perspectives (see Fig. 7).

Limitations

As our study is exploratory, several limitations must be considered. Its primary aim was to gain an initial qualitative understanding of chemistry students' ideas regarding models and reaction mechanisms at an epistemic level (MMK and SMMK). As the students in our study had not yet received formal instruction on reaction mechanisms, the results are not representative of students who already have more experience in organic chemistry. In particular, methodological perspectives may be less developed than would be expected after instruction, assuming that the lecture addresses these aspects. The findings should therefore be interpreted as initial insights into the ideas students bring with them when entering the OC1 lecture and the perspectives that instruction may need to build upon.

The findings are based on the ideas students activated during the interview, which may not fully reflect their overall conceptions about models and modeling. Moreover, because SMMK was examined without reference to a specific chemical reaction, the type of resources activated may have been influenced by this lack of contextualization, and students' ideas might vary depending on the reaction considered. The interview design also introduces potential contextual effects: ideas activated in the SMMK section may have influenced both students' activities in the subsequent SMP part and their later statements in the MMK part, while the SMP part itself may also have further shaped students' statements on MMK through priming (Schacter and Buckner, 1998). Although we placed the MMK part at the end to facilitate discussion with existing literature, such effects cannot be fully excluded. In addition, the use of pre-formulated sentence-starters in the MMK section may have subtly guided students' responses, as they prestructured the syntactic form of the answers. Finally, while students occasionally expressed ideas aligned with different levels within certain aspects, each participant was assigned one representative level per aspect for analytical clarity. This coding decision may have reduced some within-aspect nuance in students' statements.

Conclusion

Reaction mechanisms are theoretical constructions that both aim to depict reaction pathways and model them to explain, predict, or control chemical reactions (Goodwin, 2017). While the specific meta-modeling knowledge (SMMK) comprises epistemic ideas about reaction mechanisms as models, the general meta-modeling knowledge (MMK) concerns uncontextualized models more broadly. Both dimensions may shape one another, yet they are not identical due to the context- and discipline-dependence as reported in previous literature (Gobert *et al.*, 2011; Grünkorn *et al.*, 2014b; Krell *et al.*, 2015b; Krell and Krüger, 2017). Variance across different status groups within the MMK dimension has already been extensively investigated (*e.g.*, Grosslight *et al.*, 1991; Treagust *et al.*, 2002; Crawford and Cullin, 2005; Schwarz and White, 2005; Van der Valk *et al.*, 2007; Gobert *et al.*, 2011; Grünkorn *et al.*, 2014b; Krell *et al.*, 2015b; Krell and Krüger, 2016; Krell and Krüger, 2017; Lazenby *et al.*, 2020).

Our study, conducted before chemistry students attended the organic chemistry lecture, examined their ideas within the SMMK regarding reaction mechanisms, how they perceive the modeling character, and how these ideas appear in relation to their ideas within the MMK. Our findings show that students possessed a broad range of SMMK ideas (see Table 2), spanning from viewing reaction mechanisms as accurate depictive representations to understanding them as theoretical constructs for generating knowledge. Overall, media-oriented ideas dominated in the aspects *nature* and *purpose of reaction mechanisms*, emphasizing the function of mechanisms as (idealized) representations for illustrating reaction pathways or supporting understanding. These findings complement earlier studies, in which students showed difficulties recognizing the purpose of reaction mechanisms beyond describing reactions (Anderson and Bodner, 2008) or often did not use them in a model-based manner (Popova and Bretz, 2018). Nevertheless, even though students had not attended OC1 and therefore had only a rudimentary introduction to reaction mechanisms so far, many already demonstrated methodological perspectives. In the aspects *multiple*, *testing*, and *changing reaction mechanisms*, students' ideas displayed a more balanced distribution between media-oriented and methodological perspectives, with greater variation among students. This is encouraging and provides a solid foundation for further instruction. It highlights the importance of building on students' prior experiences and ideas when teaching reaction mechanisms.

To explore patterns between students' SMMK and MMK and whether they recognize and incorporate the modeling character of reaction mechanisms, especially given prior findings that MMK is context-dependent (*e.g.*, Krell, 2019; Ke and Schwarz, 2021), we identified four groups reflecting distinct conceptual patterns across both dimensions (see Fig. 7).

Some students expressed consistently media-oriented (Group 1) or consistently methodological perspectives (Group 4) across both dimensions, indicating a coherent connection and transfer of resources (Hammer *et al.*, 2005). Prior research in general chemistry has shown that many students focus primarily on the representational, media-oriented perspective on models in chemistry (Lazenby *et al.*, 2020). These findings are consistent with our results from Group 1. However, it is important to emphasize that methodological perspectives are not inherently superior to media-oriented ones; both can be equally valuable when they are meaningfully connected (Krell *et al.*, 2014). The connection of resources from decontextualized MMK and SMMK, as in Group 4, suggests flexible resource activation and transfer from decontextualized to contextualized settings. A well-developed (specific) meta-modeling knowledge and its contextual embedding are assumed to support students' understanding of scientific ideas (Taber, 2017) and scientific inquiry processes (Upmeier zu Belzen and Krüger, 2010; Schwartz, 2019). Moreover, acknowledging reaction mechanisms as models, including their epistemic underpinnings from a methodological perspective, may support the development of chemical thinking (Talanquer, 2021; Talanquer, 2025). Students in Groups 2 and 3 showed variation in their ideas within the MMK and SMMK dimensions. Students in Group 2 described the *testing* and *changing models* in a hypothesis-driven manner and conceptualized reaction mechanisms primarily within a verification-oriented perspective (*i.e.*, experimental verification of known synthesis steps). Nevertheless, both dimensions showed a strong link between *testing* and *changing*, extending previous findings on MMK (*e.g.*, Krell and Krüger, 2016; Lazenby *et al.*, 2020). This connection is valuable because it indicates that students already relate two key epistemic features of scientific knowledge: its testable and revisable nature (Windschitl *et al.*, 2008). Students in Group 3, by contrast, demonstrated elaborated methodological ideas within SMMK but did not express those same ideas in their general perspective of models.

Taken together, the present study supports the aspect-dependent view of both SMMK and MMK (*e.g.*, Crawford and Cullin, 2005; Krell *et al.*, 2014; Upmeier zu Belzen *et al.*, 2019), as differences emerged across individual aspects. It also reinforces the context-dependency of MMK (Gobert *et al.*, 2011; Grünkorn *et al.*, 2014b; Krell *et al.*, 2015b; Krell and Krüger, 2017), given that students showed notable discrepancies between their ideas about models in general and about reaction mechanisms. Our study further aligns with findings by Krell *et al.* (2013), who reported that students expressed ideas about the purpose of models in specific contexts that extended beyond descriptive accounts. By contrast, decontextualized prompts tended to elicit predominantly media-oriented perspectives. In our sample as well, students more frequently expressed methodological perspectives in the context of reaction mechanisms. This supports the inclusion of the SMMK dimension as a contextualization of the MMK dimension. Rather than revealing a single coherent pattern, the data indicate that students' ideas were linked in diverse ways. The findings may suggest that an integration of SMMK and MMK is not automatically achieved at this stage, prior entering organic chemistry lectures. This could indicate that uncontextualized MMK does not directly transfer to specific contexts such as reaction mechanisms, which leads to implications for both teaching and research.

Implications for teaching

Our study showed that there is no uniform pattern in how students' ideas within the SMMK dimension connect to their ideas within the MMK dimension. While most students already demonstrated basic ideas that align with the media-oriented perspective on models and reaction mechanisms, instruction, particularly in Organic Chemistry 1, should explicitly address the modeling character of reaction mechanisms to strengthen the connection between SMMK and MMK. As Heinrich *et al.* (2026) found, epistemic operations such as testing hypotheses (related to *testing* and *changing reaction mechanisms*) are rarely emphasized in OC1 lectures by instructors, even though they represent core practices of scientific inquiry. However, these operations should be explicitly foregrounded to promote MMK, which encompasses the scientific practices involved in working with models. Moreover, the instructor could explicitly highlight that reaction mechanisms are not certain constructs but rather provisional in nature (*nature* and *purpose of reaction mechanisms*) to avoid oversimplification (Talanquer, 2025) and to promote multivariate reasoning (Kraft *et al.*, 2010). This aligns with the need documented in chemistry education research to support early development toward relativistic thinking, which enables one to flexibly apply different concepts depending on the context to make sense of chemical reactions (Grove and Bretz, 2010). For faculty professional development, it may also help if instructors are aware that students exhibit varying patterns and connect reaction mechanisms to models in varying ways.

Since students also showed variation in their ideas within the SMMK dimension (see Fig. 4), the five different aspects should be addressed repeatedly throughout the lecture series or in laboratory courses. Aligning lecture content with laboratory work is essential for enabling authentic engagement in scientific practices. Considering the present findings, laboratory courses offer particular potential to support certain aspects of students' SMMK regarding reaction mechanisms. For instance, the aspect of *testing reaction mechanisms* can be addressed by engaging students in formulating hypotheses about reaction pathways and evaluating them based on experimental data generated in the laboratory. Moreover, laboratory work provides opportunities to engage with the aspect of *multiple reaction mechanisms*, as variations in product yields or competing reactions can be explored empirically. Rather than merely learning about scientific practices, the laboratory thus offers the opportunity in chemistry to engage in them directly (Carnduff and Reid, 2003; Hofstein and Lunetta, 2004; Reid and Shah, 2007). Within lecture series, these aspects could be further supported by explicitly framing reaction mechanisms as models (*nature of reaction mechanisms*) and by highlighting their applications in research or industrial contexts, as well as to mention well-known products resulting from such syntheses.

Implications for research

Our study showed that students in their second year of chemistry studies expressed diverse ideas regarding both their SMMK and MMK. These findings raise the question about how such ideas are shaped by either prior school experiences and how they develop or shift over the course of university education, especially how students' SMMK and MMK develop throughout the Organic Chemistry 1 lecture. It is particularly unclear to what extent ideas in the SMMK might expand or diversify, given that OC1 lectures tend to focus less on epistemic operations related to scientific inquiry and more on describing mechanistic steps (Heinrich *et al.*, 2026). With respect to MMK, explicit instruction is also likely limited in organic chemistry, raising the question of whether students' ideas about models and modeling remain rather unchanged in the absence of authentic modelling practices. Monitoring students' development of ideas in their SMMK or MMK during the organic chemistry courses could provide additional insights into these developments throughout the lecture, and if elaborated ideas are actually an asset in learning organic chemistry. For instance, how thinking *about* models (MMK) and thinking *about* reaction mechanisms (SMMK) influence thinking *with* reaction mechanisms across task contexts (specific modeling practices; SMP) (Gouvea and Passmore, 2017). This would help clarify which meta-modeling resources students activate when working on mechanistic problems in organic chemistry (Dood and Watts, 2022b). For example, when evaluating alternative reaction pathways, students' ideas regarding *multiple reaction mechanisms* may guide or prevent productive approaches when they compare and assess possible reaction outcomes. In this sense, a well-developed SMMK in the context of reaction mechanisms may support students' abilities to build mechanistic explanations and foster conceptual learning, similar to findings reported for more decontextualized modeling knowledge (Baek and Schwarz, 2015; Schuchardt and Schunn, 2016). Beyond analyzing students' argumentation in such contexts (*e.g.*, Lieber and Graulich, 2022), future research could therefore focus on the extent to which epistemic ideas about reaction mechanisms influence or complement the use of conceptual resources.

Furthermore, it would be valuable to develop a quantitative instrument to assess students' SMMK, enabling systematic evaluation and potential use in the context of OC1 instruction. While quantitative approaches for measuring MMK already exist (*e.g.*, Treagust *et al.*, 2002), comparable approaches could be adapted for the SMMK regarding reaction mechanisms. A more detailed understanding of how thinking *about* models (MMK) and thinking *about* reaction mechanisms (SMMK) influence thinking *with* reaction mechanisms across different task contexts (specific modeling practices; SMP) would help clarify which meta-modeling resources students activate when working on mechanistic problems in organic chemistry (Gouvea and Passmore, 2017; Dood and Watts, 2022b).

Author contributions

Sarah Saupe: conceptualization, data curation, investigation, methodology, project administration, visualization, writing – original draft preparation. Leonie Lieber: conceptualization, methodology. Nicole Graulich: supervision, conceptualization, methodology, project administration, writing – review and editing.

Conflicts of interest

There are no conflicts to declare.

Data availability

The interview data are not publicly available as the participants did not consent for their data to be shared publicly.

Appendices

Appendix A: interview guide for the SMMK part

To enhance transparency regarding the data collection procedure, the interview questions used in the SMMK section are provided below. The interview was conducted in a semi-structured format. Therefore, the questions listed represent the core prompts used to initiate discussion, while additional follow-up questions were asked depending on the participants' responses to encourage clarification and elaboration. The prompts were related to the five respective aspects of SMMK. As all interviews were performed in German, the questions presented here are translations of the original interview guide.

- How would you define the term ''reaction mechanism'' and what do you understand by the term?
- What is represented by a reaction mechanism?
- How would you describe the relationship between the written reaction mechanism and what happens in a reaction vessel?
- For what purposes are reaction mechanisms used?
- How are reaction mechanisms developed?
- What makes a reaction mechanism good or poor in your view?
- How can reaction mechanisms be tested in general?
- How can scientists test/evaluate reaction mechanisms?
- When/How does a reaction mechanism need to be revised or modified?
- Imagine two scientists propose different reaction mechanisms for an unknown reaction. In what ways might their mechanisms differ?
- How could such differences be addressed?

Appendix B: group-level distribution of students' ideas within the MMK dimension

The overall distribution of assigned levels 0 to 3b within the MMK dimension can be found in Table 3, and a brief description of the most prevalent student ideas is provided in Table 3. Across the aspects *nature of models*, *multiple models*, and *purpose of modeling*, most ideas students expressed were assigned to the media-oriented perspective. Regarding the *nature of models*, many students described models as highly accurate or idealized representations of phenomena, reflecting an understanding of models as tools for depicting scientific phenomena. In the aspect *purpose of modeling*, the focus lay on the description of phenomena as the most frequent idea, whereas some students also emphasized the explanatory function in the sense of promoting an understanding. In the aspect *multiple models*, most students expressed that multiple models are needed because a single model cannot capture all aspects of a complex original. This reflects an appreciation for the complementary nature of multiple models and their usefulness in addressing distinct aspects of a phenomenon.

In contrast, the aspects *testing models* and *changing models* were dominated by the perspective of models as tools within scientific inquiry processes, for example, in testing and modifying hypotheses or theories. Similar to the SMMK, these two aspects were closely connected and difficult to distinguish. In many cases, students related the testing and changing to scientific research in general rather than to individual-level actions, such as selecting a specific model to work on a task. Accordingly, *testing models* was described in terms of evaluating the correctness of the scientific knowledge represented by a model, rather than, for example, its suitability for a specific context or task (level 2).

Table 3 Distribution of assigned levels within the five aspects of the meta-modeling knowledge (MMK)

	Media-oriented perspective			Methodological perspective	
Aspect	Level 0	Level 1	Level 2	Level 3a	Level 3b
Nature of models	0	8	9	0	5
Multiple models	0	2	15	5	0
Purpose of modeling	0	13	5	1	3
Testing models	0	2	7	7	6
Changing models	0	2	4	11	5

Appendix C: coding manual for the SMMK dimension

In the data analysis section, the coding manual for the aspect *purpose of reaction mechanisms* was already presented as an example. Tables 4–7 now provide the corresponding coding manuals for the remaining four aspects of SMMK. Each coding manual includes the code, a description of the code, and an illustrative example from the data.

Table 4 Coding manual for the aspect nature of reaction mechanisms within the SMMK dimension

Level	Code	Description	Example
0	Reaction mechanisms (=RM) as fictional reaction pathways that do not occur in reality	RM are viewed as fictional constructs. Reactants and products are considered real and observable, whereas everything in between is assumed to be purely theoretical as mental aid	"*[reaction mechanisms] are only theoretical in nature, because we cannot practically verify in any way what we have described actually happens like that.*" (Loretta)
1	Reaction mechanisms as copies of reaction pathways	RM are understood as copies of reaction pathways that actually occur but cannot be directly observed. They are considered as complete and as close to reality as possible, depicting the sequence of reaction steps accurately	"*With reaction mechanisms, it's more, I would almost say, a graphical or visual kind of representation, in a pictorial way. [. . ..]*" (Victoria)
2	RM as idealized representations of reaction pathways	RM simplify and generalize reaction processes to enhance understanding, functioning as explanatory models or "recipes" of reaction pathways. Mechanisms may present shortened representations or focus on specific aspects that are represented accurately	"*Well, when you write down [reaction mechanisms], that is kind of a model. You somehow try to sketch it for yourself in a way that makes it understandable, so that you can actually understand what is happening in the vessel.*" (Jasmine)
3a	RM as best explanations of reaction pathways	RM are considered provisional and uncertain due to the limited observability of the submicroscopic level. Based on the porperties of the substances involved, mechanisms are selected as idealized representations that, after evaluation, provide the most plausible explanatory account of the reaction process	"*You always try to explain [the reaction steps] further in some way. It is simply part of being human to want to know things in more detail. [. . .] Nevertheless, they provide a good explanation, probably the best one we can offer at the moment.*" (Nora)
3b	RM as epistemic artifacts to achieve specific goals related to the purpose of RM	RM are understood as purpose-driven epistemic artifacts based on the current state of knowledge. They are used to achieve specific goals, such as formulating hypotheses about products or product distributions, or planning chemical syntheses	"*It's obviously not a direct depiction of reality, but a simplification. I don't have weird orbitals or anything like that [. . .] but rather what's relevant to me first. [. . .] If I want to produce a substance, I'm primarily interested in the path that leads to it.*" (Lily)

Table 5 Coding manual for the aspect multiple reaction mechanisms within the SMMK dimension

Level	Code	Description	Example
0	No plausible reaction mechanism (=RM) for a reaction; the reaction proceeds directly from reactants to products without mechanistic steps	RM are understood solely as fictional cognitive aids that do not occur in reality. Instead, chemical reactions are assumed to proceed directly from reactants to products without any mechanistic steps or intermediates	Not present in the data
1	Only one plausible RM for a reaction pathway from reactants to products with only one representation	It is assumed that there is only one plausible reaction mechanism for a given reaction pathway from the reactants to the products. Students explicitly state that there is exactly one correct way to represent a mechanism, and this representation cannot be altered	Not present in the data
2	Only one plausible RM for a reaction pathway from reactants to products, which can be presented through different representations	It is assumed that there is only one plausible reaction mechanism for a given reaction pathway from the reactants to the products. The mechanism may be presented using different representations or levels of detail	"*All molecules from the reactants that take part in the reaction follow the same pattern. So that, in the end, the product we observe is formed.*" *(Zoey)*
3a	Multiple RM and reaction pathways for a chemical reaction due to varying conditions	Multiple RM are assumed to be possible for a reaction depending on the reaction conditions. Different mechanisms can proceed parallel, leading to different reaction products and product distributions	"*So, that there are different pathways leading to different products, [. . .] and that there can be the same principle leading to different products*" *(Becky)*
3b	Multiple competing RM for one reaction pathway of a chemical reaction none of which has been disproven yet	Multiple competing reaction mechanisms are assumed for a single reaction pathway from the same reactants to the same products. These mechanisms may proceed parallel, or none of them have been ruled out yet	"*There are probably reaction steps that are simply less likely [. . .] and therefore occur very infrequently, whereas a mechanism that proceeds from A to B in a certain way occurs more often and is more probable.*" *(Lily)*

Table 6 Coding manual for the aspect testing reaction mechanisms within the SMMK dimension

Level	Code	Description	Example
0	Reaction mechanisms (=RM) don't need to be tested at all	RM are not considered testable or in need of testing. They are taken as given constructs, without being examined for correctness, plausibility, or empirical support. Or the student doesn't know how to test RM	"*But I would not know how one could further verify [a reaction mechanism].*" (Victoria)
1	Testing the representation in terms of coherence, correctness and formalisms (*e.g.*, EPF)	Given RM are only examined with respect to the coherence, correctness, and formal aspects of its representation. Testing focuses on whether the mechanism adequately connects reactants to products, typically by selecting an appropriate known mechanism from an existing repertoire. Evaluation is limited to checking for obvious conceptual or formal errors, without further empirical verification	"*You are familiar with the mechanisms. [...] You should perhaps have gone through them beforehand and then choose one. [...] Then I look at it and think, okay, does this reaction mechanism fit, or does this one fit, or does it not fit?*" (Judy)
2	Testing RM in terms of conceptual plausibility (application of concepts: *e.g.*, nucleophilicity/ electrophilicity) and verifying the RM with experimental evidence	RM are tested in terms of their conceptual plausibility by applying chemical concepts and by verifying them using experimental evidence. Testing is understood as verification of a proposed mechanism rather than as a comparative evaluation of alternatives and may involve examining individual mechanistic steps through a combination of conceptual reasoning and experimental findings	"*Well, I think that probably many things have already been done, documented, and observed. [...] So, if it is properly published, then it will be like that. But if I am doing experimental research, then I definitely have to try it out myself, because I need to check whether it actually happens that way.*" (Robin)
3a	Testing if a RM is the most plausible possible reaction pathway in terms of chemical concepts and experimental evidence	RM are tested by weighing multiple alternative pathways to determine which is the most plausible based on chemical concepts and experimental evidence. The focus lies on evaluation as a process of knowledge generation, assuming that substances react in specific ways due to their structures and properties	"*There are certain rules, perhaps, how substances react with one another. And then someone carries out a reaction and is asked to write down the reaction mechanism. You have to sit down and think about what exactly happens when one substance is combined with another – where bonds are formed, where something is eliminated. So this really emerges from someone performing a reaction and reflecting on how that reaction takes place.*" (Janet)
3b	Testing new RM by empirical investigation of derived hypotheses (*e.g.*, product distributions of unknown syntheses, transition states)	New RM are tested through empirical investigation of derived hypotheses, such as observations of product distributions or transition states in unknown syntheses. Testing involves an iterative interplay between conceptual reasoning and experimental work and is understood as the development of new mechanistic knowledge rather than the verification of an existing mechanism	"*You can probably formulate a lot of hypotheses and make assumptions about what should or might happen. [...]. And I start by forming well-founded assumptions. [...] I test them in small series by thinking [...]. And with that, I try to interact somehow, and then I look to see whether something different happens when I use a stronger substituent. And of course, the question is always at which position on the molecule this takes place. And then I believe all those methods like spectroscopy, crystallography, and so on, become relevant.*" (Lily)

Table 7 Coding manual for the aspect changing reaction mechanisms within the SMMK dimension

Level	Code	Description	Example
0	Reaction mechanisms (=RM) don't need to be changed at all	RM are regarded as fixed and unchangeable. Once established, they are not modified or revised, regardless of new considerations or evidence	"*Maybe there are some things that could really be wrong [...]. But I think sometimes there isn't really a [...] wrong, it might also depend on what you want to convey with it.*" (Rhonda)
1	Enhancing the representation of a RM in terms of coherence, correctness, and formalisms (*e.g.*, EPF)	RM are modified only to correct formal or conceptual errors in their representation. Changes aim at improving coherence, correctness, or adherence to formal conventions, without altering the underlying mechanistic idea	"*[If] certain principles are not fulfilled and therefore there is no theoretical correctness. [...] Conversely, if [reaction mechanisms] are consistent with the principles [...], then things already look good.*" (Kyle)
2	Changing RM to align them with chemical concepts and known evidence	RM are changed when they are found to be inconsistent with chemical concepts or established evidence. Revisions are based on identifying incorrect assumptions through theoretical reasoning or experimental investigation	"*I would say it depends on the step where the error might occur [...]. That you might be able to fix this error using chemical knowledge, or conceptual knowledge, if that is actually the case.*" (Tracy)

Table 7 (*continued*)

Level	Code	Description	Example
3a	Changing RM because alternative reaction pathways are more plausible by considering chemical concepts and new experimental evidence	RM are changed when alternative reaction pathways become more plausible based on chemical concepts and new experimental evidence. Modifications arise from the integration of new insights, leading to optimized mechanisms, for example through the inclusion of catalysts or adaptations to different reaction conditions	"*If [. . .] one then arrives at a reaction product other than the actual product, [. . .] then one might need to extend reaction mechanisms, I would not say change them but rather extend them.*" (Stuart)
3b	Revising new RM due to the falsification of derived hypotheses or new experimental evidence	RM are revised when derived hypotheses are falsified or when new experimental evidence becomes available. Changes are made to incorporate observed results and to update the mechanism accordingly	"*I think about what I want to find out with the experiment. [. . .] Then I carry out the experiment, observe what I see [. . .] and afterwards I think about, based on the knowledge I already have, how this could be connected and what might have happened in this reaction.*" (Ted)

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