

SEMESTER: EVEN, 2020-21

PAPER CODE: PT-810B (ELECTIVE, COMPUTER AIDED DRUG DESIGN)

Date	Unit/ Item	Video link	Power point Link	Study Material	Supplementary material, if any
13.04.2021	1 (introduction to Drug discovery and development)	https://youtu.be/vHLW9YMKmRg	https://drive.google.com/file/d/1cx9oKxEbgnfNAcGteCuLUA3LZ_hHlgZI/view?usp=sharing	https://drive.google.com/drive/folders/1jN5YdR5C41Mj4q82Lo_B3PQ8D5p25KZb?usp=sharing	Book 1) Hugo and kubiyanis Book https://drive.google.com/file/d/1uikpgnENd2-SFhRZTeCg0CIKhQdhZYF/view?usp=sharing Book 2) Fundamentals of Medicinal Chemistry https://drive.google.com/file/d/1dFVs8n4TEM_g_T7suPya4nybXjAgCheZ/view?usp=sharing
16.04.2021	1 (do)	https://youtu.be/zPR4UwHZXEI	https://drive.google.com/file/d/1cx9oKxEbgnfNAcGteCuLUA3LZ_hHlgZI/view?usp=sharing	do	do
22.04.2021	1 (do)	https://www.youtube.com/watch?v=e0d	https://drive.google.com/file/d/1cx9oKxEb	do	do

		bhZQem2U	gnfNAcGteCu LUA3LZ_hHI gZI/view?usp =sharing		
27.04.2021	1 (do)	https://youtu.be/iZ7U7DISpVs	https://drive.google.com/file/d/1cx9oKxEbgnfNAcGteCuLUA3LZ_hHIgZI/view?usp=sharing	https://drive.google.com/drive/folders/1jN5YdR5C41Mj4q82Lo_B3PQ8D5p25KZb?usp=sharing	do
30.04.2021	1 (do)	https://youtu.be/rdm8ZoK74L4	https://drive.google.com/file/d/1wMZcJIV9bE7LdkkyVuFx7bxtSZBmaJzw/view?usp=sharing	https://drive.google.com/file/d/1X48oV82-JZkRyRDRu9coGF_9jvSpNmEU/view?usp=sharing	do
04.05.2021	2 (QSAR) (Introduction to QSAR, descriptors, Log P, Hammett Analysis)	http://www.youtube.com/watch?v=4VQgImV51y0	do	https://drive.google.com/file/d/1zEIY2zTcG59C2MRBU_sYf2t_SxZ_LLyUb/view?usp=sharing	Do
05.05.2021	2 (QSAR) (Hammett Analysis, Hansch Analysis)	http://www.youtube.com/watch?v=GbvYWO_Oh5Q	https://drive.google.com/file/d/1IM7jDVd7En0DnzMM_rKhvHgxmFFPIYs/view?usp=sharing	https://drive.google.com/file/d/1zEIY2zTcG59C2MRBU_sYf2t_SxZ_LLyUb/view?usp=sharing ALSO READ THE KUBIYANI BOOK THAT I HAVE SHARED WITH YOU. THE SECOND BOOK IS ALSO GOOD TO GROW	Now as a third book I am posting Medicinal Chemistry by Asutosh Kar . The first few chapters are on drug design and QSAR. You will get entire syllabus from here including QSAR and descriptors. Follow the link

				CONCEPTS	https://drive.google.com/file/d/11h1En67Nql3e4mx1407ZchrsjCu2rHNR/view?usp=sharing
07.05.2021	2 (QSAR, Steric parameters, Taft Steric parameter, Molar refractivity,)	http://www.youtube.com/watch?v=AALa8URf0PI	https://drive.google.com/file/d/1Ccf2Yskg7svj7_e9TvdiqRAMCGqzQMVM/view?usp=sharing	Follow the books carefully that I posted. Everything is written inside the books. Also see the slides the I have posted. This is for your study material only	do
11.05.2021	2(QSAR), Branching index, ETSA, MLR	http://www.youtube.com/watch?v=55Yms0MU33Q	See the previous slides I have given and see the QSAR model building with Linear regression		
13-05-2021	3 (QSAR), MLR, Free Wilson Analysis (starting), Biological activity	http://www.youtube.com/watch?v=uQ9u1DTZQPs	do		
18-05.2021	(QSAR) Free Wilson Analysis	http://www.youtube.com/watch?v=ZTJXAzliYXQ	https://drive.google.com/file/d/1r8Du93MTlaEZK7ipKrjG1y6dcxOPs5cM/view?usp=sharing	https://drive.google.com/drive/folders/1y_idm7M7uCXbgFfcNLwgt3CHippsDkW6?usp=sharing	Same books Especially read this paper to have a very good concept how practically the things are

					done: https://drive.google.com/file/d/100AfIWHEdA2kFsbNXJL0J46RzYGMCGs8/view?usp=sharing
25.05.2021	QSAR (Fujita Ban Analysis)	http://www.youtube.com/watch?v=elb0m5s6Vz8			Read the books
28-05-2021	3D QSAR (COMFA)	http://www.youtube.com/watch?v=7rNvkvtSZyM		https://drive.google.com/drive/folders/1huq3cGp4jJgJOArtdT-K9CAYJOO4En?usp=sharing	https://www.youtube.com/watch?v=pVYWEEXks0j8 See this supplementary information
01-06-2021	COMFA (continued)	http://www.youtube.com/watch?v=zZQKZfJ1C58		See the previous notes	
03.06.2021	3D-QSAR (COMSIA), Introduction to virtual screening	https://youtu.be/Of6_rBzSvl https://youtu.be/Of6_rBzSvl	https://drive.google.com/file/d/1KetNSKaBclyzcolGDU NH2LqBnsDJoIDU/view?usp=sharing	Please find two things for COMSIA from the following link: 1) one book chapter written by Klebe on COMSIA 2) The original Klebe COMSIA paper at 1994 in Journal of	https://www.youtube.com/watch?v=9wOUAzTXeZo

				<p>Medicinal Chemistry The link is 1) https://drive.google.com/file/d/18nHjuGieBlaNFQG1JHMwSiCFfZ_rb_uot/view?usp=sharing</p> <p>2) https://drive.google.com/file/d/1ErX0USP6tRG44HmPHXIOezuP6CyfR7jw/view?usp=sharing</p>	
08.06.2021	Virtual screening (introduction to docking)	http://www.youtube.com/watch?v=rf8QJ4S_ON4			
09.06.2021	Virtual Screening (docking continued)	http://www.youtube.com/watch?v=Eytgun3ic4s		http://www.youtube.com/watch?v=Eytgun3ic4s	<p>Dear Students, for Virtual screening learning, please visit my two videos from my youtube channel And make notes apart from what I am providing to you</p> <p>https://www.youtube.com/watch?v=yrSKWc2xKKQ</p> <p>https://www.y</p>

					outube.com/watch?v=NaJakEloe6c&t=130s
15.06.2021	Virtual Screening (Docking)	http://www.youtube.com/watch?v=SzfQ6hVt3AQ		Please go through the previous notes on virtual screening and docking. Together, please see this lecture material, https://drive.google.com/file/d/1E-L-i_Drpl9wJOYCJm115iHIVOjjJcu/view?usp=sharing	
17.06.2021	Virtual Screening (Pharmacophore based)	http://www.youtube.com/watch?v=96ibkwNjEKw		https://drive.google.com/file/d/1otnNQWjvhzGpRF7jkCLCWcO2AQ8q1dd/view?usp=sharing https://drive.google.com/file/d/1A8NkFLece07kVQpfjcP7lqd4zi_7r7-4/view?usp=sharing	
18.06.2021	Virtual Screening, Cheminformatics, ADME databases	http://www.youtube.com/watch?v=t8kuc_dyplA			

13.07.2021	Bioinformatics and Molecular modelling			https://drive.google.com/drive/folders/1OsQjSpqpTcrSsBv_z5etlZDPlwqcdVzI?usp=sharing	
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