

Off Target Prediction & Polypharmacology — Hands-on

Learn how to profile off target risks and polypharmacology in discovery pipelines. You will work with chemogenomic style data, similarity and simple network views to understand how compounds may engage multiple targets, summarize potential liabilities and communicate risk aware design suggestions to project teams.

Off Target Prediction & Polypharmacology

Help Desk · WhatsApp

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Networks | Session 3 — Polypharmacology Profiles & Workflows | Session 4 — Mini Capstone: Off

Target & Polypharmacology Brief

Session 1

Fee: Rs 8800 Apply Now

Off Target Concepts & Liability Landscape

On target vs off target actions in discovery

efficacy vs safety perspectives safety pharmacology focus (conceptual) role in series triage

Key classes of off targets and liability themes

enzymes (conceptual) simple risk categories

Chemogenomic style data and panels (overview)

notions panel based thinking

Session 2

Fee: Rs 11800 Apply Now

Target Panels, Similarity & Networks

Target panel style data organisation

activity tables and matrices thresholds and flags (conceptual) heatmap style views

Similarity and substructure search for off targets

scaffold ideas simple analogue reasoning

Network style views of compound-target space

bipartite network concepts hub targets and hubs compounds visual inspection of risk clusters

Session 3

Fee: Rs 14800 Apply Now

Polypharmacology Profiles & Workflows

Desired vs adverse polypharmacology (conceptual)

multi target efficacy ideas side effect and liability themes series level patterns

Building simple polypharmacology profiles

count and intensity style metrics target class based summaries traffic light style scoring

Workflows for off target and polypharmacology triage

panel and similarity inputs summary tables and plots prioritisation of compounds and series

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Off Target & Polypharmacology Brief

Assemble an off target and polypharmacology panel for a small series

Theory + Practical

Summarise risks and opportunities at series level

heatmaps and panel tables traffic light risk views short prioritisation notes

Deliverables: off target panel, polypharmacology snapshot & narrative

spreadsheet and plots one page briefing slide PDF or HTML summary