Online Course Chapters

No. of Chapter	Name of the Chapter
1	Brief Introduction of QSAR and its workflow
2	Structure drawing with ACD Lab Chemsketch/ ChemOffice, download, installation, creating new molecules and playing with various parameters to edit the molecule, switch between 2D and 3D parameters
3	In silico drug likeliness testing, application of Lipinsky Rule of Five, Using Molinspiration server, in silico toxicity testing, using admetSAR, to screen drug molecules
4	Concept of Docking
5	Working with PDB, protein structure search, downloading protein structure in PDB format
6	Working protein structure in UCSF chimera, add hydrogens, delete native water molecules, preparation of final protein structure in .pdb format
7	Predicting biological activity of selected compounds by molecular docking with SWISSDOCK or PARDOCK, counting the docking scores, analysing protein-ligand binding interactions with UCSF Chimera
8	Building up 2D QSAR model equation with biological acitivity (predicted) and molecular descriptors, using REGRESSION ANALYSIS and ARRAY FORMULA
9	Validating QSAR model, comparison between OBA and PBA by ANOVA (Student t-test)
10	Basic Bioinformatics Working with gene and protein sequences from NCBI, downloading gene and protein sequences