DIPARTIMENTO MATEMATICA

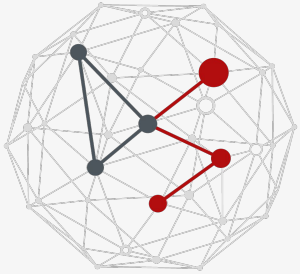
Residue Interaction Network Generator (RING)

Computer Science - Structural Bioinformatics

2020

UNIVERSITÀ DEGLI STUDI DI PADOVA

DIPARTIMENTO MATEMATICA



DATA SCIENCE
UNIVERSITY OF PADOVA

Residue Interaction Network Generator
- RING -

Master of Science in Data Science

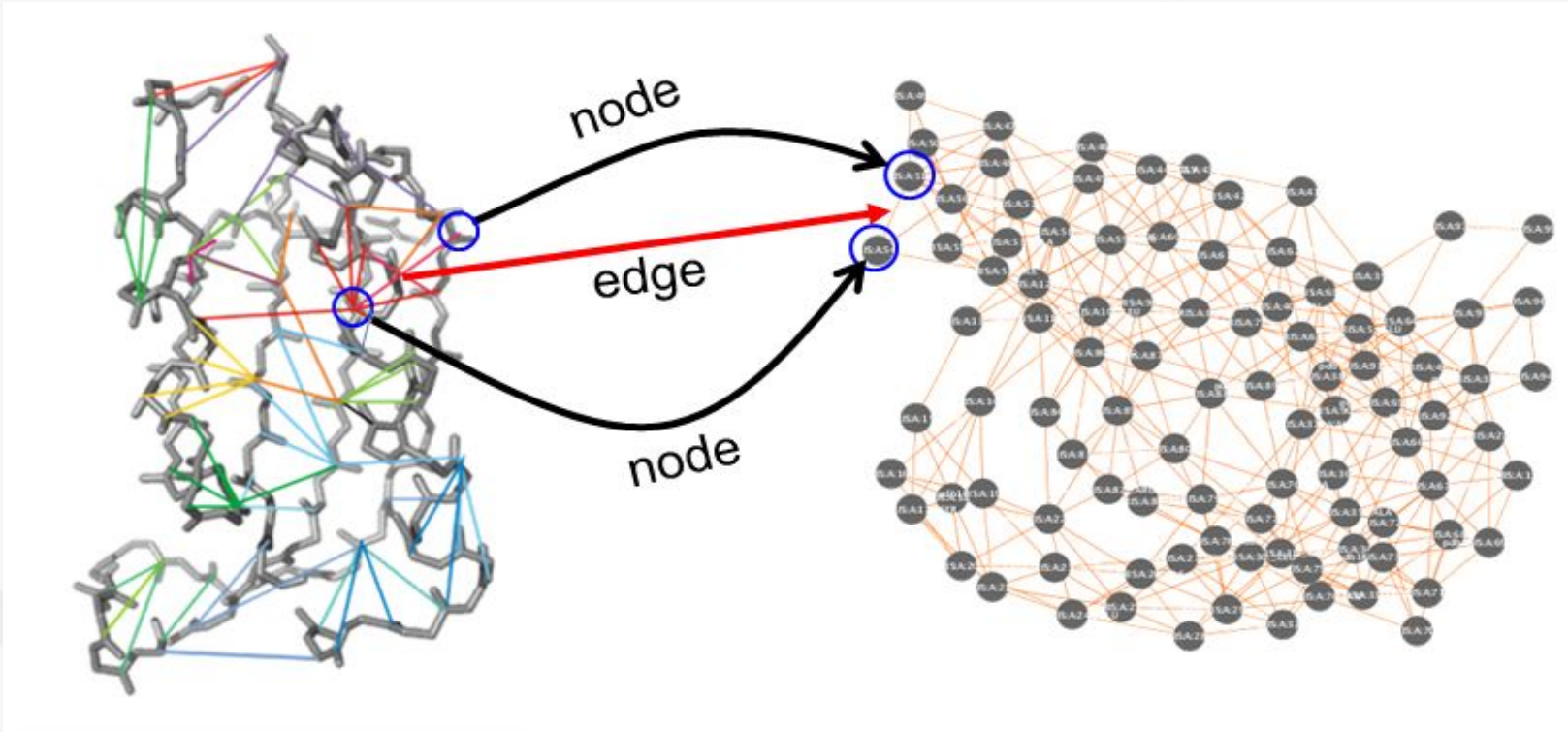
Damiano Piovesan

Concept

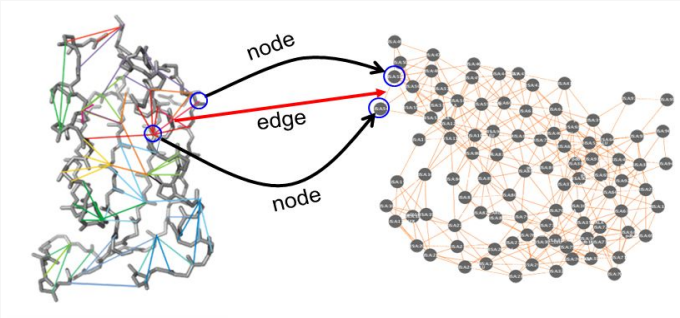
DIPARTIMENTO MATEMATICA

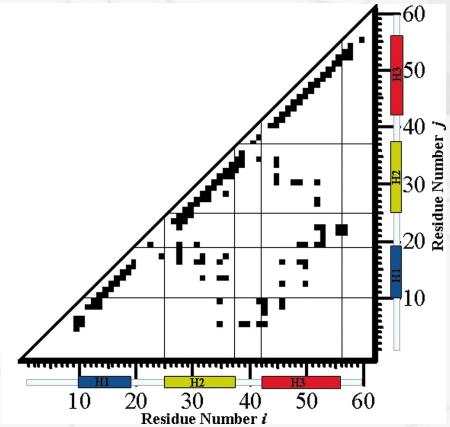
3D coordinates (PDB)

Contacts (Graph)



RIN and contact maps





DIPARTIMENTO MATEMATICA

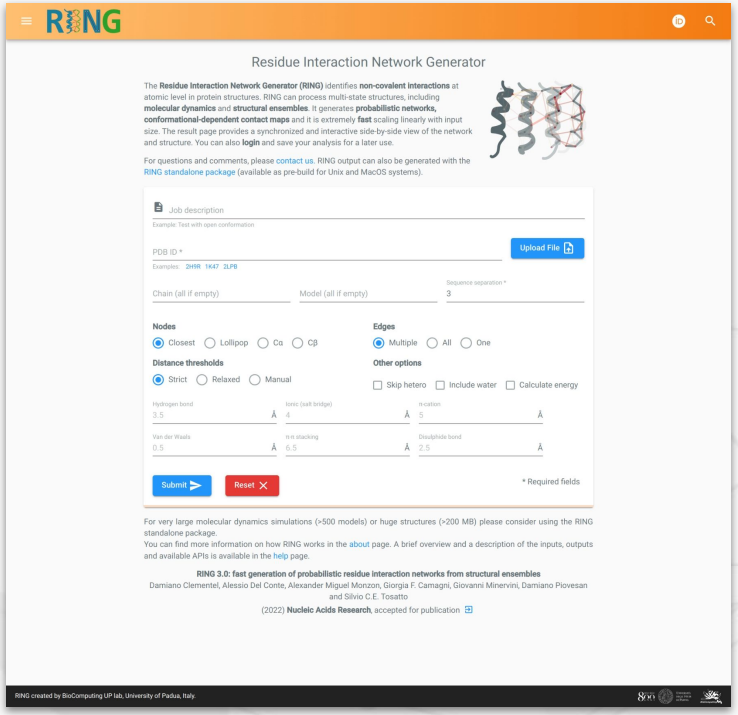
Why RINs?

- Functional features
- Effect of mutations
- Protein folding
- Intra protein domain–domain communication
- Catalytic activity
- Machine learning features (ex. contact maps)
- Molecular Dynamics Analysis

RIN generator software

- PIC (2007)
- RING (2011 – first release)
- RINerator/RINalyzer (2014)
- NAPS (2016)

Web server

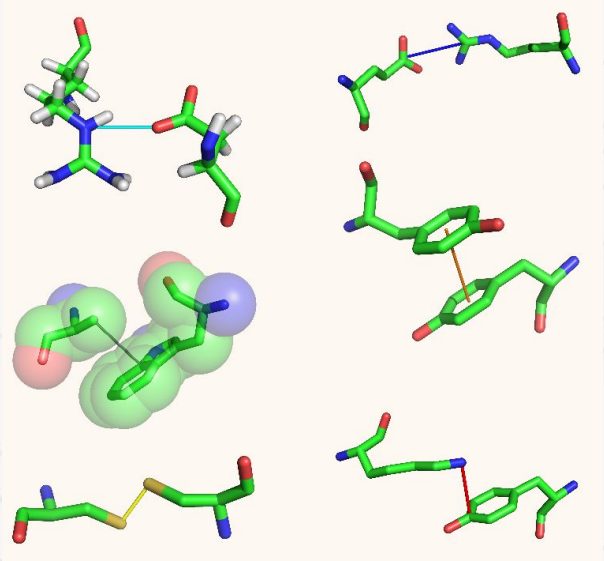


https://ring.biocomputingup.it

RING 3.0: fast generation of probabilistic residue interaction networks from structural ensembles. Clementel et al., **NAR**, 2022, 44(W1), W367–W374

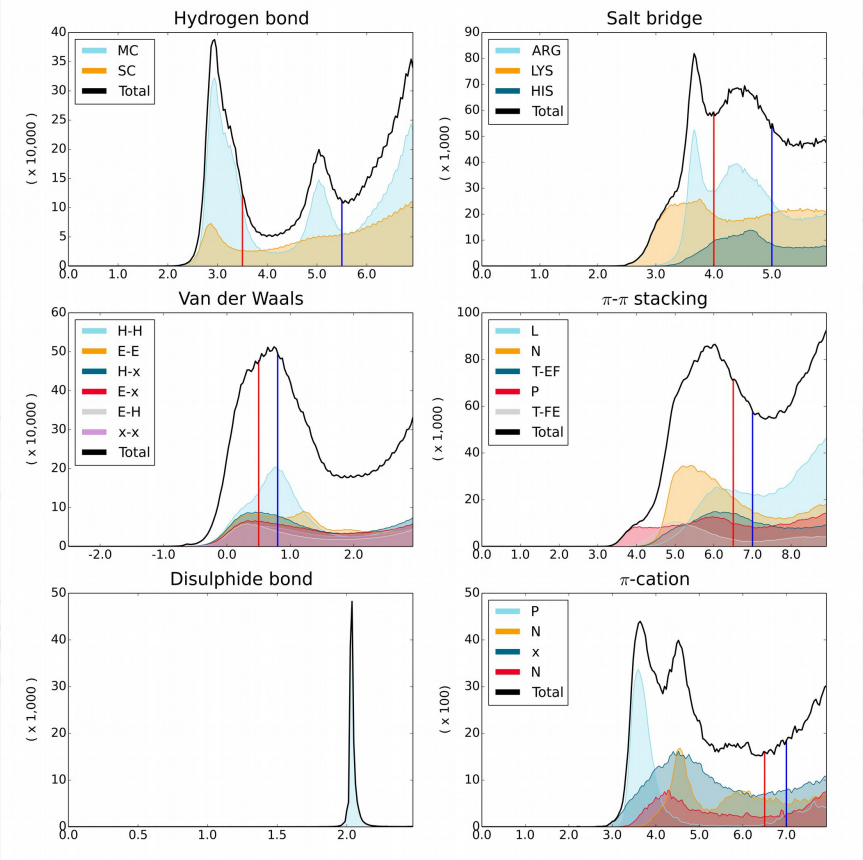
Types of interactions

- **Hydrogen bond** (HBOND)
- **Van der Waals interactions** (VDW)
- **Disulfide bridges** (SBOND)
- **Salt bridges** (IONIC)
- **π-π stacking** (PIPISTACK)
- **π-cation** (PICATION)
- **Inter-Atomic Contact** (IAC), close residues but untyped interaction



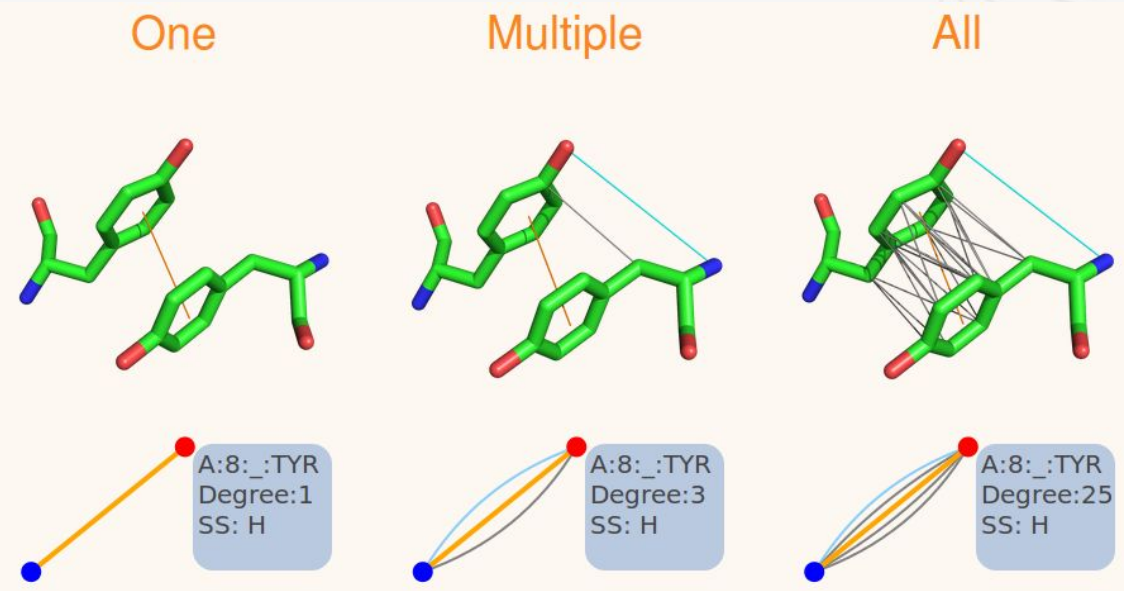
Distance cutoff

- Relaxed
- Strict (default)



The RING-2.0 web server for high quality residue interaction networks. Piovesan D, Minervini G, Tosatto, SCE. **NAR**, 2016, 44(W1), W367-74

Number of interactions per residue



DIPARTIMENTO MATEMATICA

RING Output

- Edge file (TSV)
- Node file (TSV)
- Network file (JSON, nodes + edges)

NodeId1	Interaction	NodeId2	Distance	Angle	Energy	Atom1	Atom2	Donor	Positive	Cation	Orientation	Model
A:7:_:ILE	VDW:SC_SC	B:23:_:LEU	3.863	NaN	6	CD1	CD2					1
A:10:_:GLY	HBOND:MC_MC	A:14:_:LEU	3.12	11.827	17	O	N	A:14:_:LEU				1
A:18:_:TYR	PIPISTACK:SC_SC	A:33:_:PHE	5.469	163.303	9.4	-18.707,-13.286,-31.383	-15.420,-9.669,-33.838				P n2.26,p4.98	1
A:18:_:TYR	PIPISTACK:SC_SC	A:37:_:TYR	5.594	157.475	9.4	-18.707,-13.286,-31.383	-14.451,-11.910,-28.023				P n1.33,p4.66	1
A:18:_:TYR	PIPISTACK:SC_SC	A:38:_:PHE	4.872	140.138	9.4	-18.707,-13.286,-31.383	-15.755,-16.713,-29.572				T-FE n4.66,p0.97	1
A:18:_:TYR	PIPISTACK:SC_SC	B:38:_:PHE	6.48	42.081	9.4	-18.707,-13.286,-31.383	-18.269,-19.119,-34.170				L n4.73,p6.40	1
A:32:_:ASP	IONIC:SC_SC	B:42:_:ARG	3.658	41.722	20	-10.655,-13.491,-40.731	CZ		B:42:_:ARG			2

Edge file for 2H9R

PyMOL plugin (work in progress…)

- https://github.com/BioComputingUP/ring-pymol