Supporting Information for CLEAN

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Bernd Jastorff, Reinhold Störmann und Johannes Ranke

Thinking in Structure-Activity Relationships – A Way Forward Towards Sustainable Chemistry

Electronic Supporting Information

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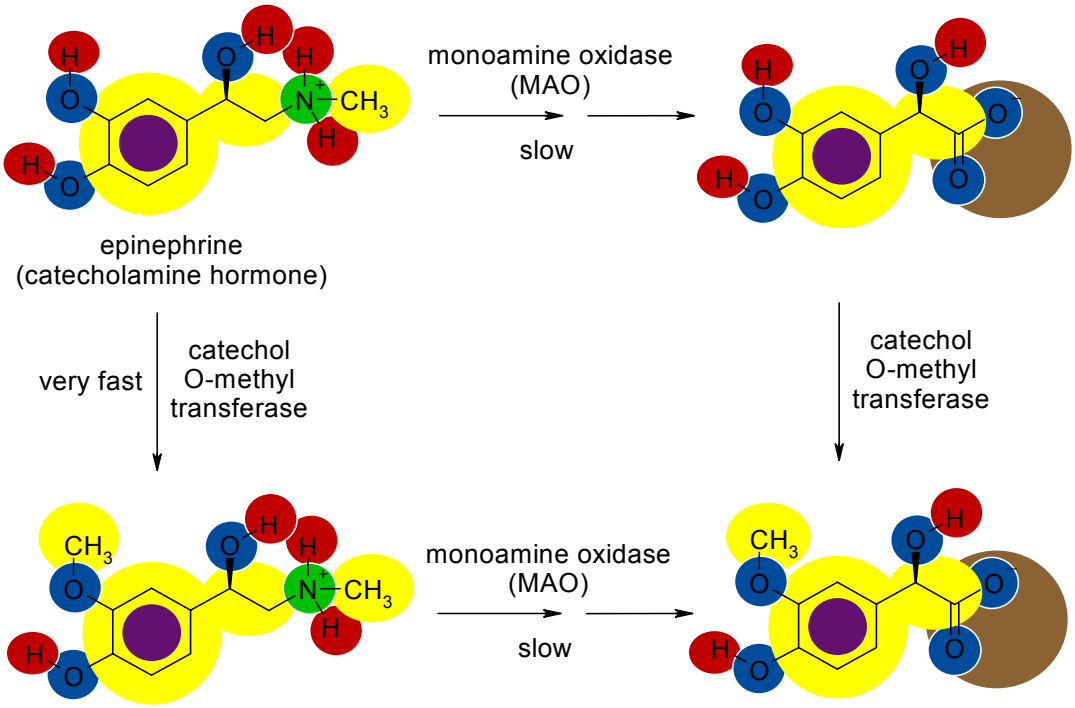
Color Code for Molecular Interactions and Supplementary Figures 1–2

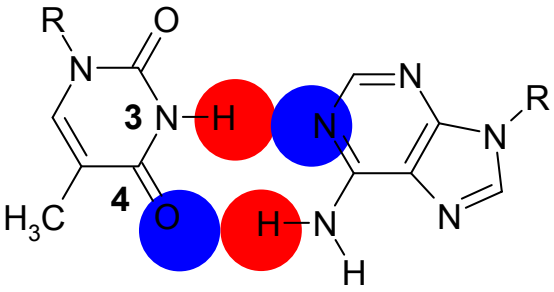
To facilitate the association of molecular interaction potentials with the drawn molecule, defined color codes for each type of interaction potential have been defined and are used to emphasize the importance of these interactions:

Charge transfer	violet
H-Acceptor	blue
H-Donor	red
Hydrophobic potential	yellow
Negative Charge	brown
Positive Charge	green

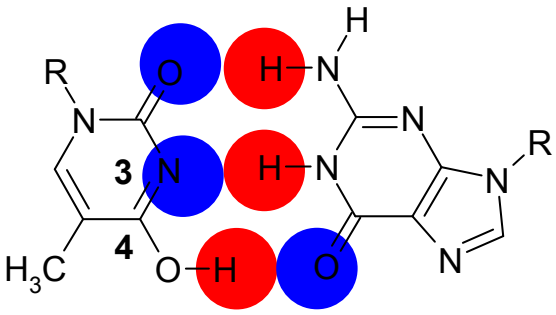
There is no one-to-one relation between atom type and interaction potential. For example, the color code for a hydrogen atom can be red or yellow depending on the neighboring atom and the polarization of the bond to it.



Supplementary Figure 1. „Switching off“ epinephrine in the human body. One metabolic pathway replaces the positive charge on epinephrine by a negatively charged group, the other pathway works by transforming a phenolic OH-group from a H-bond donor into a hydrophobic methyl ether. Both transformations cause a drastically lower affinity to the catecholamine receptor.



thymine adenine base pair
(TA)



thymine* guanine base pair
(T*A)

Supplementary Figure 2. Illustration of the pairing of thymine with adenine as normally present in DNA (left). To the right, an abnormal pairing of the enol form of thymine with guanine is shown, which leads to mutations in the genome.