LEARNING USING SOFTWARES

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN (AUTONOMOUS), SIVAKASI – 626 123.

(Affiliated to Madurai Kamaraj University, Re-accredited with A Grade by NAAC,
College with Potential for Excellence by UGC and Mentor Institution under UGC PARAMARSH)

2017-2018

M.Sc MICROBIOLOGY

MOLECULAR DOCKING STUDY OF NATURAL AND SYNTHETIC COMPOUNDS AS NOVEL INHIBITORS OF NON STRUCTURAL PROTEIN (NS5) AND STRUCTURAL PROTEIN OF DENGUE VIRUS

Project Report submitted to

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN (AUTONOMOUS)

(Affiliated to Madurai Kamaraj University, Reaccredited with 'A' Grade by NAAC and College with Potential for Excellence by UGC)

SIVAKASI

in partial fulfillment of the requirements for the Degree of

MASTER OF SCIENCE

in

MICROBIOLOGY

by

MISS.V.GOKILA

16PX002

Under the guidance of

MRS.G.SONA, M.Tech,

DEPARTMENT OF MICROBIOLOGY

APRIL 2018

BONAFIDE CERTIFICATE

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN (AUTONOMOUS)

(Affiliated to Madurai Kamaraj University, Reaccredited with 'A' Grade by NAAC and College with Potential for Excellence by UGC)

SIVAKASI

DEPARTMENT OF MICROBIOLOGY

Certified that this is a bonafide record of the

Project work done by

V.Gokila (16PX002)

at

The Standard Fireworks Rajaratnam College for Women (Autonomous), Sivakasi

during the year 2017-2018.

Place: Sivakasi

HOD

Date: 2.4.2018

Department of Microbiology

Submitted for the Viva – Voce Examination held at

The Standard Fireworks Rajaratnam College for Women (Autonomous), Sivakasi on 3.5.2018.

Internal Examiner

External Examiner

ABSTRACT

Dengue virus is one of the most important global pathogens and represents a global pandemic. Dengue virus causes dengue fever, an acute febrile infectious disease. Dengue is usually transmitted by the mosquito *Aedes aegyti*. Mosquitoes generally transmit the virus while feeding on the blood of an infected human host. After virus incubation for eight to ten days, an infected mosquito is capable, during probing and blood feeding, of transmit the virus to their offspring by transovarial transmission, but the role of this in sustaining transmission of the virus to humans still remains undefined. Envelope protein and NonStructure5 protein are shown to be elevated during the progression of dengue disease, which made effective drug targets for treating dengue disease. The goal of this study to screen group of natural compounds, which have effective inhibitory activity against Envelope protein and NonStructure5 protein and control the mechanism of upregulation of Envelope protein and NonStructure5 protein in the pathogenesis of dengue disease. The plant based natural compounds were used as in dengue diseases and sources are used as natural ligand for molecular docking process with protein drug targets using glide (version5.5) of Maestro (9.0) (Schrodinger suite). In this study, a natural compound were found to be good Envelope protein and NonStructure5 protein inhibitors. The natural bio-drug namely Glycyrrhizic acid isolated from the *licorice root* which is a medicinal plant have a good inhibition effect on Envelope protein. The synthetic compounds namely Rosmarinic acidic isolated from the rosemary (*Rosmarinus officinalis*) which is variety plant have a good inhibition. Here by it is conclude that these natural compounds when screened with all other natural and synthetic compounds were found to posses good binding affinity with these proteins and considered to be effective drug targets for treatment of dengue disease.

Keywords: Dengue Disease, Envelope protein, NonStructure protein5, Natural compounds

Rosmarinic acidic compounds comes as first hit with hydrogen bond interactions with residues of NonStructural protein5 and hydrophobic interaction was observed.

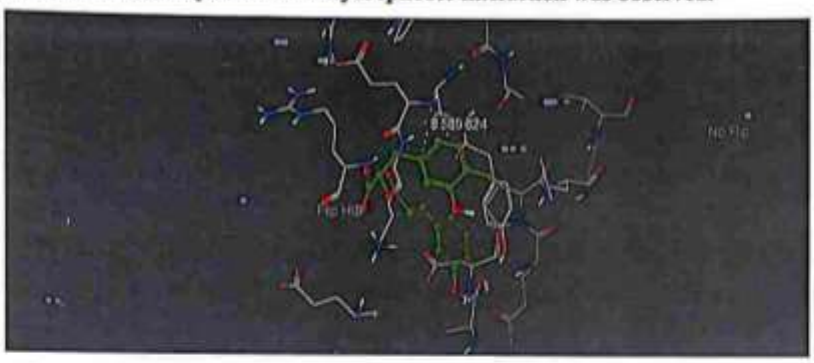

Figure 4: H-Bond interaction between Active site residues of NonStructural protein 5 of dengue and Rosmarinic acidic.

The Genistein compounds comes as second hit with hydrogen bond interactions with residues of NonStructural protein5 and hydrophobic interaction was observed.

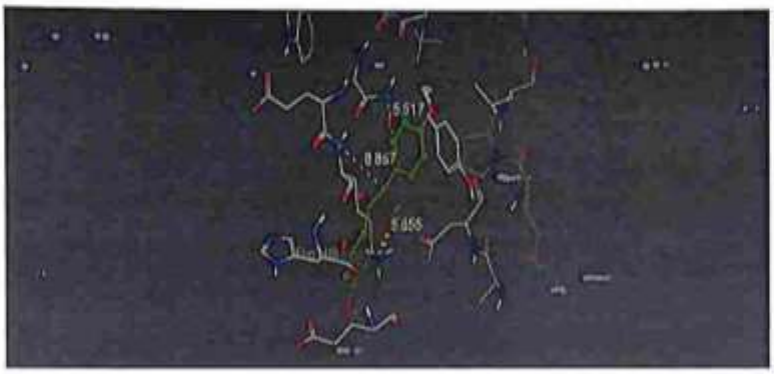

Figure 5: H-Bond interactions between Active site residues of NonStructural protein 5 of dengue and Genistein.

2016-2017

M.Sc MICROBIOLOGY

MOLECULAR DOCKING OF NATURAL AND SYNTHETIC COMPOUNDS AGAINST

VASCULAR ENDOTHELIAL GROWTH FACTOR AND CREATINE KINASE PROTEINS:

DRUG DESIGN FOR BRAIN CANCER

Project Report submitted to

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN (AUTONOMOUS)

(Affiliated to Madurai Kamaraj University, Reaccredited with 'A' Grade by NAAC and College with Potential for Excellence by UGC)

SIVAKASI

in partial fulfillment of the requirements for the Degree of

MASTER OF SCIENCE

in

MICROBIOLOGY

by

MISS. A. SANTHANA LAKSHMI

(Register No. 15PX011)

Under the guidance of

Mrs. G. SONA, M. Tech.,

DEPARTMENT OF MICROBIOLOGY

APRIL 2017

BONAFIDE CERTIFICATE

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SIVAKASI

DEPARTMENT OF MICROBIOLOGY

Certified that this is a bonafide record of the

Project work done by

Miss. A.SANTHANA LAKSHMI (Register No: 15px011)

at

The Standard Fireworks Rajaratnam College for Women (Autonomous), Sivakasi

during the year 2016-2017.

S.S.R

Place: Sivakasi

Date: 01.04.17

HOD/Co- ordinator

Department of Microbiology

Submitted for the Viva - Voce Examination held at

The Standard Fireworks Rajaratnam College for Women (Autonomous), Sivakasi on

02.05.17.

Sonaly 2/5/17

Internal Examiner

5.2.17

External Examiner

ABSTRACT

Brain tumor is one of the most common brain diseases which has affected and devastated many lives. Brain tumor poses unique challenges due to its distinct biology, genetics, treatment response, and survival. Brain tumors can be malignant (cancerous) or benign (non-cancerous) can affect both children and adults. Together, the brain and spinal cord (the central nervous system (CNS)) control the physiological and psychological functions of the body. The Vascular Endothelial Growth Factor Receptor-2 that are involved in the breakdown of blood vessels and breakdown of basement membrane in the first step of angiogenesis and finally in the initiation of cell proliferation and cell migration. Creatine kinase plays an important role in the buffering and transport of high energy phosphates via phosphocreatine to sites of ATP utilization where the enzyme is associated with ATP dependent processes. In this study docking analysis was carried out using Maestro (10.2) Schrodinger suite. The docking process was performed between natural and synthetic compounds with vascular endothelial growth factor receptor-2 and creatine kinase. The plant and animal derived natural and synthetic compounds were used as natural and synthetic ligands. The result of this study, Myricetin is a flavonoid compound derived from herbs which have a good binding affinity to the vascular endothelial growth factor receptor-2. Etoposide, a natural compound derived from *berberidaceae* which is an ornamental tree; it has a good binding affinity to the creatine kinase.

The first hit was Myricetin, a flavonoid derived from herbs which is a plant with a glide score of -13.6 which exhibits 8 hydrogen bond interactions residues of vascular endothelial growth factor receptor-2 of brain tumor and hydrophobic interaction was not observed.

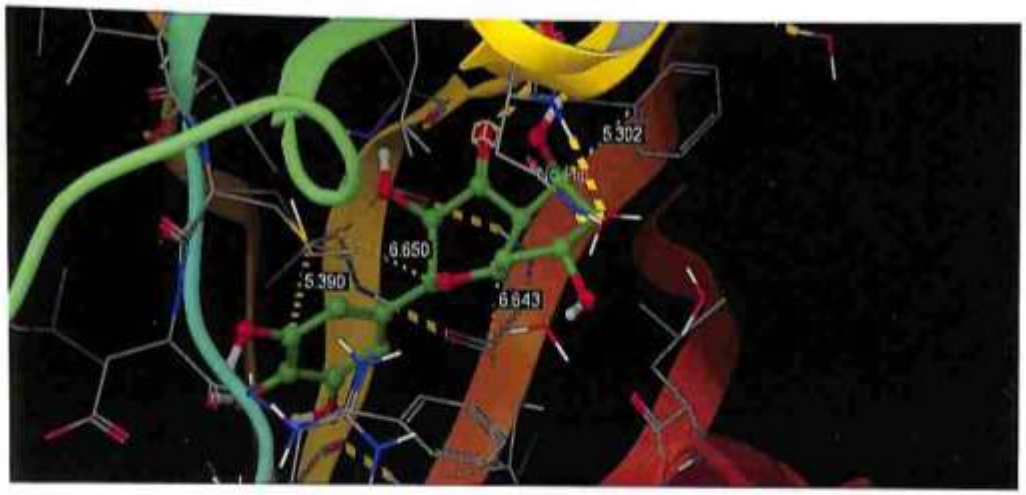


Plate1: H-Bond interaction between Actives site residues of vascular endothelial growth factor receptor-2 of brain tumor and Myricetin.

The third hit was tretinoin is a natural compound derived from *camptotheca acminata*, which is an ornamental tree with glide score -10.62 and it exhibits 10 hydrogen bond interaction residues of vascular endothelial growth factor receptor-2 and absence of hydrophobic interaction was observed.

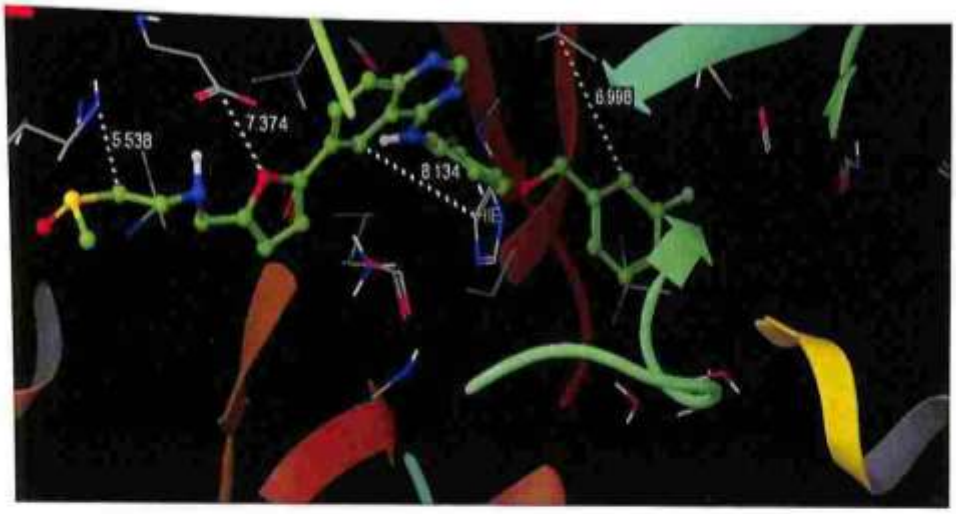


Plate3: H-Bond interaction between Actives site residues of vascular endothelial growth factor receptor-2 of brain tumor and Tretinoin.

2016-2017

IN SILICO SCREENING OF NATURAL AND SYNTHETIC COMPOUNDS AS ALDOSE REDUCTASE AND MATRIX METALLOPROTEINASES INHIBITORS: DRUG DESIGN FOR DIABETIC RETINOPATHY

Project Report submitted to

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN (AUTONOMOUS)

(Affiliated to Madurai Kamaraj University, Reaccredited with 'A' Grade by NAAC and College with Potential for Excellence by UGC)

SIVAKASI

in partial fulfillment of the requirements for the Degree of

MASTER OF SCIENCE

in

MICROBIOLOGY

by

MISS. M. SYEDALIFATHIMA

(Register No. 15PX013)

Under the guidance of

MRS. G. SONA, M.Tech.,

DEPARTMENT OF MICROBIOLOGY

APRIL 2017

ABSTRACT

Diabetic retinopathy (DR) is a micro-vascular complication of diabetes and one of the leading causes of blindness. In diabetic retinopathy oxygen supply to the part of the retina is decreased which blocks the blood vessels causing hypoxic condition. To compensate from this condition a signal sent by the retina for the formation of new blood vessels are leaky, fragile and having thin wall which leak the blood on the surface of eye and blindness takes place. Accumulation of intracellular sorbitol due to increased Aldose reductase activity has been implicated in the development of various secondary complication of diabetes and the MMP proteins found in the vitreous eyes with proliferative diabetic retinopathy. Three of the possible candidate proteins contributing to the development of diabetic retinopathy are Aldose reductase, Matrix metalloproteinase-2 and Matrix metalloproteinase-9. In the current study plant derived medicinal compounds and chemical compounds are studied by Docking analysis that are carried out using Maestro (10.2) (Schrodinger suite).The screened compounds were found to possess good binding affinity with these proteins and hence they are considered as diabetic retinopathy inhibitors. In this study, Chlorogenic acid, a plant green coffee bean isolated from leaves of *Hibiscus sabdariffa* was found to have high Binding Affinity and was proved to be the naturally available novel inhibitor of Aldose reductase. Acarbose is a starch blocker and inhibits alpha glucosidase, an intestinal enzyme that releases glucose from larger carbohydrates. It was found to have high Binding Affinity to the Matrix metalloproteinase-2 and -9 drug targets. From this study it is concluded that these natural compounds were found to have good binding affinity with these target proteins and considered to be effective drug targets for treatment of diabetic retinopathy (DR).

The β-valerolactone comes as the third hit and has 8 hydrogen bond interactions residues of Aldose reductase (1ADS) protein.

Plate 3: H-Bond Interactions between Active site residues of ALR2 (1ADS) protein and β -valerolactone.

2015-2016

MOLECULAR DOCKING OF NATURAL AND SYNTHETIC COMPOUNDS AGAINST CULTURE FILTRATE PROTEIN AND TYROSINE PHOSPHATASE PROTEIN : DRUG DESIGN FOR TUBERCULOSIS

Project report submitted to

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN, SIVAKASI

An Autonomous Institution

Affiliated to Madurai Kamaraj University

Reaccredited with A Grade by NAAC & CPE Status by UGC

The requirements for the

Degree of

MASTER OF SCIENCE

IN

MICROBIOLOGY

By

Miss. M.VANITHA

Reg. No. 14PX011

POST GRADUATE DEPARTMENT OF MICROBIOLOGY

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN (Autonomous)

SIVAKASI – 626 124

APRIL – 2016

THE STANDARD FIREWORKS RAJARATNAM COLLEGE FOR WOMEN

SIVAKASI

(An Autonomous Institution, Affiliated to Madurai Kamaraj University andReaccredited with 'A' Grade status by NAAC and CPE Status by UGC)

CERTIFICATE

This is to certify that the project work entitled"**MOLECULAR DOCKING OF NATURAL AND SYNTHETIC COMPOUNDS AGAINST CULTURE FILTRATE PROTEIN AND TYROSINE PHOSPHATASE PROTEIN:DRUG DESIGN FOR TUBERCULOSIS"**is a bonafide work done by **M.VANITHA (14PX011)**submitted to the Department of Microbiology, The Standard Fireworks Rajaratnam College for Women, Sivakasi, in partial fulfillment of the requirements of the award of the degree of M. Sc., Microbiology.

Sonaly 26/4/16
Internal Guide

S.S.R
Head of the Department

Submitted for Viva-voce held on 26/4/16

Sonaly 26/4/16
Internal Examiner

External Examiner

ABSTRACT

Tuberculosis is an infectious airborne disease caused by a bacterial infection that affects the lungs and other parts of the body. Tuberculosis is a bacterial disease usually affecting the lungs (pulmonary TB). Other parts of the body can also be affected, for example lymph nodes, kidneys, bones, joints, etc. (extrapulmonary TB). Tuberculosis can affect anyone of any age. Tuberculosis is spread through the air when a person with untreated pulmonary TB coughs or sneezes. The symptoms of TB include a low-grade fever, night sweats, fatigue, weight loss and a persistent cough. A person with TB disease may remain contagious until on appropriate treatment for several weeks. a person with latent TB infection, but not disease, cannot spread the infection to others, since there are no TB germs in the sputum. Culture filtrate protein10ESAT6 complex and Tyrosine phosphatase protein are considered to be elevated during the progression of tuberculosis, which made effective drug targets for treating tuberculosis. Isoniazid is used to treat tuberculosis (TB). Isoniazid is effective drug. Isoniazid, also known as isonicotinylhydrazide (INH), is an antibiotic used as a first-line agent for the prevention and treatment of both latent and active tuberculosis. TB is a bacterial infection which mostly affects the lungs, but which can affect any part of your body. It is treatable with a course of medicines which usually lasts for six months in total. Although isoniazid is a very effective medicine, it can sometimes cause damage to peripheral nerves (such as numbness and tingling sensations in the hands and feet).The goal is to screen the group of natural compounds, which have effective inhibitory activity against culture filtrate protein complex which can be used to control the mechanism of upregulation of culture filtrate protein10ESAT6 complex and Tyrosine phosphatase protein isolated from *Opium* in the pathogenesis of tuberculosis. The natural compounds were found to be good culture filtrate protein10ESAT6 complex and Tyrosine phosphatase protein. The natural aminoglycosides namely amikacin isolated from the *streptococcus aureus* which is medicinal plant have a good inhibition effect on culture filtrate protein10ESAT6 complex. Thus, it is concluded that these natural compounds and synthetic compounds docking with these proteins and considered to be effective drug targets for treatment of tuberculosis.

The kanamycin comes as the second hit and has 10 hydrogen bond interactions residues of culture filtrate protein 10 ESAT6 and absence of hydrophobic interaction was observed.

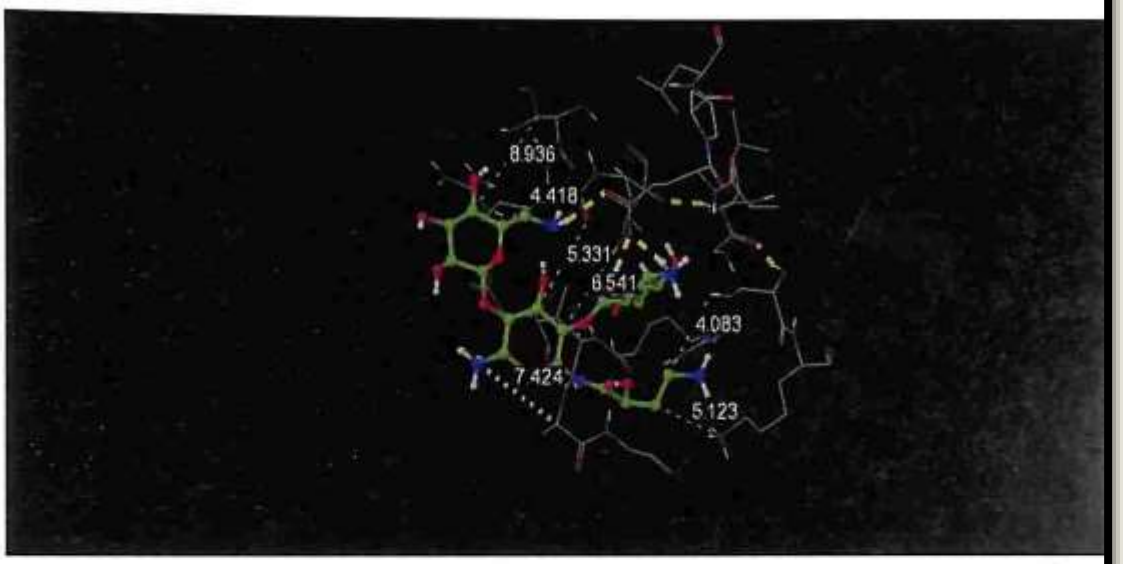
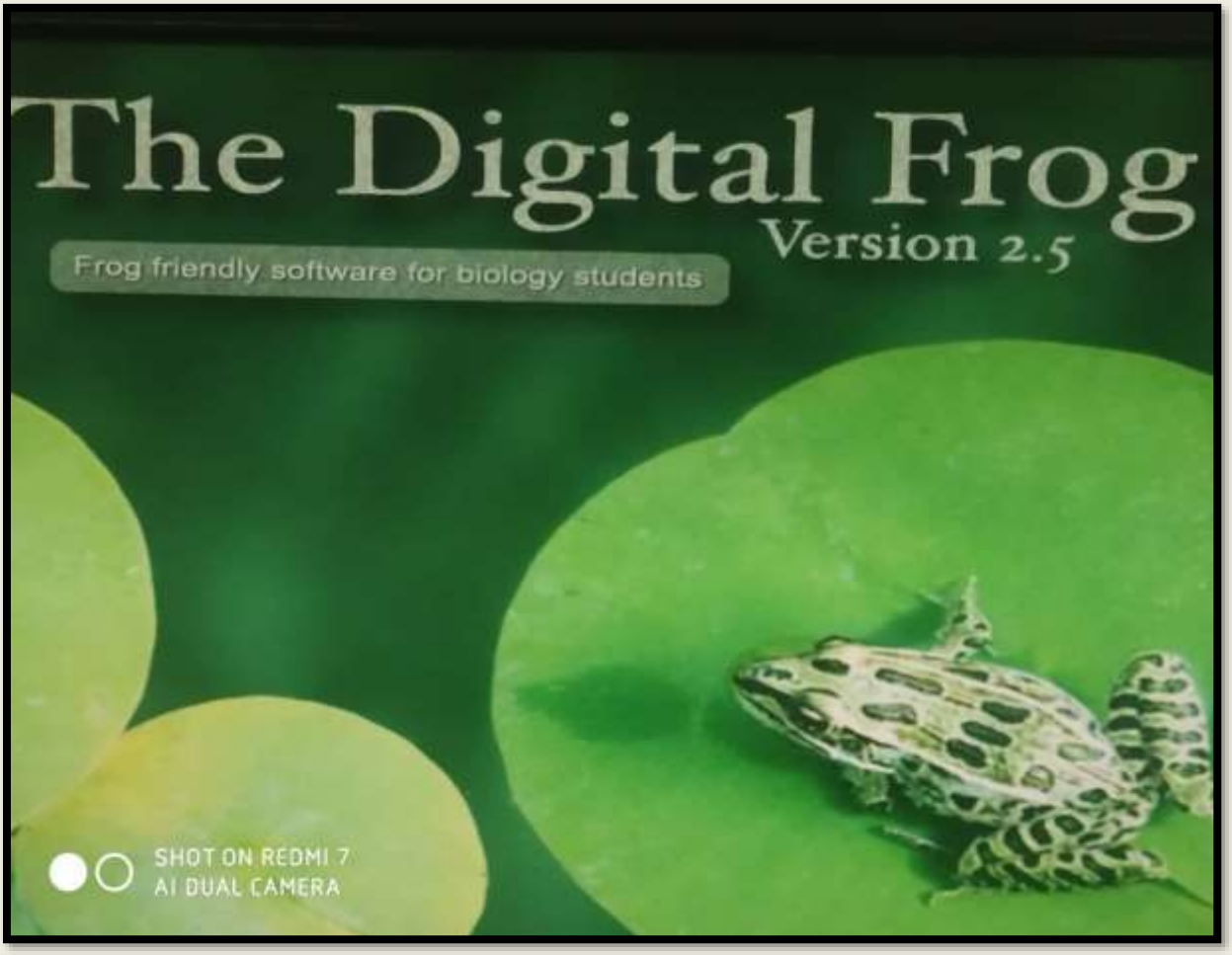
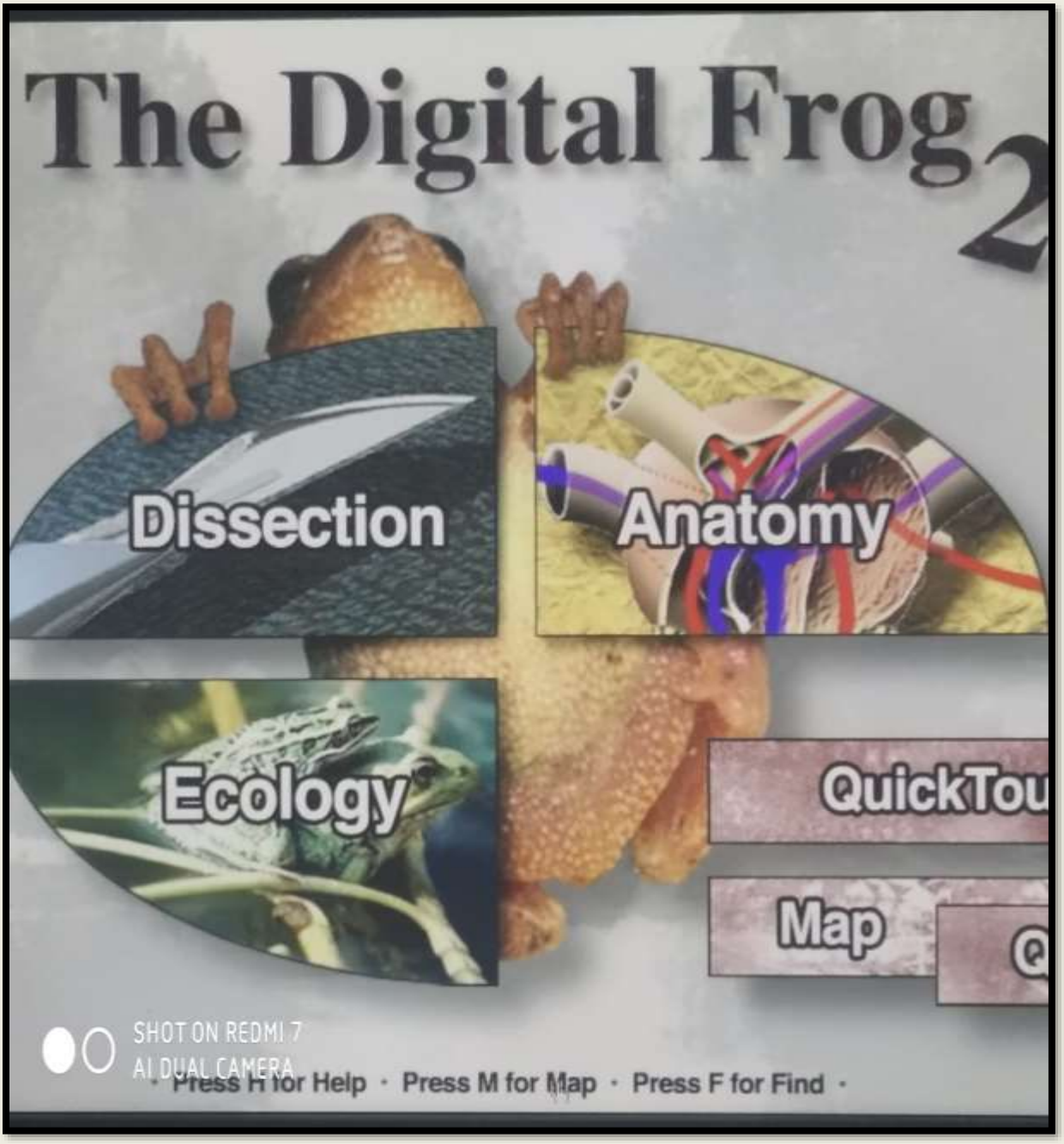
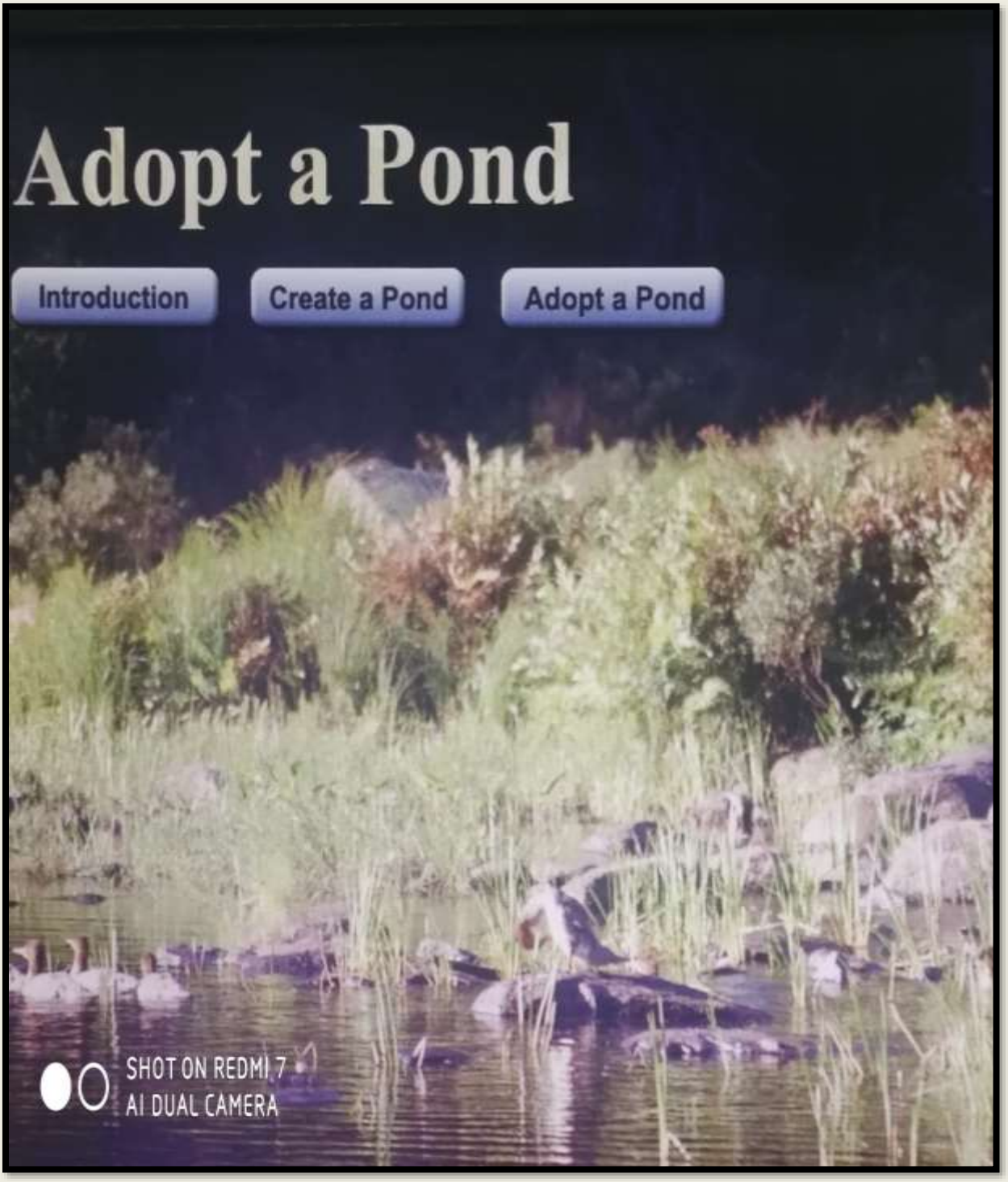


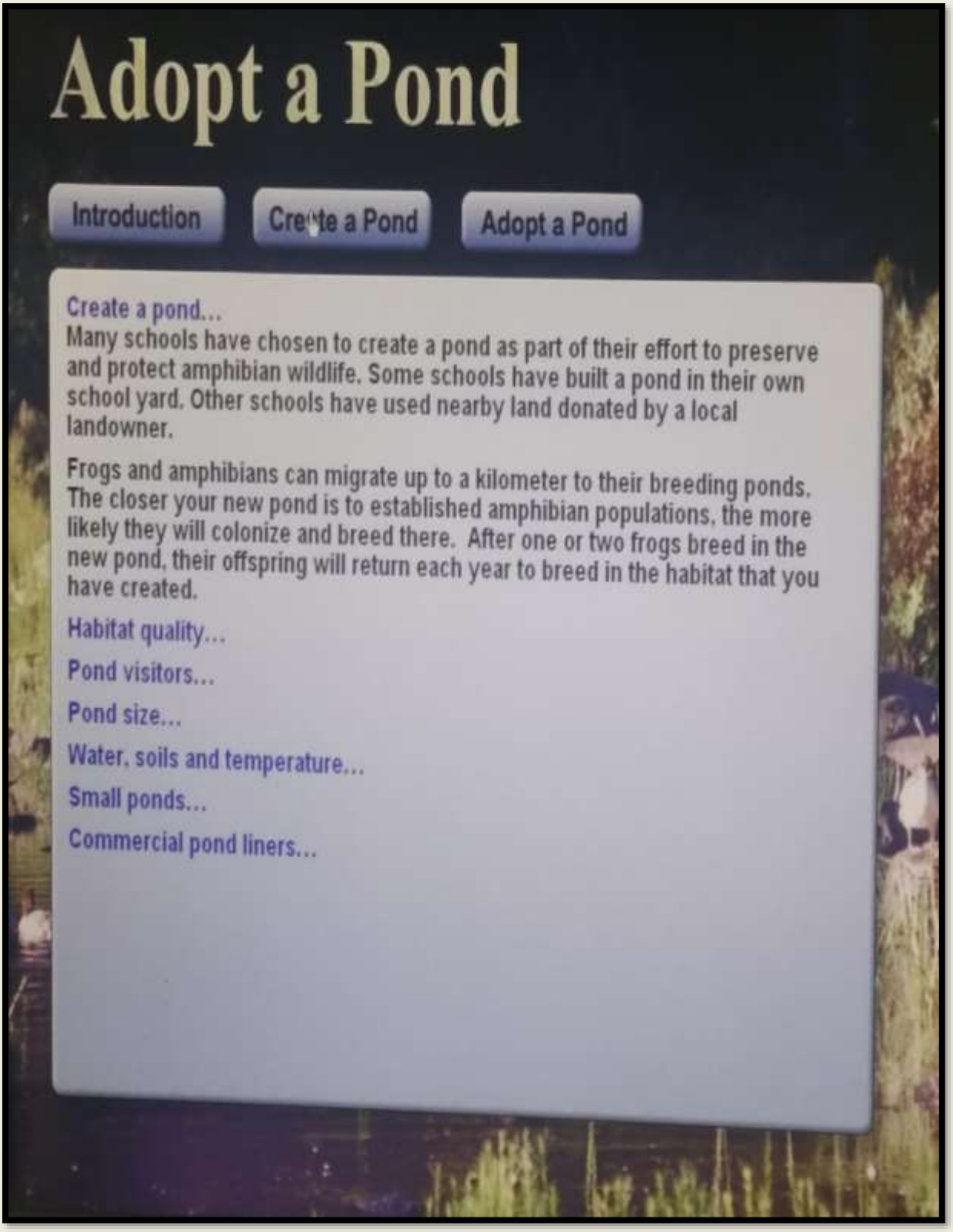
Figure 2:H-Bond interactions between Active site residues of culture filtrate protein 10 ESAT6 and kanamycin

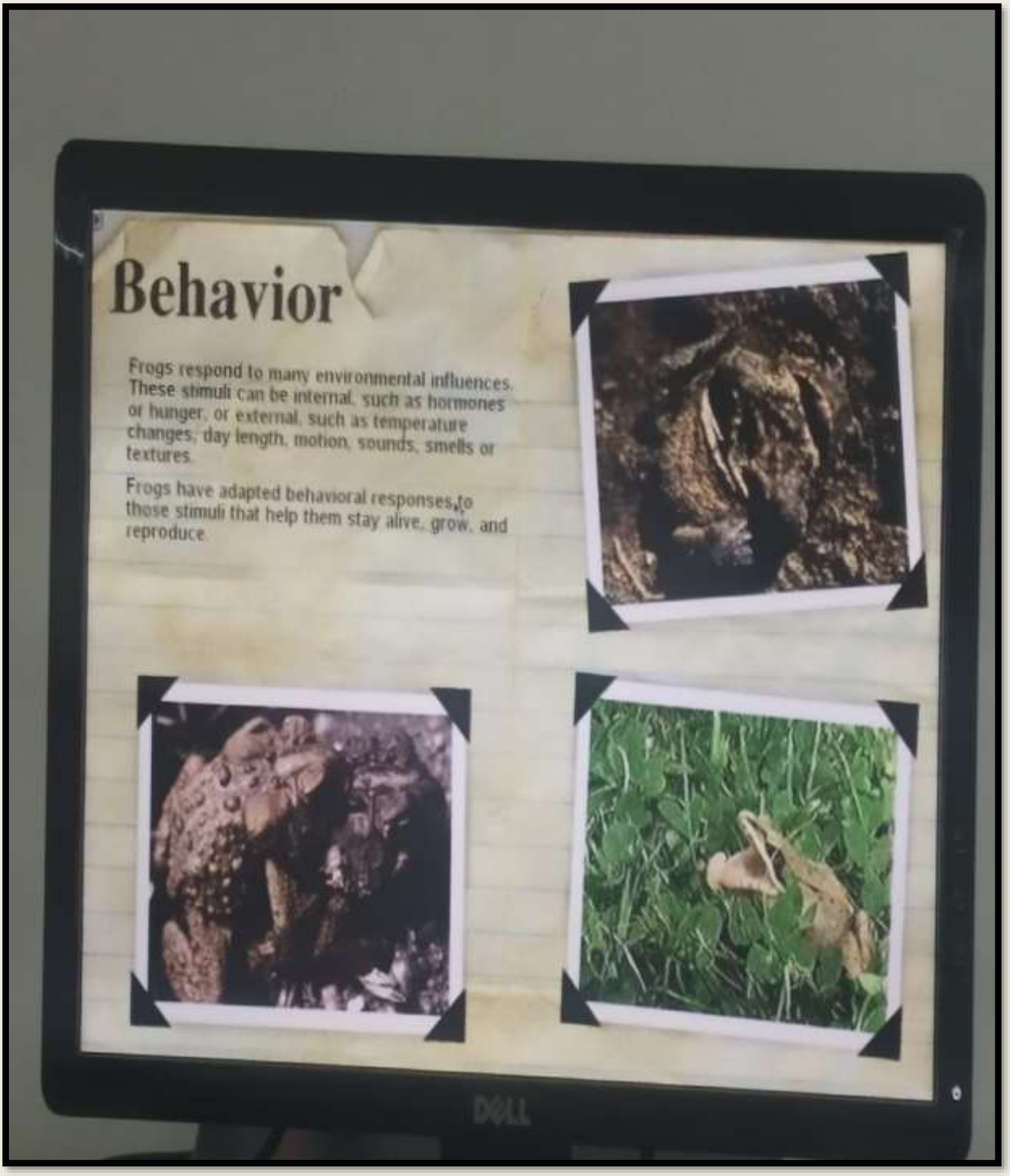
DIGITAL FROG SOFTWARE

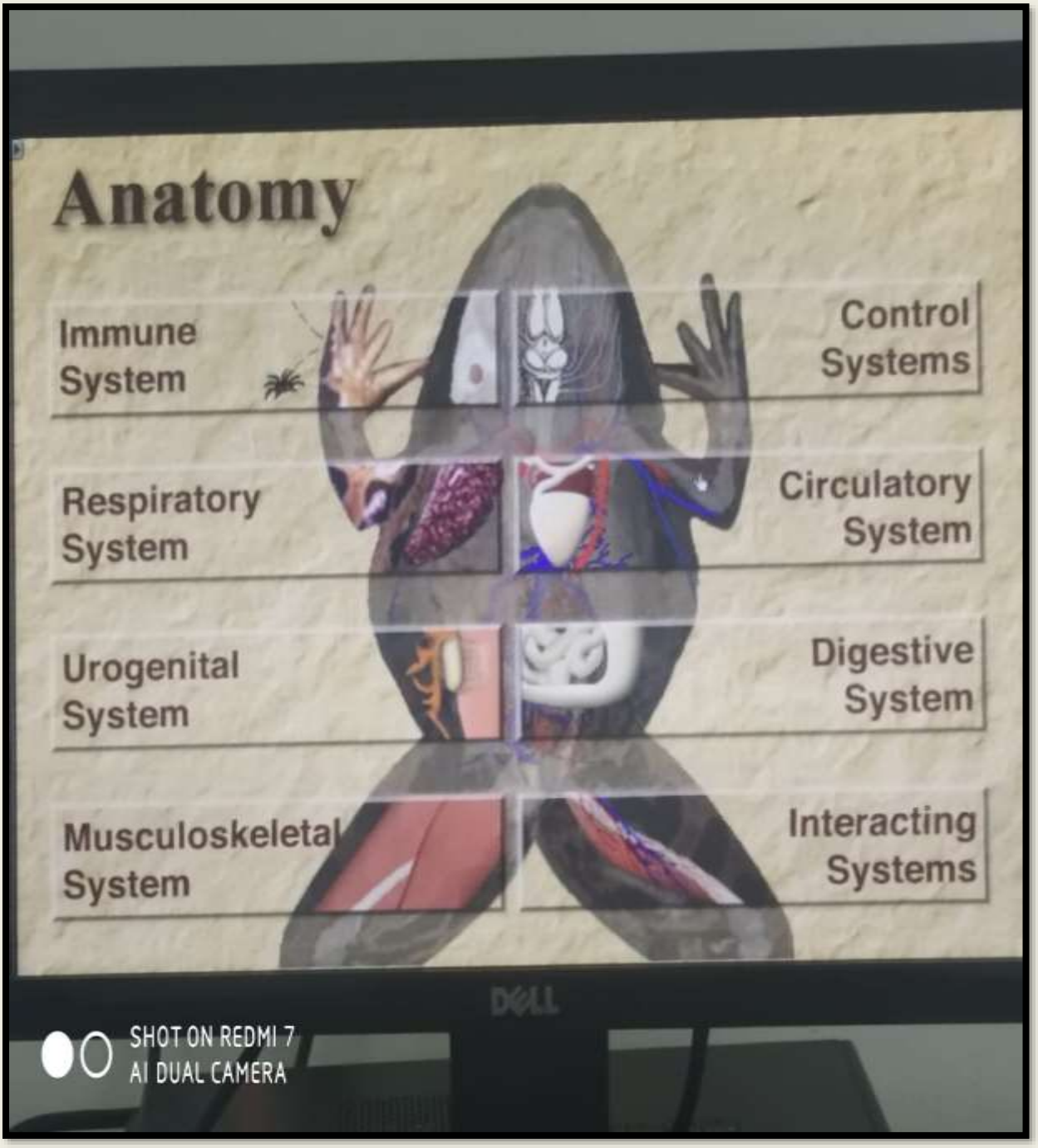

The Digital Frog
Version 2.5
Frog friendly software for biology students
SHOT ON REDMI 7
AI DUAL CAMERA

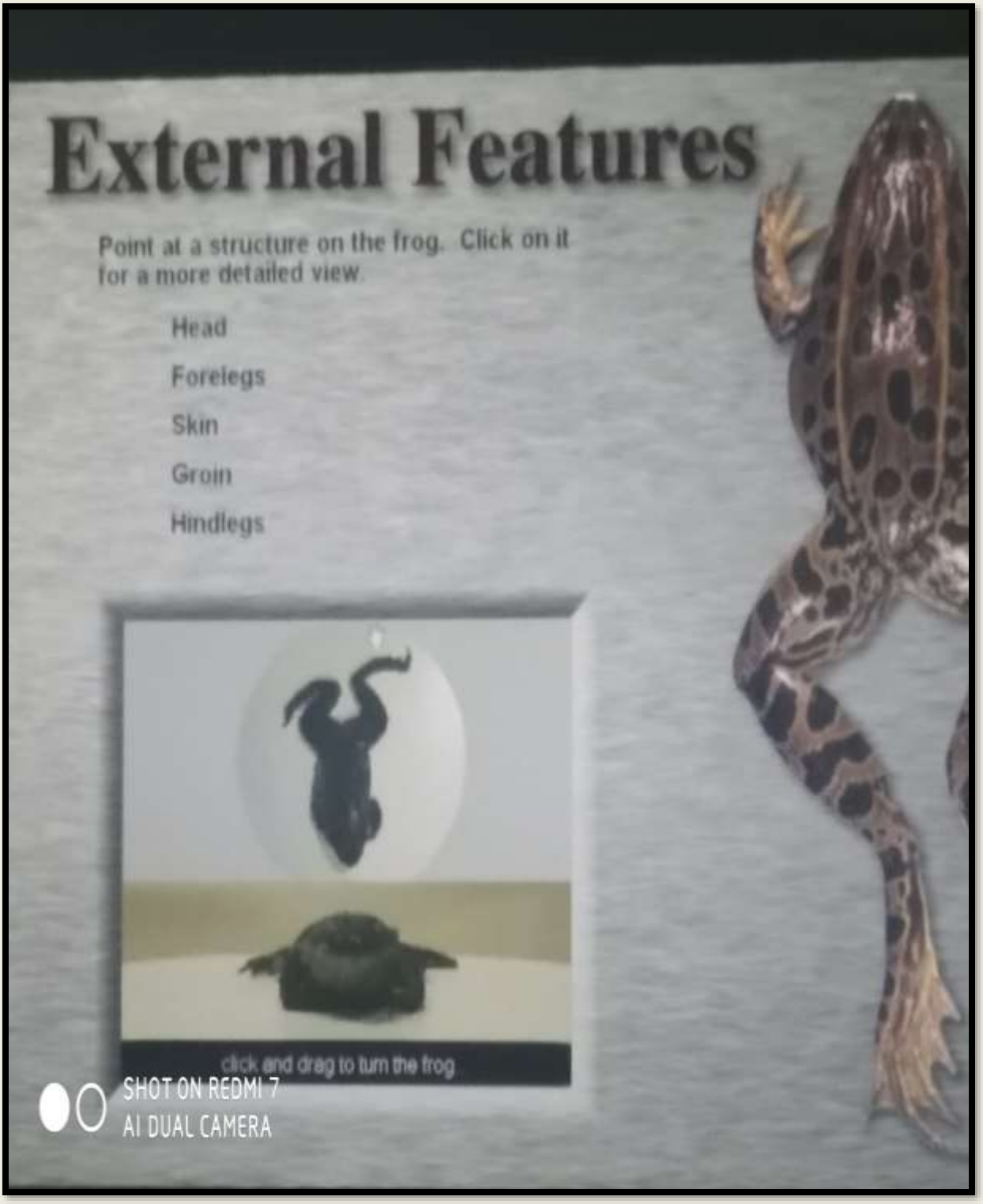

The Digital Frog 2
Dissection
Anatomy
Ecology
QuickTou
Map
SHOT ON REDMI 7
AI DUAL CAMERA
Press H for Help · Press M for Map · Press F for Find ·

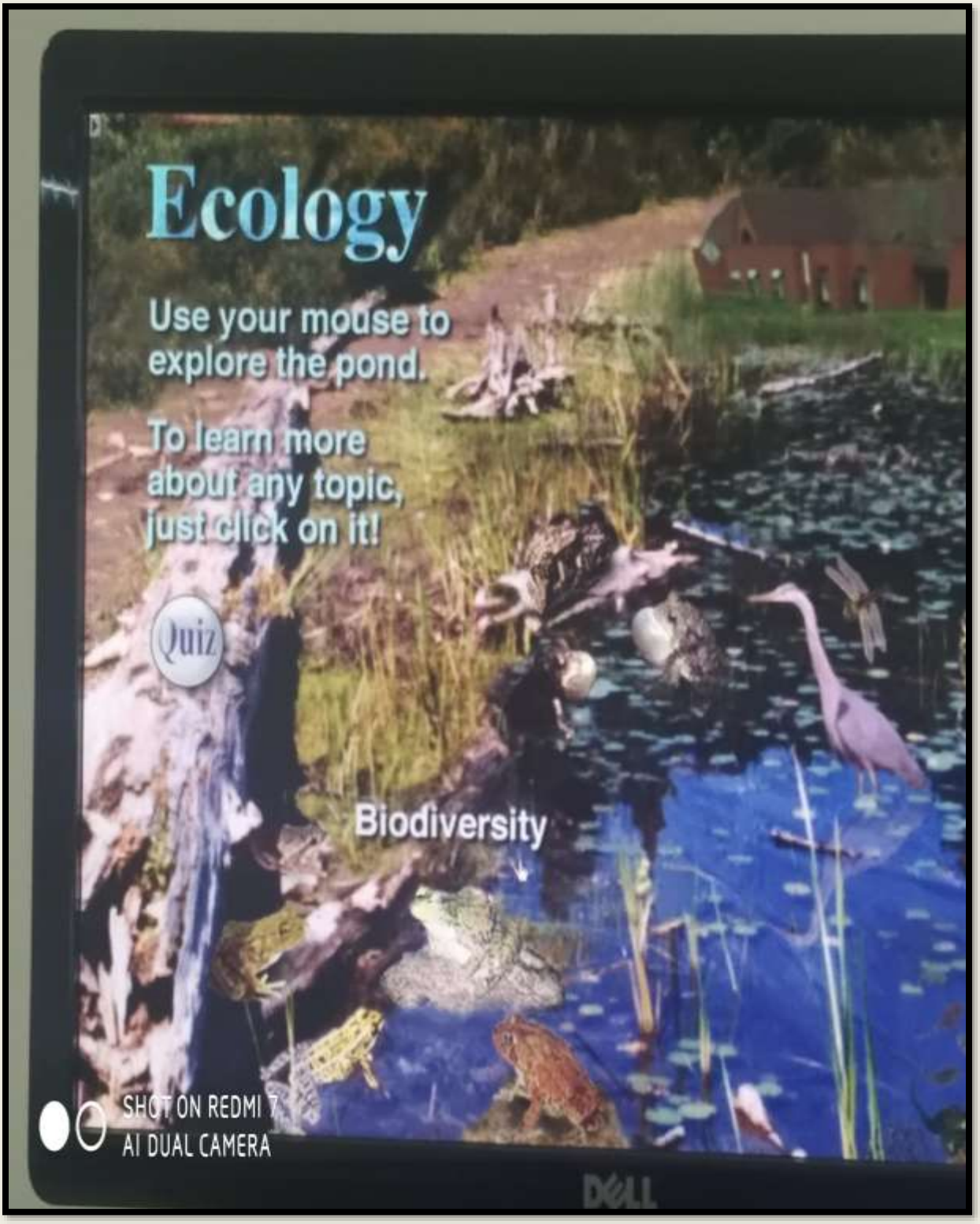

Adopt a Pond
Introduction
Create a Pond
Adopt a Pond
SHOT ON REDMI 7
AI DUAL CAMERA


Adopt a Pond
Introduction
Create a Pond
Adopt a Pond
Create a pond...
Many schools have chosen to create a pond as part of their effort to preserve and protect amphibian wildlife. Some schools have built a pond in their own school yard. Other schools have used nearby land donated by a local landowner.
Frogs and amphibians can migrate up to a kilometer to their breeding ponds. The closer your new pond is to established amphibian populations, the more likely they will colonize and breed there. After one or two frogs breed in the new pond, their offspring will return each year to breed in the habitat that you have created.
Habitat quality...
Pond visitors...
Pond size...
Water, soils and temperature...
Small ponds...
Commercial pond liners...


Behavior
Frogs respond to many environmental influences. These stimuli can be internal, such as hormones or hunger, or external, such as temperature changes, day length, motion, sounds, smells or textures.
Frogs have adapted behavioral responses to those stimuli that help them stay alive, grow, and reproduce.
DELL


Anatomy
Immune System
Control Systems
Respiratory System
Circulatory System
Urogenital System
Digestive System
Musculoskeletal System
Interacting Systems
SHOT ON REDMI 7
AI DUAL CAMERA


External Features
Point at a structure on the frog. Click on it for a more detailed view.
Head
Forelegs
Skin
Groin
Hindlegs
click and drag to turn the frog
SHOT ON REDMI 7
AI DUAL CAMERA


Ecology
Use your mouse to explore the pond.
To learn more about any topic, just click on it!
Quiz
Biodiversity
SHOT ON REDMI 7
AI DUAL CAMERA
DELL


The Digital Frog


External Features