N

- **Narumi–Katayama index** → vertex degree
- **NASAWIN descriptors** → substructure descriptors (⊙ fingerprints)
- **Natural Bond Orbital analysis** → quantum-chemical descriptors
- **NCD descriptors** → molecular descriptors (⊙ invariance properties of molecular descriptors)
- ***ND* indices** → spectral indices (⊙ A_{xi} eigenvalue indices)

Nearest Neighboring Code (*NNC*)

This is a → *local vertex invariant* derived both from the → *H-filled molecular graph* and the → *Graph of Atomic Orbitals* and defined to distinguish the different atom types in the framework of the → *OCWLI* approach [Toropov and Toropova, 2002a; Toropov, Nesterov *et al.*, 2003a]. From the H-filled molecular graph, it is calculated as

$$NNC_i = 100 \cdot \delta_i + 10 \cdot \delta_i(\mathrm{C}) + \delta_i(\mathrm{H})$$

where δ_i is the total number of neighbors of the *i*th atom, that is, its → *vertex degree*, and δ_i(C) and δ_i(H) are the number of neighbors of the *i*th atom, which are carbon and hydrogen atoms, respectively.

The Nearest Neighboring Code of the *i*th vertex in the Graph of Atomic Orbitals is calculated as [Toropov and Toropova, 2004]:

$$^{GAO}NNC_i = 100 \cdot \delta_i + 10 \cdot \delta_i(2\mathrm{p}^2) + \delta_i(1\mathrm{s}^1)$$

where δ_i is the total number of neighbors of the *i*th atom, and $\delta_i(2p^2)$ and $\delta_i(1s^1)$ are the number of neighbors that correspond to $2p^2$ atomic orbitals and the number of neighbors that correspond to $1s^1$ atomic orbitals in the graph, respectively.

- **negative predictive value** → classification parameters
- **negentropy** ≡ *total information content* → information content
- **neighborhood-distance map matrix** → biodescriptors (⊙ proteomics maps)
- **neighborhood Euclidean matrix** ≡ *neighborhood geometry matrix* → molecular geometry
- **neighborhood geometry matrix** → molecular geometry
- **neighborhood information content** → indices of neighborhood symmetry
- **neighborhood matrices** → matrices of molecules
- **neighborhood of a vertex** → indices of neighborhood symmetry

Molecular Descriptors for Chemoinformatics, Volume I: Alphabetical Listing
Roberto Todeschini and Viviana Consonni

ISBN: 978-3-527-31852-0

- **neighborhood total information content** → indices of neighborhood symmetry
- **net atomic charges** ≡ *atomic charges* → charge descriptors
- **NICS index** → delocalization degree indices
- **Nikolić–Trinajstić–Randić index** → Wiener index
- **NOAEL** ≡ *No-Observed-Adverse-Effect Level* → biological activity indices (⊙ toxicological indices)
- **NOEL** ≡ *No-Observed-Effect Level* → biological activity indices (⊙ toxicological indices)
- **nonadjacent number** → Hosoya Z index
- **nonerror rate** → classification parameters
- **non-Omega polynomial** → Omega polynomial
- **nonoverlapping volume** → minimal topological difference
- **nonoverlap steric volume** → molecular shape analysis (⊙ common overlap steric volume)
- **No-Observed-Adverse-Effect Level** → biological activity indices (⊙ toxicological indices)
- **No-Observed-Effect Level** → biological activity indices (⊙ toxicological indices)
- **normal boiling point** → physico-chemical properties (⊙ boiling point)
- **normalized atomic walk count** → walk counts
- **normalized centric index** → centric indices (⊙ Balaban centric index)
- **normalized extended connectivity** → canonical numbering (⊙ Morgan's extended connectivity algorithm)
- **normalized fragment topological indices** → fragment topological indices
- **normalized Laplacian matrix** → Laplacian matrix
- **normalized molecular moment** → moment indices
- **normalized number of ring systems** → ring descriptors
- **normalized quadratic index** ≡ *quadratic index* → Zagreb indices
- **normalized root mean square deviation** ≡ *normalized root mean square error* → regression parameters
- **normalized root mean square error** → regression parameters
- **normalized Szeged property matrices** → Szeged matrices
- **normalized vertex distance complexity** → topological information indices
- **normalized Wiener index** → Wiener index
- **Norrington lipophilic constant** → lipophilicity descriptors (⊙ Hansch–Fujita hydrophobic substituent constants)
- **N_t index** → spectral indices
- **nuclear information content** → atomic information indices
- **nucleophilic atomic frontier electron density** → quantum-chemical descriptors
- **nucleophilic charge** → quantum-chemical descriptors (⊙ nucleophilic atomic frontier electron density)
- **nucleophilic frontier electron density index** → quantum-chemical descriptors (⊙ nucleophilic atomic frontier electron density)
- **nucleophilic indices** → reactivity indices
- **nucleophilicity–electrophilicity index** → quantum-chemical descriptors (⊙ Fukui functions)
- **nucleophilic substituent constant** → electronic substituent constants (⊙ resonance electronic constants)
- **nucleophilic superdelocalizability** → quantum-chemical descriptors
- **nucleus-independent chemical shift index** ≡ *NICS index* → delocalization degree indices

- **number of atoms in substituent specific positions** → steric descriptors
- **number of ring systems** → ring descriptors
- **number of terms in the model** → model complexity
- **Nys–Rekker hydrophobic fragmental constants** → lipophilicity descriptors