Computer-Aided Molecular Design: Fundamentals, Methods, and Applications

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Nomenclature

A	Helmholtz free energy
A_k	Matrix of number of occurrences of molecular groups in molecule k
ACO	Ant colony optimization
ADI	Absorption-desorption index
AHP	Analytic hierarchy process
a_{mn}	Group-group interaction parameter used in calculation of γ_i^c
AUP^M	Augmented property index
AP	Augmented penalty
ASOG	Analytical Solution of Groups
BB	Branch and bound
BM	Big-M formulation
b_{mn}	Group-group interaction parameter for higher order approximation used in calculation of γ_i^c
C	Vector of concentration of components/molecules
CADD	Computer-aided drug design
CAM^{b}D	Computer-aided mixture design
CAMD	Computer-aided molecular design
CAMPCD	Computer-aided molecular, process and control design
CAMPD	Computer-aided molecular and process design
CAM^{R}D	Computer-aided molecular design for reactions
CAM^{u}D	Computer-aided molecular design under uncertainty
CAOS	Computer-aided organic synthesis
C_j	Cluster for property j
c_k	Concentration of k^{th} component/molecule
c_{mn}	Group-group interaction parameter for higher order approximation used in calculation of γ_i^c
CoMT	Continuous molecular targeting
COSMO	Conductor-like Screening Model
D	Vector of design variables
DEA	Data envelopment analysis
DFO	Derivative-free optimization
DFT	Density functional theory
d_i	i^{th} design variable
D_j	Contributions of second-order groups
E	Vector of disturbances
EACO	Efficient ACO
EBS	Environmentally benign solvent
E_l	Contributions of third-order-groups
EoS	Equation of state
ER	Equality relaxation
F	Vector of objective functions
F_j	j^{th} objective function
GA	Genetic algorithms
GBD	Generalized Benders decomposition
GC	Group contributions