

A Team-Based Learning Activity with AI-Supported Reasoning for Teaching Molecular Dynamics

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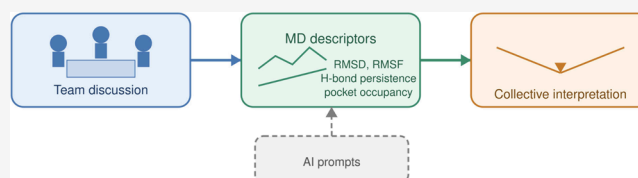
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ABSTRACT: Molecular dynamics (MD) simulations are increasingly included in chemistry and life science curricula, yet students often struggle to interpret outputs and to integrate multiple descriptors into coherent explanations. This paper presents a Team-Based Learning (TBL) activity for a graduate-level physical chemistry course for biotechnology students designed to support this process. The activity emphasizes comparison and integration of protein and ligand root-mean-square deviation (RMSD) time series, regional RMSF values, key hydrogen-bond persistence and pocket occupancy. It also requires collective justification under interpretative ambiguity and uses a deliberately constrained AI-based tutor as a reflective scaffold to prompt explanation without providing authoritative answers. Team discussions during the activity typically involved comparing these indicators and developing collective explanations for alternative molecular scenarios. Student feedback was generally favorable toward the collaborative TBL structure, whereas perceptions of the AI tutor were mixed, indicating that its perceived usefulness varied among students.

KEYWORDS: Graduate Education, Physical Chemistry, Cooperative Learning, Problem Solving, Molecular Dynamics, Artificial Intelligence



INTRODUCTION

Molecular dynamics (MD) simulations play an increasingly important role in physical chemistry and related fields by providing access to molecular behavior beyond static representations alone. As a result, MD has become a common component of undergraduate and graduate curricula in chemistry and the molecular life sciences.¹ Despite this, MD poses substantial educational challenges, particularly when students are required to interpret simulation outputs and integrate multiple quantitative descriptors.

In life science-oriented physical chemistry courses, MD is typically introduced as a conceptual framework for understanding biologically relevant molecular systems rather than as a computational specialization.² Instruction therefore emphasizes reasoning about simulation outputs rather than executing the simulations. Commonly used descriptors include RMSD, the root-mean-square deviation of a selected set of atoms from a reference structure after structural alignment; RMSF, the root-mean-square fluctuation of an atom or residue about its mean position over the trajectory; and interaction persistence, the percentage of analyzed frames in which a specified interaction is present. In this activity, interaction persistence referred to a key protein–ligand hydrogen bond. These descriptors do not provide direct or unequivocal interpretations. The same trend may reflect different molecular behaviors depending on context, time scale, or reference structure.

Interpreting these descriptors therefore requires reasoning about dynamic molecular behavior rather than simply reading

graphs. MD analysis can thus be viewed as an interpretative practice in which multiple pieces of evidence, such as global structural deviation, local flexibility, hydrogen-bond persistence, and pocket occupancy, must be coordinated to support a plausible explanation.

Research in molecular life science education highlights the challenges of reasoning about dynamic molecular processes and coordinating multiple representations and levels of description³, a challenge shared with other areas of physical chemistry. At the same time, this interpretative complexity also represents an opportunity: meaningful engagement with MD depends on integrating heterogeneous evidence and justifying conclusions.^{4,5}

Although the teaching and learning of chemistry pose well-documented challenges,^{6,7} active and collaborative instructional approaches support learning, particularly in domains characterized by abstraction and interpretative ambiguity.^{8,9} TBL combines individual accountability with application tasks requiring collective decision making.^{10–12} It was selected for this activity because students were required to compare alternative interpretations of the same data and agree on a

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Structure of the TBL activity

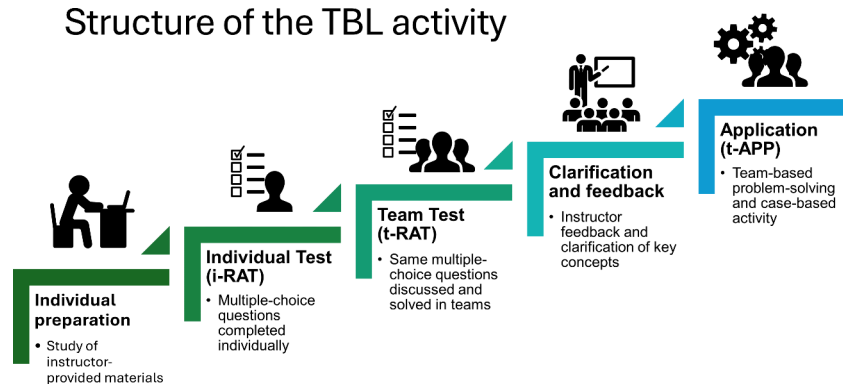


Figure 1. Structure of the TBL activity.

shared, evidence-based choice. TBL has also been applied to promote problem solving, peer explanation, and argumentation in chemistry education.^{13–18} Collaborative discussion can play an important role by making students' reasoning explicit and by encouraging comparison between alternative interpretations.

Emerging digital technologies, including artificial intelligence (AI), have recently attracted attention as potential tools for supporting learning in chemistry education.¹⁹ However, concerns persist regarding over-reliance and reduced engagement with disciplinary reasoning.²⁰ Recent discussions emphasize the importance of designing AI-supported environments that stimulate reasoning rather than provide solutions.^{21–23} When carefully constrained, AI can act as a prompt for explanation and evaluation rather than a source of answers.

Recent reviews on AI in collaborative learning environments^{24,25} suggest that AI can support peer learning most effectively when it is used to provide adaptive prompts, feedback, and process-oriented guidance rather than direct answers. In these contexts, AI agents can play multiple roles, including supporting reasoning, facilitating discussion, and prompting reflection, but their educational value depends strongly on how they are framed within the instructional design. At the same time, this literature highlights important challenges, including the risk of over-reliance and the need to preserve students' autonomy and epistemic agency. These considerations are particularly relevant in domains characterized by interpretative complexity and the integration of multiple sources of evidence, where AI may be most productively used as a deliberately constrained scaffold embedded within peer interaction rather than as an answer-providing tutor.

While AI-supported collaborative learning has been increasingly explored, its integration within structured TBL settings, particularly in discipline-specific contexts such as STEM, remains less clearly developed. This paper describes the design and implementation of a TBL activity in a graduate-level physical chemistry course for biotechnology students. The activity engages students in interpreting MD descriptors through comparison of alternative scenarios and collective justification of decisions. A deliberately constrained AI tutor was integrated to prompt reflection without providing direct solutions. The proposed materials and instructional structure may help support introducing MD as an interpretative practice within collaborative learning environments.

COURSE CONTEXT AND PARTICIPANTS

The activity was implemented within a graduate-level course, *Physical-Chemical Models and Methods for Biological Systems*, in a

biotechnology degree program. Students had not received prior formal instruction in MD. Their initial preparation on the topic consisted of independent study of the materials assigned 1 week before the first classroom session. The activity focused on the conceptual interpretation of MD trajectories and structural descriptors rather than on the technical setup or execution of simulations.

The cohort consisted of 13 students, reflecting the typical course size. Students had heterogeneous academic backgrounds (biological sciences and biotechnology) and varied prior exposure to physical chemistry. This heterogeneity supported an instructional design focused on collaborative interpretation and comparison of reasoning strategies.

For the TBL activity, students were organized into three teams of four, four, and five members. Team formation followed TBL principles to maximize heterogeneity within groups.¹⁰

Information on students' academic backgrounds, prior preparation, work experience, age, personal interests, and other background characteristics was collected through a preliminary questionnaire (Supporting Information S1) and used to balance the teams. These characteristics were considered together to distribute disciplinary knowledge, experiences, and perspectives across teams and thereby maximize within-team heterogeneity. The questionnaire responses were used for team formation and were not analyzed as study outcomes.

- Although smaller than typical TBL teams, these groups suited the exploratory, reasoning-focused nature of the activity.

All teams worked on the same MD data set and identical application task, enabling comparison of responses based on interpretation and reasoning rather than on task conditions.^{10,12}

Participation was voluntary and involved no activities beyond normal course practice. The researcher was also the instructor. Students were informed about the study aims and provided informed consent. In line with local institutional practice, formal ethics approval was not required for this low-risk educational research. Data were analyzed in anonymized form after course completion.

Safety

No unexpected or unusually high safety hazards were encountered during the implementation of this classroom activity.

OVERVIEW OF THE TBL ACTIVITY

The activity followed a structured TBL sequence consisting of individual preparation, readiness assurance process, and an in-

class application phase.^{10,26} An overview of the sequence of phases is provided in Figure 1.

The activity was implemented over two class sessions. One week before the first session, students were assigned preparatory material introducing the basic concepts required to interpret MD trajectories and common structural descriptors used in MD analysis.^{27,28}

At the beginning of the first session, students completed an individual readiness assurance test (iRAT) based on the assigned preparatory material. Consistent with the standard TBL readiness assurance process, they then reconsidered and answered the same items through team discussion in the team readiness assurance test (tRAT).^{10,26} Each team agreed on a shared set of answers, which was submitted through one designated member. Consequently, the recorded tRAT score represents the collective response of the team rather than the individual performance of the student who entered the answers. This phase allowed students to compare interpretations and clarify key concepts before proceeding to the main activity. A short instructor-led clarification session followed the readiness assurance process to address common difficulties revealed by students' responses, resolve misconceptions, and reinforce the concepts required for the application activity.

The second session was held 2 days after the first and was devoted to the team application activity (tAPP), in which teams interpreted MD data, compared alternative molecular scenarios, and committed to a collective decision supported by explicit justification. In line with TBL principles, all teams worked on the same data set and addressed identical prompts, enabling comparison across teams and whole-class discussion focused on differences in reasoning and evidence integration rather than on correctness alone.

Design and Learning Goals of the MD Application Task

The tAPP was conceived as a research-inspired interpretative activity aimed at engaging students in reasoning with simulation-derived data within a realistic scientific context. The task design was informed by a published MD study investigating ligand binding and structural stability in a viral protease system.²⁹ The instructional goal was not to train students in the technical aspects of running simulations, but to engage them in reasoning about what different descriptors can reveal about molecular behavior. In particular, students were asked to compare alternative interpretations of the data and to identify the scenario that most plausibly explained the observed patterns (see Supporting Information S2 for a table summarizing how key elements of the original research study were mapped onto the tAPP activity).

A research-inspired framing was adopted to situate the task within a realistic decision-making scenario. Students were positioned as members of a multidisciplinary research consortium engaged in the early stage selection of candidate inhibitors for a viral protease. Within this scenario, teams were asked to evaluate multiple ligand-bound systems and to consider the qualitative effects of a targeted residue substitution on binding stability. To support this design, synthetic instructional data sets were generated specifically for the activity (see Supporting Information S3). The instructional data sets included separate RMSD time series for the protein and ligand in each WT and mutant complex, RMSF values for three predefined protein regions, and summary indicators of key hydrogen-bond persistence, pocket occupancy, and ligand exit events.

ChatGPT 5.1 was used as a design aid to generate simplified data showing contrasting RMSD profiles, region-specific RMSF patterns, and differences in hydrogen-bond persistence and pocket occupancy across the alternative scenarios. The data sets did not derive from MD simulations and were not intended to represent physically validated simulation trajectories. They were reviewed visually to confirm the presence of the intended qualitative patterns, but no physical or statistical validation was performed. Students were explicitly informed that the data sets were synthetic and intended solely for instructional use.

To support this process, the activity materials were designed so that no single descriptor provided a definitive answer. Instead, meaningful interpretation required considering the combined behavior of several metrics and discussing alternative explanations within the team.

AI-SUPPORTED TUTORING

The AI-supported tutoring component was designed as an optional part of the tAPP activity, with the explicit goal of supporting students' reasoning without providing authoritative interpretations or solutions. To this end, a custom generative AI-based conversational agent, named *Isacco*, was developed, and embedded within the tAPP phase of the activity.

Isacco was implemented as a custom ChatGPT-based agent whose behavior was defined through a dedicated set of system-level instructions. To ensure coherence with students' preparatory work, the agent was granted access to the same learning materials provided to the class, including the introductory scientific articles,^{27,28} the course slides, and the research article that inspired the design of the application task.²⁹

Isacco was explicitly prevented from functioning as an automated problem solver. Instead, its contributions were limited to targeted prompts intended to elicit explanation, encourage comparison across metrics, and highlight potential inconsistencies in students' interpretations. The full set of system instructions defining these constraints is provided in Supporting Information S4. The configuration can be adapted to other disciplinary contexts by replacing the task-specific materials and references while retaining the general constraints that require the agent to elicit justification and avoid providing direct solutions. This design approach is informed by prior research on dialogic and intelligent tutoring systems, which indicates that question-driven interactions can support learning while preserving students' responsibility for interpretation and decision making.^{22,23}

Responsibility for interpreting the MD data remained entirely with the student teams, in line with TBL principles and with broader recommendations for responsible and constrained use of AI in educational settings.^{30,31}

CLASS IMPLEMENTATION AND STUDENTS' RESPONSES

The activity was distributed over two consecutive weeks. Students first completed the assigned preparatory work independently during the week preceding the classroom implementation. The in-class component consisted of two sessions of approximately 2 h each. The first session included the individual and team readiness assurance tests, feedback, and instructor-led clarification of concepts needed for the application activity. The second session was devoted primarily to the team application activity, including analysis of the MD data, consultation of the AI tutor when considered useful by the

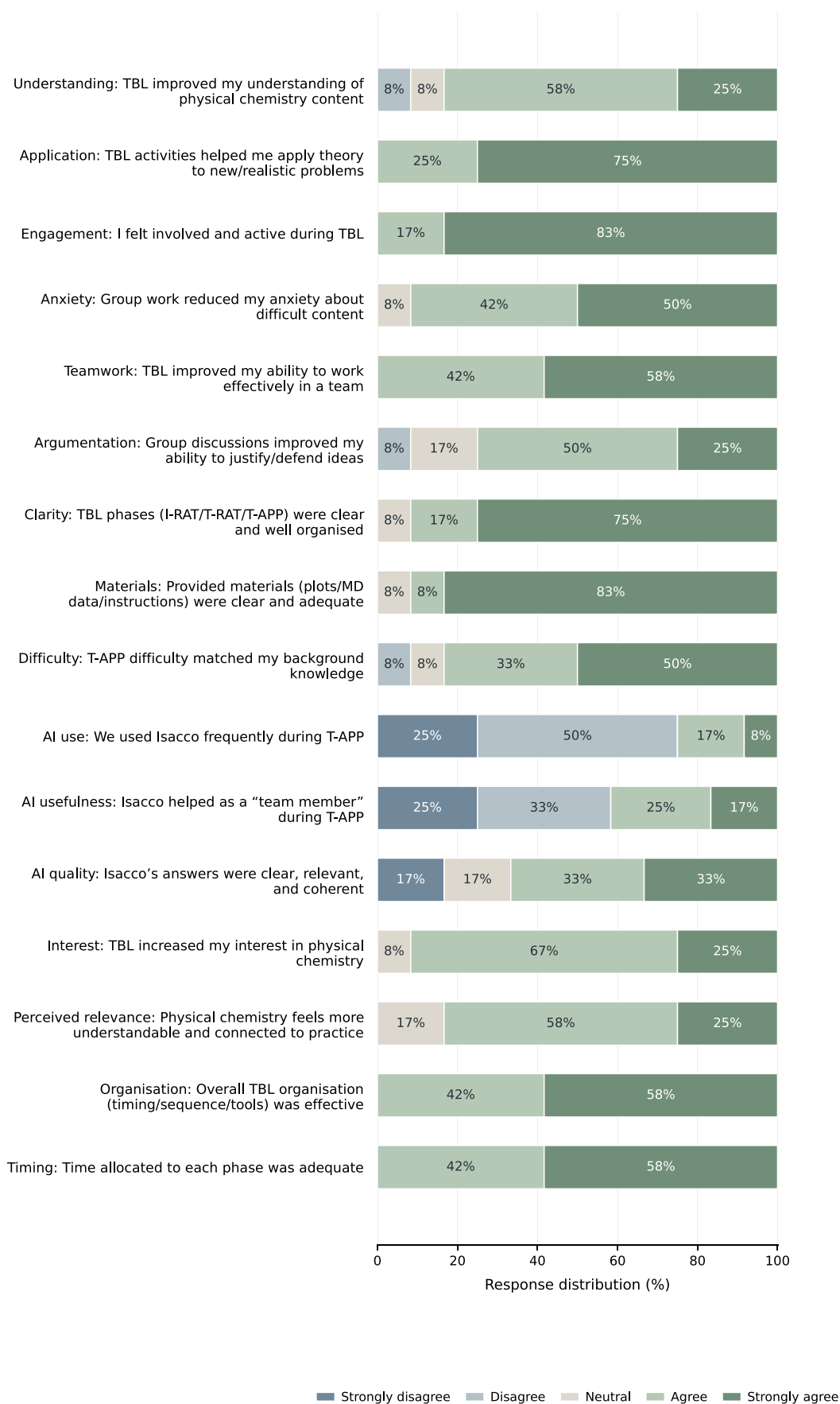


Figure 2. Distribution of student responses to the items of the feedback questionnaire ($n = 12$). Bar widths represent the percentage distribution across the five-point Likert scale, while the numbers within the segments indicate the corresponding response counts.

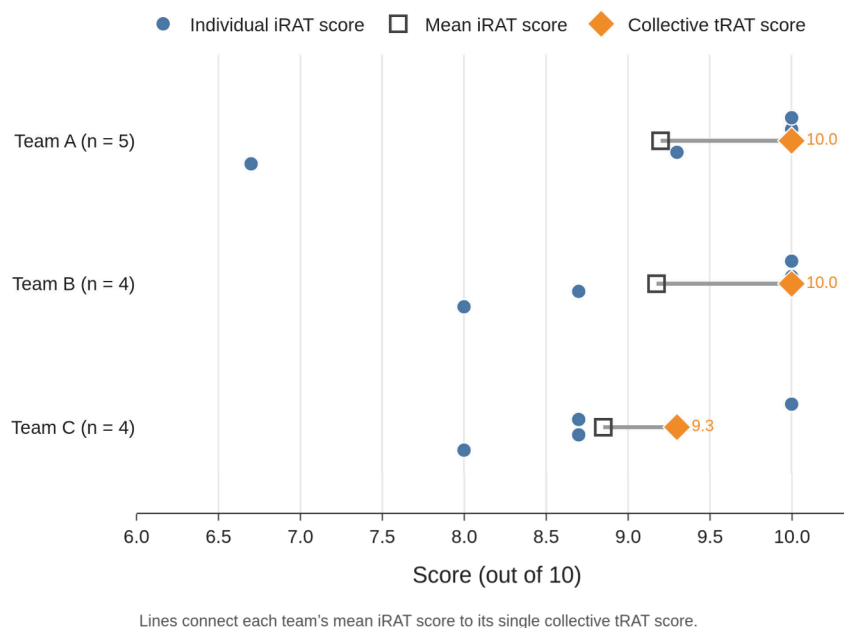


Figure 3. Individual and collective readiness assurance scores by team. Circles represent the individual iRAT scores of the students assigned to each team, open squares indicate the corresponding mean iRAT score, and diamonds show the single collective tRAT score submitted by each team. Lines connect each team mean to its collective tRAT score and are intended only as a descriptive comparison. Scores are reported on a 10-point scale, and team sizes are indicated on the y-axis. The tRAT scores represent collective team responses rather than individual post-test results.

teams, preparation of a shared decision, and simultaneous reporting and discussion of the teams' responses. All teams worked on the same MD data set and addressed the same application task.

To gather students' perceptions of the activity, at the end of the session 12 of the 13 students completed a short anonymous questionnaire providing feedback on the perceived usefulness of the activity and the role of the AI tutor. The questionnaire was intended to document students' perceptions of the activity and was not designed as a direct measure of learning outcomes. Figure 2 shows the distribution of responses to the feedback questionnaire.

Readiness Assurance Phase

Within the standard TBL sequence, the iRAT and tRAT served complementary functions: the iRAT documented students' individual readiness after the preparatory work, whereas the tRAT required each team to reconsider the same items and agree on a collective response.

Figure 3 presents the iRAT scores of all 13 students according to team membership, together with the corresponding mean iRAT score and the collective tRAT score for each team. The collective tRAT score was therefore higher than the corresponding mean iRAT score for each of the three teams.

This phase also served an instructional role by allowing students to clarify key concepts before engaging with the more demanding application task. Discussion during the team test often focused on the interpretation of commonly used descriptors such as RMSD and RMSF, helping students establish a shared understanding before proceeding to the analysis of the simulation data.

The readiness assurance test items are provided in Supporting Information S5, and the anonymized individual and team scores underlying Figure 3 are provided in Supporting Information S6.

Team Reasoning during the Application Activity

During the application phase, teams analyzed the MD descriptors and discussed possible interpretations of the simulated protein–ligand behavior. Rather than focusing on a single metric, teams typically considered multiple descriptors when constructing their explanations.

For example, some teams initially interpreted relatively stable RMSD values as evidence of strong ligand binding. During discussion, however, they reconsidered this interpretation after examining RMSF patterns and indicators of interaction persistence, which suggested localized flexibility near the binding pocket. Comparing these different descriptors often prompted teams to revise their initial explanations and to explore alternative interpretations before reaching a collective decision.

Although the level of detail in the explanations varied between teams, the activity generally prompted students to coordinate different sources of information rather than relying on a single descriptor. In several cases, explanations remained partially descriptive, focusing on individual metrics rather than fully articulated mechanistic interpretations. Nevertheless, these responses often revealed emerging attempts to relate different descriptors to one another, suggesting transitional forms of reasoning that are pedagogically informative in this domain.

The requirement to produce a shared team decision encouraged students to articulate and justify their reasoning explicitly during the discussion.

Student Perceptions of the Activity

Student feedback suggested that the structured sequence of individual preparation, readiness assurance, and collaborative application supported engagement with the task. Several students reported that the team discussion helped them better understand the meaning of the MD descriptors and the relationships between different metrics. Some comments also emphasized the value of comparing different descriptors during

the group discussion, which helped students move beyond a purely descriptive reading of the simulation plots.

Responses concerning the AI tutor were more mixed than those concerning the TBL structure. Some students perceived the tutor as useful for checking the coherence of an interpretation or considering alternative explanations, whereas neutral and negative responses, including some strong disagreement, were also recorded for items concerning its usefulness, quality, and role during the tAPP. The AI tutor therefore did not represent an equally valuable resource for all participants and functioned as a supplementary scaffold rather than as a central component of the collaborative reasoning process.

Overall, the activity was perceived as useful for understanding how MD data can be interpreted in the context of biomolecular systems, although some students also highlighted its cognitive complexity.

CONCLUSIONS

This work describes the design and classroom implementation of a TBL activity to support students' interpretation of MD data in a graduate-level physical chemistry course for life science students. The activity emphasized interpretation, integration of multiple metrics, and collective justification of decisions, while a deliberately constrained AI-supported tutor was included to prompt reflection without providing authoritative answers.

The activity illustrates how structured collaborative tasks can support students in approaching MD analysis as an interpretative practice. In particular, the design encouraged students to consider multiple descriptors, such as RMSD, RMSF, and indicators of interaction persistence, and to compare alternative interpretations before reaching a shared decision. Even when reasoning remained partially descriptive, students were prompted to coordinate heterogeneous sources of information during group discussion.

Student feedback indicated that participants generally perceived the structured TBL sequence as supporting engagement with the task and helping them navigate interpretative ambiguity. In contrast, perceptions of the AI-supported component were mixed: it was regarded as a useful supplementary resource by some students, while others expressed neutral or negative views. Its role should therefore be interpreted as exploratory and secondary to the TBL structure, rather than as evidence of a general learning benefit. Although implemented in a single course with a small cohort and supported by descriptive evidence, the activity has several limitations. In particular, because all questionnaire items were positively worded, acquiescence bias in students' responses cannot be excluded. Moreover, the questionnaire documented students' perceptions and should not be interpreted as direct evidence of learning outcomes. Nevertheless, the design principles and materials presented here may support adoption and adaptation in other instructional contexts. Future work may explore implementation in larger cohorts, variations in task design, or alternative forms of AI-supported scaffolding within collaborative learning environments.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.6c00082>.

Student background questionnaire (PDF)

Table mapping key elements of the original research study onto the tAPP activity (PDF)

Synthetic instructional data sets for tAPP (XLSX)

System instructions for the AI tutor (TXT)

Readiness Assurance Test items (PDF)

Scores for iRAT and tRAT (XLSX)

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The author declares no competing financial interest.

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