

**Course name: Basic programming with Python and its application in database management, artificial intelligence and machine learning (AI/ML).**

**Level of the course:** Certificate

**Course objective:** To teach the students of Pharmacy Python programming language as well as to train them in database management, artificial intelligence/machine learning using Python to improve their career opportunities.

**Proposed course structure:**

| Class         | Content/Topic                                                                                                                                             | Required Time (in hour)/Credit hour | Year                  |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------|-----------------------|
| <b>Unit 1</b> | <b>Introduction to Python</b>                                                                                                                             |                                     | <b>2<sup>nd</sup></b> |
| 1             | History, use and basics of Python                                                                                                                         | 1                                   | 2 <sup>nd</sup>       |
| 2             | Data types: Understanding different data-types, size and use                                                                                              | 1                                   | 2 <sup>nd</sup>       |
| 3             | Operators: Explanation about relational, conditional, logical, modulo-division, Boolean operators with different examples and programming implementations | 1                                   | 2 <sup>nd</sup>       |
| <b>Unit 2</b> | <b>Conditional statement</b>                                                                                                                              |                                     | <b>2<sup>nd</sup></b> |
| 1             | Conditional statement -1: Explaining the syntax of if, if-else and elif                                                                                   | 1                                   |                       |
| 2             | Conditional statement -2: Programming examples and implementation of all the conditional statements.                                                      | 1                                   | 2 <sup>nd</sup>       |
| <b>Unit 3</b> | <b>Loop</b>                                                                                                                                               |                                     |                       |
| 1             | Loop-1: Introduction to <i>while</i> loop with different examples and programming implementation.                                                         | 1                                   | 2 <sup>nd</sup>       |
| 2             | Loop-2: Introduction to <i>for</i> loop with different examples and programming implementation.                                                           | 1                                   | 2 <sup>nd</sup>       |
| 3             | Loop-3: Use of range functions in <i>for</i> and <i>while</i> loop with different examples and programming implementation.                                | 1                                   | 2 <sup>nd</sup>       |
| <b>Unit 4</b> | <b>Lists, Tuple and Dictionary</b>                                                                                                                        |                                     |                       |
| 1             | Lists-1: Lists constructs, syntax and use                                                                                                                 | 1                                   | 2 <sup>nd</sup>       |
| 2             | Lists-2: Use of lists in <i>for</i> and <i>while</i> loop with different examples and programming implementation                                          | 1                                   | 2 <sup>nd</sup>       |

|               |                                                                                                                                                                                                                       |   |                 |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---|-----------------|
| 3             | Tuple: Tuple constructs, syntax and use with programming examples                                                                                                                                                     | 1 | 2 <sup>nd</sup> |
| 4             | Dictionary: Dictionary constructs, syntax and use with programming examples                                                                                                                                           | 1 | 2 <sup>nd</sup> |
| <b>Unit 5</b> | <b>Functions and Class</b>                                                                                                                                                                                            |   |                 |
| 1             | Functions-1: Introductions to functions, use and classifications of functions                                                                                                                                         | 2 | 2 <sup>nd</sup> |
| 2             | Functions-2: Programming examples and implementations of built-in functions and user-defined functions                                                                                                                | 2 | 2 <sup>nd</sup> |
| 3             | Class concepts: Introduction to object-oriented programming (OOP) with Class with programming implementations                                                                                                         | 2 | 2 <sup>nd</sup> |
|               | Exam-1                                                                                                                                                                                                                | 2 | 2 <sup>nd</sup> |
| <b>Unit 6</b> | <b>Important python packages</b>                                                                                                                                                                                      |   |                 |
| 1             | NumPy: Introduction to numPy, numPy array, uses of NumPy in mathematical calculations.                                                                                                                                | 1 | 2 <sup>nd</sup> |
| 2             | SciPy: Introduction to SciPy and uses of SciPy in mathematical calculations.                                                                                                                                          | 1 | 2 <sup>nd</sup> |
| 3             | Database management with Pandas: Introduction to Pandas and its uses in database handling. Introduction to different data formats (e.g., .csv, .xlsx).                                                                | 1 | 2 <sup>nd</sup> |
| 4             | Database management with Pandas: How to import/export the different data types with Pandas and how to edit the data and obtain statistical results                                                                    | 1 | 2 <sup>nd</sup> |
| <b>Unit 7</b> | <b>Artificial Intelligence and Machine Learning</b>                                                                                                                                                                   |   |                 |
| 1             | AI/ML: Introduction to AI and ML +concepts about supervised and unsupervised learning.                                                                                                                                | 1 | 2 <sup>nd</sup> |
| 2             | ANN: Basic concept of artificial neural network, introduction to Perceptron.                                                                                                                                          | 1 | 2 <sup>nd</sup> |
| 3             | Perceptron: How to write a basic program for Perceptron with Python                                                                                                                                                   | 2 | 2 <sup>nd</sup> |
| 4             | MLP and DNN: Concepts of Multilayer Perception and Deep Neural Network                                                                                                                                                | 2 | 2 <sup>nd</sup> |
| <b>Unit 8</b> | <b>Applications of AI/ML in Pharmacy</b>                                                                                                                                                                              |   |                 |
| 1             | Databases in Pharmacy and Bioinformatics: Collection and curation of chemical/pharmaceutical datasets for a specific biological target from ChEMBL and Binding Database (using Pandas and NumPy) and other databases. | 2 | 2 <sup>nd</sup> |

|   |                                                                                                                                                                              |           |                 |
|---|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|-----------------|
| 2 | Cheminformatics: Basic concepts of cheminformatics and how to calculate molecular descriptors and fingerprints using various non-commercial packages.                        | 2         | 2 <sup>nd</sup> |
| 3 | Rdkit and molecular descriptors: Introduction to Python based Rdkit program to import data, convert data formats and calculations of molecular descriptors and fingerprints. | 2         | 2 <sup>nd</sup> |
| 4 | How to use Scikit-learn for developing ANN models for the pharmaceutical datasets.                                                                                           | 2         | 2 <sup>nd</sup> |
| 5 | How to use Tensorflow for developing ANN models for the pharmaceutical datasets.                                                                                             | 2         | 2 <sup>nd</sup> |
| 6 | Transformer-CNN: Development of Transformer-CNN models using SMILES notations of chemical compounds.                                                                         | 2         | 2 <sup>nd</sup> |
|   | Exam-2                                                                                                                                                                       | 2         | 2 <sup>nd</sup> |
|   | <b>Total</b>                                                                                                                                                                 | <b>40</b> |                 |

**Requirement:**

Human resource: Will be conducted by selected faculties of Dr. B. C. Roy College of Pharmacy and A. H. S. (BCRCP)

Course coordinators: (a) Mr. Soumen Banerjee, Assistant Professor, BCRCP

(b) Dr. Amit Kumar Halder, Associate Professor, BCRCP

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