Datastat Research
Building Capacity in Training and Research

DATASTAT TRAINING IN

OFFICIAL COURSE PROSPECTUS

Center for Advanced Research & Professional Development

Nairobi Training Center • Global Virtual Academy • Corporate On-Site

BIOTECHNOLOGY AND PHARMACEUTICAL DEVELOPMENT

Advanced Medicinal Chemistry for Undruggable Targets Training Course

Comprehensive Course Syllabus, Practical Modules & Upcoming Schedules

PROGRAM SPECIFICATIONS & HIGHLIGHTS

- **DURATION**
  10 Days Practical Hands-on
- **DELIVERY MODES**
  In-Person Class & Live Virtual
- **CERTIFICATION**
  Accredited Certificate of Completion
- **INTAKES / DATES**
  Multiple Cohort Schedules Included

PREPARED FOR:

Valued Participant

Email: training@datastatresearch.org | Issued: November 21, 2026

Academic & Professional Training Year: 2026

DATASTAT TRAINING INSTITUTE

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Advanced Medicinal Chemistry for Undruggable Targets Training Course

Biotechnology and Pharmaceutical Development • 10 Days Intensive • Accredited Certification

Course Overview

Advanced Medicinal Chemistry for Undruggable Targets Training Course is designed to equip R&D scientists with the advanced knowledge and practical computational chemistry skills needed to pioneer next-generation therapies, specifically leveraging novel mechanisms of action to address diseases with high unmet medical needs, such as aggressive cancers and neurodegeneration

Key Skills & Software Tools Covered

Molecular modeling • SAR analysis • cheminformatics software

Upcoming Training Schedules

Confirmed cohort intakes and venues. Both physical in-person classroom and live virtual online seats are available.

TRAINING DATES	LOCATION / VENUE	FORMAT / DURATION	INVESTMENT (FEE)
29 Dec 2025 – 9 Jan 2026	Nairobi	Classroom / 10d	**$4,000 USD / KES 250,000**
29 Dec 2025 – 9 Jan 2026	Kigali	Classroom / 10d	**$6,000 USD / KES 110,000**
29 Dec 2025 – 9 Jan 2026	Dubai	Classroom / 10d	**$10,000 USD / KES 110,000**
29 Dec 2025 – 9 Jan 2026	Cape Town	Classroom / 10d	**$9,000 USD / KES 110,000**
29 Dec 2025 – 9 Jan 2026	Addis Ababa	Classroom / 10d	**$6,000 USD / KES 110,000**
29 Dec 2025 – 9 Jan 2026	Singapore	Classroom / 10d	**$10,000 USD / KES 110,000**
29 Dec 2025 – 9 Jan 2026	Istanbul	Classroom / 10d	**$10,000 USD / KES 110,000**
29 Dec 2025 – 9 Jan 2026	Bangkok	Classroom / 10d	**$10,000 USD / KES 110,000**
29 Dec 2025 – 9 Jan 2026	Accra	Classroom / 10d	**$8,000 USD / KES 110,000**
12 Jan 2026 – 23 Jan 2026	Nairobi	Classroom / 10d	**$4,000 USD / KES 250,000**
12 Jan 2026 – 23 Jan 2026	Kigali	Classroom / 10d	**$6,000 USD / KES 110,000**
12 Jan 2026 – 23 Jan 2026	Dubai	Classroom / 10d	**$10,000 USD / KES 110,000**

* Corporate discounts and customized cohort scheduling are available for teams of 3 or more participants.

Course Curriculum & Modules

Advanced Medicinal Chemistry for Undruggable Targets Training Course

Introduction

In the pursuit of novel therapeutics, modern Medicinal Chemistry has transitioned from traditional enzyme and receptor targets to the vast, complex space of the undruggable proteome. This paradigm shift is driven by the reality that over 80% of disease-relevant proteins, including critical Transcription Factors, Protein-Protein Interactions, and Intrinsically Disordered Proteins, lack the well-defined, hydrophobic binding pockets required for conventional Small Molecule Drugs. Success in this frontier demands the mastery of cutting-edge modalities and data-driven strategies. Advanced Medicinal Chemistry for Undruggable Targets Training Course is designed to equip R&D scientists with the advanced knowledge and practical computational chemistry skills needed to pioneer next-generation therapies, specifically leveraging novel mechanisms of action to address diseases with high unmet medical needs, such as aggressive cancers and neurodegeneration.

The training will provide a rigorous, translational deep dive into revolutionary techniques that are redefining what is "druggable." Key among these are Targeted Protein Degradation, utilizing PROTACs and Molecular Glues, as well as Covalent Inhibitors and the exciting field of RNA-Targeting Small Molecules. The curriculum focuses on integrating AI-driven drug design and Fragment-Based Drug Discovery with advanced chemical synthesis to accelerate the identification and optimization of leads against historically challenging targets like KRAS and MYC. By emphasizing real-world case studies, this course ensures participants are not only theoretically proficient but also skilled in applying these Next-Generation Therapeutics to shorten drug discovery timelines and unlock new therapeutic possibilities for complex biological systems.

Course Duration

10 days

Course Objectives

Upon completion of this course, participants will be able to:

- Master the principles of Targeted Protein Degradation and differentiate the design of PROTACs vs. Molecular Glues.
- Apply AI-Driven Drug Design and Machine Learning algorithms to predict new binding pockets on IDPs.
- Design and optimize Covalent Inhibitors to target non-catalytic cysteine residues, focusing on irreversible binding kinetics.
- Evaluate and apply Fragment-Based Drug Discovery and Structure-Based Drug Design for shallow or planar protein surfaces.
- Develop lead compounds against key Oncogenic Transcription Factors previously deemed intractable.
- Characterize and modulate difficult Protein-Protein Interactions using macrocycles and stabilized Peptide Therapeutics.
- Identify and synthesize small molecules that selectively target disease-relevant non-coding RNA and mRNA structures.
- Utilize advanced Cheminformatics and High-Throughput Screening data to navigate the "dark chemical space."
- Interpret and optimize ADMET and Physicochemical Properties specifically for Bifunctional Modalities
- Analyze the mechanism of action for allosteric modulators as an alternative strategy for undruggable targets.
- Implement specialized synthetic methods for the rapid library generation of novel scaffolds.
- Translate preclinical findings using Target Engagement assays like CETSA to validate on-target mechanism in a cellular context.
- Drive innovation in neglected disease areas by applying these technologies to targets in Neurodegeneration and Autoimmune Diseases

Target Audience

- Medicinal & Organic Chemists.
- Computational Chemists/Data Scientists.
- Pharmacologists & Biologists.
- R&D Group Leaders/Managers.
- Postdoctoral Researchers.
- Biotech & Pharma Executives.
- Process/Analytical Chemists.
- Clinical/Translational Scientists.

Course Modules

Module 1: The Undruggable Proteome: Challenges and Opportunities

- Defining the "Undruggable" space: TFs, IDPs, and non-catalytic PPIs.
- Lack of deep, hydrophobic binding pockets.
- Biological significance of key undruggable targets
- The shift from "Blockade" to "Degradation" and "Redirection."
- Case Study: The journey to drug KRAS G12C

Module 2: Fundamentals of Targeted Protein Degradation

- Mechanism of action for PROTACs and the E3 Ligase Recruitment paradigm.
- Key E3 Ligases in drug discovery
- Linker length, warhead-ligand pairing, and cooperativity.
- Pharmacokinetics and cell permeability challenges for large degraders.
- Case Study: Design and optimization of the first clinical PROTAC

Module 3: Molecular Glues and Alternative TPD Modalities

- Stabilizing neo-substrate interactions with E3 Ligases.
- Thalidomide and the discovery of Molecular Glues.
- Design strategies for identifying novel glues
- Introduction to non-PROTAC TPD
- Case Study: The mechanism and clinical success of Lenalidomide

Module 4: Covalent Inhibitors for Undruggable Targets

- Kinetics and advantages of irreversible inhibitors.
- Targeting non-active site cysteine residues

- Warhead selection and balancing reactivity/selectivity.
- Chemoproteomics techniques for identifying and validating covalent targets.
- Case Study: The development of BTK and EGFR Covalent Inhibitors

Module 5: Computational Drug Design and AI/ML

- Advanced Virtual Screening (VS) techniques.
- AI/Machine Learning for De Novo Design and property prediction
- Molecular Dynamics (MD) simulations to predict target flexibility and cryptic pockets.
- Free Energy Perturbation (FEP) for highly accurate binding affinity prediction.
- Case Study: Utilizing AI to accelerate hit-to-lead for novel kinase inhibitors.

Module 6: Fragment-Based Drug Discovery (FBDD)

- Screening small fragments to find high-quality starting points.
- X-ray Crystallography, NMR, SPR for fragment screening.
- Fragment evolution strategies.
- Combining FBDD with SBDD for shallow/planar binding sites.
- Case Study: FBDD success in targeting BCL-2

Module 7: Modulating Protein-Protein Interactions (PPIs)

- Characteristics of PPI interfaces.
- Stabilized Peptides/Macrocycles and Allosteric Modulators.
- Conformational restraint techniques to enhance cell permeability.
- Computational approaches for identifying hot spots and cryptic sites on PPIs.
- Case Study: Development of a stapled peptide inhibitor for the p53-MDM2 interaction.

Module 8: The Rise of RNA-Targeting Small Molecules

- Targeting structures on non-coding and messenger RNA.
- Achieving selectivity, binding affinity, and cell permeability.
- Screening methodologies.
- Targeting splice-site regulation and ribosomal function.
- Case Study: Development of Risdiplam and its mechanism of action.

Module 9: Designing for Pharmacokinetics (PK) in Novel Modalities

- Specialized ADMET considerations for PROTACs and large molecules.
- Addressing poor permeability and rapid metabolism in Peptide/Macrocycle therapeutics.
- Strategies for achieving brain-penetrant small molecules.
- In silico and in vitro assays for profiling absorption and stability.
- Case Study: Tuning the PK properties of a PROTAC to improve oral bioavailability.

Module 10: Advanced Synthetic Methods in Medicinal Chemistry

- C-H Activation and other late-stage functionalization techniques.
- Application of Flow Chemistry and automation in drug discovery synthesis.
- Click Chemistry and biocompatible ligations for rapid library synthesis.
- Techniques for synthesizing isotopically labeled compounds for ADMET studies.
- Case Study: Using advanced catalysis to synthesize novel constrained macrocycles.

Module 11: Undruggable Targets in Oncology

- Detailed focus on the RAS family and strategies beyond the G12C mutation.
- Targeting MYC and other key Transcription Factors via degradation or disruption.
- Developing inhibitors for the Kinome and Phosphatome using allosteric sites.
- Targeting the Tumor Microenvironment and cancer-immune interactions.
- Case Study: New modalities for targeting MYC.

Module 12: Undruggable Targets in Neurodegeneration and Inflammation

- Targeting aggregation-prone proteins in the CNS.

- Strategies for crossing the Blood-Brain Barrier (BBB) with novel compounds.
- Targeting the inflammasome and other chronic inflammation pathways.
- Utilizing Radiopharmaceuticals and Theranostics for CNS disease.
- Case Study: The challenge of targeting Tau and Alpha-Synuclein in Alzheimer's/Parkinson's.

Module 13: Target Engagement and Cellular Efficacy Validation

- Importance of establishing Target Engagement (TE) in the cellular environment.
- CETSA, nanoBRET, Thermal Shift Assays.
- Assessing Efficacy in relevant cellular and phenotypic models.
- Translational biomarkers and their role in early clinical development.
- Case Study: Using CETSA to validate the cellular activity of a new TPD molecule.

Module 14: Safety, Selectivity, and Off-Target Effects

- Strategies for maximizing selectivity against highly homologous protein families.
- Profiling and mitigating potential off-target toxicity and Drug-Drug Interactions
- In Silico Tox prediction and High-Content Screening for safety.
- Ethical and regulatory considerations for novel modalities.
- Case Study: Analyzing the off-target toxicity profile of an early-stage PROTAC candidate.

Module 15: Course Synthesis and Future Directions

- Choosing the right therapeutic approach for the target.
- The future of Combinatorial Chemistry and automation in the undruggable space.
- Emerging technologies: Antibody-Drug Conjugates and Gene-Targeting agents.
- Designing a strategy to drug a newly nominated undruggable target
- Case Study: Analyzing the regulatory and market landscape for Next-Generation Therapeutics.

Training Methodology

This course employs an intensive Blended Learning approach combining didactic, interactive, and problem-solving elements to ensure maximum retention and practical skill development:

- Interactive Lectures.
- Hands-on Workshops.
- Case Study Analysis.
- Team-Based Problem Solving.
- Q&A with Subject Matter Experts.

Register as a group from 3 participants for a Discount

Send us an email: info@datastatresearch.org or call +254724527104

Certification

Upon successful completion of this training, participants will be issued with a globally- recognized certificate.

Tailor-Made Course

We also offer tailor-made courses based on your needs.

Key Notes

a. The participant must be conversant with English.

b. Upon completion of training the participant will be issued with an Authorized Training Certificate

c. Course duration is flexible and the contents can be modified to fit any number of days.

d. The course fee includes facilitation training materials, 2 coffee breaks, buffet lunch and A Certificate upon successful completion of Training.

e. One-year post-training support Consultation and Coaching provided after the course.

f. Payment should be done at least a week before commence of the training, to DATASTAT CONSULTANCY LTD account, as indicated in the invoice so as to enable us prepare better for you.

Certification & Learning Methodology

- Hands-on practical delivery with real-world datasets, case studies, and lab exercises.
- Post-training mentorship, access to class resources, and customized follow-up support.
- Participants who successfully complete the course receive an accredited Datastat Certificate of Completion.

How to Enroll & Reserve Your Seat

1. Online Registration: Visit https://datastatresearch.org/courses/advanced-medicinal-chemistry-for-undruggable-targets-training-course to register online.
2. Email Booking: Send participant details to training@datastatresearch.org for official invoice & reservation.
3. Support & Assistance: Inquire via phone +254 724 527 104 | +254 734 969 612.