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A Bio-Edutainment System to Virus-Vaccine Discovery based on Collaborative Molecular in Real-Time with VR

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[Abstract]

An edutainment system aims to help learners to recognize problems effectively, grasp and classify important information needed to solve the problems and convey the contents of what they have learned. Edutainment contents can be usefully applied to education and training in the both scientific and industrial areas. Our present work proposes an edutainment system that can be applied to a drug discovery process including virtual screening by using intuitive multi-modal interfaces. In this system, a stereoscopic monitor is used to make three-dimensional (3D) macro-molecular images, with supporting multi-modal interfaces to manipulate 3D models of molecular structures effectively. In this paper, our system can easily solve a docking simulation function, which is one of important virtual drug screening methods, by applying gaming factors. The level-up concept is implemented to realize a bio-game approach, in which the gaming factor depends on number of objects and users. The quality of the proposed system is evaluated with performance comparison in terms of a finishing time of a drug docking process to screen new inhibitors against target proteins of human immunodeficiency virus (HIV) in an *e*-drug discovery process.

▸ **Key words**: Edutainment, Docking Simulation, Multimodal interface, Virus, Bio-Game

[요 약]

에듀테인먼트 시스템은 학습자가 문제를 효과적으로 인식하고, 문제를 해결하는 데 필요한 중요한 정보를 파악 분류하고, 배운 내용을 전달할 수 있도록 돕는 것을 목표로 한다. 에듀테인먼트를 활용한 콘텐츠는 과학 및 산업 분야의 교육 및 훈련에 유용하게 적용될 수 있다. 본 논문에서는 직관적인 멀티 모달 인터페이스를 활용하여 신약개발에서 활용되고 있는 가상스크리닝에 적용될 수 있는 에듀테인먼트 시스템을 제안한다. 본 연구에서는 분자 구조의 3D 모델을 효과적으로 조작하기 위해 입체 모니터를 활용하여 3차원(3D)거대 분자 모델링을 시각화 하였으며, 멀티 모달 인터페이스를 활용하여 분자 모델을 조작하고 있다. 본 시스템은 신약 개발 혹은 백신 개발에 있어 매우 중요한 방법 중의 하나인 가상 약물 선별 방법 중 하나 인 도킹 시뮬레이션 실험을 게임적 요소를 활용하여 쉽게 해결하는 방법을 제안하고 있다. 레벨 업 개념은 게임 요소가 객체와 사용자의 수에 의해 의존되는 바이오 게임 접근법을 활용하여 구현하였다. 실험 방법으로는 제안된 시스템의 신약 개발 과정에서 인간 면역 결핍 바이러스 (HIV)의 새로운 후보물질을 활용하여 바이러스의 활동 억제를 스크리닝하는 도킹 과정에서의 시간 측정으로 성능 비교 평가하였다.

▸ **주제어**: 에듀테인먼트, 도킹 시뮬레이션, 멀티모달 인터페이스, 가상 약물 스크리닝, 바이오-게임

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I. Introduction

Computer games have been widely used for people including children and the elderly in daily life. There have been several approaches using these computer games to attain educational purpose [1-3]. Typical games are only focused on entertainment with deriving some side-effects such as addiction, violence and nudity. However recent advances in games show that users are able to gain some good influences including learning and training beside entertainment while playing the game. We called this is "Serious Game" or "Edutainment".

In the edutainment research area, final goals are improving user's ability to solve problem or educating students to understand special subjects [4, 5]. There are interesting research issues using edutainment contents such as helping elderly people to understand and use computer easily [6]. In particular, Nintendo Wii was proposed as a new attractive tool for edutainment contents [7, 8]. It also may be adapted to scientific areas for the purpose of educating and training the users who need a virtual reality environment.

In this paper, we propose a bio edutainment content to utilize molecular modeling and docking which is an important part of *e*-drug discovery process. A molecular modeling is the research tool to operate three dimensional molecular structures in a computational manner. Structural biologists are able to simulate their experiments with equations of quantum and/or molecular mechanics in virtual reality. Usually molecular docking is used to develop new materials or new drugs against special binding site of a target protein [9]. Currently many tools to support molecular modeling works are available in the both public and commercial field. However it is still difficult to understand and use the modeling software for beginners or even for expert computational biologists. To solve this problem, we suggest specialized bio edutainment content which supports users to learn, enjoy and get feedback.

For the edutainment system, virtual reality platform is developed with stereoscopic functionality in order to actualize more immersive environment. Also, we used the WiiRemotes as interfaces to manipulate *in silico* molecular models in a user-friendly way. Using these tools, we think bio edutainment system contribute for the *e*-drug discovery areas especially to beginners and normal users.

In the next section, we present related works for edutainment and molecular modeling areas. In the Bio Edutainment System section, the proposed system and methods are presented. The presented system is evaluated in the following section

II. Related works

A game derives users participate in it through interesting challenges if they gain a success in the goal. In progress with the game, users acquire basic information and accomplish some sub-subjects which are essential conditions to approve the goal [12]. Since a VR game with immersive senses motivates its user to solve problem and to perform various approaches actively, it can be practically applied to another areas beside entertainment, called *serious game* [13]. The edutainment is similar to the serious game, but it focuses on more educational goals [14]. Nowadays, WiiRemote becomes a famous multi-modal interface which is an enabling tool to play various games with physical activities [15]. Shirai et al [8] suggested WiiMedia to adapt various areas such as game, media arts and training with physical interactions based on human motions.

In molecular modeling process, a success of work is depend on user's experience on the skill to get biological information from given three dimensional molecular model and compound data. It is a kind of empirical science. There are several researches to support molecular modeling. 3D visualization tools provide convenient virtual reality environment for easy interaction [10, 11]. To calculate the molecular

structure in real time, grid or distributed computing applications have been suggested [16, 17]. Some tools are running on the web for easy access [18, 19]. Also, collaborative platforms were suggested for internet environment [20, 21].

Foldit [22] is an interesting online game which combined with bioinformatics and emulates the process of creating folded conformation of unknown proteins. It provides a tutorial for beginners and teaches users how to rotate and move sub-models to make correct in silico molecular system. Users can play game to make appropriate ligand after finishing the tutorial jobs and they get scores by time and correctness. However, Foldit supports single user mode alone when they playing game and only allows a mouse as an interface. Although the 3D view for the molecular structure is very important, Foldit just supports non stereoscopic mode. These weaknesses may diminish effectives for the both entertainment and education.

Cai et al.[28] proposed an immersive and interactive bio game to educate young students for learning bio-molecular structures called X games. It provides an active stereoscopic mode and interactive 3D interfaces. However, their 3D interfaces such as Cyber Glove are too expensive to be used by general users.

In this paper, we introduced edutainment contents for molecular dockings to *e*-drug discovery. This edutainment system is attainable to play with Wii Remote by touches, gestures and a stereoscopic display to provide more detailed information on the molecular model. The suggested system simulates a docking process which is one of the best and the efficient ways to screen new drug candidates using computers.

III. Bio edutainment system

The proposed system is briefly described in Fig. 1. This system consists of six components: WiiRemotes, Sensor Manager, Feedback Manager, Molecular Simulator, Rendering Manager and Animation Controller. *WiiRemotes* receives user's input information via the Bluetooth communication with *Sensor Manager*. *Feedback Manager* reads the information from *Sensor Manager* to convert original data to meaningful data such as 3D info of molecules, feedback, changing rendering module, and so on. *Molecular Simulator* calculates potential energy of the molecular structure, which is game clear conditions, and sends it to *Rendering Manager* and *Feedback Manager*. *Rendering Manager* and *Animation Controller* visualizes and animates the consequence effects for input behaviors of users. *Feedback Manager* reads resulting physical data from the *Molecular Simulator* and converts to three feedbacks including sound, visual and force effects.

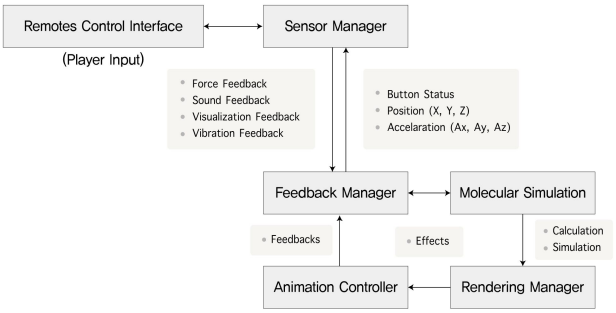

Fig. 1. System Overview

3.1 Multi-modal Interaction using WiiRemote as an interface

Multi-modal interactions can be processed in our suggested system as follows:

Action	Interactions
Inputs	The system receives 3D position values using WiiRemotes and its infrared sensor bar.
	The system receives Euler angle values from gyro sensors of WiiRemotes.
Outputs	The system provides a haptic feedback through WiiRemotes to denote success or failure.
	The system provides an audio feedback through WiiRemote to present success or failure.

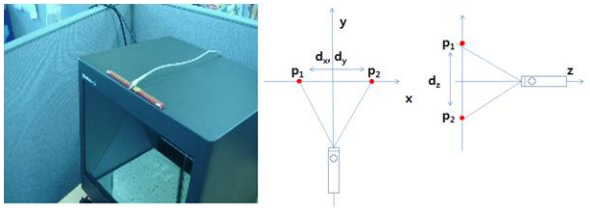

Fig. 2. (A) An infrared sensor bar (B) and tracking algorithm

The WiiRemote extracts 3D position values of user's inputs from the two LED light sources as shown in Figure 2 (B). The algorithm distinguishes the points of the LED sources p1 and p2 as two dimensional coordinates, where locations on the plane was projected as z is zero. In this case, the values of p1 (which consists of p1x, p1y) and p2 (which consists of p2x, p2y) are changed by variation of every input data from WiiRemote. So, we get displacements dx and dy using changes of p1 and p2. Finally, the x and y values are calculated by getting a middle point of dx and dy. Since WiiRemote only provides two dimensional coordinates, we used an approximated equation to obtain distance value dz between two positions using dx and dy. Also, a threshold value was utilized for presentation minus coordinate. The whole formulae are described in equation (1) as follows:

$$\begin{aligned} d_x &= p2x + p1x \\ d_y &= p2y + p1y \\ d_z &= \sqrt{d_x^2 + d_y^2} \\ x &= d_x / 2 \\ y &= d_y / 2 \\ z &= d_z + t \end{aligned} \qquad (1)$$

Sensor Manager reads the Euler angles using gyro sensors in WiiRemote. In output stage, *Sensor Manager* provides a force feedback with vibrators and a sound signals with speaker equipped in WiiRemote. The information about feedback is defined by system, in which the feedback will be triggered by behaviors of results from input data.

Molecular Simulator calculates game simulation with input data and decides on the state is success, fail or progress and this information is stored in *Feedback Manager*. In *Feedback Manager*, the state information is converted to three types of feedbacks; visual, force, and sound feedback. Each *Rendering Manager* and *Animation Controller* shows visualization and animation of visual feedback, respectively. The *Feedback Manager* also sends force and sound feedback to WiiRemote through *Sensor Manager* and a Bluetooth communication. This feedback information is described in Table 1.

Table 2. The result of processing time for the simulation between two groups.

Users		1	2	3	4	5
A	1	3:25	2:26	2:21	2:16	1:58
	2	3:15	2:22	2:13	1:57	1:55
	3	4:54	4:11	3:56	3:44	3:20
	4	4:23	3:45	3:10	2:53	2:43
B	1	5:32	5:21	4:22	3:52	3:48
	2	5:10	4:50	4:14	4:04	3:40
	3	7:28	7:14	7:01	6:41	6:54
	4	6:50	6:34	6:29	6:25	6:01

3.2 Real-Time Game Play

The main purpose of bio edutainment system is developing a game which enhances the performance of the molecular modeling process including docking simulation to virtual drug screening. The docking procedure aims to find a candidate molecular (a ligand) which can be combinded with a receptor protein at a specific position called an active site, Generally, Lemma1 and Lemma2 calculate docked structures in real time, when the receptor and the ligand are combined during the docking simulation as shown in Fig.3[20].

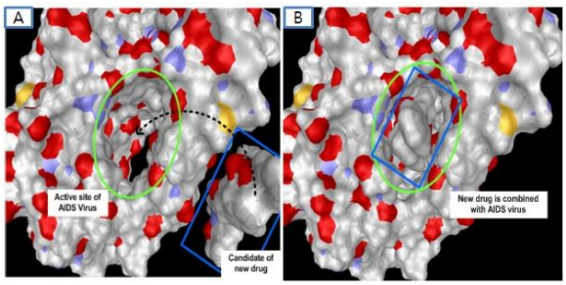

Fig. 3. (A) Before an HIV protease target model and a new drug model are combined (B) After the HIV protease tartget model and the new drug model are combined.

Since Lemma 1 is widely used in molecular docking process, we used this intermolecular energy algorithm in equation (2), which is condition to clear game.

Lemma1. An active site locates a special position which is stabilized between two molecules by the calculation so called intermolecular energy equation [16].

Lemma2. When the ligand molecule is combined onto the active site of receptor protein, the geometry information of two molecules is appeared complementarily [23].

$$E_{elec} = \sum_{excl(i,j)=1} \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

$$E_{vdw} = \sum_{excl(i,j)=0} \left(\left(\frac{v_i + v_j}{r_{ij}} \right)^{12} - \left(\frac{v_i + v}{r_{ij}^{6}} \right. \right.$$

$$E_{total} = E_{charge} + E_{vdw} \qquad (2)$$

where

i : i_{th} atom of virus
j : j_{th} atom of ligand
q : amount of electric charge by elemen
v : radius of vanderwaals by elementary
r_{ij} : distance between atom i and atom
e : epsilon

The proposed system provides an immersive gaming environment to understand hidden information in the molecular models using a stereoscopic display. Since Lemma 2 is important factor to modelers, users obtain 3D geometry information of molecules during participating in a bio game with stereoscopic display.

The level-up concept was also designed for entertainment's purpose beside education more complex methods of molecular modeling. The level design is consists of followings factors:

a. In level 1, user only manipulates one molecular model.
b. In level 2, user operates two molecules with two WiiRemotes in each hand.
c. In level 3, two users co-work game whit their respective 3D molecular models.

Users are trained to learn basic concept about molecular modeling and method in the Wii Remote in level 1. Next, he or she manipulates two molecules simultaneously with two Wii Remotes. In the final level, two people participate in the game each one Wii Remote. Players can chat and give some feedbacks such as vibration sound through Wii Remote to solve the problems.

3.3 Game Visualization

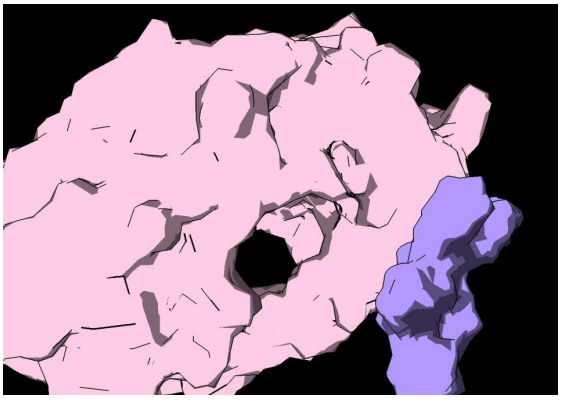

Fig. 4. Cartoon shading result with simplified mesh model(10%)

To provide entertainment factors for users who are participating in our bio edutainment contents, the proposed system should support innovative methods to distinguish this system among the other molecular modeling software. We utilized a cartoon rendering technique [24, 25] which is a kind of a non-photo realistic rendering method and simplified the original meshes [26] of molecular models. Even though the meshes are visualized with cartoon rendering, users may recognize the shapes of the molecular models which are similar to the original models. The simplified mesh models of the target protein and ligand molecules are rendered by cartoon shading as shown in Figure 4.

3.4 Game Cycle

First, the goal of game is selected for molecular docking process of target protein of HIV virus and

ligand [27]. A user takes advantage of a stereoscopic display for viewing 3D model in the game and WiiRemote (an input and output device) to manipulate the model and to receive haptic and sound feedbacks.

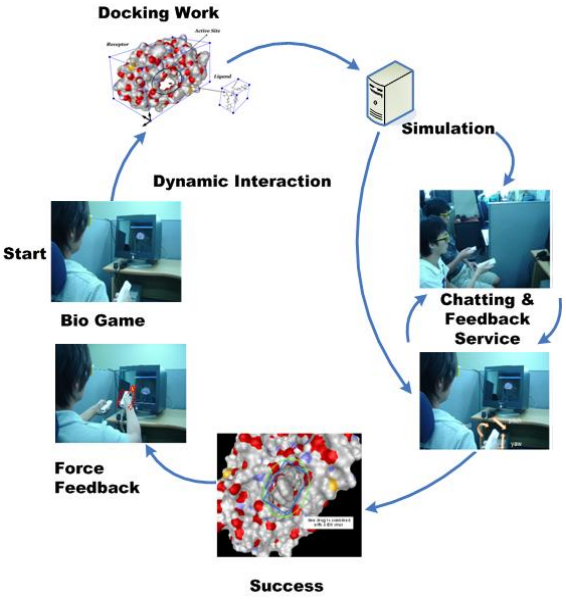

Fig. 5. Game cycle of the present bio game

As shown in Fig. 5, he or she operates the viral protein and the ligand. Energy calculation for the molecular motion is executed by the *Molecular Simulator*. Several users are able to perform collaborative work using WiiRemotes while more difficult level is going on. The results are delivered to the players and received feedback as result of the game.

IV. Experimental results

It is trivial that the proposed system shows educational affect as compared to previous approaches. We conducted various experiments to reveal possibilities of the proposed system. The following four types of experiments were exercised:

a. Checking educational effects of the game.
b. Comparing the WiiRemote and mouse.
c. Checking average clear time in each level.
d. Performing interviews to measure subjective opinions.

4.1 Evaluation of educational experiment.

We evaluated educational effects on accomplishment to both trained users who played our proposed system and other users who were only learned general process of molecular modeling. Also, we assumed that different result might be appeared between the general and novice people. We tested this experiment with eight users who tried these techniques for the first time. The users were divided into two groups; group A used our proposed game and experiment molecular modeling [11] and another group B conducted the molecular modeling after learned general lectures, such as presentation and movie. Each group consist of both general and novice users. We numbered two general users have one and two, who are undergraduate students majored in biological science. Other numbers three and four were selected for general users in major of computer science.

In group A, each user learned a manipulating method of WiiRemote for molecular modeling and played the proposed edutainment contents. The group B users studied molecular modeling process and method with the lecture, movie or manual instead of game play (Fig. 6). After first work, all members of groups tried 5-times of real molecular modeling jobs and the finishing time was recorded until docking is complete.

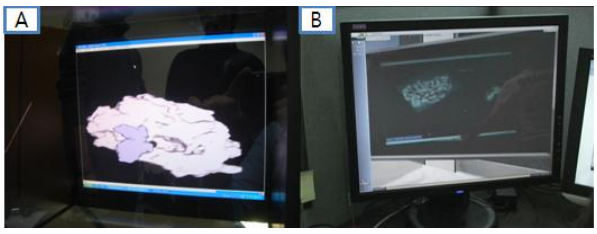

Fig. 6. Experiment environment (A) Playing a bio edutainment (B) Learning molecular modeling process from prerecorded movie.

Table 2. The result of numbers of conflicts and average clear time.

Users		BioGame Conflicts	BioGame ClearTime	Simulation Conflicts	Simulation Time
A	1	15	3:26	7	3:10
	2	12	3:42	8	2:57
	3	10	4:13	6	2:24
B	1	5	4:21	10	4:32
	2	9	4:10	11	6:28
	3	6	3:44	9	4:10

Table 2 shows the result of performance testing. The technique group A showed faster accomplishment than previous lecture. This result represents that game-based learning or training could be adapted to the real experiment quickly. Moreover we obtained interesting result from table 2 for distinguishing both general and novice users with showing novice users generally his experiment earlier than the general in both two groups and the general people. Anybody who tried our proposed system in group A showed better adaptive result as compared to another group.

4.2 Comparing WiiRemote with mouse for ability of adaption.

We divided two groups A for playing with WiiRemote and B for playing with mouse which consists of different 6 general volunteer users from previous experiment. Users re-played 5 times using both our proposed system and molecular docking process under detailed and precise simulation environment. The numbers of conflicts were measured as an index for unexpected errors originated from user's input and average clear time.

Molecular modeling environment provides more precise simulation and gives real-time visual with haptic feedbacks from chemical structure calculation. This environment supports a Head Mounted Display (HMD) as an output device to realize immersive environment. Haptic interfaces were also adapted as both input and output devices for the analyzing user's detailed input coordinates and interactive force feedbacks [10, 21].

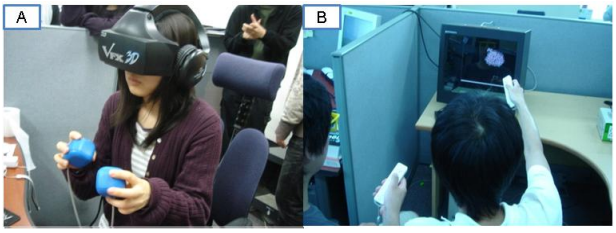

Fig. 7. Environment of molecular modeling (A) molecular modeling, Haptic Interface and HMD (B) immersive environment with two users game play

After playing the proposed system, users were able to learn the process and methods of molecular docking simulation. User-friendly molecular docking process is shown in Fig. 7(A). We also measured numbers of conflicts and average docking time. Table 3 shows results of this experiment. According to table 3, modeling job with the mouse showed better performance in terms of stability and accuracy because general users feel more comfortable when they use mouse operation rather than WiiRemote. However, WiiRemote realized interactive manipulation, which enables to operate two molecular models with each corresponding WiiRemote. Therefore, modeling job with the WiiRemote showed faster error recovering rates from conflicts. Consequently, average clear times were similarly.

In other hands, the results of simulation showed that users using WiiRemote ranked higher scores compared with users with mouse in terms of stability and accuracy, because molecular simulation environment provided stable human-computer interactions and two input haptic interfaces to simultaneous manipulation of two molecules. Users using mouse generally need more time to adapt this characteristic.

4.3 Evaluation of average clear time in each level.

We checked the clear time while they playing three-levels of the proposed system. Average times spent to play game were measured five times per each level. In level1, user utilizes own WiiRemote and user manipulates two WiiRemotes in each hand, finally two users are co working in level 3 (In Figure 7.(B)). We found that users were able to gain learning effect while they were playing the games.

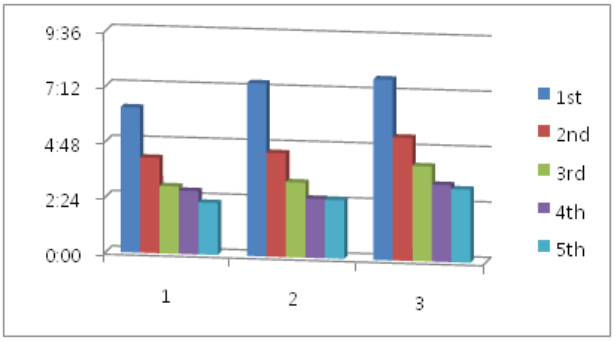

Fig. 8. Average clear time on different levels

As Fig. 8 shows, clearing the subject was very slow in the beginning. However, they finished it about 2.8-fold faster in the end. The most interesting stage for users was the level three because they could chat and gave feedbacks to each other using WiiRemote.

4.4 User satisfaction.

Satisfaction index was surveyed in terms of usability during the subjects (Fig. 9). We measured degree of satisfaction in the field of manipulation, entertainment, and application. The users mentioned that they satisfied by manipulating the molecular model using WiiRemote.

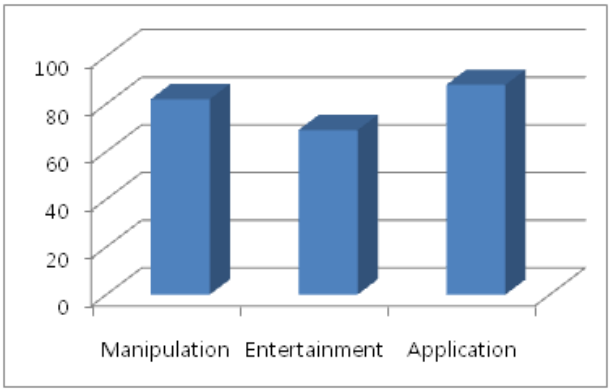

Fig. 9. User satisfaction surveyed in terms of manipulation, entertainment and application

However, most users felt that our system needs to be improving game facts, such as competition concepts or more interactive feedback, for realistic edutainment. The subjects expected that the proposed system would become more applicable to not only practical molecular docking but also computer aided *e*-drug design areas.

V. Conclusions

We introduced bio edutainment system to effective learn of virtual drug design including molecular docking or *e*-drug screening in easy way. The present system used WiiRemote as an interactive interface for easy and interesting manipulation by both single and multi users. It provided a stereoscopic display to obtain 3D hidden geometry information of molecules under immersive environment. The level-up concept was implemented in the edutainment system for both training and entertaining purpose.

The evaluation of the system revealed that the proposed system could enhance learning effects of users. The bio game system can be applied to other scientific application areas such as computer aided drug design, because users are able to learn theory and know-how about molecular design by playing or enjoying the game. The collaborative molecular docking supported by the game system may increase the efficiency of the *e*-drug discovery. The team-works of researchers in pharmaceutical companies and universities can be greatly improved by training the researchers with the bio game.

As future work, we are trying to apply the techniques to game effects, for example, collaboration and competition mode through internet and game effects like particle. For more interactive manipulation, we are developing additional and more detailed feedbacks.

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