COMPUTER AIDED DRUG DESIGN

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INTENDED AUDIENCE : Biotech/Pharmaceuticals/Bioinformatics /Chemistry and allied programmes and research scientists in biotechnology and pharma industries and clinicians/medical practioners

PRE-REQUISITES : Prior knowledge of biochemistry, bioinformaticsl

INDUSTRIES APPLICABLE TO : Pharmaceutical industries/Biopharma/biotech

COURSE OUTLINE :

Drug discovery and development is a time consuming and expensive process., taking about 10 years and costing about US 1.0 B dollars. Several candidates that enter clinical trials fail because of several reasons. Computer assisted drug design can speed up the process, reduce surprises and predict the properties, thereby reduce the cost of R&D. The course will cover structure and target based design, molecular modeling, quantum mechanics, drug likeness properties, QSAR and pharmacokinetic and dynamics using several softwares that are freely available.

ABOUT INSTRUCTOR :

Mukesh Doble: Professor at the department of Biotechnology at IIT Madras. Has previously worked in Imperial chemical Industries(ICI) and General Electric(GE) for 20 years . Areas of research are Biomaterials, Biopolymers and Drug design. Published 270 papers and 10 books and filed 10 patents (including two US). Has delivered on line video courses in Downstream processes and Biostatistics.

COURSE PLAN :

Week 01 : Introduction to drug discovery
Week 02 : Structure and property
Week 03 : ADME-rules
Week 04 : Force field/MM/QM
Week 05 : Boundary conditions/Conformation
Week 06 : QSAR/Pharmacophore
Week 07 : Enzymes/proteins structures/docking
Week 08 : PK/PD