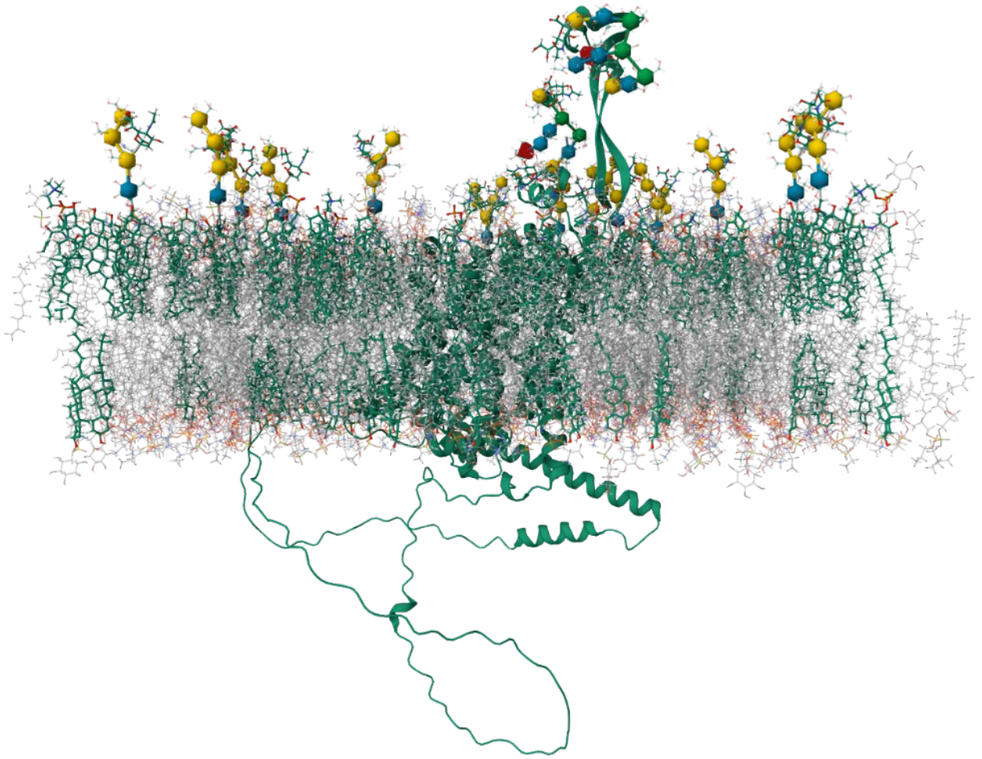
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MANIA

A reproducible residue interaction network pipeline for molecular dynamics analysis of the tumor-associated transporter NaPi2b (*SLC34A2*)



A. A. Illarionov, N. I. Akberova, R. A. Vlasenkova

Institute of Fundamental Medicine and Biology
Kazan Federal University, Kazan, Russia

Motivation and development





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Structural measures and residue interaction networks provide complementary views of protein dynamics. Their combined analysis helps describe conformational changes and contact rearrangements.

Goal: integrate these analyses in a configurable workflow with explicit measurement rules and traceable results.

MANIA 0.2.0: development since abstract submission

	Submitted workflow	Current core
Architecture	NaPi2b-focused pipeline	Independent core with optional profiles
Analysis	RIN, fingerprints and state analysis	Structural measures, partner contacts and replica aggregation
Traceability	Manifest and output status	Checked identities, frame evidence and result validation

The computational core

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Molecular inputs

Topology and trajectory
GROMACS / NAMD

Configuration

Selected methods
Atoms and physical time

MANIA Core

Input and applicability checks

Contacts, structure and networks

State analysis and comparisons

Results

CSV / JSON tables
Method status

Provenance

Settings, versions
Identities, hashes

Optional profile

NaPi2b

External applications and research

WANIA visualization

FAIR research project

Analysis capabilities

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Molecular contacts

Protein, lipid and glycan contacts
Geometric interaction types

Contact dynamics

Occupancy, episodes and lifetimes
Replay from saved observations

Structural measures

Radius of gyration
RMSD with a declared reference

Networks and frame patterns

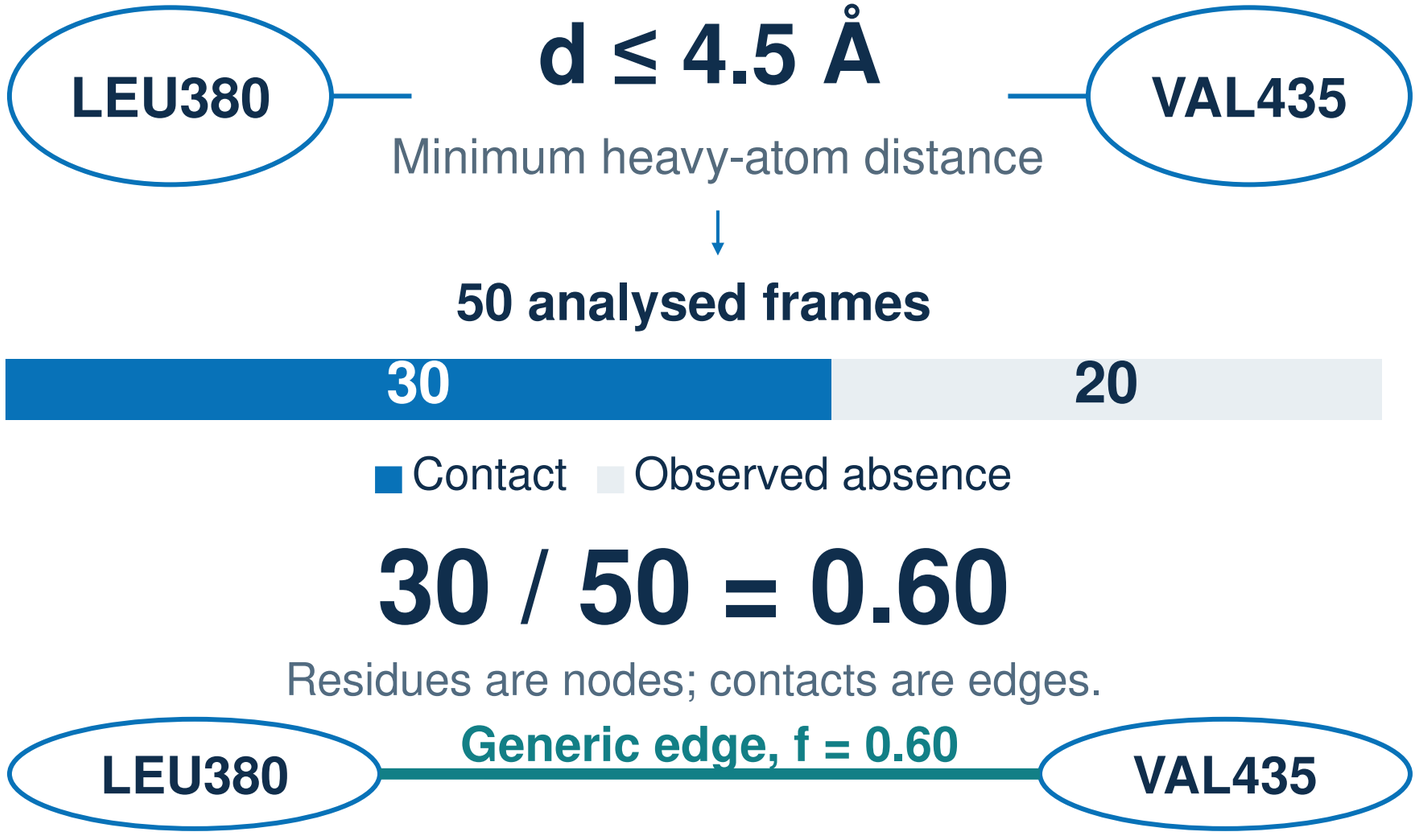
Static and temporal RIN
Centralities and communities
Fingerprints, PCA and clustering

Conditions and replicas

Matched condition metrics
Compatible replica summaries

Contact calculation

Testing: 50 frames from a 100 ns simulation



Scientific rigor and reproducibility

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Measurement rule

d ≤ 4.5 Å

Minimum heavy-atom distance
Declared atom selections
Explicit RMSD reference

→

Valid observations

Contact observed

Observed absence

Unavailable frame

Availability determines the valid denominator

→

Traceable result

Input identities
Effective settings
Software versions
Hashes and method status

Technical status and scientific qualification

Tested here: contacts and static RIN; one replica, 50 sampled frames.

RAW / Prepared	Frames	Residues	RIN edges	Frequencies	Centralities
Matched sample	50 / 50	690 / 690	4099 / 4099	**Identical**	**Identical**

Current limitations

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Area	Current boundary
Scientific qualification	Qualification of all methods on real trajectories is incomplete
Coordinates	Strict runs require suitable nonperiodic or externally prepared coordinates
Statistical inference	Condition comparisons provide descriptive summaries General p-values and confidence intervals are unavailable
Methods in development	RMSF, SASA and secondary structure

Exploratory outputs retain an explicit unvalidated status

Conclusions and next steps





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MANIA combines contact, structural and network analyses in a configurable modular core, with explicit method dependencies and reusable outputs.

Explicit atom selections, geometric definitions, physical time and observation availability define how measurements are obtained. Input identities, settings, versions and hashes preserve the origin of results.

In a NaPi2b test using 50 frames from a 100 ns trajectory, RAW and Prepared runs produced matching contact frequencies and centralities. Both all-type RINs contained 690 residues and 4,099 edges.

This demonstrates consistency for one replica. Next priorities are independent reference comparisons, cutoff and sampling sensitivity tests, and additional prepared trajectories. Planned developments include RMSF for local flexibility, SASA for solvent exposure, secondary structure analysis, and reusable extensions.