Metrics

**Molecular Formula (MolForm):**

Molecular formula determined by Compound Identification Algorithm, determined using the program Formularity. [Tolic et al., 2017](https://pubs.acs.org/doi/abs/10.1021/acs.analchem.7b03318)1

**Aromaticity Index (AI):**



When the numerator or denominator is ≤0, aromaticity is 0. When aromaticity >0.5 a compound is considered not aromatic, 0.5≤aromaticity <0.67a compound is aromatic, and when aromaticity ≥0.67a compound is a condensed aromatic. [Koch & Dittmar, 2006](https://onlinelibrary.wiley.com/doi/abs/10.1002/rcm.2386)2 [Erratum](https://onlinelibrary.wiley.com/doi/full/10.1002/rcm.7433)3

**Modified Aromaticity Index (AI\_Mod):**



When the numerator or denominator is ≤0, modified aromaticity is 0. When modified aromaticity >0.5 a compound is considered not aromatic, 0.5≤ modified aromaticity <0.67a compound is aromatic, and when modified aromaticity ≥0.67 a compound is a condensed aromatic. [Koch & Dittmar, 2006](https://onlinelibrary.wiley.com/doi/abs/10.1002/rcm.2386)2 [Erratum](https://onlinelibrary.wiley.com/doi/full/10.1002/rcm.7433)3

**Double Bond Equivalent (DBE):**

Also known as the degree of unsaturation. Calculated as:



[Koch & Dittmar, 2006](https://onlinelibrary.wiley.com/doi/abs/10.1002/rcm.2386)2 [Erratum](https://onlinelibrary.wiley.com/doi/full/10.1002/rcm.7433)3

**Double Bond Equivalent minus Oxygen (DBE\_O):**

An alternative way of calculating DBE. Calculated as:



[Koch & Dittmar, 2006](https://onlinelibrary.wiley.com/doi/abs/10.1002/rcm.2386)2 [Erratum](https://onlinelibrary.wiley.com/doi/full/10.1002/rcm.7433)3

**Nominal Oxidation State of Carbon (NOSC):**

Calculated as:



[Koch & Dittmar, 2006](https://onlinelibrary.wiley.com/doi/abs/10.1002/rcm.2386)2 [Erratum](https://onlinelibrary.wiley.com/doi/full/10.1002/rcm.7433)3

**Gibbs Free Energy (GFE or Gibbs):**

Cox Gibbs Free Energy. Calculated as: 60.3−28.5∗NOSC [LaRowe & Van Cappellen, 2011](https://www.sciencedirect.com/science/article/pii/S0016703711000378)4

**Kendrick Defect (kdefect or KenDef):**

Kendrick Defect = Nominal Kendrick Mass - Kendrick Mass [Hughey et al., 2001](https://pubs.acs.org/doi/pdf/10.1021/ac010560w)5

**Kendrick Mass (kmass or KenMass):**

*IUPACmass∗(14/14.01565)*, where IUPAC mass is based on the 12C atomic mass as exactly 12 Da. [Hughey et al., 2001](https://pubs.acs.org/doi/pdf/10.1021/ac010560w)5

**Boundary Sets (bs1\_class, bs2\_class, and bs3\_class)**

These are boundary sets which are used to assign compound classes to molecular formula. Boundary sets 1 and 2 are both Van Krevelen-based (Kim et al., 2003 & Bailey et al., 2017) while boundary set 3 further integrates stoichiometry to assign modified compound classes (Rivas-Urbach et al., 2018). [Kim et al., 2003](https://www.ncbi.nlm.nih.gov/pubmed/14710810)6 [Bailey et al., 2017](https://www.sciencedirect.com/science/article/pii/S0038071716306447)7 [Rivas-Urbach et al., 2018](https://pubs.acs.org/doi/abs/10.1021/acs.analchem.8b00529)8

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