3.8.2020

MARCH

Friday 28

WK 13 • 087-278

APRIL 2014

M	T	W	T	F	S	S
7	1	2	3	4	5	6
14	8	9	10	11	12	13
21	15	16	17	18	19	20
28	22	23	24	25	26	27
	29	30				

SCI643 BIOMOLECULAR STRUCTURE INTERACTIONS AND DYNAMICS

TAUGHT BY

- prof. B gopalakrishnan

COURSE TOPICS

1-2 Structure & properties of biomolecules

- steric & electronic effects
- electrophiles
- nucleophiles
- acids, bases, and salts
- buffers

3 interactions between biomolecules

- hydrogen bonding & solvation
- examples of structure property correlation

2014

MARCH

29 Saturday

088-277 • WK 13

4-7 properties of ensembles of biomolecules

9

- elementary concepts of chemical thermodynamics

10

- equilibrium & kinetics

11

- ionic equilibrium & chemistry in aqueous solution

12

- application to stability of proteins, nucleic acids, and their interactions

1

2

8-9 reactions & reaction mechanisms

3

- classification of reactions and their mechanisms
- application to classification of biochemical reactions and their enzymes

30 10-12 important biochemical reactions

Sunday

- examples from enzyme classes
- active site
- target specificity
- inhibition & activation

3.8.2020

3 MARCH

Monday 31

WK 14 • 090-275

APRIL 2014

M	T	W	T	F	S	S
7	1	2	3	4	5	6
14	8	9	10	11	12	13
21	15	16	17	18	19	20
28	22	23	24	25	26	27
	29	30				

- reactions involved in storage and retrieval of energy
- enzyme kinetics

13-18 exploration and analysis of biomolecular structures and interactions

- experimental methods and techniques for analyzing structures and interactions
- NMR, ESR, X-ray, CD, fluorescence, etc.
- detailed structural analysis of some representative proteins
- analysis of DNA and RNA structures

19-24 molecular modeling & docking, concepts and techniques

- useful concepts in molecular modeling
- tasks and techniques in molecular modeling
- identification of tasks, e.g. alignment, minimization, conformational search, dynamics and simulation, etc.

2014

3.8.2020

- methods of analyzing structures
- methods of prediction & validation of structures

25-28 databases & tools

- classification of databases
- databases of structures and functions
- CATH
- SCOP
- PFAM
- functional domain
- analysis servers

LABORATORY

1. visualization & rendering
2. building molecules
   - physical (ball & stick, paper models)
   - in silico

3. rendering of various aspects of structures of biomolecules
   - web-based tools

4. query tools
   - sequence retrieval
   - structure retrieval

5. protein structure analysis tools
   - structure alignment
   - homology search
   - domain assignment
   - fold recognition and analysis

6. structure prediction tools
   - secondary structure prediction
   - protein structure
   - RNA structure

APRIL

3 Thursday

093-272 • WK 14

3.8.2020

7. molecular modeling tools

- threading
- comparative modeling (Swiss Mod)

8. computational tools

- geometry optimization & energy minimization
- molecular dynamics simulation

TEXT BOOKS

- bio-chemistry ; lehninger
- bio-chemistry ; stryer
- bio-chemistry ; voet, voet, and pratt.

2014