BioSol Centre
BIOLOGICAL SOLUTION CENTRE

PROGRAMME PROSPECTUS · FOR SUPERVISORS AND FUNDING APPROVAL

Machine Learning & AI-Based Drug Design

A three-tier professional training programme in computer-aided drug discovery, molecular dynamics and bioinformatics — from a five-day introduction to a six-month supervised research project ending in a peer-reviewed submission.

Organised by	BioSol Centre (Biological Solution Centre)
Training and content	Foysal Ahammad, Founder & CEO
Founded	October 2019 · Jashore & Dhaka, Bangladesh
Delivery	Online, worldwide · hosted laboratory provided
Contact	biosolcentre@gmail.com · +880 1783 541054

SECTION 1

Executive summary

One page for a supervisor or department head deciding whether to approve attendance and release funds.

WHAT IS BEING PROPOSED

Participation in a structured, hands-on training programme in machine learning and AI-based drug design, delivered online by BioSol Centre and taught by Foysal Ahammad. The programme is offered at three levels, so the cost and the time commitment can be matched to what the researcher actually needs. It is open to every academic level — undergraduate, MSc, MPhil, PhD, postdoctoral and faculty — as well as to industry scientists; the only prerequisite is basic Python.

300+	20+	30+	100%
Trained since 2019	Papers co-authored with participants	Guided to funded scholarships abroad	Open-source software, no licences

TRACK RECORD

Since October 2019 BioSol Centre has trained more than **300 students, researchers and teachers**; co-authored over **20 peer-reviewed papers** with trained participants in Q1, Web of Science and Scopus-indexed journals; and guided more than **30 participants** into funded scholarship places in the USA, Canada, Australia and elsewhere. Those figures describe one pipeline: participants arrive to learn a method, many co-author the work they produced during or after the training, and some use that publication to win a funded place abroad.

WHY IT IS WORTH APPROVING

- **Transferable capability, not a certificate.** Participants return able to run docking, MD simulation, QSAR and ADMET prediction independently, on the group's own targets.
- **No software budget required.** The whole stack is open source — RDKit, AutoDock Vina, GROMACS, PyTorch, REINVENT. No Schrödinger or MOE licence is needed for any exercise.
- **No hardware required.** A hosted laboratory environment is provided; long jobs run on the course server.
- **Output the group keeps.** Curated datasets, validated protocols, trained models, trajectories and publication-quality figures — all reproducible from a supplied Docker image.
- **A route to publication.** The top tier is supervised research ending in a submitted manuscript, with authorship governed by ICMJE criteria.

COST AT A GLANCE

FEES BY TIER — BANGLADESH AND INTERNATIONAL RATE CARDS

Tier	Duration	Bangladesh	International	Instalments
1 — Basic	5 days · 30 h	**BDT 4,500**	**USD 95**	Single payment
2 — Advanced	4 weeks · 60 h	**BDT 15,000**	**USD 320**	2 payments
3 — Professional	6 months	**BDT 55,000**	**USD 1,100**	3 payments

Student rates, early-bird and group discounts reduce these further. Scholarships above 70 % are available to students resident in Bangladesh on request, and institutional purchase orders are accepted with thirty-day payment terms. Section 7 has the full price list.

> **WHAT THIS PROGRAMME DOES NOT CLAIM**
>
> No in-silico result replaces an assay, and no tier guarantees a publication. These methods reorder and prioritise chemical space; they do not confirm activity. Participants finish able to state this clearly — which is itself part of the training.

PROSPECTUS

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SECTION 2

The organisation

BioSol Centre — Biological Solution Centre — is a biotechnology and bioinformatics research organisation in Bangladesh, founded in October 2019.

ORGANISATION DETAILS

Full name	BioSol Centre (Biological Solution Centre)
Founded	October 2019
Founder	Foysal Ahammad
Field	Biotechnology and bioinformatics research, training, and analysis services
Main location	Jashore University of Science and Technology (JUST) Campus Road, Jashore, Bangladesh
Administrative	Dhaka, Bangladesh
Team	11–50 people, including student researchers and trainees
Status	Private educational and biotechnology research organisation
Partnerships	Academic researchers internationally; local organisations including SeqBee Bioscience for joint workshops and computational drug design training
Email	structuralbiologyai@gmail.com
Phone / WhatsApp	+880 1783 541054
Online	facebook.com/biosolcentre · linkedin.com/company/biosol-centre · researchgate.net/lab/BioSol-Centre-Foysal-Ahammad

What the Centre does

- **Structured training** — three tiers of hands-on training in AI-based drug design, from a five-day introduction to a six-month supervised project.
- **Supervised research** — collaborative computational projects run to publication, with authorship determined by contribution.
- **Analysis services** — molecular docking, MD simulation, virtual screening, multi-omics, epigenomics, exome sequencing and publication support, delivered for research groups directly.
- **Institutional cohorts** — private training for departments and companies, on site or online, with the teaching target replaced by one of the group's own.

Accessibility commitments

Training is priced against two rate cards, so participants are charged against the economy they live in rather than a single global price. Scholarships above 70 % are available to Bangladeshi students on request, need-based waivers are reserved in every cohort, and instalments are offered without interest or credit checks on every paid tier.

SECTION 3

The instructor and research record



Foysal Ahammad

Founder, BioSol Centre · Course content and training

All course material, laboratory design and supervision for this programme are developed and delivered by Foysal Ahammad, a computational biologist and bioinformatician. His work spans computational drug discovery — molecular docking, virtual screening, molecular dynamics and binding free energy — and bioinformatics, including multi-omics, epigenomics and sequencing data analysis.

He founded BioSol Centre in October 2019 and serves as its Chief Executive Officer, leading its training programmes and research collaborations. He is a researcher at Hamad Bin Khalifa University (HBKU) in Qatar, working on a QNRF-funded project investigating paediatric cerebral palsy through whole-genome and epigenome sequencing.

Positions and education

Current position	Researcher and Research Assistant, Hamad Bin Khalifa University (HBKU), Qatar — QNRF-funded paediatric cerebral palsy genomics project
Founder & CEO	BioSol Centre, Jashore, Bangladesh — since October 2019
MSc	Biological Science — King Abdulaziz University, Saudi Arabia
BSc	Genetic Engineering and Biotechnology — Jashore University of Science and Technology (JUST), Bangladesh
Previous roles	Research Assistant at King Abdulaziz University; International Islamic University Malaysia (IIUM); Malaysia Genome and Vaccine Institute
Research areas	Computational drug discovery, molecular dynamics, machine learning, structural biology, genomics and epigenomics, neurobiology, microbiology
Published work includes	Multi-epitope vaccine design against SARS-CoV-2; fish disease technology; antiviral and anti-inflammatory compounds from mangrove and medicinal plants; AI/ML-driven drug discovery and clinical risk modelling

Peer-reviewed publications — selected, 2021–2026

The methods taught in this programme are the methods used in the work below.

2026 · FEATURED

Machine learning-driven modeling of synergistic perinatal risk profiles in early-onset pediatric cerebral palsy

BMC Medical Informatics and Decision Making

doi:10.1186/s12911-026-03710-y

2025

Molecular docking, QSAR, and simulation analyses of EGFR-targeting phytochemicals in non-small cell lung cancer

Journal of Molecular Structure

doi:10.1016/j.molstruc.2024.139924

2025

Investigating new drugs from marine seaweed metabolites for cervical cancer therapy by molecular dynamic modeling

Scientific Reports

doi:10.1038/s41598-024-82043-0

2024

Cheminformatics-based identification of phosphorylated RET tyrosine kinase inhibitors for human cancer

Frontiers in Chemistry

doi:10.3389/fchem.2024.1407331

2023

The ortholog of human ssDNA-binding protein SSBP3 influences neurodevelopment and autism-like behaviors in *Drosophila melanogaster*

PLOS Biology

doi:10.1371/journal.pbio.3002210

2021

Pharmacoinformatics and molecular dynamics simulation-based phytochemical screening of neem plant against human cancer

Briefings in Bioinformatics

doi:10.1093/bib/bbab098

PROFILES

ORCID	0000-0001-7313-4729 — orcid.org/0000-0001-7313-4729
Google Scholar	scholar.google.com — search "Foysal Ahammad"
PubMed	pubmed.ncbi.nlm.nih.gov — Ahammad F[Author]
ResearchGate lab	researchgate.net/lab/BioSol-Centre-Foysal-Ahammad
Portfolio	structuralbiologyai-art.github.io/portfolio

Citation counts change constantly and are therefore not quoted. The Google Scholar record is the authoritative source for current citations, h-index and newly indexed work.

SECTION 4

Programme structure and the three tiers

One curriculum taught at three depths. A participant who starts low and works up never repeats a session, and the fee already paid is credited in full.

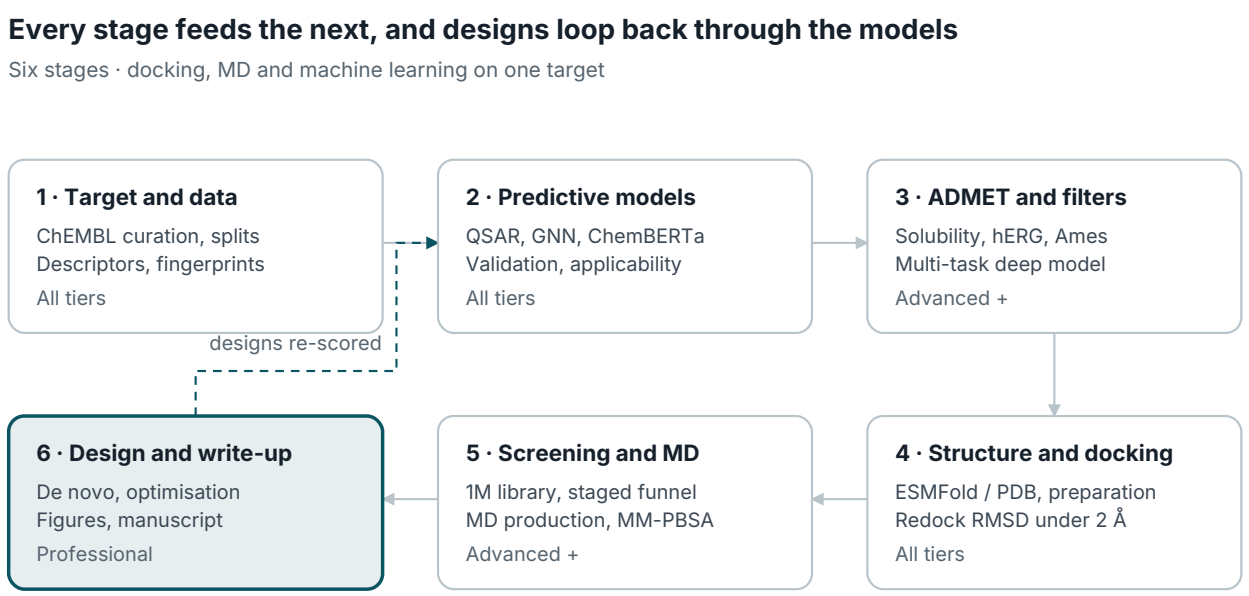

Figure 1 — The programme pipeline. One target is chosen at the start and carried through every stage, so each stage's output is the next stage's input. The dashed loop is the design–make–test cycle: generated molecules go back through the predictive models and the validated docking protocol before anyone calls them candidates.

TABLE 4.1 — TIER COMPARISON

	Tier 1 — Basic	Tier 2 — Advanced	Tier 3 — Professional
Purpose	Learn the tools	Run a full campaign	Publish with supervision
Best for	Undergraduate, MSc, PhD, postdoc	MSc, PhD, postdoc, faculty with a target	Any level needing a publication
Duration	5 days · 30 h	4 weeks · 60 h	6 months · 60 h + supervision
Delivery	Live online or on site	Weekend intensive, online	Weekly 1:1 + fortnightly group
Cohort size	Up to 40	Up to 25	8 only
Docking	Single target	Validated, 1M library	Publication-grade
MD simulation	Demonstration	100 ns + MM-PBSA	3 × 200 ns + free energy
Machine learning	QSAR, random forest	+ GNN, ChemBERTa, ADMET	Built for the manuscript
Generative design	Overview	Hands-on	If the project needs it
Manuscript support	—	One session	Drafting to submission
Outcome	Certificate, 30 h	Complete in-silico campaign	Co-authored manuscript

Tier 1 — Basic · 5 days, 30 hours

Five days with no project attached. Participants finish able to curate a bioactivity dataset, build and validate a QSAR model, prepare a protein and dock a ligand — and able to read a computational drug design paper critically.

Day	Content	Hours
1	Drug discovery pipeline and where AI fits; RDKit; molecular representation	6
2	ChEMBL extraction; curation and standardisation; descriptors and fingerprints	6
3	QSAR with random forest and XGBoost; validation basics	6
4	Protein preparation, binding-site definition, molecular docking	6
5	Pose analysis and visualisation; MD and generative design demonstrations	6

Deliberately excluded: redocking validation, enrichment testing, production MD, free-energy calculation and publication support. These belong to the higher tiers and the exclusion is stated in advance.

Tier 2 — Advanced · 4 weeks, 60 hours

Four weekends, with participants bringing their own protein from week two after a feasibility check. This is the tier that includes molecular dynamics properly — a 100 ns production run the participant sets up, launches and analyses, followed by MM-PBSA binding free energies.

Week	Content	Hours
1	Data curation at depth; QSAR; scaffold and time splits, Y-randomisation, applicability domain, conformal intervals, SHAP	15
2	Graph neural networks in PyTorch Geometric; ChemBERTa fine-tuning; multi-task ADMET; uncertainty by ensembling	15
3	Structure preparation; redocking and cross-docking validation; retrospective enrichment with decoys; 1M-compound staged screen; ML rescoring and consensus ranking	15
4	MD — force field, solvation, ions, minimisation, NVT/NPT equilibration, 100 ns production; RMSD, RMSF, Rg, SASA, H-bond and PCA analysis; MM-PBSA; figures; writing workshop	15

Deliverable: a complete in-silico campaign on one target — curated dataset, validated predictive model, validated docking protocol, ranked hit list, 100 ns trajectory with analysis, MM-PBSA energies and publication-quality figures. In practice this is the results section of a paper.

Tier 3 — Professional · 6 months + revision support

Eight participants, one supervised research project each, ending with a manuscript submitted to a peer-reviewed journal with the participant as an author. The taught content is the Advanced curriculum, delivered alongside the project.

Month	Milestone	Contact
0	Admission interview; target and research question agreed in writing before payment	One 45-min call
1	Taught modules; literature review written; dataset curated and documented	Weekly 1:1 + group
2	Predictive model built and validated; docking protocol validated by redocking and enrichment	Weekly 1:1
3	Large-scale screening; hit selection; MD systems built and equilibrated	Weekly 1:1
4	3 × 200 ns replica simulations; full trajectory analysis; MM-PBSA / MM-GBSA	Weekly 1:1
5	Figures finalised; first full draft written by the participant; author order agreed in writing	Weekly 1:1
6	Internal review, journal selection, submission; data and code deposited publicly	Weekly 1:1
7–12	Revision support until the first editorial decision is answered	As needed, no fee

Project types offered: structure-based virtual screening against a disease target; repurposing screen of an approved-drug library; machine-learning ADMET profiling of a compound series; comparative MD study of resistance or activating mutations; natural-product library screen with MD and free-energy validation. Participants may propose their own, with feasibility decided at interview rather than after payment.

SECTION 5

Full curriculum — 24 modules

Every module exists once. A tier is a selection from this list, so an upgrading participant never repeats a session.

TABLE 5.1 — MODULE COVERAGE BY TIER

#	Module	Basic	Advanced	Professional
M1	Drug discovery pipeline and where AI fits	Full	Full	Full
M2	Molecular representation and RDKit	Full	Full	Full
M3	Bioactivity data extraction and curation	Full	Full	Full
M4	Descriptors and fingerprints	Full	Full	Full
M5	Splitting data honestly — scaffold, time, random	Short	Full	Full
M6	Classical QSAR — RF, XGBoost, SVM	Full	Full	Full
M7	Validation and the applicability domain	Short	Full	Full
M8	Interpreting a model — SHAP, fragments, MMP	—	Full	Full
M9	Graph neural networks	Overview	Full	Full
M10	Chemical language models — ChemBERTa, MolFormer	Overview	Full	Full
M11	Multi-task ADMET and uncertainty	Overview	Full	Full
M12	Protein structures and AI prediction	Full	Full	Full
M13	Protein preparation and site definition	Full	Full	Full
M14	Molecular docking	Full	Full	Full
M15	Validating a docking protocol	—	Full	Full
M16	Large-scale screening and ML rescoring	Demo	Full	Full
M17	Setting up an MD simulation	Demo	Full	Full
M18	Production MD and trajectory analysis	—	100 ns	3 × 200 ns
M19	Binding free energy — MM-PBSA, MM-GBSA, FEP	—	Full	Full
M20	Generating and optimising molecules	Overview	Full	If needed
M21	Synthesisability and retrosynthesis	—	Full	If needed
M22	Publication-quality figures	—	Full	Full
M23	Writing a CADD manuscript	—	One session	Full, iterative
M24	Reproducibility and data deposit	—	Short	Full

Full — taught and run by the participant. **Short** — condensed treatment. **Demo** — the instructor runs it while participants watch. **—** — not included at that tier.

Accompanying tutorials

Twenty-four runnable notebooks, each with a marked minimum path and optional extensions. Solutions are released at the end of each session. Notebooks remain available for twelve months.

#	Tutorial	Produces
T1–T5	RDKit essentials · ChEMBL extraction · curation pipeline · descriptors and fingerprints · split comparison	Clean, split dataset
T6–T9	QSAR baselines · nested CV and Optuna · applicability domain and conformal intervals · SHAP and fragment attribution	Validated model + model card
T10–T12	GNN from scratch · ChemBERTa fine-tuning · multi-task ADMET profiling	Benchmark table, ADMET profile
T13–T18	Protein preparation · docking and pose inspection · redocking validation · retrospective enrichment · 1M staged screen · ML rescoring and consensus	Validated protocol, ranked hits
T19–T21	MD system building and equilibration · production MD and trajectory analysis · MM-PBSA free energy	Trajectory, plots, energies
T22–T24	Generative design with a composite objective · retrosynthesis route search · figures and reproducibility packaging	Designed set, submission package

SECTION 6

Software, datasets and compute

Everything is free for academic use. No licence purchase is required for any exercise, and no participant needs to own hardware.

TABLE 6.1 — SOFTWARE STACK

Component	Tools used	Licence
Cheminformatics	RDKit, Open Babel, MolVS, SELFIES	BSD / free
Descriptors	Mordred, PaDEL, RDKit 2D	Free
Classical ML	scikit-learn, XGBoost, LightGBM, Optuna, SHAP	Free
Deep learning	PyTorch, PyTorch Geometric, DeepChem	Free
Pretrained models	ChemBERTa, MolFormer	Free weights
Structure prediction	ESMFold, Boltz, AlphaFold DB	Free / non-commercial
Protein preparation	PDBFixer, OpenMM, fpocket	Free
Docking	AutoDock Vina, smina, QuickVina-W, GNINA	Free
Molecular dynamics	GROMACS, OpenMM, AmberTools, MDAnalysis	Free
Free energy	MM-PBSA / MM-GBSA tooling	Free
Generative design	REINVENT 4, SAFE, CReM, AiZynthFinder	Free
Visualisation	PyMOL (open source), py3Dmol, NGLView	Free

TABLE 6.2 — DATASETS

Dataset	Content
ChEMBL	Curated bioactivity records for the chosen targets
Therapeutics Data Commons	ADMET and toxicity benchmark endpoints
MoleculeNet	Standard benchmark tasks for model comparison
Protein Data Bank, PDBbind	Structures and complexes with measured affinities
DUD-E, DEKOIS 2.0	Known actives with property-matched decoys
Enamine REAL subset	One million purchasable compounds for screening
ZINC in-stock	Alternative screening library

COMPUTE PROVIDED

A hosted laboratory environment is supplied to every participant — log in and run every step in the browser. Long jobs, including the million-compound screen and MD production runs, execute on the course server. Participants keep a Docker image and `environment.yml` that rebuild the entire stack locally in one command.

SECTION 7

Fees, instalments and scholarships

Two rate cards, published openly. Residence decides the rate, not nationality.

BANGLADESH RATE (BDT)

Tier	Standard	Student
Basic	**4,500**	**3,500**
Advanced	**15,000**	**12,000**
Professional	**55,000**	**45,000**

INTERNATIONAL RATE (USD)

Tier	Standard	Student
Basic	**95**	**70**
Advanced	**320**	**250**
Professional	**1,100**	**900**

Instalments

Tier	Plan	Bangladesh	International	Due
Basic	Single payment	**BDT 4,500**	**USD 95**	At registration
Advanced	2 instalments	**2 × BDT 7,800**	**2 × USD 165**	Registration, before week 3
Professional	3 instalments	**3 × BDT 19,000**	**3 × USD 380**	Months 0, 3 and 5

No interest and no credit check. Where a scholarship is awarded it is applied to the total first, and the reduced balance is split across the same number of instalments.

Discounts

Discount	Amount	Conditions
Student rate	**See price list**	Valid student ID at registration
Early bird	**About 12 %**	Paid four or more weeks before the cohort begins
Group of 3–5	**10 % each**	Same institution, registered together
Group of 6 or more	**20 % each**	Same institution, registered together
Upgrade credit	**100 % of lower fee**	Moving up a tier within 12 months
Returning participant	**15 %**	Completed a previous cohort
Need-based waiver	**Up to 100 %**	Two seats per Basic cohort, one per Advanced cohort

Scholarships

Students resident in Bangladesh may apply for a scholarship of **more than 70 %** on any tier, including the Professional publication track. There is no application fee, no separate deadline and no quota announced in advance. Applications are made by email with a short paragraph and proof of enrolment, and answered within one week.

Tier	Full BDT fee	At 70 % scholarship
Basic	4,500	**1,350**
Advanced	15,000	**4,500**
Professional	55,000	**16,500**

Bangladeshi early-career researchers within three years of graduating may receive up to 50 %; international applicants in financial hardship up to 40 %; and applicants from low-income countries may be charged on the Bangladesh rate card on request.

Payment and invoicing

From Bangladesh	bKash, Nagad or Rocket to **+880 1783 541054** (Personal / Send Money), or bank transfer on request
International	Card or PayPal through the registration platform, or SWIFT bank transfer
Institutions	Purchase orders accepted; invoice payable within thirty days; the seat is held on the purchase order rather than on payment
Receipts	A numbered receipt with a programme reference is issued for every payment, for departmental reimbursement

Refunds

Cancellation	Basic and Advanced	Professional
More than 14 days before	Full refund less 10 % handling	Full refund less 10 % handling
7 to 14 days before	50 % refund	50 % refund
Under 7 days or after start	No refund; one free transfer	No refund once project assigned
Cancelled by BioSol Centre	Full refund	Full refund

SECTION 8

Assessment, certification and deliverables

Assessment is built from work participants already produce, so nothing extra is added to the week.

TABLE 8.1 — ASSESSMENT SCHEME

Component	Weight	When
Daily exit criteria (5 × 6 %)	**30 %**	End of each day
Model card (Day 2 / Month 2)	**15 %**	Following session
Docking validation report	**15 %**	Following session
Capstone campaign and notebook	**25 %**	Final session
Capstone presentation, incl. stated weakness	**15 %**	Final session

Pass mark 60 %. Certificates name the modules covered and the total contact hours, and carry a verification code tied to the participant record. Professional certificates additionally name the project and the manuscript.

What the participant brings back to the group

- [ ] Their own curated dataset with full provenance, reusable on the group's targets
- [ ] A validated predictive model with an honest metric, applicability domain and model card
- [ ] A validated docking protocol with its redocking RMSD recorded
- [ ] MD trajectories, analysis plots and binding free energies they generated themselves
- [ ] A ranked hit list with scores, interaction fingerprints and rationale
- [ ] The complete annotated notebook set with released solutions
- [ ] A Docker image and `environment.yml` rebuilding the whole stack in one command
- [ ] Five one-page protocol sheets written as checklists for real projects
- [ ] A reading list of the key papers behind every method taught
- [ ] A verifiable certificate naming the modules and contact hours

> **WHY THE "STATED WEAKNESS" SLIDE CARRIES THE MOST MARKS**
>
> In the capstone, each team must present one slide identifying the single biggest weakness in their own pipeline. A team that correctly identifies a fatal flaw in its own work has understood more than a team with a prettier hit list — and that habit is what makes a researcher useful to a group rather than merely productive.

SECTION 9

Authorship and research-integrity policy

This policy governs the Professional tier and is published in full. What is sold is supervision; authorship follows from the work, not from the invoice.

WHAT IS PROMISED

- A defined research project, agreed in writing before payment is taken
- Supervision at every stage, including methods review and manuscript editing
- Submission to a peer-reviewed, recognised and indexed journal agreed with the participant
- Authorship for every participant who meets the criteria below
- Revision support until the first editorial decision is answered, at no extra charge

WHAT IS NOT PROMISED

- **Acceptance.** No supervisor controls a reviewer, and the fee buys none of that influence.
- **A named journal or impact factor.** The target journal is chosen when the results are in.
- **First authorship by default.** Author order follows contribution and is agreed in writing at the start of month five.
- **Publication in a predatory outlet.** Journals are selected from recognised indexes; a request to use a disreputable venue is refused.

AUTHORSHIP CRITERIA

Each author must meet all four ICMJE conditions: a substantial contribution to the design or the analysis; drafting the work or revising it critically; approval of the final version; and agreement to be accountable for it. A participant who does not run their own analyses and does not write is **acknowledged, not listed**. This is explained at the admission interview and repeated in the written agreement.

INTEGRITY RULES

- No ghostwriting — the participant drafts, the supervisor edits
- No gift, guest or honorary authorship, for anyone, including the organisation's own staff
- No fabricated or selectively reported results; negative findings are published as negative
- Data and code deposited publicly with every submission
- Any AI assistance in writing disclosed exactly as the target journal requires
- Article processing charges are the participant's responsibility, or the project targets a no-fee journal — decided at interview and written into the agreement

A NOTE FOR SUPERVISORS

If your student is considering any provider that promises a guaranteed acceptance, a named impact factor, or authorship on a manuscript they did not work on, that provider is selling something that can be retracted later with your institution's name attached. Ask any provider — including this one — to put their authorship criteria in writing before funds are released. This section is that document.

SECTION 10

Research and analysis services

For groups that need the result rather than the skill, BioSol Centre runs the analysis directly. Quoted individually, with a free feasibility check first.

TABLE 10.1 — SERVICES OFFERED

Service	Scope
Molecular docking and virtual screening	Receptor preparation, site definition, redocking and cross-docking validation, retrospective enrichment, staged screening funnels from hundreds to millions of compounds, ML rescoring, consensus ranking, interaction analysis
Molecular dynamics simulation	System building and parameterisation, equilibration, production runs from 100 ns to 1 µs with replicas, RMSD / RMSF / Rg / SASA / H-bond / PCA / free-energy landscape analysis, convergence assessment
Binding free energy	MM-PBSA and MM-GBSA with per-residue decomposition; free-energy perturbation and umbrella sampling on request
QSAR and ML models	Data curation, model building across classical and deep architectures, rigorous validation, applicability domain, calibrated uncertainty, SHAP interpretation
ADMET and drug-likeness	Solubility, permeability, hERG, CYP, clearance, mutagenicity; drug-likeness and structural alerts; per-compound profiles
Multi-omics analysis	Bulk and single-cell RNA-seq, proteomics, metabolomics, and integrated multi-layer analysis through to pathway enrichment and network construction
Epigenomics	DNA methylation (WGBS, RRBS, arrays), ChIP-seq, ATAC-seq; differential methylation and peaks, annotation, motif discovery, integration with expression
Exome and genome sequencing	GATK best-practice pipelines; germline and somatic SNV, indel and CNV calling; annotation, filtering and ACMG-guided interpretation; trio analysis
Network and systems biology	Protein–protein interaction networks, network pharmacology, target fishing and reverse docking, gene-regulatory networks, biomarker candidates
Publication support	Manuscript structuring, methods writing, figure preparation, journal selection, cover letters, reviewer responses, data and code deposit
Generative and de novo design	Multi-objective molecular generation, scaffold hopping, R-group optimisation, retrosynthesis and synthetic-accessibility assessment
Structure prediction	Homology modelling and AI prediction with AlphaFold, ESMFold and Boltz, with honest confidence assessment

HOW A SERVICE ENGAGEMENT RUNS

1. **Describe the question** — a short email about the system, the data and what needs to be shown.
2. **Free feasibility check** — an honest answer about whether the data can answer the question, including when it cannot.
3. **Written proposal and fixed quote** — scope, methods, deliverables, timeline, price, and authorship position if the work is headed for publication.

4. **Analysis with checkpoints** — intermediate results shared; validation metrics reported as they happen.
5. **Delivery** — results, figures, methods text, code and parameters, all reproducible.
6. **Follow-up** — clarifications and reviewer-driven reanalysis within the agreed scope, at no extra charge.

Bangladeshi academic groups and self-funded students are quoted against the local rate card; a reduced academic rate applies internationally.

SECTION 11

How to enrol, pay and claim reimbursement

Steps for the applicant

1. **Email the course address** at structuralbiologyai@gmail.com stating the tier, your position, your institution and your country of residence. Cohort dates for the next intake are sent by return.
2. **Complete the screening step** — none for Basic; a twenty-minute online task for Advanced; a forty-five-minute interview for Professional, at which the project and the article-processing-charge arrangement are agreed in writing.
3. **Request a scholarship or an instalment plan** if needed, before paying. Scholarship decisions are returned within one week.
4. **Receive the invoice or payment details**, including a formal invoice for institutional payment or departmental reimbursement.
5. **Pay and confirm** — a numbered receipt with a programme reference is issued for every payment.
6. **Complete the environment check** one week before the cohort begins; failures are fixed individually by email.

For the institution

Purchase orders	Accepted; the seat is held on the purchase order rather than on payment
Payment terms	Invoice payable within thirty days
Formal invoice	Issued on request with institution name, participant, tier and dates
Group registration	10 % each for 3–5 participants; 20 % each for 6 or more from the same institution
Private cohort	On site or online for a closed group, with the teaching target replaced by one of the institution's own; from BDT 250,000 or USD 5,500
Certificates	Verifiable, naming modules and contact hours, suitable for training records

Contact

Email	structuralbiologyai@gmail.com — answered within two working days
Phone / WhatsApp	+880 1783 541054
Organisation	BioSol Centre, JUST Campus Road, Jashore · Dhaka, Bangladesh

ANNEX A

Template letter to a supervisor

Adapt the text below and send it with this prospectus attached. Replace the highlighted parts.

Dear [Professor [Name]],

I am writing to request approval and funding to attend the **[Tier] tier** of the Machine Learning and AI-Based Drug Design training programme run by BioSol Centre, at a cost of **[amount]**. The full prospectus is attached.

What it covers. The programme is hands-on training in computer-aided drug discovery: data curation, QSAR and machine-learning models with rigorous validation, protein preparation and molecular docking, large-scale virtual screening, molecular dynamics simulation with trajectory analysis and MM-PBSA binding free energy, ADMET prediction, and generative molecular design. It runs for [duration] with [hours] contact hours.

Why it is relevant to our work. [One or two sentences linking the methods to a specific project or target in the group — for example: "This would let me run the docking and MD validation for the [target] project in-house rather than waiting on a collaborator."]

What the group gets. I would return with a validated docking protocol, a trained and documented predictive model, MD trajectories with full analysis, and a reproducible software environment that rebuilds in one command. All of it transfers directly to our own targets. The entire software stack is open source, so there is no licence cost to the department, and the hosted computing environment is included in the fee — no hardware purchase is required.

Time commitment. [For Basic: five consecutive days. For Advanced: four weekends, so no working days are lost. For Professional: six months alongside normal work, with one supervision call per week.]

Cost and payment. The fee is [amount]. [If applicable: I have applied for a scholarship, which would reduce this to [amount].] BioSol Centre accepts institutional purchase orders with thirty-day payment terms and issues a formal invoice and a numbered receipt for reimbursement. Instalments are available at no additional interest.

On the publication track, if relevant. [For the Professional tier only: The programme includes a supervised research project ending in a manuscript submission. Authorship is governed by ICMJE criteria and is explicitly not guaranteed by payment — the policy is set out in full in Section 9 of the attached prospectus, and I would be glad to discuss it with you before committing.]

I would be happy to summarise what I learn for the group afterwards, and to run the methods on [project/target] on my return.

Kind regards,
[Your name]
[Position, Department]