Nanotechnology-Enabled Medical Informatics: From Atomistic Mechanisms to Intelligent Nanosystems and Accountable Clinical Decisions

Table S1. Clinical application matrix for nanotechnology-enabled medical informatics

Clinical area	Nanosystem role	Main data streams	Informatics task
Oncology	Targeted probes, nanocarriers, contrast agents	Imaging, liquid biopsy, pathology, genomics	Response prediction, delivery modelling
Cardiometabolic	Electrochemical sensors, plaque imaging agents	Continuous glucose/lactate, troponin, vitals	Trend detection, dosing support
Infection and AMR	Rapid pathogen assays, antimicrobial coatings	Point-of-care results, host response, epidemiology	Diagnosis, stewardship, surveillance
Neurology	Nanostructured electrodes, BBB-crossing carriers	Electrophysiology, imaging, behaviour	Seizure detection, closed-loop stimulation
Regenerative medicine	Nanofibre scaffolds, responsive matrices	Spatial omics, microscopy, biomechanics	Linking structure to repair
Dentistry and oral health	Remineralisation agents, implant coatings, salivary sensors	Intraoral scans, salivary markers, behaviour	Caries and periodontal risk, implant surveillance
Point-of-care and low-resource care	Paper-based, microfluidic, plasmonic tests	Offline results, delayed sync, images	Robust interpretation, quality flags

AMR, antimicrobial resistance; BBB, blood–brain barrier.

Table S2. The NanoMed-Info framework linking nanoscale evidence to clinical translation

Layer	Representative descriptors	Required metadata	Clinical purpose
Atomistic identity	Composition, facets, defects, protonation state, ligands	Simulation and characterization provenance	Reproducible material definition
Physicochemical product	Size, shape, charge, porosity, stability, dissolution	Batch, protocol, storage and uncertainty	Batch release and comparability
Biological interface	Corona, membrane contact, uptake, trafficking, clearance	Specimen and exposure context	Mechanistic safety and targeting
Device or formulation	Sensitivity, release, imaging, heating or delivery	Calibration and operating conditions	Analytical validation
Data and algorithm	Preprocessing, features, models and confidence	Version, training domain and drift	Reliable, calibrated interpretation
Clinical utility	Decision, workflow, outcome, usability and cost	Population and comparator	Benefit in the intended use
Lifecycle governance	Security, equity, updates, surveillance and disposal	Audit trail and accountability	Sustained safety and trust

Table S3. Proposed minimum reporting checklist for nanosystem-derived clinical data

Domain	Minimum items to report
Material identity	Composition; core and hydrodynamic size distributions; shape; surface chemistry and ligand density; surface charge; batch identifier
Preparation and storage	Synthesis route; purification; sterilisation; storage conditions and duration; ageing or oxidation checks
Biological context	Specimen type; exposure medium and time; corona characterisation method; donor or population characteristics
Simulation (if used)	Software and version; force field or functional; system size; sampling length; convergence and uncertainty estimates
Device and calibration	Transduction principle; device and firmware version; calibration lot; LoB, LoD, LoQ; working range; drift
Data processing	Raw-data retention; preprocessing steps and code version; quality flags; handling of missing data
Model	Model type and version; training and test populations; split strategy; calibration; subgroup performance; abstention rule
Clinical use	Intended use; target population; comparator; decision threshold; clinical action; outcomes measured
Interoperability	Data standard (e.g., FHIR); terminology codes (LOINC, SNOMED CT); units (UCUM); provenance record
Governance	Consent and privacy model; cybersecurity controls; change-control plan; post-market surveillance plan