



7 – Pharmacophore Modeling, Virtual Screening, and Customized Development

1 WEEK 1 – Pharmacophore Fundamentals & Identification

Day	Core Course Activity (FULL TITLES)	Lecture Duration (per lecture)	Core Duration (Real Sum)	Book Reading	Reading Duration	Quiz	Assignment	<input checked="" type="checkbox"/>	Notes
Saturday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	ثابت
Sunday	Pharmacophore – The Core of Drug Activity Part 1	58:09		Daily Book Reading	30 min	—	—	<input type="checkbox"/>	
	Pharmacophore – The Core of Drug Activity Part 2	01:10:04	≈ 2:08 hr					<input type="checkbox"/>	Unit 1 مكتمل
Monday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—
Tuesday	Pharmacophore Mapping	42:51		Daily Book Reading	30 min	—	—	<input type="checkbox"/>	
	Pharmacophore Identification	53:23	≈ 1:36 hr					<input type="checkbox"/>	Unit 2 مكتمل
Wednesday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—
Thursday	Live Session: Pharmacophore Concepts, Mapping & Identification + Q&A	2 hrs	2 hrs	Daily Book Reading	30 min	Week 1 Quiz	—	<input type="checkbox"/>	Live
Friday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—



1 WEEK 2 – MOE Foundations & Ligand-Based Pharmacophore Modeling

Day	Core Course Activity (FULL TITLES)	Lecture Duration (per lecture)	Core Duration (Real Sum)	Book Reading	Reading Duration	Quiz	Assignment	<input checked="" type="checkbox"/>	Notes
Saturday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	ثابت
Sunday	Theoretical of Practical: Pharmacophore Modelling in MOE	46:25		Daily Book Reading	30 min	—	—	<input type="checkbox"/>	
	Practical 0: MOE Installation, Setup & Interface	29:19						<input type="checkbox"/>	
	Case Study: Celecoxib as a Selective COX-2 Inhibitor	13:58	≈ 1:30 hr					<input type="checkbox"/>	Unit 3 (part)
Monday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—
Tuesday	Practical 1: Multi-Ligand Pharmacophore Modelling – Training Set Alignment	01:18:28		Daily Book Reading	30 min	—	—	<input type="checkbox"/>	
	Practical 2: Manual Pharmacophore Feature Definition	25:50	≈ 1:44 hr					<input type="checkbox"/>	Unit 4 مكتمل
Wednesday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—
Thursday	Live Session: MOE Pharmacophore Workflow & Ligand-Based Modeling + Q&A	2 hrs	2 hrs	Daily Book Reading	30 min	Week 2 Quiz	—	<input type="checkbox"/>	Live
Friday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—



WEEK 3 – Structure-Based Pharmacophore, Validation & Virtual Screening

WEEK 3 – UNIFIED OPERATIONAL TABLE (REAL CALCULATION)

Day	Core Course Activity (FULL TITLES)	Lecture Duration (per lecture)	Core Duration (Real Sum)	Book Reading	Reading Duration	Quiz	Assignment	<input checked="" type="checkbox"/>	Notes
Saturday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	ثابت
Sunday	Practical 3: Structure-Based Pharmacophore Generation	41:28		Daily Book Reading	30 min	—	—	<input type="checkbox"/>	SB-Pharmacophore
	Practical 4: Pharmacophore Validation – Actives from PubChem & Decoys from DUD-E	34:12						<input type="checkbox"/>	Validation
	Practical 5: The Power of Google Colab – Cloud Drug Discovery	19:28	≈ 1:35 hr					<input type="checkbox"/>	Unit 5 (part)
Monday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—
Tuesday	Practical 6: Pharmacophore Validation – Active & Decoy Dataset Integration and Virtual Screening	~45:00		Daily Book Reading	30 min	—	—	<input type="checkbox"/>	Virtual Screening
	Virtual Screening Analysis & Hit Selection (Guided)	~30:00						<input type="checkbox"/>	Post-screening
	Pharmacophore Optimization & Iteration Strategy (Guided)	~30:00	≈ 1:45 hr					<input type="checkbox"/>	Unit 6 مكتمل
Wednesday	—	—	—	Daily Book Reading	30 min	—	—	<input type="checkbox"/>	—
Thursday	Live Session: Structure-Based Pharmacophore → Validation → Virtual Screening Workflow + Q&A	2 hrs	2 hrs	Daily Book Reading	30 min	Week 3 Quiz	Pharmacophore Final Project	<input type="checkbox"/>	Live
Friday	—	—	—	Daily Book Reading	30 min	—	Project Deadline	<input type="checkbox"/>	Submission