

Capstone End-to-End Cheminformatics Project — Hands-on

Bring together the ideas from the cheminformatics, ADMET and safety modules into one integrated project. You will scope a realistic case, organise a curated dataset, apply QSAR and virtual screening concepts at a high level, summarise ADMET and safety flags, and produce a concise, traceable project pack suitable for internal review and learning. No synthesis, purchasing or regulatory advice is covered.

Capstone End-to-End Cheminformatics Project

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Session 1

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Project Scoping & Dataset Assembly

Selecting a realistic cheminformatics case theme

simple discovery or safety context **clear question and scope statement** **boundary of what will be done in silico**

Assembling and curating a starting dataset (conceptual)

structures and key properties table **basic standardisation and QC ideas** **metadata and simple**

lineage notes

Planning the overall project flow and milestones

from data curation to summary pack **inputs,**
intermediate outputs and checks **responsible and**
transparent analysis plan

Session 2

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Descriptors, QSAR Ideas & Screening Flow

Descriptor and feature choices at a high level

simple 0D–2D descriptor concepts **property and**
fingerprint style views **feature awareness and**
limitations

QSAR and model use at concept level (non advisory)

training, evaluation and simple checks **applicability**
and uncertainty notions **responsible communication**
of outputs

High level virtual screening and prioritisation flow

sequence of filters and ranking ideas **hit lists and**
shortlists (conceptual) **no procurement or synthesis**
decisions

Session 3

Fee: Rs 14800 Apply Now

ADMET Flags, MPO Style Views & Safety Notes

Summarising ADME related properties and flags responsibly

exposure relevant properties overview **simple flag**
and traffic light views **clear caveats on in silico**
outputs

MPO style multi property summaries (idea level only)

balanced profile tables and grids **comparison of series or subsets** **non prescriptive design language**

Safety oriented narrative notes (educational, non regulatory)

describing patterns and concerns **highlighting gaps for expert review** **avoiding legal or regulatory advice**

Session 4

Fee: Rs 18800 Apply Now

Capstone Packaging, Review & Reflection

Assembling the end to end project pack

Theory + Practical

Creating figures, tables and short report for internal use

data curation and QC summary **QSAR and screening overview plots** **ADMET and safety flag tables**

Deliverables & reflection on good practices and limits

curated dataset and project notebook **PDF/HTML summary report** **written reflection on scope and ethics**