

# Creating CDIO-Based Chemistry Research Activities for Students: A Case Study in Organic Compound Structure

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**Abstract** The chemistry program in university includes content on reaction mechanisms and IR and NMR spectroscopy. However, the laboratory conditions are limited, so students do not have access to experimental spectral data. Applying the CDIO teaching process, we designed a group activity for university students to help them improve their knowledge and ability to predict reaction mechanisms as well as use spectroscopy to confirm structures of predicted products. On that basis, there will be impact assessments on students' capacity when researching the structure of organic compounds in chemistry to take appropriate improvement measures. This activity uses spectral analysis and reaction mechanisms in an exercise. Students are tasked with predicting the reaction mechanism to identify the products of an organic chain reaction. Then, they analyze the provided IR and <sup>1</sup>H NMR spectra and match each spectrum with the appropriate product.

**Keywords:** CDIO, organic compound structure, reaction mechanisms, NMR Spectroscopy, IR Spectroscopy

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## 1. Introduction

CDIO stands for the English phrase Conceive - Design - Implement - Operate. CDIO is an initiative of the engineering departments of the Massachusetts Institute of Technology (MIT), USA, in collaboration with Swedish universities. This is a solution to improve training quality to meet social requirements on the basis of determining output standards to design training programs and methods according to a scientific process [1,2].

CDIO is logically constructed and has a generalized approach to it that can be used to develop standard procedures for a variety of training fields outside of engineering (with necessary modifications and additions), including the pedagogical field.

Until now, the network of universities applying CDIO in the world is increasing, especially in the US. Up to this point, there have been more than 100 universities around the world applying the program in Physics, Electronic Engineering and Machine Engineering [3].

The CDIO-based teaching process is carried out through the following steps:

**Conceive:** Form ideas on the basis of analyzing teaching content.

**Design:** Design activities based on proposed ideas.

**Implement:** Organize and carry out activities based on the teaching plan.

**Operate:** Evaluate impact, perfect teaching process,

constantly improve teaching activities.

Based on this process, the study will guide students in group activities to learn about the structure of organic compounds based on data on infrared spectroscopy and nuclear magnetic resonance spectroscopy.

## 2. Content and Research Methods

### 2.1. Conceive

Teaching infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy is an essential component of undergraduate curricula [4] and part of an important program for students in Vietnam. Additionally, using a reaction mechanism to predict the chemical structures of products in organic synthesis plays an equally important role. When students study organic chemistry, they learn the fundamentals of reaction mechanisms and IR and NMR spectroscopy, particularly <sup>1</sup>H NMR. However, the use of experiments to analyze products requires laboratory time and an NMR spectrometer, and multiple experiments are needed to generate a variety of compounds for spectroscopic analysis. To address these challenges, an activity in class involving exchange and group activities was applied to introduce upper-division undergraduate students to the broader applications of IR and NMR spectroscopy. This activity helps students synthesize and evaluate organic compounds without requiring laboratory time or IR and NMR spectrometers. The students should

be able to predict the products on the basis of the reaction mechanism and then confirm the structure of the organic compounds by analyzing  $^1\text{H}$  NMR and IR spectra, identifying splitting patterns by taking into account nuclear spin and interpreting the  $^1\text{H}$  NMR spectra of organic molecules. Thus, students will be able to confidently confirm whether the reaction mechanisms predicted are correct or not.

## 2.2. Design

This activity is constructed to follow a fundamental lecture on IR and NMR spectroscopy and reaction mechanisms. Students are provided with a chain reaction (Figure 1). They work in groups of 3-4. The activity takes approximately 2 hours to complete and can be broken into hour-long segments when needed. First, the students individually predict the mechanism of each reaction and write the reactions. Then, they use existing knowledge of IR and  $^1\text{H}$  NMR fundamentals and reference materials that provide approximate chemical shifts to predict splitting patterns and signals in IR and  $^1\text{H}$  NMR spectra and then discuss their predictions within their group. After that, they are provided with the IR and  $^1\text{H}$  NMR spectra and asked to match each molecule with the proper spectrum to confirm the compound structures. Finally, they assign peaks and briefly reflect on their discussion in writing.

The exercise uses a constructivist model to encourage retrieval of prerequisite knowledge before scaffolding new but related concepts [8,9].

Students must carefully consider solvent signals, longer-range couplings that are sometimes not predicted in simulations, and instrumental resolution because none of the spectra used in the exercise were simulated (rather, they were experimentally obtained). The writing prompt is constructed to ask students what they understood, what they did not understand, why, and how a gap in understanding could be addressed [7]. This metacognitive element to the exercise is designed to prompt student reflection for increased knowledge retention [8-10]. As a class, students then discuss what may have surprised them. The class discussion can be expanded to include the underlying principles of  $^1\text{H}$  NMR couplings.

## 2.3. Implement

We predict the reaction mechanism from compound (C) to compound (D) (Figure 2) and write the reaction (Figure 3). Then, we analyze the IR and  $^1\text{H}$  NMR spectra to confirm the structure of compound (D). The students will do the same with the other reactions in the exercises.

This is consistent with the synthesis of 1,3,4-oxadiazole-2-thiol heterocyclic compounds from hydrazide and carbon disulfide [11,12].

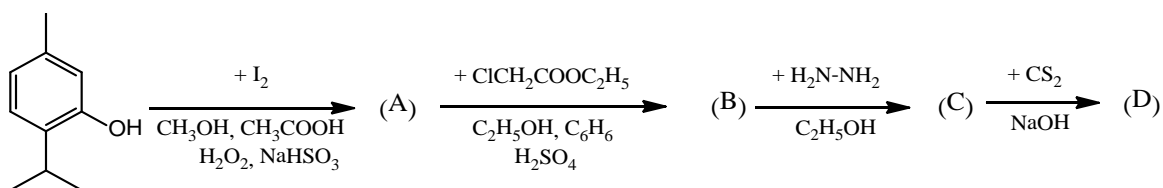


Figure 1. The chain reaction exercise

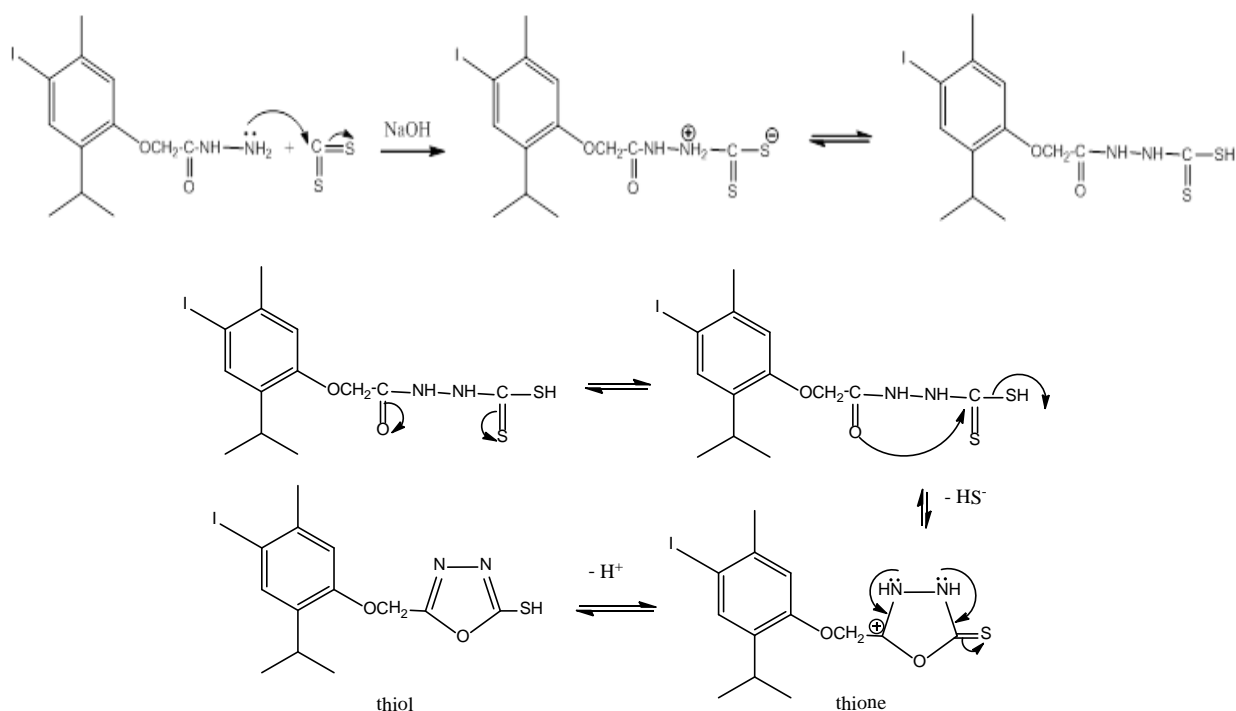


Figure 2. The reaction mechanism for the reaction between compound (C) and  $\text{CS}_2$  to yield compound (D)

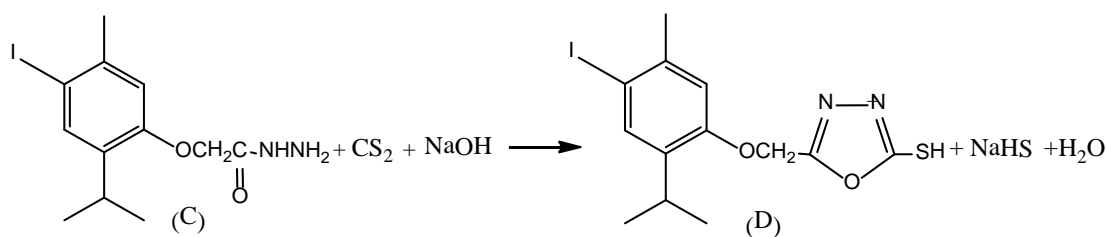


Figure 3. The reaction between compound (C) and  $\text{CS}_2$  to yield compound (D)

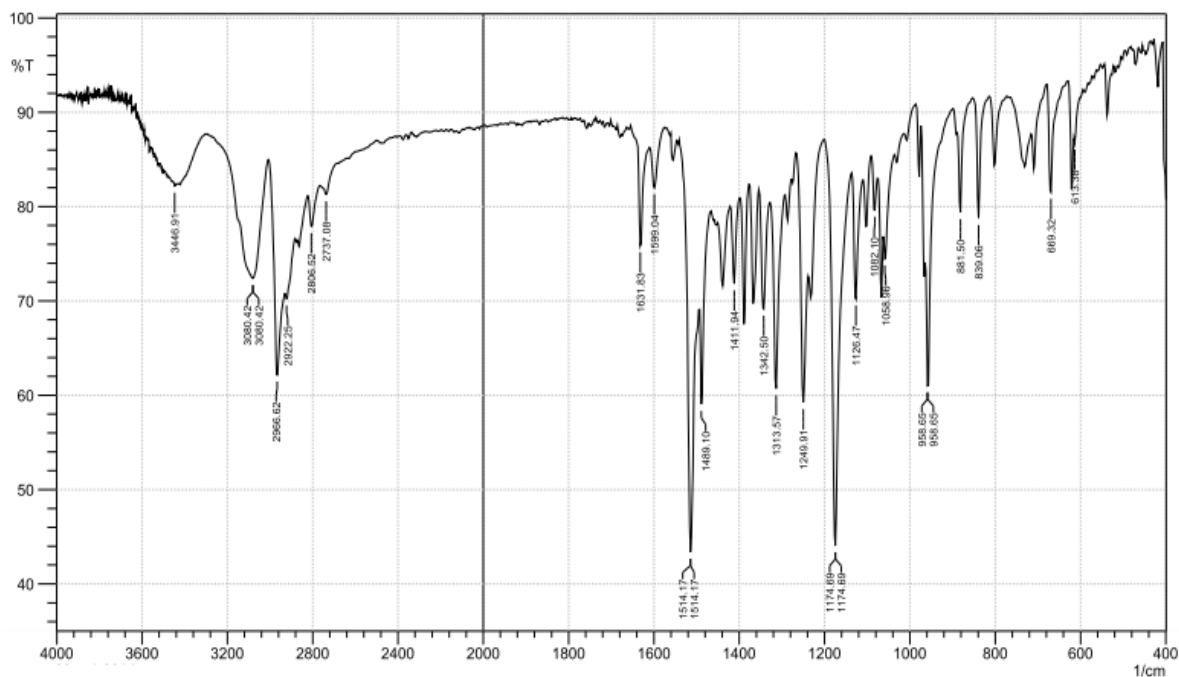


Figure 4. IR spectrum of a KBr pellet of compound (D) (50/60 Hz)

### 2.3.1. Analysis of the IR Spectrum

This IR spectrum (Figure 4) showed no peaks at  $1678.13\text{ cm}^{-1}$  ( $\text{C}=\text{O}$  signal, strong peak) or at  $3313.82\text{--}3200\text{ cm}^{-1}$  ( $-\text{NH}-\text{NH}_2$  signal, strong broad peak), demonstrating the transformation of carbonyl and hydrazyl groups. In addition, a variety of strong, broad peaks from  $2700\text{ cm}^{-1}$  to  $2966.62\text{ cm}^{-1}$  were observed, especially at  $2720\text{ cm}^{-1}$  (weak peak), consistent with a thiol vibration signal. Strong absorption was observed in the frequency range from  $3080\text{ cm}^{-1}$  to  $3200\text{ cm}^{-1}$ , indicating the presence of a particular  $-\text{N}-\text{H}$  bond in the compound. Furthermore, peaks were observed at  $2966.62\text{ cm}^{-1}$ ,  $1599.04\text{ cm}^{-1}$  and  $1514.17\text{ cm}^{-1}$  ( $\text{C}=\text{C}$  of the aromatic ring). In addition, an absorption peak at  $1631.83\text{ cm}^{-1}$  was indicative of the presence of a  $\text{C}=\text{N}$  bond, and strong signals from  $1126.47\text{ cm}^{-1}$  to  $1174.69\text{ cm}^{-1}$  indicated the presence of a  $\text{C}=\text{S}$  bond. All the IR spectral data mentioned provide evidence of an oxadiazole skeleton and confirm the existence of two tautomers, thione and thiol [13].

### 2.3.2. Analysis of the $^1\text{H}$ NMR Spectrum

Triple-bond JHH coupling constants in  $^1\text{H}$  NMR are typically on the order of 7 Hz [14].  $^1\text{H}$  NMR spectroscopy (Figure 5 and Figure 6) revealed signals at a high magnetic field that were consistent with alkyl substituents,

such as methyl and isopropyl groups, on the benzene ring. Six  $\text{H}_{2b}$  and  $\text{H}_{2c}$  protons gave rise to a doublet peak ( $J = 7.0\text{ Hz}$ ) at a chemical shift at  $\delta = 1.180\text{ ppm}$  due to a spin-spin interaction with  $\text{H}_{2a}$ . In addition, the signal of the  $\text{H}_{2a}$  proton was observed at  $3.190\text{--}3.245\text{ ppm}$  (multiplet peak). Three protons of the methyl substituent gave rise to a peak at  $2.391\text{ ppm}$  (singlet peak). Furthermore, methylene  $\text{H}_{1a}$  bonded with the heteroatom oxygen and the 1,3,4-oxadiazole scaffold, leading to a resonance at  $5.030\text{ ppm}$  (singlet peak). Compared to the  $\text{H}_{1a}$  signal of the ester ethyl thymoxyacetate ( $\delta = 4.787\text{ ppm}$ ), the  $\text{H}_{1a}$  signal in this compound was shifted to a lower magnetic field, which was consistent with the electrophilic 1,3,4-oxadiazole discussed in the introduction. In the specific  $^1\text{H}$  NMR spectral range for arene, there are two singlet peaks at  $6.776\text{ ppm}$  and  $7.596\text{ ppm}$  representing 2 protons,  $\text{H}_6$  and  $\text{H}_3$ , of the benzene ring. Moreover, at  $10\text{--}10.5\text{ ppm}$ , a broad peak for the  $\text{H}_7$  proton appeared. To summarize, all spectral  $^1\text{H}$  NMR data provided evidence for the predicted structure.

## 2.4. Operate

We conducted pedagogical experiments and a test to evaluate the feasibility and effectiveness of the activity. The experiment involved 117 students in the control group (Co) and 117 students in the experimental group (Ex). All

students were in Vietnam. Students in the Co group completed individual activities and multiple tests (the total score of the tests was 10). Students in the Ex group

complete a combined activity with only one test (the score of the test was 10). The results are summarized in Table 1 and Table 2.

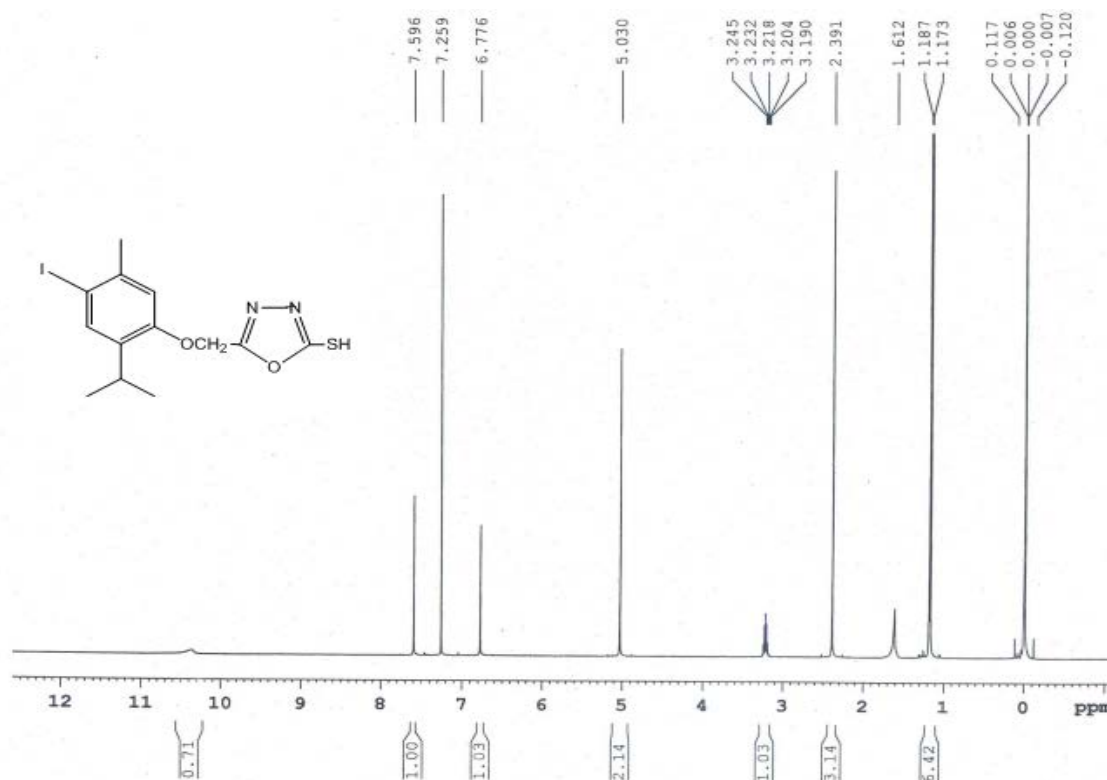


Figure 5.  $^1\text{H}$  NMR spectrum in DMSO of compound (D) (500 MHz) at 0–12 ppm

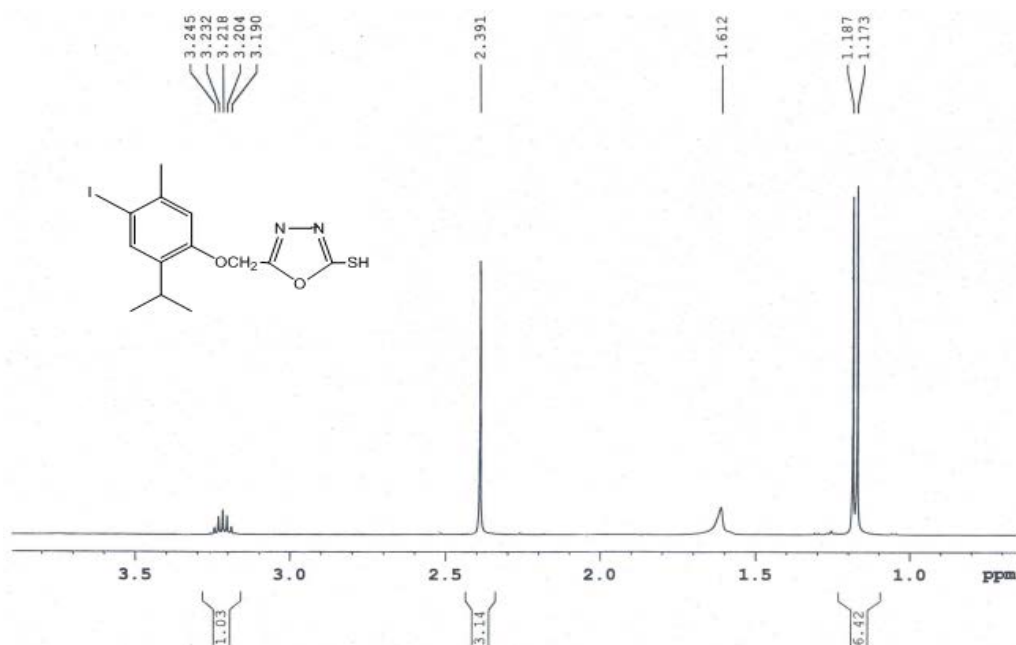


Figure 6.  $^1\text{H}$  NMR spectrum in DMSO of compound (D) (500 MHz) at 1.0–3.5 ppm

Table 1. Summary of Test Scores

Group		Score $X_i$									
Number of students		2	3	4	5	6	7	8	9	10	
Ex	Number	0	4	6	11	14	17	14	13	23	15
	117 %	0.00	3.42	5.13	9.40	11.97	14.53	11.97	11.11	19.66	12.82
Co	Number	0	23	17	15	15	14	13	14	6	0
	117 %	0.00	19.66	14.53	12.82	12.82	11.97	11.11	11.97	5.13	0.00

**Table 2. Cumulative Frequencies Table**

Group	% Students receive a score of Xi or below									
	1	2	3	4	5	6	7	8	9	10
Ex	0.00	3.42	8.55	17.95	29.91	44.44	56.41	67.52	87.18	100.00
Co	0.00	19.66	34.19	47.01	59.83	71.79	82.91	94.87	100.00	100.00

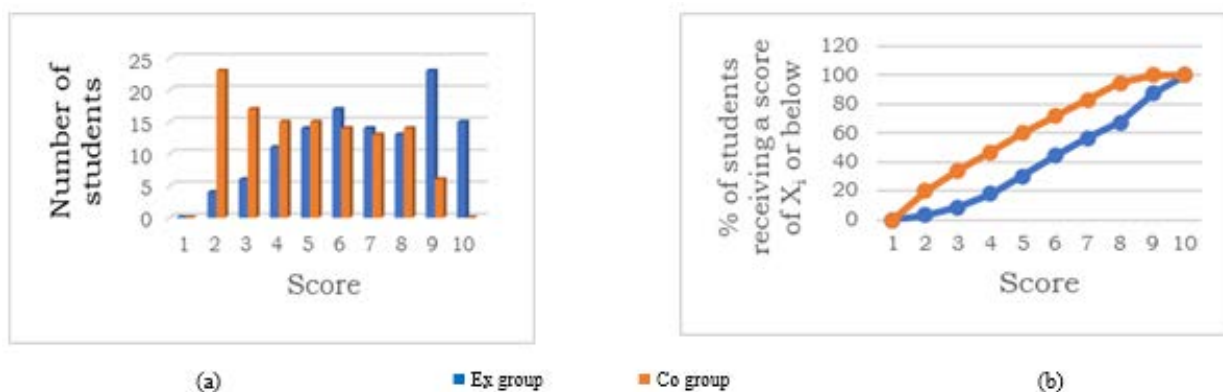
**Table 3. Summary of Specific Data**

Group	Number of students	$\bar{X}$	$S^2$	S	CV	k	t	$t_{\alpha,k}$	ES	Influence
Ex	117	6.85	5.22	2.28	33.36	232	6.60	1.97	0.87	Large
Co	117	4.90	4.97	2.23	45.53					

( $\bar{X}$ : the average test score value; S: the criterion deviation value; CV: the coefficient of variation; k: degrees of freedom; t: Student's t-distribution;  $\alpha = 0.05$ ; ES: effect size)

**Table 4. Summary of t-Test Data**

Variances	Levene's Test for Equality of Variances		t-test for Equality of Means						
	F	Sig.	t	df	Sig (p)	Mean Difference	Std. Error Difference	95% Confidence Interval of the Difference	
								Lower	Upper
Equal variances assumed	0.04	0.85	6.60	232	0	1.95	0.30	1.37	2.53
Equal variances not assumed			6.60	232	0	1.95	0.30	1.37	2.53

**Figure 7.** Diagram of test scores (a); graph of cumulative frequencies (b)

According to the diagram of test scores and the average test score values (Figure 7, Table 3), we found that the average test scores of the control group were lower than those of the experimental group. In the graph of cumulative frequencies, the line for the experimental group is to the right and below the line for the control group, confirming that the outcomes of the students in the experimental group are higher than those of the students in the control group. According to the data in Table 3, the criterion deviation (S) value and the coefficient of variation (CV) are relatively small ( $S_{Ex} < S_{Co}$  and  $CV_{Ex} < CV_{Co}$ ), so the data are less dispersed. The average test score values ( $\bar{X}$ ) have high reliability. We hypothesize the following:  $H_0$  – the difference between the values of  $\bar{X}_{Ex}$  and  $\bar{X}_{Co}$  is not statistically significant;  $H_1$  – the difference between the values of  $\bar{X}_{Ex}$  and  $\bar{X}_{Co}$  is statistically significant. The value of t (Student's t-distribution) is greater than  $t_{\alpha,k}$  ( $\alpha = 0.05$ ). Therefore, we can reject hypothesis  $H_0$  and accept hypothesis  $H_1$ . This means that students in the experimental group have better advancement than students in the control group [15]. The value of ES is large [16]. By using a t-test (Table 4), we found that the (p) Sig. values were less than the value of  $\alpha$  ( $= 0.05$ ), indicating that the difference in the distribution

of test scores between the control and experimental groups is due to the impact of the combined activity, not an accident [17].

Through observing the developments in class, we found the following: (1) In the control group, the learning attitude of the students was not positive, and the students were quite quiet and less proactive in participating in the lesson. Completing the exercises was not voluntary. It depended on the score. (2) In the experimental group, the students' attitude were more positive. They were very interested in performing the exercises.

### 3. Conclusion

Applying a teaching process based on CDIO, helps students work actively in groups and enjoy determining the structure of organic compounds based on spectroscopic data. In contrast to individual activities, this activity helps students improve their ability to predict the products of organic reactions by predicting reaction mechanisms and analyzing IR and  $^1H$  NMR spectra to confirm the structure of the predicted substances. This activity incorporates aspects of peer-to-peer learning and

metacognition to increase student understanding and retention of knowledge. We recommend evaluating future iterations of this activity despite the small sample size, as this will help track student progress in mastering the use of organic reaction mechanisms to predict products and the ability to confirm the structure of the compounds by analyzing IR and  $^1\text{H}$  NMR spectroscopic data. To make this activity more effective, we recommend collecting  $^{13}\text{C}$  NMR spectra to further help students confirm the structure of the predicted compounds accurately and reliably.

Thereby confirming that when teaching chemistry content associated with complex experiments, if teaching activities are designed based on the CDIO approach, it will help students develop chemical competencies and, moreover, teaching organization competencies.

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## Statement of Competing Interests

The Authors have no competing interests.

## List of Abbreviations

CDIO - Conceive - Design - Implement – Operate  
Ex - Experimental Group  
Co - Control Group

## References

- [1] E. Crawley, J. Malmqvist, S. Ostlund, D. Brodeur, *Rethinking Engineering Education: The CDIO Approach*, Springer.
- [2] Svante Gunnarsson, et. al., "Large Scale Use of The CDIO Syllabus In Formulation of Program and Course Goals", *Proceedings of the 3rd International CDIO Conference*, MIT, Cambridge, Massachusetts, June 11-14, 2007.
- [3] <http://www.cdio.org/cdio-vision>, accessed May 2022.
- [4] Soulsby, D.; Wallner, A. S. Introduction to NMR Spectroscopy in the Undergraduate Curriculum. In *NMR Spectroscopy in the Undergraduate Curriculum: First-Year and Organic Chemistry Courses Volume 2*; Soulsby, D., Wallner, A.S., Eds.; ACS Symposium Series, American Chemical Society: Washington, DC, 2016; pp 1–10.
- [5] National Research Council. *How People Learn: Brain, Mind, Experience, and School: Expanded Edition*; National Academies Press: Washington, DC, 2000.
- [6] Karpicke, J. D.; Roediger, H. L. The Critical Importance of Retrieval for Learning. *Science* 2008, 319 (5865), 966–968.
- [7] Rocks, S. S.; Stockland, R. A. NMR Structure Elucidation in the Presence of Heteroatoms: An In-Class Activity. *J. Chem. Educ.* 2020, 97 (2), 479–483.
- [8] Nückles, M.; Hübner, S.; Renkl, A. Enhancing Self-Regulated Learning by Writing Learning Protocols. *Learn. Instr.* 2009, 19 (3), 259–271.
- [9] Conner, L. N. Cueing Metacognition to Improve Researching and Essay Writing in a Final Year High School Biology Class. *Res. Sci. Educ.* 2007, 37 (1), 1–16.
- [10] Berthold, K.; Nückles, M.; Renkl, A. Do Learning Protocols Support Learning Strategies and Outcomes? The Role of Cognitive and Metacognitive Prompts. *Learn. Instr.* 2007, 17 (5), 564–577.
- [11] Joshi, S. D.; Vagdevi, H. M.; Vaidya, V. P.; Gadaginamath, G. S. Synthesis of New 4-Pyrrol-1-yl Benzoic Acid Hydrazone Analogs and Some Derived Oxadiazole, Triazole and Pyrrole Ring Systems: A Novel Class of Potential Antibacterial and Antitubercular Agents. *Eur. J. Med. Chem.* 2008, 43 (9), 1989–1996.
- [12] Joshi, D. G.; Oza, H. B.; Parekh, H. H. Synthesis of Some Novel 1,3,4-Oxadiazoles and 5-Oxo-Imidazolines as Potent Biologically Active Agents. *Heterocycl. Commun.* 1997, 3 (2), 169–174.
- [13] Burcu Arslan, N.; Özdemir, N.; Dayan, O.; Dege, N.; Koparr, M.; Koparr, P.; Muğlu, H. Direct and Solvent-Assisted Thione–Thiol Tautomerism in 5-(Thiophen-2-yl)-1,3,4-Oxadiazole-2(3H)-Thione: Experimental and Molecular Modeling Study. *Chem. Phys.* 2014, 439, 1–11.
- [14] Levitt, M. H. *Spin Dynamics: Basics of Nuclear Magnetic Resonance*, 2nd ed.; John Wiley & Sons Ltd.: West Sussex, England, 2008.
- [15] Haynes, W. Student's t-Test. *Encyclopedia of Systems Biology*. 2013, 2023–2025.
- [16] Cohen, J. *Statistical Power Analysis for the Behavioral Sciences*, 2nd ed.; Lawrence Earlbaum Associates: Hillsdale, NJ, 1988.
- [17] Levene, H. Robust Tests for Equality of Variances. In *Contributions to Probability and Statistics: Essays in Honor of Harold Hotelling*; Olkin, I., Ghurye, S.G., Hoeffding, W., Madow, W.G., Mann, H.B., Eds.; Stanford University Press: Stanford, CA, 1963; pp 62–62.



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