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Uncritical Inference Test in Developing Basic Knowledge and Understanding in the Learning of Organic Spectroscopy

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ABSTRACT

The learning of spectroscopic techniques for structural elucidation of unknown compounds is of profound importance to students. At present, there have been limited exercises associated with basic knowledge in the organic spectroscopy course. In this paper, through the implementation of Uncritical Inference Test (UIT) along with the teaching of organic spectroscopy course, this activity has enabled students to revise on their basic knowledge and understanding, as well as to enable the course instructor to check and rectify any weaknesses in the subsequent lessons. Three case studies based on lessons associated with Mass Spectroscopy (MS), Infrared (IR) and Nuclear Magnetic Resonance (NMR) were designed for this study. Based on the students' reflective writing, the UIT has promoted several positive learning outcomes, which includes a deeper understanding of a concept, improved thinking skills, motivated to study, fun-filled learning, peer learning and autonomous learning, which further encouraged the use of UIT in the teaching of other subjects.

Keywords: Uncritical inference test, Basic knowledge and understanding, Organic spectroscopy, Reflective writing

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INTRODUCTION

Organic spectroscopy is an important course in the undergraduate chemistry program as it has wide applications encompassing all fields of chemistry.(Gurst, 1981; Sweeting, 1998) Currently, there is an effort to introduce the topic of Nuclear Magnetic Resonance (NMR) into the content of high school curricula, which is indicative of its significance in research and teaching. (Bonjour, Hass, Pollock, Huebner, & Frost, 2017) The NMR spectroscopy when used in complement with other organic analytical techniques, such as Infrared (IR) and Mass Spectrometry (MS), enables structural elucidation of unknown compounds (Kandel & Tonge, 2001). The organic spectroscopy course is a key subject and it is commonly taught to students in their second year of study, both in the classroom and laboratory. (Donald, Lampman, & George, 1988; Feist, 2004; Goodrich, Parker, & Phelps, 1993; Horowitz, 2000; Svoronos & Sarlo, 1993)

The organic spectroscopy course could be difficult for students to learn as it requires not only the understanding of theories, but also a lot of practice in spectra problem solving.(Karatjas, 2014) As a result, students have developed a negative attitude towards this subject as there has been limited availability of spectral exercises and lack of spectral analyzing questions in the exams for students to attempt and relate to their theoretical knowledge.(Angawi, 2014; Merlic, Fam, & Miller, 2001) To this end, efforts have been made to overcome this situation by supplementing methods to help students to master structural elucidation skills. (Graham, McIntee, & Schaller, 2016; McClusky, 2007; Wist & Patiny, 2012) However, exercises that enable students to test their basic knowledge associated with IR, NMR and MS are still lacking.

Our approach to organic spectroscopy teaching is consistent with the goals reported in a previous publication, which is to enable students to develop basic understanding associated with IR, NMR and MS, to motivate students' learning, recall and relate previous knowledge in problem solving and also to develop their thinking skills required in analyzing problems.(Iler, Justice, Brauer, & Landis, 2012; Schoffstall & Gaddis, 2007) Previously, the Uncritical Inference Test (UIT) activity was implemented in the author's classroom to instill deeper learning and interest in the basic organic chemistry course among students and the result showed that students developed positive learning through this activity.(Cha, Kan, & Chia, 2016; Kan, Cha, & Chia, 2015) In this paper, we would like to report on the implementation of the UIT along with the teaching of organic spectroscopy in the author's classroom. Apart from cultivating interest and creating deeper learning among students in this course, the authors would like to reinforce basic knowledge and to check on students' understanding of previous lessons, so that the course instructor can rectify the students' misconception and weaknesses in the subject. The students' learning outcomes were also investigated as described in this paper.

MATERIALS AND METHOD

This activity was conducted for the 90 students enrolled into the organic spectroscopy course, semester II 2016/17 session, at the Universiti Malaysia

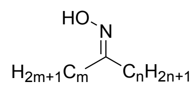
Terengganu, and have not participated in the UIT activity. This course comprised of one two-hour lesson and one one-hour lesson per week for 14 weeks. Before conducting the UIT activity, students have learnt the basic knowledge associated with NMR, IR and MS from the class instructor. The IR spectrum was obtained from an experimental data performed at the Universiti Malaysia Terengganu and ^{1}H- and ^{13}C- NMR spectra were simulated from the Chemdraw® software. The UIT activity was conducted after each lesson and the last 15 mins of the lecture was reserved for this activity. Students were given a set of statement and a case study at a time for them to review on the previous lesson. They were required to decide on a statement based on the information presented whether it is true, false or not sure. Students were required to mark true if a statement is true based on the case study and facts. A false statement is neither supported by facts nor information as provided in the case study. On the other hand, a "not sure" answer is indicative of a statement that could be either true or false to a certain degree. In total, three sets of case studies were developed for this study and a closed book session was conducted throughout the whole activity. Students were allowed to discuss their answer with their peers. After 10 mins, the course instructor invited students to share their answers during the open discussion session. Finally, all the answer scripts were collected at the end of the activity and analyzed by the course instructor.

In order to review the students' feedback on this activity, students were encouraged to submit an anonymous reflective writing, though it was not compulsory. These were collected after all three UIT case studies were conducted. A systematic network was built based on the collected reflective writing so as to understand the effectiveness of this activity in organic spectroscopy course. In total, 82 students participated in the reflective writing.

RESULTS AND DISCUSSION

Case study #1.

Compound Z



(m+n = 5)

M^{+} = 115

m/z: 100 (16 %), 73 (100 %), 58 (12 %).

Statement to readers:

1. The parent ion is at the m/z: 73.
2. The homolytic alpha cleavage at m/z: 100 produces methyl radical.
3. The m/z at 58 produces a carbocation with chemical formula $C_2H_4NO^+$.
4. The m/z at 73 consists of radical cation of C_3H_7NO.
5. McLafferty rearrangement occurs at m/z: 58.
6. 2 M of H_2SO_4 was used to induce the formation of amide later.
7. Compound Z is an oxime compound.
8. Compound Z has an aromatic substituent.

Figure 1. The GC-MS data of compound Z in case study 1

After the end of the MS lesson, UIT#1 (Figure 1) was carried out with an intention to recapture students' basic knowledge in this subject. As the discussion progressed, students showed enthusiasm by actively participating and exchanging views, thereby creating an active learning environment. After 10 mins of discussion, students were invited for answers and to provide their reasoning for the answer chosen. To further promote intellectual exchange, the course instructor directed the questions to the class for alternative ideas and then provided the correct answers (Table 1), along with the explanation for each statement at the end of each UIT actvity.

Table 1
Students' response to the statements in case study 1

Statements		Number of individuals		
		True	False	Not Sure
1.	The parent ion is m/z: 73	17	83*	0
2.	The homolytic alpha cleavage at m/z: 100 produces methyl radical.	53*	37	0
3.	The m/z at 58 produces a carbocation with chemical formula $C_2H_4NO^+$.	52*	38	0
4.	The m/z at 73 consist of radical cation of C_3H_7NO.	36*	54	0
5.	The McLafferty rearrangement occurs at m/z: 58.	47	43*	0
6.	2 M of H_2SO_4 was used to induce the formation of amide later.	4	0	86*
7.	Z is an oxime compound.	88*	2	0
8.	Z has an aromatic substituent.	3	87*	0

*correct answers

In case study 1, it was encouraging to note that the majority of students were able to answer question 1 correctly as evident in the classroom discussion and in the collected answer scripts. However, about 19% of the students developed misconception between parent ion and base peak. Students thought that the m/z at 73 with 100% abundancy was the parent molecular ion. The misconception was later explained in the class by the course instructor. Students found it challenging to work out the chemical formula of compound Z according to the students' comment during the open discussion in the class. Most of the students managed to work out the chemical formula by screening a combination of possibility (m:n = 1:4 or 2:3) and matched it to the fragment in the GC-MS spectrum. The correct answer is m:n = 1:4 or 4:1. In questions 2 and 3, students' understanding on the alpha homolytic cleavage was evaluated here. Students were able to comprehend this concept as evident in the students' answer scripts, about 59% and 57% of the students marked the correct answer for questions 2 and 3 respectively. In questions 4 and 5, the percentage of students who answered correctly was low, which was recorded at 40% and 48%, respectively. Some students explained that they were unable to recall the concept of McLafferty rearrangement during the classroom discussion. Students' inabillity to recall facts from previous lessons was consistent with a previous publication (Bligh, 2000; Kiewra, 2002), where without regular revision, students' knowledge retention declined 20% after 3 weeks. To overcome this problem, the course instructor advised students to make regular revision on previous lectures for sustainable memory. For questions 6, 96% of the students marked the correct answer, where they realized that there was insufficient information regarding the oxime and sulphuric acid reaction and thus marked "not sure" as answer. For questions 7 and

8, the percentage of students who marked the correct answers were recorded at 98% and 97%, respectively. Students realized that compound Z is an oxime and the total number of carbon for compound Z is five, as evident in their answer scripts. As a result, this has eliminated the possibility of having benzene substituent in compound Z. Overall, students responded well to this activity and showed great enthusiasm to learn more about organic spectroscopy. Figure 2 shows a sample of a student's answer in the UIT activity.

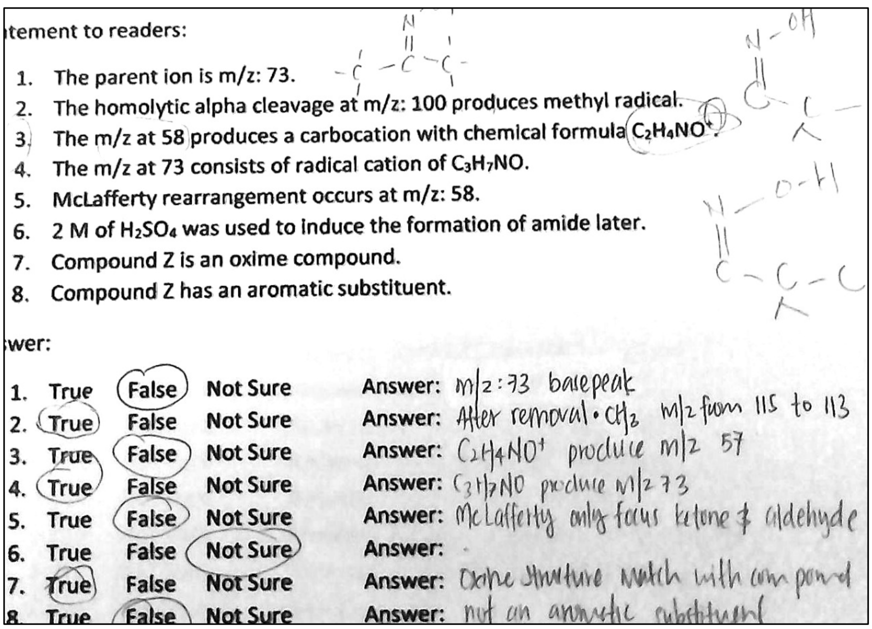


Figure 2. One of the students' sample answer to case study 1 in the UIT activity

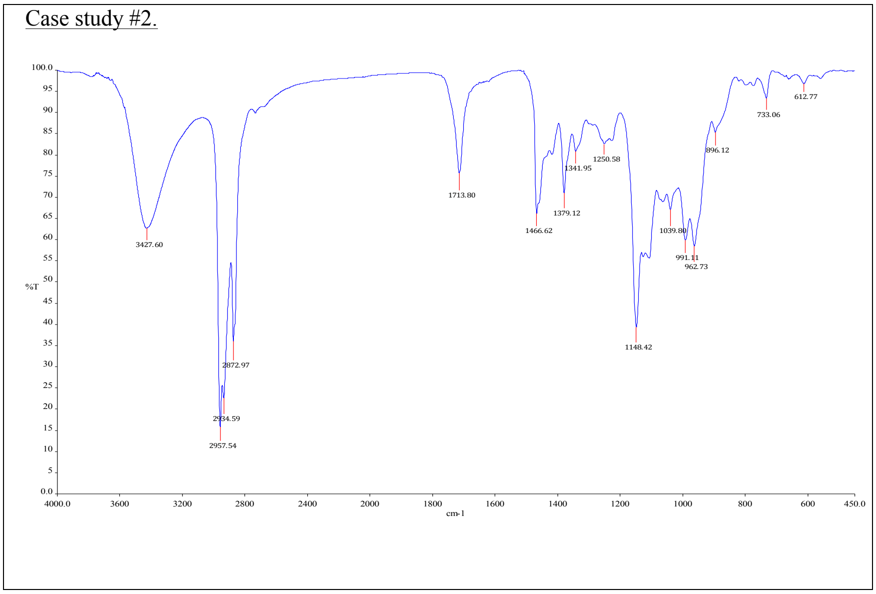


Figure 3. IR spectrum of compound X

Case study 2 (Figure 3) was designed and directed to students so as to revise their basic understanding on the IR topic. After the completion of the IR lesson, students' understanding on the IR topic was evaluated in the UIT activity. Based on Table 2, students had no difficulty in answering statements 9 to 16, where they were able to justify their answers during the classroom discussion. Based on Table 2, students marked the correct answers for most questions, except for question 14 which required students to have a deeper understanding of the statement. About 87% students marked the correct answer for question 9 and made the correct justification as evident in their answer scripts. It was encouraging to notice that 93% of the students were able to understand the IR absorption by alcohol O-H functional group (question 10). The course instructor then further elaborated that the alcohol O-H stretch has a broad signal from 3600 to 3200 cm^{-1}, while carboxylic acid O-H stretch shows an even broader signal from 3400 to 2400 cm^{-1}. A few students were unable to differentiate between an alcohol O-H stretch and a carboxylic O-H stretch and thus marked "not sure" as the answer. This was evident in one of the student's answer scripts as shown in Figure 4. For question 11, 91% of the students were able to determine the correct answer, either by positive identification thinking that the broad and singlet signal at 3427 cm^{-1} was due to alcohol O-H stretch or through negative identification thinking that a tertiary amine does not show any N-H stretch in IR spectroscopy, thus marked "false" as the correct answer. Likewise, students did not have difficulty in distinguishing the IR absorption by sp^2 and sp^3 C-H stretch, which occurs at 3100-3000 cm^{-1} and 3000-2850 cm^{-1}, respectively. For questions 12, 13 and 15, the percentage of students who marked the correct answer were recorded at 86%, 80 % and 88 %, respectively. For question 14, 96% of the students realized that there was insufficient information to confirm that compound X is hept-1-ol, therefore marked "not sure" as the answer. Last but not least, 92% of the students have marked the correct answer for question 16, which was related to the proton-deuterium exchange reaction.

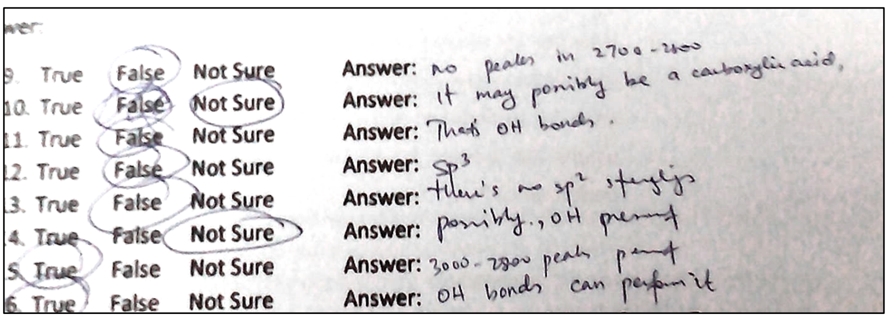


Figure 4. One of the students' answer to case study 2 in the UIT activity

Table 2
Students' response to the statements in case study 2

Statements		Number of individuals		
		True	False	Not Sure
9.	Compound X is an aldehyde compound.	12	78*	0
10.	Compound X is an alcohol compound.	84*	2	4
11.	The broad and singlet signal at 3427 cm^{-1} is due to the presence of tertiary amine.	8	82*	0
12.	The IR absorption at 2957-2871 cm^{-1} is due to the sp^2 C-H stretching	23	77*	0
13.	The benzene substituent is present in compound X	18	72*	0
14.	The compound X is hept^{-1}-ol.	4	0	86*
15.	The compound X possess sp^3 carbon.	79*	11	0
16.	Compound X is capable to undergo the hydrogen-deuterium exchange reaction.	83*	7	0

*correct answers

Case study #3.

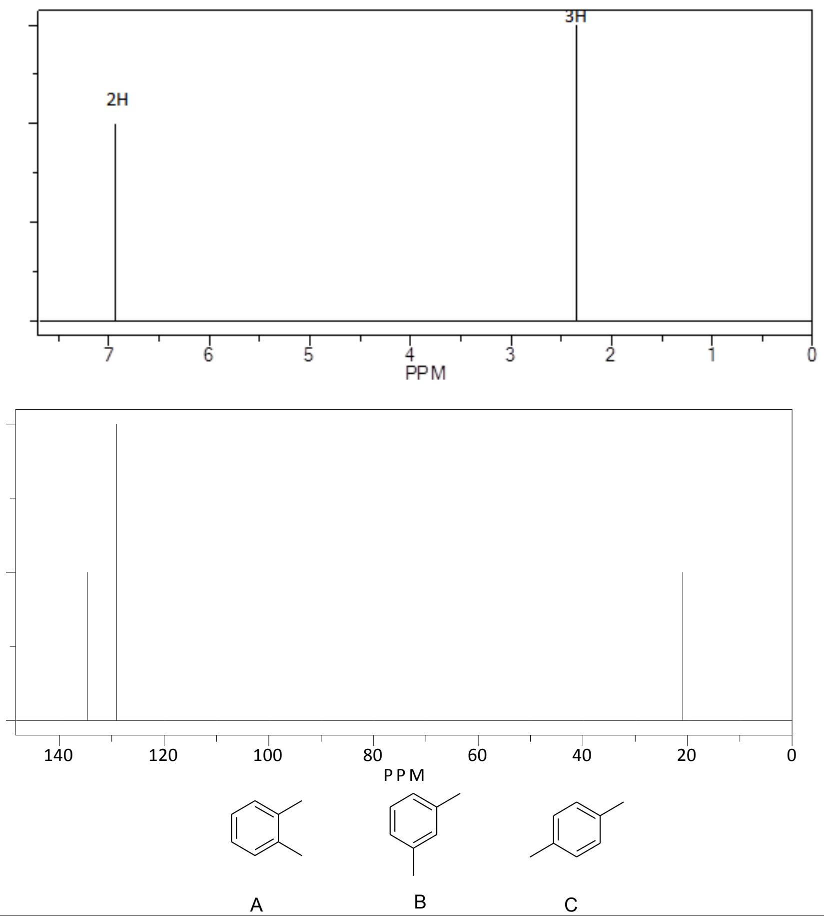


Figure 5. [1]H and [13]C-NMR spectra of Compound Y

In case study 3 (Figure 5), 10 statements were formed based on the [1]H- and [13]C-NMR spectroscopy chapter and students need to have prior knowledge on this topic before answering these statements. Undoubtedly, all A, B and C structures possess at least a plane of symmetry, therefore the correct answer for question 25 is "true". Based on Table 3, 98% of the students marked the correct answer for this question. For questions 17 to 22, students' basic understanding in organic chemistry was examined, which required them to identify the number of plane of symmetry and relate this to the number of different magnetic environment of proton and carbon in structures A to C. The number of different magnetic environment of proton for structures A to C are 3, 4 and 2 respectively, thus statements 17 to 19 are true. Students who have marked the correct answer were recorded to be at 76%, 81% and 91% respectively, as reflected in their answer scripts together with the appropriate explanation to their answers. On the other hand, 73%, 78% and 74% of the students have clear understanding of the number of different magnetic environment of carbon in structures A to C (statements 20 to 22), which are 3, 5 and 4 respectively. On the contrary, students did not have difficulty in choosing the correct answers for questions 23 and 24, as indicated by the fact that 79% and 98% of the students' answers were correct. Finally, based on the information in the spectra, students were asked to match the correct structure to the spectra provided (statement 26). It was promising to note that 84% of the students marked the correct answer. Overall, students gave a good appreciation to the objective of the UIT activity in the organic spectroscopy course, which was to enable them to revise their basic knowledge, recall and to apply previous knowledge in problem solving. Figure 6 shows one of the student's sample answers for case study 3.

Table 3
Students' response to the statements in case study 3

Statements		Number of individuals		
		True	False	Not Sure
17.	Structure C has two different magnetic environment of protons in the ^{1}H-NMR.	68*	22	0
18.	Structure B has four different magnetic environment of protons in the ^{1}H-NMR.	73*	27	0
19.	Structure A has three different magnetic environment of protons in the ^{1}H-NMR.	82*	8	0
20.	In the ^{13}C-NMR, structure C has three magnetic environment of carbons including non-protonated carbons.	66*	24	0
21.	In the ^{13}C-NMR, structure B has three magnetic environment of carbons including non-protonated carbons.	20	70*	0
22.	In the ^{13}C-NMR, structure A has three magnetic environment of carbons including non-protonated carbons.	24	66*	0
23.	Structure B and C can be distinguished using NMR spectroscopy.	71*	29	0
24.	The ^{1}H-NMR spectrum of compound Y shows the presence of methyl signals.	88*	2	0
25.	All the structures A, B and C possess at least a plane of symmetry.	87*	3	0
26.	The ^{1}H- and ^{13}C-NMR spectrums of compound Y match with the structure of B.	14	76*	0

*correct answers

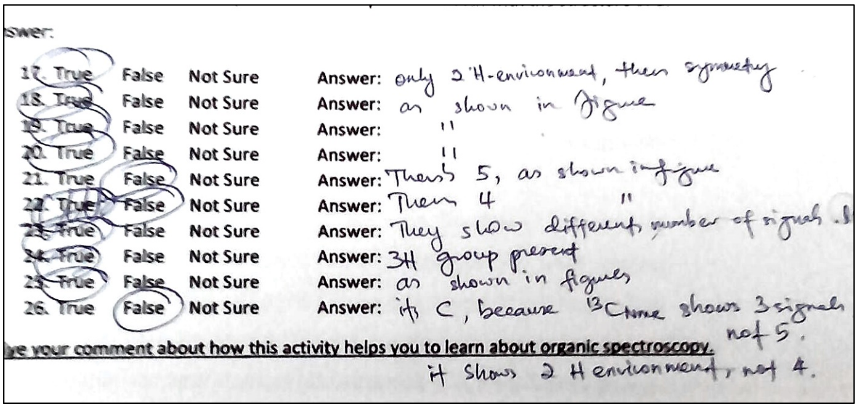


Figure 6. A student's sample answer for case study 3

Analysis on Students' Reflective Writing

Prior to the commencement of this activity, the author has thought about using pre- and post-testing which would ideally be a good measurement or assessment to gauge student's understanding before and after the administration of UIT in the organic spectroscopy course. However, considering the fact that there was only one organic spectroscopy class, with no other similar course taught in parallel by the same lecturer or by the author's colleagues during the same period, the pre- and post-testing offers little useful information in our study if there is no control group. In contrast, the author has employed reflective writing as a tool to understand students' perspective on this activity. It is imperative for students to have self-realization that they are responsible in their own learning by active participation, understand the changes in their learning under the intervention and the progress they made by reflecting deeply on this activity. The pre- and post-testing would only allow the researchers to keep the growth and challenges to themselves most of the time. The analysis should also be made valuable to both researchers and students. In this case, by having students to submit a reflective writing, students are able to reflect about their own learning progress, strengths, weaknesses and celebrate their growth. The author believed that a reflective writing would allow students to be more confident in their ability to learn.

Students' feedback on the UIT activity in the spectroscopy course was analyzed and a systemic network (Figure 7) was formed in an attempt to learn about the benefits of the UIT activity towards students' learning. In Figure 7, students' feedback was analyzed and categorized based on Bloom's taxonomy. In the cognitive domain, 8 students responded that the UIT activity have benefited them in previous knowledge recall (C1), such as revision on the previous knowledge associated with MS, IR and NMR. It was noteworthy that 37 students responded that this activity enabled them to think deeply in the concepts associated with IR, MS and NMR and to apply them in problem solving (C2). On the other hand, two students have benefited in developing thinking skills which enhanced their decision making (C3). Undoubtedly, one needs to be equipped with a strong basic understanding of a subject, recall and to apply it in problem solving.

In the affective domain, students who paticipated in this activity were motivated as reflected in 27 students' reflective writing (A1). Three students experienced joy in studying the organic spectroscopy course incorporated with the UIT activity (A2). In the group learning domain, three students have benefited from their peers (peer learning) (G1). Finally, this activity has positively aided two students to study independently as reflected in their reflective writing (G2). Figure 8 shows a student's reflective writing on the implemented UIT activity and some students' comments on the UIT activity are included as follows:

> *It is helpful to get better understanding of this organic spectroscopy course. To think critically to get an accurate answer.*
>
> *This activity gives me flash back memories of what I've learnt in chapter 1, as well as other chapters too.*
>
> *Managed to perform problem solving by discussing with fellow friends.*
>
> *This activity enables me to improve my thinking skills and apply all the skills that I learnt to determine a chemical structure.*

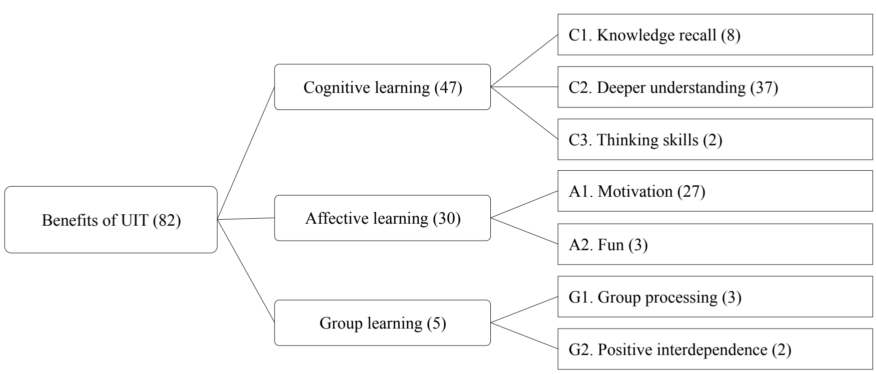


Figure 7. Students' feedback on the UIT activity as represented by the network diagram

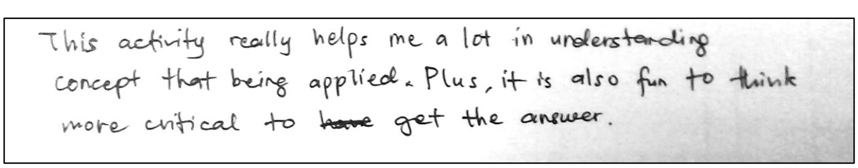


Figure 8. A sample of student's reflective writing towards the implemented UIT activity in the organic spectroscopy course

CONCLUSION

Three case studies associated with the MS, IR and NMR lessons were directed to students to reinforce their basic understanding in these topics. Through the incorporation of UIT activity in the classroom teaching of organic spectroscopy course, it has promoted several positive learning outcomes, which includes a deeper understanding of a concept, improved thinking skills, motivated to study, fun-filled learning, peer learning and autonomous learning. It has also helped students to revise on their basic understanding in the organic spectroscopy course and monitor their learning progress, as reflected in their reflective writing. The current study has proved that UIT can be applied not only in the teaching of basic organic chemistry but also in promoting understanding in organic spectroscopy. This will further encouraged the use of UIT in the teaching of other subjects.

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