MERSY descriptors

MerSy (MERA Symmetry) descriptors are calculated usung 3D representation of molecules in the framework of MERA algorithm and include the quantitative estimations of molecular symmetry with respect to symmetry axes from C2 to C6 and to inversion-rotational axis from S1 to S6 in the space of principal rotational invariants about each orthogonal component. Additionally the molecular chirality is quantitatively evaluated in agreement with the negative criterion of chirality (the absence of inversion-rotational axes in the molecular point group).

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All MerSy descriptors vary in the range from 0 to 1 and possess a meaning of the presence of the symmetry element.

- SYMC2X is the C2 point group of symmetry about the first (X) rotational invariant.
- SYMC2Y is the C2 point group of symmetry about the second (Y) rotational invariant.
- SYMC2Z is the C2 point group of symmetry about the third (Z) rotational invariant.
- SYMC2 is the aggregate estimate of the C2 point group presence.

- SYMC3X is the C3 point group of symmetry about the first (X) rotational invariant.
- SYMC3Y is the C3 point group of symmetry about the second (Y) rotational invariant.
- SYMC3Z is the C3 point group of symmetry about the third (Z) rotational invariant.
- SYMC3 is the aggregate estimate of the C3 point group presence.

- SYMC4X is the C4 point group of symmetry about the first (X) rotational invariant.
- SYMC4Y is the C4 point group of symmetry about the second (Y) rotational invariant.
- SYMC4Z is the C4 point group of symmetry about the third (Z) rotational invariant.
- SYMC4 is the aggregate estimate of the C4 point group presence.

- SYMC5X is the C5 point group of symmetry about the first (X) rotational invariant.
- SYMC5Y is the C5 point group of symmetry about the second (Y) rotational invariant.
- SYMC5Z is the C5 point group of symmetry about the third (Z) rotational invariant.
- SYMC5 is the aggregate estimate of the C5 point group presence.

- SYMC6X is the C6 point group of symmetry about the first (X) rotational invariant.
- SYMC6Y is the C6 point group of symmetry about the second (Y) rotational invariant.
- SYMC6Z is the C6 point group of symmetry about the third (Z) rotational invariant.
- SYMC6 is the aggregate estimate of the C6 point group presence.
- SYMS1X is the S1 point group of symmetry about the first (X) rotational invariant (plane of symmetry YOZ).
- SYMS1Y is the S1 point group of symmetry about the second (Y) rotational invariant (plane of symmetry XOZ).
- SYMS1Z is the S1 point group of symmetry about the third (Z) rotational invariant (plane of symmetry XOY).
- SYMS1 is the aggregate estimate of the S1 point group (plane of symmetry) presence.

- SYMS2 is the aggregate estimate of the S2 point group presence. S2 point group is the center of symmetry which is independent from axes.

- SYMS3X is the S3 point group of symmetry about the first (X) rotational invariant.
- SYMS3Y is the S3 point group of symmetry about the second (Y) rotational invariant.
- SYMS3Z is the S3 point group of symmetry about the third (Z) rotational invariant.
- SYMS3 is the aggregate estimate of the S3 point group presence.

- SYMS4X is the S4 point group of symmetry about the first (X) rotational invariant.
- SYMS4Y is the S4 point group of symmetry about the second (Y) rotational invariant.
- SYMS4Z is the S4 point group of symmetry about the third (Z) rotational invariant.
- SYMS4 is the aggregate estimate of the S4 point group presence.

- SYMS5X is the S5 point group of symmetry about the first (X) rotational invariant.
- SYMS5Y is the S5 point group of symmetry about the second (Y) rotational invariant.
- SYMS5Z is the S5 point group of symmetry about the third (Z) rotational invariant.
- SYMS5 is the aggregate estimate of the S5 point group presence.

- SYMS6X is the S6 point group of symmetry about the first (X) rotational invariant.
- SYMS6Y is the S6 point group of symmetry about the second (Y) rotational invariant.
- SYMS6Z is the S6 point group of symmetry about the third (Z) rotational invariant.
- SYMS6 is the aggregate estimate of the S6 point group presence.

CHIR is the chirality of a molecule estimating as a probability of absence of inversion-rotational axes in the molecular point group (the negative criterion of chirality).