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FEASIBILITY OF COMPUTATIONAL CHEMISTRY-BASED LEARNING MEDIA ON THE SUBJECT OF HYDROCARBONS

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Abstract

This study aims to determine the feasibility of computational chemistry-based learning media on the subject of hydrocarbons. This research is classified as development research developed with the ADDIE model consisting of analyze, design, development, implementation, evaluation. Data collection in this study was carried out by research instrument methods in the form of material and media validation questionnaires. The location of this study is SMA Negeri Modal Bangsa Arun. In this study, material expert validation was tested by four material experts and media expert validation was tested by one media expert. The results of the research obtained in the form of computational chemistry-based learning media received an assessment from material experts obtaining a percentage of scores of 88.92% for the feasibility aspect of content, 97.37% for the feasibility aspect of language, and 90.75% for the feasibility aspect of presentation. All three aspects fall into the "decent" category with minor revisions. Meanwhile, the results of research obtained for the feasibility of learning media by media experts obtained a percentage of value of 90% into the "feasible" category. Based on the value of the overall percentage of material and media feasibility is high, it shows that computational chemistry-based learning media on the subject of hydrocarbon as a learning medium is feasible to use.

Keywords: hydrocarbons, feasibility of learning media, computational chemistry

1 Introduction

Chemistry learning includes three aspects of study that must be understood, namely macroscopic, microscopic, and symbolic aspects. On the macroscopic aspect, teachers often implement it because this level covers real chemical phenomena directly or indirectly on the daily experience of learners. Meanwhile, for microscopic aspects teachers very rarely implement it into learning, because at this level real chemical phenomena are shown at the particular level, so they cannot be seen such as the movement of electrons, molecules, particles, or atoms. Then, for the symbolic aspect, teachers also often implement it because this is related to forms in the form of pictures, counts and graphs.

One of the chemicals included in the three aspects above is Hydrocarbons. Hydrocarbons are one of the SMA chemicals with basic competence (KD.3.1), namely analyzing the structure and properties of hydrocarbon compounds based on understanding the peculiarities of carbon atoms and the classification of compounds. In this material there is also a sub-material about isomerism in alkanes, alkenes, and alkynes.

Based on observations and interviews with chemistry teachers at SMA Negeri Modal Bangsa, Arun said learning hydrocarbon material at the high school level requires more effort because students must understand molecular structure and naming. This makes students less understanding of microscopic concepts and can also cause misconceptions about chemistry learning. Students also do not understand properly about the structure of existing compounds. This is in accordance with the opinion that students learn to interpret the visualized molecular structure as a simple line drawing is a difficult thing to deal with [1]. Chemistry lessons study a substance which includes the composition, structure, properties, changes, dynamics and energetics of substances involving skills and reasoning [2]. Factors that cause chemistry is difficult to study because chemistry requires the ability to think abstractly for study materials for example, atomic structure, chemical bonds and molecular shapes [3].

In addition to abstract and complex chemical materials, it turns out that learning media to improve the quality of learning is still inadequate. The media used is still very limited, teachers only present structural images obtained from the internet. Then, the textbooks used also do not display the 3-D structure of hydrocarbon compounds. Thus, almost all students do not know the shape of 3-D structures or molecules. Therefore, this has not been able to increase the knowledge of students to be able to visualize molecular structures in three dimensions. The importance of using learning media in addition to increasing students' knowledge can also arouse new desires and interests, generate learning motivation, and even bring psychological influence on students [4]. The use of appropriate learning media is essential when learning, because it has various advantages, namely resulting in abstract and complete principles becoming something clear, simple, and planned [5].

The difficulties encountered can be minimized by the use of learning media such as computational chemistry. According to him, computational chemistry is one branch of chemistry that uses chemical materials inserted into computer programs with the aim of being able to calculate the properties of molecules (atomic structure, energy and energy difference, charge, dipole moment, reactivity, vibration frequency, and other spectroscopic quantities) and their changes. Computational chemistry can forecast the structure, mechanism and energy of reactions, so users can design structures and forecast the properties of a compound accurately and provide data at the microscopic level. The use of software in computational chemistry helps learners understand material about molecular structure. This is because software in computational chemistry is able to visualize molecular structures in three dimensions. The use of computational chemistry is a very motivating means to make learners involved in chemistry in creating more realistic and real models of molecular structure [6]. Some softwares computational chemistry such as, Jmol, Marvin Sketch, HyperChem, Chemdraw, NWChem, and Avogadro which can visualize microscopic matter into reality [7], [8].

There are several studies that have been carried out on the use of computational chemistry such as the research of using hyperchem computational media on molecular form materials [9]. The use of hyperchem is considered relatively easy and can directly show the appearance of the structure to be made. The use of Hyperchem is suitable for the subjects of atomic structure, periodic properties, molecular geometry, energy and thermodynamics and chemical laboratories, while for subjects such as acid-base and physical and chemical properties of substances are not very suitable. Then, according to the results of ChemLab software is also able to represent macroscopic aspects to bridge chemical practices in the laboratory, such as color changes, phase changes, such as liquids, gases and solids [10].

From this explanation, it can be seen that computational chemistry can be used as an alternative learning medium to help increase students' understanding of chemical materials optimally [11]. Computational chemistry can support concrete chemistry learning, learners in hands-on experience in rotating and translating structures. 3D visualization reinforces submicroscopic level illustrations [12]. The same thing was also explained that computational studies to understand the nature and changes in macroscopic systems through simulations based on the laws of interaction in the system [13]. For example, the properties of molecules (energy, structure, dipole moment, polarity, or hyperpolarization) can be incorporated into the calculation.

Previous research stated that learning media with computational methods on haloalkane material received an average percentage of 92.6%, which means it is very feasible to use [14]. The same is the case with research on learning media based on computational methods using Software NWCHem. In electrolyte and non-electrolyte solution materials, an average percentage of 87.50% was obtained with the category of very feasible [15]. Based on the results of research that that the use of NWChem software in learning molecular form material contributes very high compared to using Chemsketch software [16]. Learning media using NWChem can improve student learning outcomes because in this media students can learn molecular shapes with pictures and video animations of molecular shapes.

Previous research conducted by using avogadro software, explained that this software is able to bring students closer to molecules, reveal details at the microscopic level, and understand more about chemical laws, chemical properties, chemical reactions, and other chemical phenomena [17]. Meanwhile, another research concluded that the use of visualization media using Avogadro software to describe the shape of molecules in 3 Dimensions (3D) is proven to attract students' learning interest and understanding [18]. This software can clarify the understanding of abstract concepts so that it can be more concrete, easily captured by the students' brains and fun to follow the explanation. In accordance with the characteristics of the basic competence of hydrocarbon materials and media needs in the teaching and learning process, researchers are interested in conducting research on the use of computational chemistry with Avogadro, NWChem, and Jmol software.

2 METHODOLOGY

This research is research and development (Research &; Development). Research and development (R&D) is a research method used to produce certain products and test the effectiveness of those products. In this case, the resulting product is a learning media based on computational chemistry assisted by Microsoft Sway for the subject of hydrocarbons. The development model used in this study is ADDIE with the following stages: 1. Analysis; 2. Design; 3. Development; 4. Implementation; 5. Evaluation. The data collection techniques used in this study were questionnaires and observations. Questionnaires are given to material expert validators and media experts to test the validity of the instrument. The research instruments used will be presented in Table 1.

Table 1. *List of research instruments*

No	Instrument Name	Contents/Aspects assessed
1.	Material Expert Validation Instrument Assessment Sheet Based on the National Education Standards Agency (BSNP)	Aspects of content feasibility, language, and presentation
2.	Media Expert Validation Assessment Sheet on the Development of Computational Chemistry-Based Learning Media	Aspects of Guide and Information, Aspects of Program Performance, and Aspects of Systematics, Aesthetics, and Design Principles

The data analysis technique used in this study is a quantitative descriptive analysis technique, which describes the product to be tested for feasibility. Data analysis is in the form of a product development process, namely description data from media experts and material experts as well as data on the feasibility assessment of learning media products by media experts and material experts. In this study, media expert validation was tested by one media expert and material expert validation was tested by 4 material experts. The calculation of descriptive analysis techniques for the feasibility of material in computational chemistry-based learning media is as follows:

$$\text{Eligibility percentage (\%)} = \frac{\text{observed score}}{\text{expected score}} \text{ x } 100\%$$

Based on the results the percentage is compared with the criteria as presented in Table 2.

Table 2. *Eligibility category criteria*

Achievement Percentage (%)	Information
76-100	Proper
56-75	Quite decent
40-55	Less viable
0-39	Not worth it

As for Calculation of descriptive analysis techniques for the feasibility of computational chemistry-based learning media as follows:

$$x = \frac{\sum X}{n}$$

Information:

X = average score of each assessment component

$\sum X$ = Number of scores per assessment component

n = number of statement points

Convert the average score result of each component. The average of each component is compared to the criteria as presented in Table 3.

Table 3. *Interpretation of the feasibility of multimedia learning*

No	Interval Mean Score	Information
1	1.00-2.49	Not worth it
2	2.50-3.32	Less viable
3	3.33-4.16	Proper
4	4.17-5.00	Very decent

3 RESULTS

The development of learning media based on computational chemistry assisted by Microsoft Sway has been carried out on the subject of hydrocarbons. Media development is carried out based on the stages of the ADDIE model. The analysis phase is carried out a needs analysis of the learning media used during the learning process. It turns out that it has never used computational chemistry-based learning media during the learning process, especially for materials that require three-dimensional images of molecules. Furthermore, in the second phase, namely design, design activities are carried out including making instruments, designing the structure of compounds to be made based on computational chemistry. Making the structure of the compound with NWChem, namely structure of the compound C_2H_6, C_3H_8, C_2H_4, C_3H_6, C_4H_8, C_3H_4, C_4H_6, dan C_5H_8.

The result of the calculations using the NWChem version 6.6 software to obtain the calculated data using the Unrestricted Hartree-Fock (UHF) method with a base set of 3-21 G. the results of the calculations of C_2H_6 (ethane) and C_3H_8 (propane) compounds which are alkanes, using NWChem software, are then visualized using Jmol software in 3 Dimensional (3D) from as presented in the Figure 1.

***Figure 1**. The Structure of the Visualization (a) Ethane; (b) Propane*

The calculation results of C_2H_4, C_3H_6, and C_4H_8 compounds which are alkene, using NWChem software, are then visualized using Jmol software in 3 Dimensional (3D) from as presented in the Figure 2.

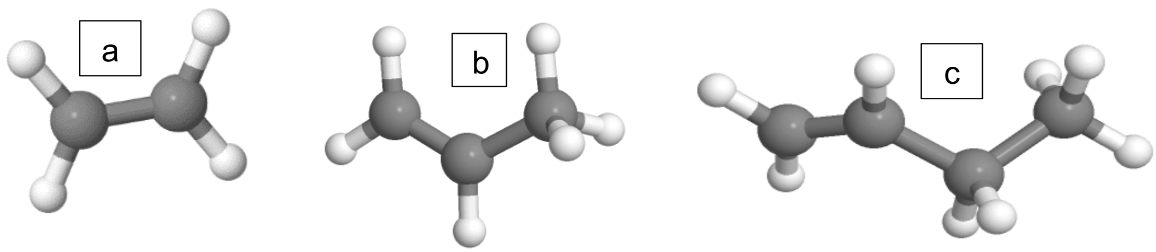

***Figure 2**. The Structure of the Visualization (a) C_2H_4; (b) C_3H_6; (c) C_4H_8*

The calculation results of C_3H_4, C_4H_6, and C_5H_8.compounds which are alkyne, using NWChem software, are then visualized using Jmol software in 3 Dimensional (3D) from as presented in the Figure 3.

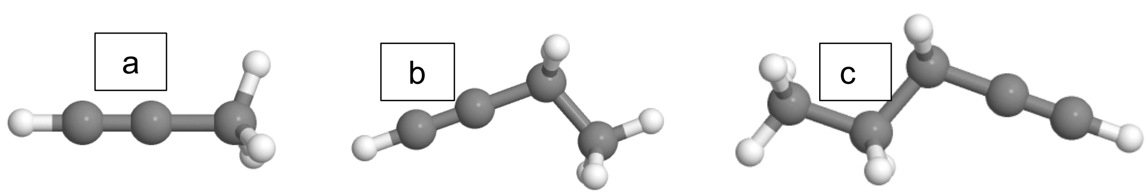

***Figure 3**. The Structure of the Visualization (a) C_3H_4; (b) C_4H_6; (c) C_5H_8*

The development stage, the third stage includes product manufacturing activities to be produced, namely learning media based on computational chemistry assisted by Microsoft Sway. In this stage, the structure of hydrocarbon compounds is made using Avogadro, then optimized molecules using NWChem, finally calculations are carried out while visualizing a stable structure using Jmol. After the three-dimensional molecular structure is produced, computational chemistry-based learning media is created using the help of Microsoft Sway for the display of hydrocarbon material presentations. The following is displayed the initial menu of the learning media that has been developed in Figure 4.

Figure 4. *Media Start Menu Display*

Figure 4 is the media start menu display showing the title and author. Furthermore, basic competencies, learning objectives, learning materials, sample questions, and exercises will be displayed. In the menu display this learning material is an implementation of hydrocarbon molecules or compounds that have been made using several software such as Avogadro, NWChem, and Jmol. Here's a look at materials based on computational chemistry as presented in Figure 5.

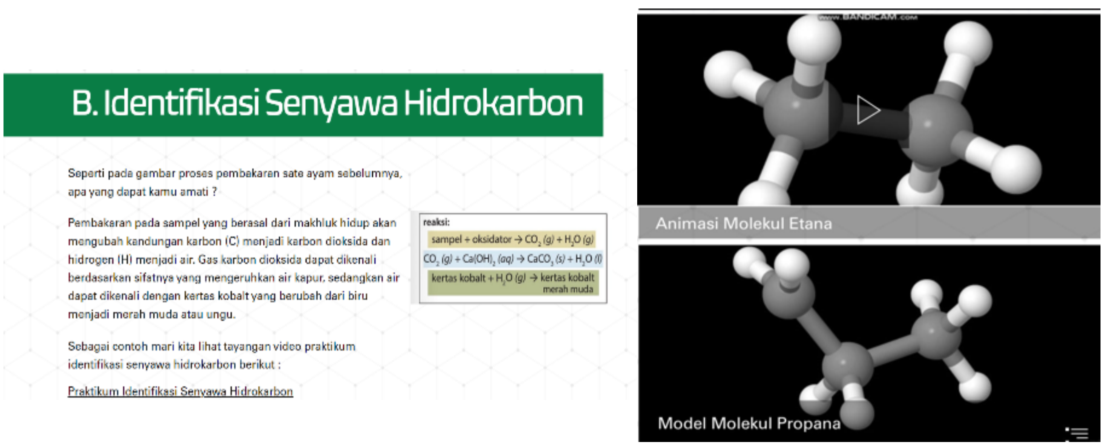

Figure 5. *Material Menu Display That Displays The Results Of Computational Chemistry*

At this stage of development, validation activities are also carried out to experts. Based on validation to validators consisting of 1 media expert and 4 material experts, the feasibility of material on learning media was obtained in terms of the feasibility of content, language, and overall presentation of 92.34% with the feasible category. While the feasibility of learning media in terms of guidance and information, program performance, and systematics, aesthetics, and design principles obtained a percentage of 90% (in an average of 4.17) with a very feasible category. The results of the material feasibility analysis can be seen in Figure 6 .

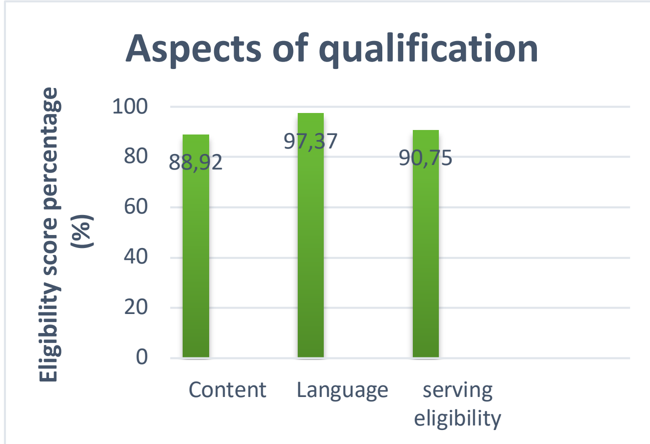

Figure 6. *Results of Feasibility Analysis of Hydrocarbon Material in Learning Media*

The feasibility aspect of the material leads to the suitability of the material contained in the computational chemistry-based learning media. The material contained is hydrocarbon material at competence (KD) 3.1. The feasibility aspect of the content is an assessment in terms of material coverage, material accuracy, material up-to-date in accordance with the latest chemical developments, can foster the productive character of students, and stimulate students' curiosity. Based on Figure 6 on the feasibility aspect of the content, it is known that the average assessment results of the four material expert validators obtained a validity percentage of 88.92%. These results are obtained with the category of feasible. These results are in accordance with the acquisition of feasibility results in several statement items on the material feasibility validation sheet number 1, 5, 10, and 11 on the feasibility aspect of the content reads "indicators in accordance with KI and KD, writing correct question formulations, accuracy of applicable theories in accordance with their fields of science, experiments or case examples presented in reality and efficiently to increase understanding for students / media users" obtained a score of 4 from the four validators. With this percentage, it can show that the material in the resulting learning media displays a decent scope of material given to students to help understand hydrocarbon material.

The feasibility aspect of language is an assessment in terms of communicative, the language used is able to explain concepts easily so that students understand, accuracy, straightforwardness, coherence and coherence of thought flow and the use of appropriate symbols or symbols. In the language aspect, it is known that the average assessment results of the four validators obtained a validity percentage of 97.37%. The score is high in the decent category. The feasibility results are supported by the results of several statements on the validation sheet in the language aspect, namely in number 3 which reads "sentences are communicative, material descriptions, examples, and exercises are presented in interesting language and commonly used in Indonesian communication" obtaining a score of 4 from the four validators. So that the score obtains validity with a decent category. The results also state that computational chemistry-based learning media use clear and communicative sentences in order to present the material well.

The feasibility aspect of presentation is an assessment in terms of media display design, visual appearance, and easy media operation. In terms of the display of chemistry-based learning media assisted computing Microsoft Sway It should have a look that consists of color alignment, consistency of slide shapes and layouts, selection of appropriate font size and typeface, video/image/audio quality, easy menu display, and design that has appeal to learners. Based on Figure 6 on the feasibility aspect of presentation, it is known that the average assessment results of the four validators obtained a validity percentage of 90.75% with the feasible category. These results are in accordance with the acquisition of feasibility results on several statement items on the material feasibility validation sheet number 9 on the presentation aspect that reads "consistent display design, good display format, organized, and attractive" obtaining a score of 4 from the four validators. So that this score shows that the material in the resulting learning media displays the use of attractive designs to make it easier for students to learn hydrocarbon material and attract the attention of students. These results are supported by Hardianto's opinion [19] which states that the use of animation in learning media can provide a direct picture of a material concept. In addition, the existence of animation can describe a concept of material that is presented abstract so that it becomes concrete and students feel directly interacting with the concept. In addition, in the feasibility aspect of presentation, there is also an indicator component that reads "color selection and font size are appropriate", this also supports the media to look attractive. Because it is based on Gagne's theory of information processing, which states that an information / stimulus that can attract someone's attention, will be more meaningful so that the information obtained can be encoded better and will be stored in long-term memory. That way it will make the information obtained will continue to be remembered by the person. So that the hydrocarbon material that students obtain or learn through the computational chemistry-based learning media developed will be stored in the long-term memory of students and this improves the quality of receiving and processing student information.

The next feasibility assessment is the feasibility of computationally assisted chemistry-based learning media Microsoft Sway that has been developed. Aspects of program performance lead to ease of operation or use of learning media can be used in accordance with navigation instructions or existing buttons to help students learn a material presented in the learning media. Indicators in this aspect are media usage guides, ease of installation, accuracy of using media navigation symbols, ease of use of navigation buttons, accuracy of browsing and links, operating system support, hardware support needed. It can be seen that the average assessment results from media expert validators obtained an overall validity average of 4.17 with a very decent category. This can be seen in Figure 7.

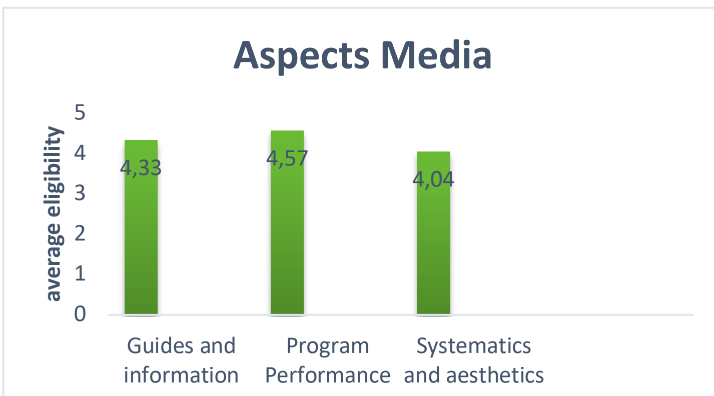

Figure 7. *Results of Learning Media Feasibility Analysis by Validators*

Result The analysis can mean that the resulting learning media displays guidance and information, appropriate program performance, and good aesthetic systematics. In accordance with that learning media is designed to be able to provide feedback quickly as if the media provides interaction to users [20]. So that good learning media is learning media accompanied by a controller so that it can quickly provide appropriate responses to the use of navigation.

4 CONCLUSIONS

The results of the research obtained in the form of computational chemistry-based learning media received an assessment from material experts who obtained a percentage score of 88.92% for the feasibility aspect of content, 97.37% for the aspect of language feasibility, and 90.75% for the feasibility aspect of presentation. All three aspects fall into the "feasible" category with minor revisions. Meanwhile, the results of research obtained for the feasibility of learning media by media experts obtained a percentage of 90% value into the "feasible" category. Based on the overall percentage value of material and media feasibility is high, it shows that computational chemistry-based learning media on hydrocarbon subjects as learning media are feasible to use.

REFERENCES

[1] M. Setyarini, K. Herlina, C. Diawati, Y. Ambarwati, and A. Saputra, "In-House Training of 3D Molecular Modeling using Avogradro for High School Chemistry TeachersIn-House Training of 3D Molecular Modeling using Avogradro for High School Chemistry Teachers," 2022.

[2] Q. Zuliatin, F. Fatayah, and I. F. Yuliana, "PENGEMBANGAN E-LKPD BERBASIS STEM (SCIENCE, TECHNOLOGY, ENGINEERING, AND MATHEMATIC) PADA MATERI STRUKTUR ATOM," *UNESA Journal of Chemical Education*, vol. 11, no. 3, pp. 195–202, 2022.

[3] S. R. Ama, S. Syutaridho, and A. K. Wardani, "Pengembangan Lembar Kerja Peserta Didik Berbasis STEM pada Materi Transformasi Geometri di Kelas XI SMA," *Jurnal of Education in Mathematics, Science, and Technology*, vol. 6, no. 1, pp. 1–10, 2023.

[4] P. W. Sasonohardjo, *Media Pembelajaran Bahan Ajar Diklat Kewidyaiswaraan Berjenjang Tingkat Pertama*. Jakarta: Lembaga Administrasi Negara., 2002.

[5] N. Nurfajriani, S. Hajar, and N. Halimah, "Pengaruh Multimedia Articulate Storyline Berbasis Discovery Learning terhadap Kemampuan Berpikir Kreatif Pada Materi Laju Reaksi.," in *Prosiding Seminar Kimia*, 2020, pp. 75–80.

[6] S. Paramita, E. V YD, N. Nasrokhah, and P. Iswanto, "Pemilihan Metode Perhitungan Kimia Komputasi Semi-Empiris Untuk Pengembangan 1, 3, 4-Thiadiazole," *Indonesian Journal of Chemical Research*, vol. 8, no. 1, pp. 51–56, 2020.

[7] I. Amalia, V. P. A. Dani, V. Tamala, and M. Musnaini, "Pemodelan Reaksi Hidrogenasi Senyawa Hidrokarbon Golongan Alkena dan Alkuna Melalui Studi Komputasi," *KATALIS: Jurnal Penelitian Kimia dan Pendidikan Kimia*, vol. 2, no. 1, pp. 33–40, 2019.

[8] L. E. Violante, D. A. Nunez, S. M. Ryan, and W. T. Grubbs, "3D printing in the chemistry curriculum: inspiring millennial students to be creative innovators," in *Addressing the Millennial Student in Undergraduate Chemistry*, 2014, pp. 125–146.

[9] A. D. Siregar and L. K. Harahap, "Pengembangan e-modul berbasis project based learning terintegrasi media komputasi hyperchem pada materi bentuk molekul," *JPPS (Jurnal Penelitian Pendidikan Sains)*, vol. 10, no. 1, pp. 1925–1931, 2020.

[10] S. Hadisaputra, L. R. T. Savalas, and S. Hamdiani, "Praktikum kimia berbasis kimia komputasi untuk sekolah menengah atas," *Jurnal Pijar Mipa*, vol. 12, no. 1, pp. 11–14, 2017.

[11] D. Y. M. Arifani, L. R. T. Savalas, A. D. Ananto, E. Junaidi, and S. Hadisaputra, " Pengembangan Modul Praktikum Kimia Berbasis Kimia Komputasi Pada Materi Asam Basa.," in *Prosiding SAINTEK*, 2021, pp. 660–666.

[12] J. Pernaa, "Possibilities and challenges of using educational cheminformatics for STEM education: A SWOT analysis of a molecular visualization engineering project," *ournal of Chemical Education*, vol. 99, no. 3, pp. 1190–1200, 2022.

[13] B. Prianto, “Pemodelan kimia komputasi. Berita Dirgantara,” *Berita Dirgantara*, vol. 8, no. 1, pp. 6–9, 2020.

[14] A. G. Marwan and A. W. Nugraha, “Pengembangan Media Pembelajaran Menggunakan Metode Komputasi pada Sub Pokok Bahasan Haloalkana di SMA,” *Humantech: Jurnal Ilmiah Multidisiplin Indonesia,* vol. 1, no. 7, pp. 927–934, 2022.

[15] A. S. Harahap, E. K. K. Hia, and A. W. Nugraha, “Pengembangan media pembelajaran berbasis metode komputasi pada materi larutan elektrolit dan non elektrolit,” *Educenter: Jurnal Ilmiah Pendidikan*, vol. 1, no. 6, pp. 683–690, 2022.

[16] S. R. Hasibuan, A. W. Nugraha, and M. Damanik, “Development of Learning Media Based on Computation Method in Molecular Shape.,” in *In The 5th Annual International Seminar on Transformative Education and Educational Leadership (AISTEEL 2020)*, Atlantis Press, 2020, pp. 107–112.

[17] C. U. H. Sinaga and A. W. Nugraha, “Determining the Most Stable Structure of Benzamided Derivatives Using Density Functional Theory (DFT),” *Indonesian Journal of Chemical Science and Technology*, vol. 4, no. 2, pp. 49–54, 2021.

[18] R. Adelina, E. Daniati, D. Nursinta, I. Sari, and H. Hasby, “Pengaruh Penerapan Aplikasi NMR Pro Trial terhadap Peningkatan Hasil Belajar Mahasiswa pada Materi Spektroskopi NMR,” *KATALIS: Jurnal Penelitian Kimia dan Pendidikan Kimia*, vol. 3, no. 1, pp. 31–38, 2020.

[19] A. Hardianto, K. Syahidi, T. Hizbi, and F. Fartina, “Pengembangan Media Pembelajaran Fisika Interaktif Berbasis Macromedia Flash 8 Materi Gerak Lurus,” *Kappa Journal*, vol. 4, no. 1, pp. 93–99, 2020.

[20] R. Fadli, M. Hakiki, S. Rahayu, and S. Astriyani, “Validitas media pembelajaran interaktif berbasis android pada mata pelajaran komputer dan jaringan dasar di sekolah menengah kejuruan,” *Jurnal Inovasi Pendidikan dan Teknologi Informasi (JIPTI)*, vol. 1, no. 1, pp. 9–15, 2020.