Category : Poster **Class: B. Pharm. .**

TITLE	**Design and Development of Augmented Computational Application Software for Interpretation of Infra-Red Spectrum of Organic Compounds**
NAME OF PI/CO-PI:	PI – Dr. Ujwala N. Mahajan , Dr. Amol Warokar Co-PI – Ms. Kirti Korade
COLLABORATOR (S), IF ANY:	Mr. Aditya Baulia : Kalyani government eng.: Electronic and communication engineering with specialization in Artificial intelligence
DURATION OF PROPOSAL:	3 Months

IDEA

- Infrared (IR) spectroscopy is one of the most common and widely used spectroscopic techniques , but due there's unavailability of computer programs for its accurate interpretation .
- Infrared spectra are "fingerprints" of molecules and eventually it leads imprecise predictions.
- If an expert looks at the infrared spectrum, there's difficulty to interpret it.
- Software are being commercialized on H-NMR but there's no such structural based software .
- Generally spectral interpretation is easily possible for simple compounds, but it is time consuming, expensive and generally limited for more complicated compounds.
- The proposed idea state benefits over theoretical basis as well prediction of vibrational frequency which depends upon force constant and reduced mass .

RATIONALE OF IDEA

❖ Although the traditional method of analyzing infra red spectrum has flaws as follows :

- **Difficulties to interpret.**
- **Manual mistakes.**
- **Overlapping spectrum of functional groups**
- **Budding graduates who had fresh exposure to IR spectrum.**
- **Hunt and peak issues** , it has to be ascertained by modern established scientific tool.

❖ The main advantage is that virtual IR spectral SEARCH is fast and can be used by less qualified personal.

❖ Limited not only for pharmaceuticals but also by Basic sciences.

AIM :- Design and Development of Augmented Computational Application Software for Interpretation of Infra-Red Spectrum of Organic Compounds

OBJECTIVES :-

- ✓ To obtain IR spectrum of organic compounds without actual instrumentation which illustrates the vibrational frequency as well as intensity of absorption of the bands of the functional group associated with organic compounds.
- ✓ To create their own spectral libraries.
- ✓ To obtain desired spectrum with customized structured of organic compounds .
- ✓ To understand the factors influencing vibrational frequency like bond strength, mass of atom, electronegativity, hybridization state of the atom constituted with the bond.

IMPORTANCE IN CURRENT CONTEXT

1. OFFLINE EXCESS : Application can work in different areas having fluctuating internet.
2. CONTENT SIMILARITY AND ACCURACY : Output has variable buttons to access specific data .
3. DATA LIBRARIES: Data being processed will be stored in files and easy accessible whenever need.
4. USER FRIENDLY : IR patterns can be easily access without actual instrumentations .
5. CONCEPT CLARITY: Probable hydrogen bonding and shifting of IR band accordingly.

WORK PLAN

1. CONCEPTS OF HOOKS LAW:

$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}}$$

$\bar{\nu}$ = wave number, in cm^{-1}, corresponding to the vibrational frequency of the bond

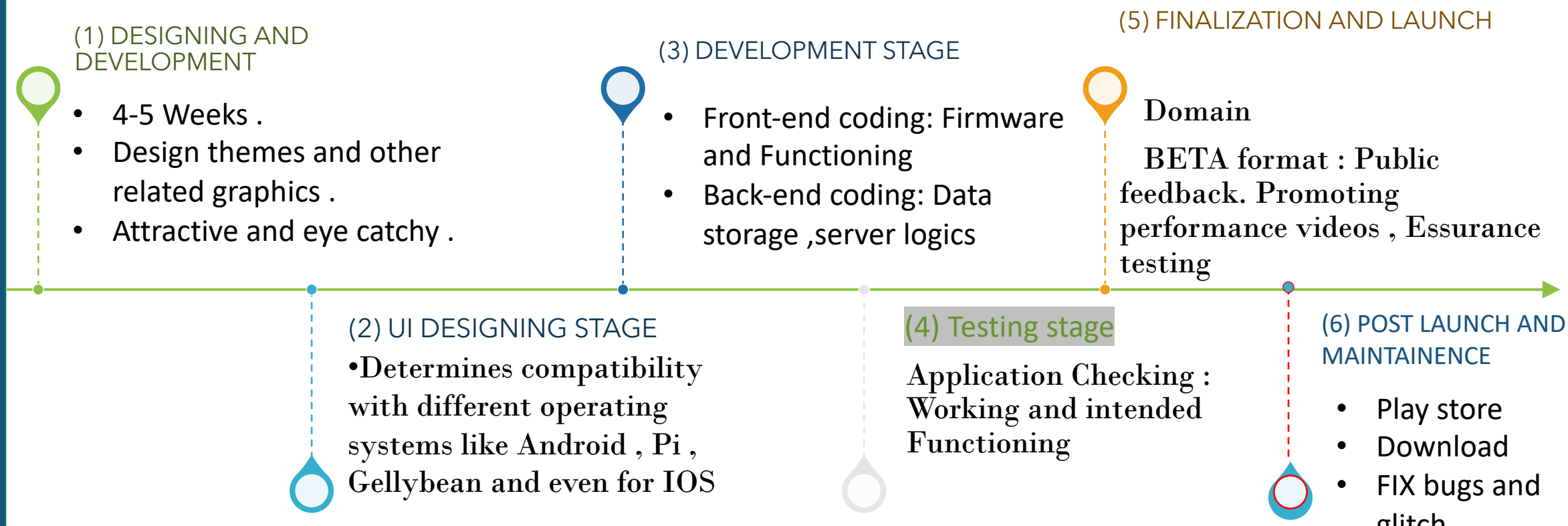
c = speed of light in cms^{-1}

K = force constant in $dynescm^{-1}$ (a measure of bond strength. The stronger the bond, the larger the K.)

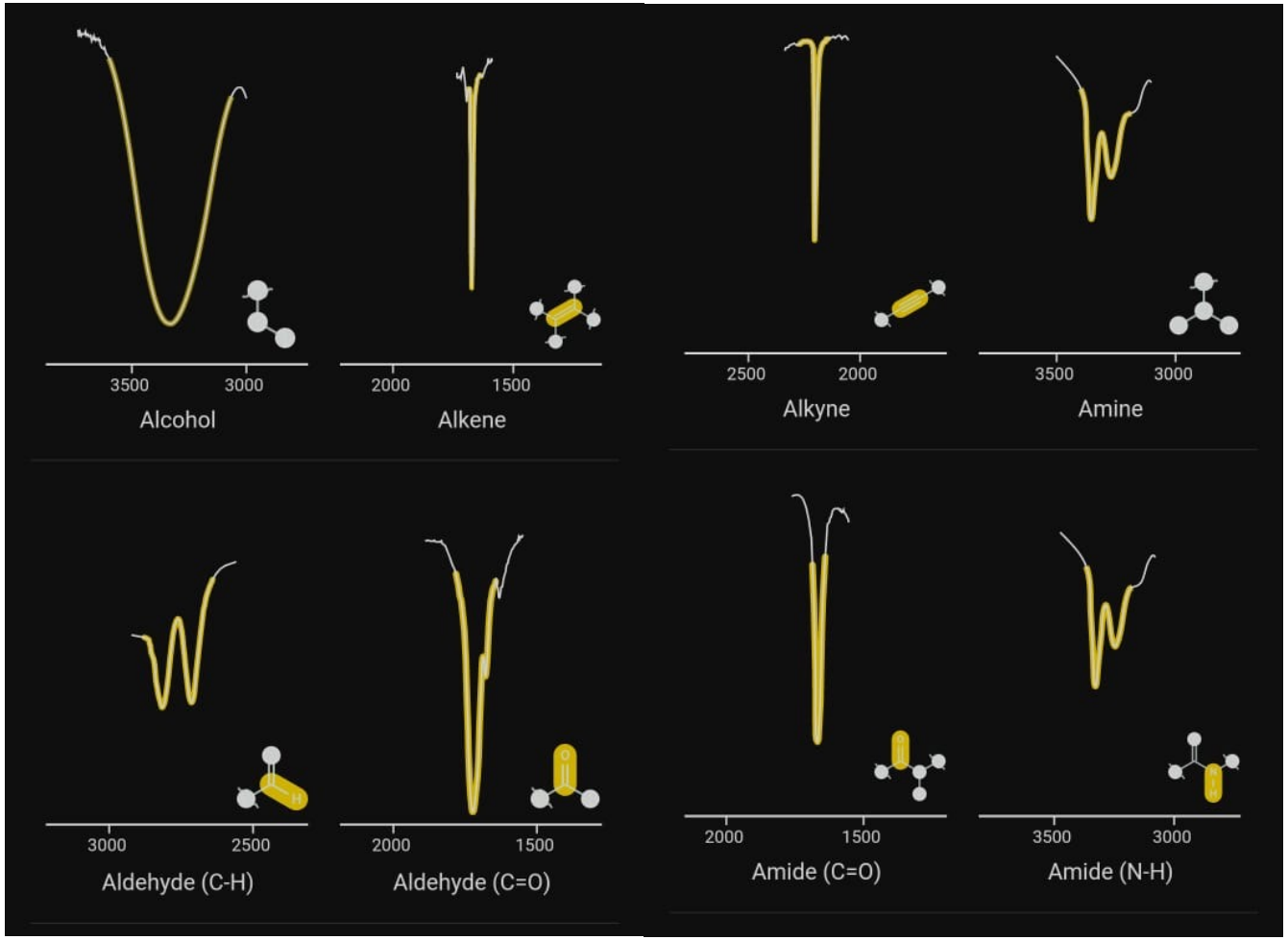
μ = reduced mass in $gatom^{-1}$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

2. CODING:


(1) DESIGNING AND DEVELOPMENT
• 4-5 Weeks .
• Design themes and other related graphics .
• Attractive and eye catchy .
(2) UI DESIGNING STAGE
•Determines compatibility with different operating systems like Android , Pi , Gellybean and even for IOS
(3) DEVELOPMENT STAGE
• Front-end coding: Firmware and Functioning
• Back-end coding: Data storage ,server logics
(4) Testing stage
Application Checking : Working and intended Functioning
(5) FINALIZATION AND LAUNCH
Domain
BETA format : Public feedback. Promoting performance videos , Essurance testing
(6) POST LAUNCH AND MAINTAINENCE
• Play store
• Download
• FIX bugs and glitch
• Updation

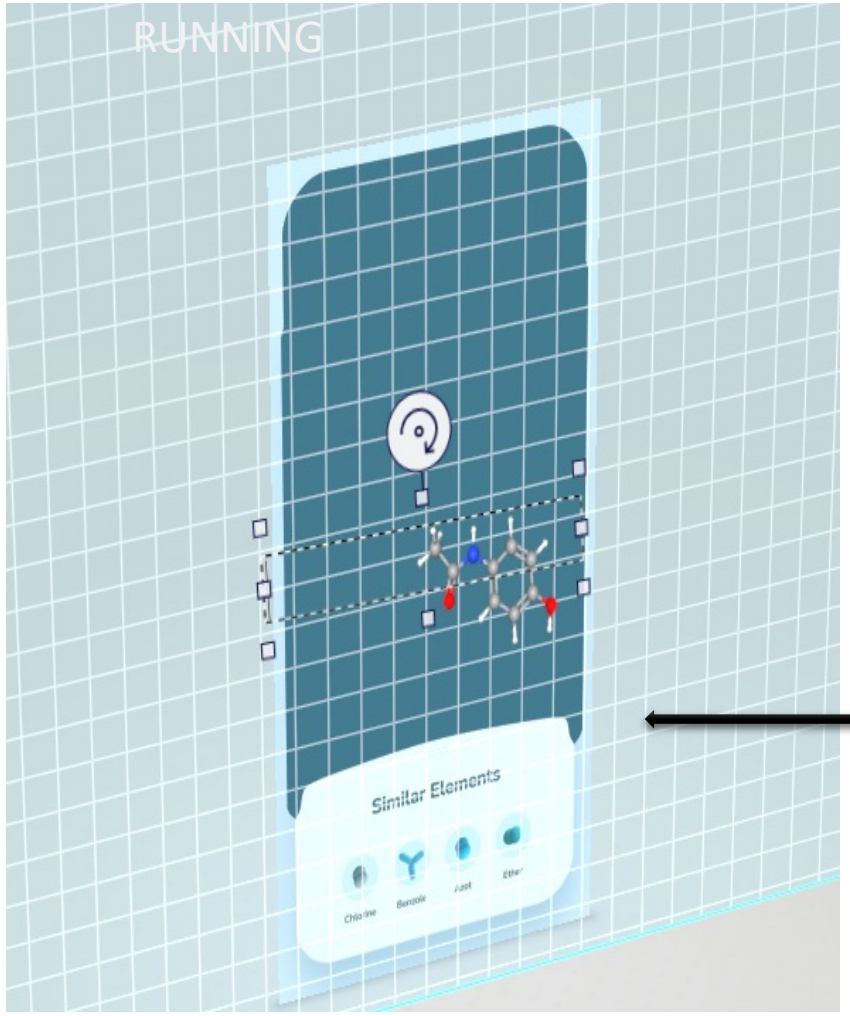
EXPECTED OUTCOME



- Different functional groups of a molecule (like –CH3, COOH, NH2) exhibit peaks at different ranges of wavenumbers.
- The peak position gives you information about sample and depends on the symmetry of the molecule, atom weight and bond strength .
- Peak intensity gives you quantitative information and depends on concentration.
- Peaks from 1400 – 650 nm can be obtained with labelling of frequencies which commercial instrument can't show.

PILOT STUDY RESULTS

CURRENT
RUNNING



A 3D demo of molecular structure obtained after sketching our pre-intended INPUT Accessible 3D Movement

GLIMSE OF CODING

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PILOT STUDY RESULTS

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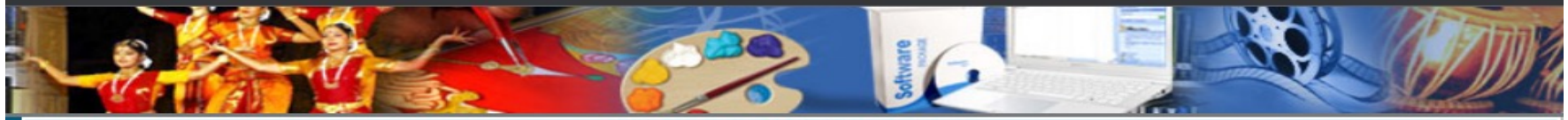

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RECEIPT NO : 68590
FILING DATE : 11/12/2022
BRANCH : Delhi
USER : Kirti29

S.No	Form	Diary No.	Request No	Title	Amount (Rupees)
1	Form-XIV	25758/2022-CO/SW	70698	DESIGN AND DEVELOPMENT OF AUGMENTED COMPUTENTIONAL SOFTWARE BASED ON INFRA-RED SPECTRUM TO INTERPRET ORGANIC COMPOUND	500
Amount in Words			Rupees Five Hundreds		500

PAYMENT MODE	Transaction Id	CIN
Online	C-0000079342	1112220004488

(Administrative Officer)

Thank You .....