

# GLOSSARY OF THE TOMOCOMD-CAMPS MuLiMs SOFTWARE

## 1. General Glossary

- **ToMoCoMD**: Topological Molecular Computational Design
- **CAMPS**: Computer-Aided Modelling in Protein Science
- **MuLiMs-MCoMPAs**: Multi-Linear Maps based on N-Metric & Contact Matrices of 3D-Protein and Amino-Acids Weightings
- **LAIs**: Local Amino acidic Invariants

### 1.1. N-Tuple

- **Two**: Two-tuples
- **Three**: Three-tuples

### 1.2. Algebraic Forms

- **B**: Bilinear
- **F**: Linear
- **Q**: Quadratic
- **Tr**: Threelinear
- **TrF**: Threelinear-linear
- **TrB**: Threelinear-bilinear
- **TrQB**: Threelinear-quadratic-bilinear
- **TrC**: Threelinear-cubic

### 1.3. Matrix Forms

- **NS**: Non-Stochastic
- **SS**: Simple-Stochastic
- **MP**: Mutual Probability

### 1.4. Cut-Off

- **KA**: Keep All
- **(LG[P]) Lag P**: Path Cut-Off (topological)
- **(LG[L]) Lag L**: Length Cut-Off (geometrical)

### 1.5. Groups

#### Amino acid-types

- **RAP**: Apolar

- **RPC:** Polar positively charged
- **RNC:** Polar negatively charged
- **RPU:** Polar uncharged
- **ARO:** Aromatic
- **ALG:** Aliphatic

#### **Secondary Structure Preference**

- **FAH:** Alpha helix favoring amino acids
- **FBS:** Beta sheet favoring amino acids
- **AFT:** Beta turn favoring amino acids
- **UFG:** Uncommon in alpha helix and/or beta sheet

#### **R group**

- **ALA:** Alanine
- **ARG:** Arginine
- **ASN:** Asparagine
- **ASP:** Aspartate
- **CYS:** Cysteine
- **GLU:** Glutamate
- **GLN:** Glutamine
- **GLY:** Glycine
- **HIS:** Histidine
- **ILE:** Isoleucine
- **LEU:** Leucine
- **LYS:** Lysine
- **MET:** Methionine
- **PHE:** Phenylalanine
- **PRO:** Proline
- **SER:** Serine
- **THR:** Threonine
- **TRP:** Tryptophan
- **TYR:** Tyrosine
- **VAL:** Valine

### **1.6. Amino acid properties**

- **MM:** Side-Chain Mass
- **MV:** Side-chain volume
- **Z1:** Z1-scale
- **Z2:** Z2-scale
- **Z3:** Z3-scale

- **ECI:** Atomic charge
- **ISA:** Isotropic surface area
- **HWS:** Hoop-Woods hydropathy index
- **KDS:** Kyte-Dolittle hydropathy index
- **PIE:** Isoelectric point
- **EPS:** Heat of formation
- **PAH:** Relative Alpha helix frequency
- **PBS:** Relative Beta-sheet frequency
- **PTT:** Relative Reverse turn frequency
- **GCP1:** Geometric compatibility parameter 1
- **GCP2:** Geometric compatibility parameter 2

### 1.7. Aggregation Operators

- **N1:** Manhattan norm
- **N2:** Euclidean norm
- **N3:** Minkowski norm
- **GM:** Geometric Mean
- **AM:** Arithmetic Mean
- **P2:** Quadratic Mean
- **P3:** Potential Mean
- **HM:** Harmonic Mean
- **V:** Variance
- **S:** Skewness
- **K:** Kurtosis
- **SD:** Standard Deviation
- **VC:** Variation Coefficient
- **RA:** Range
- **Q1:** Percentile 25
- **Q2:** Percentile 50
- **Q3:** Percentile 75
- **I50:** Inter-quartile Range
- **MX:** Maximum value
- **MN:** Minimum value
- **AC:** Autocorrelation
- **GV:** Gravitational
- **TS:** Total sum
- **MIC:** Mean Information Content
- **TIC:** Total Information Content
- **SIC:** Standardized Information Content
- **ES:** Electropotological state

## 2. MuLiMs-MCoMPAs Glossary

## 2.1. 3D-Protein Representations

- **CA:** Alpha-Carbon Atom
- **CB:** Beta-Carbon Atom
- **AB:** Amide Bond-Carbon Atom
- **AVG:** Pseudo Atom (Arithmetic mean of the spatial coordinates (x,y,z) of all amino acid atoms(heavy))

## 2.2. (Dis)-Similarity Measures

- **M01:** Minkowski metric for  $p=0.25$
- **M02:** Minkowski metric for  $p=0.50$
- **M03:** Minkowski metric for  $p=1$  or Manhattan metric
- **M04:** Minkowski metric for  $p=1.5$
- **M05:** Minkowski metric for  $p=2$  or Euclidean metric
- **M06:** Minkowski metric for  $p=2.5$
- **M07:** Minkowski metric for  $p=3$
- **M08:** Minkowski metric for  $p=\text{infinity}$  or Chebyshev metric
- **M09:** Personalized (p value) Minkowski
- **M10:** Canberra metric
- **M11:** Lance-Williams metric
- **M12:** Clark metric
- **M13:** Soergel metric
- **M14:** Bhattacharyya metric
- **M15:** Wave-Edges metric
- **M16:** Angular Separation metric
- **M17:** SL-Like metric
- **M18:** Average Euclidean metric
- **M19:** Squared Euclidean metric
- **M20:** Pearson
- **M21:** Cosine-Ochiai
- **M22:** Chord
- **M23:** Fossum
- **M24:** Tanimoto
- **M25:** Kulczynski
- **M26:** Sokal-Sneath
- **M27:** Simpson
- **M28:** Ruzicka
- **M29:** Dice
- **M30:** Identity Corrected
- **M31:** Additivity
- **M32:** Proportionality Corrected
- **M33-M34:** Triangle Area
- **M35-M36:** Triangle's Incircle Area

- **M37-M38:** Summation Sides
- **M39:** Angle between sides
- **M40:** Bond angle
- **M41-M42:** JOI RULE
- **M43-M44:** MIN RULE
- **M45-M46:** MAX-RULE
- **M47-M48:** AVE-RULE
- **M49-M50:** MED-RULE
- **M51-M52:** WAR-RULE
- **M53-M54:** ADJ-RULE
- **M55-M56:** MAH-RULE
- **M57-M58:** ADD-RULE
- **M59-M60:** SUM-RULE
- **M61-M62:** PRO-RULE
- **M63-M64:** QUA-RULE
- **M65-M66:** GEO-RULE
- **M67-M68:** RAN-RULE