

LFER studies compared to Log D data in describing the Aqueous Normal Phase ANP retention – Tips & Suggestions

Log D (*the Distribution Coefficient*) is known as the octanol : water partition coefficient which accounts for the ionization state of the **analyte**. Log D is pH dependent and is equivalent to log P for non-ionizable compounds. Log D is often used for describing reversed phase retention properties, since it is a measure of the **analyte**'s hydrophobicity.

However, log D is of limited use in describing other types of retention mechanisms such as ANP or HILIC. This is because hydrophobicity is of relatively lower importance in these mechanisms, which are primarily driven by forces of hydrogen bonding, proton donor-acceptor interactions, and/or partitioning in a water layer (in the case of HILIC). LFER can distinguish among these various interactions whereas log D cannot.

Linear Free Energy Relationships (LFER) on the other hand provide more detailed information on these types of interactions. These studies can demonstrate important theoretical models for understanding how ANP retention works as well as how it differs from the HILIC retention mode.

References:

- J. Soukup, P. Jandera, Hydrosilated silica-based columns: the effects of mobile phase and temperature on dual HILIC-RP separation mechanism of phenolic acids, *J. Chromatogr. A* 1228 (2012)125-134.
- J. Soukup, P. Jandera, The effect of temperature and mobile phase composition on separation mechanism of flavonoid compounds on Hydrosilated silica-based columns. *J. Chromatogr. A*, 1245 (2012) 98-108 .
- P. Jandera, T. Hájek, V. Škeříková, J. Soukup, Dual hydrophilic interaction-reversed phase retention mechanism on polar columns: Structural correlations and implementation for 2D separations on a single column. *J.Sep. Sci.*, 33 (2010) 841-852.

