J

- **Jaccard/Tanimoto coefficient** → similarity/diversity
- **Jaccard–Tanimoto similarity coefficient** → similarity/diversity (Table S9)
- **JEDA** ≡ *Joint Entropy-based Diversity Analysis* → cell-based methods
- **Jenkins steric parameter** → steric descriptors
- **J_p statistics** → regression parameters
- **J_t index** → Balaban distance connectivity index
- ***J′/J* index** → bond order indices (⊙ graphical bond order)
- **JJ indices** → Wiener matrix
- **Jochum–Gasteiger canonical numbering** → canonical numbering
- **Joint Entropy-based Diversity Analysis** → cell-based methods
- **joint entropy** → information content

Joshi electronic descriptors

These are molecular → *electronic descriptors* assuming that the minimum energy conformation of a molecule represents the optimal picture of the electronic charge distribution in the whole molecule [Joshi, Meister *et al.*, 1993, 1994].

The Joshi electronic descriptors (JS1–JS5) are defined as

$$JS1 = \frac{E_R}{E_H} \qquad JS2 = \frac{E_R - E_H}{E_H} \qquad JS3 = \frac{E_R - E_{HS}}{E_H}$$

$$JS4 = \frac{E_R - \sum_j E_{R_j}}{E_H} \qquad JS5 = \frac{E_R - \sum_j E_{R_j} - E_{HS}}{E_H}$$

where E is the ΔH_f conformational energy value of the global minimum energy conformer calculated by → *computational chemistry* (AM1) methods. The subscripts R, H, and HS refer to a R-substituted compound, the unsubstituted compound, and a compound for which the aromatic moiety is unsubstituted but the side chain is substituted in a similar way. E_{Rj} is the energy contribution due to the formation of the *j*th substituent group calculated by subtracting the energy value of methane from that of the corresponding substituted methane. The summation in JS4 and JS5 depends on the series of studied compounds.

- **Joshi steric descriptor** → steric descriptors
- **Julg–François index** → delocalization degree indices

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- **Jurs cost function** → regression parameters
- **Jurs shape indices** ≡ *shadow indices*