ranging from 18 to 765 g/mol (median=180); only 3% >500 g/mol. Approximately 53% of the chemicals in the database have functional groups which are ionizable in the pH range of 6 to 7.4, with 31% being appreciably ionized. The compiled log KP values ranged from −5.8 to 0.1 cm/h (median= −2.6). The selected subset of the KP data was then used to evaluate eight representative KP models that can be readily applied for HTS assessments, i.e., parameterized with KOW and MW. The analysis indicates that a version of the SKINPERM model performs the best against the selected dataset. Comparisons of representative KP models against model input parameter property ranges (sensitivity analysis) and against chemical datasets requiring human health assessment were conducted to identify regions of chemical properties that should be tested to address uncertainty in KP models and HTS exposure assessments.

Caron, G. et al. (2018). "Log *P* as a tool in intramolecular hydrogen bond considerations." *Drug Discov Today Technol* 27:65–70.

Intramolecular hydrogen bonding (IMHB) considerations are gaining relevance in drug discovery and a molecular descriptor which can predict very early the capacity of a compound to form IMHB is needed to speed up the optimization process of drug candidates. Although log *P*oct is largely used for optimization purposes, in this paper we firstly use the Block Relevance (BR) analysis to theoretically show how log *P*oct is not a convenient choice to assess IMHB properties of candidates. Then, we discuss the limits of log *P*oct and introduce Deltalog *P*oct-tol, i.e., the difference between log *P*oct and log *P*tol (the logarithm of the partition coefficient in the toluene/water system). Finally, we provided some examples also, including bRo5 protease inhibitors, to clarify how to interpret Deltalog *P*oct-tol values.

Cordero, C. et al. (2015). "Comprehensive two-dimensional gas chromatography and food sensory properties: Potential and challenges." *Anal Bioanal Chem* 407(1):169–191.

Modern omics disciplines dealing with food flavor focus the analytical efforts on the elucidation of sensory-active compounds, including all possible stimuli of multimodal perception (aroma, taste, texture, etc.) by means of a comprehensive, integrated treatment of sample constituents, such as physicochemical properties, concentration in the matrix, and sensory properties (odor/taste quality, perception threshold). Such analyses require detailed profiling of known bioactive components as well as advanced fingerprinting techniques to catalog sample constituents comprehensively, quantitatively, and comparably across samples. Multidimensional analytical platforms support comprehensive investigations required for flavor analysis by combining information on analytes' identities, physicochemical behaviors (volatility, polarity, partition coefficient, and solubility), concentration, and odor quality. Unlike other omics, flavor metabolomics and sensomics include the final output of the biological phenomenon (i.e., sensory perceptions) as an additional analytical dimension, which is specifically and exclusively triggered by the chemicals analyzed. However, advanced omics platforms, which are multidimensional by definition, pose challenging issues not only in terms of coupling with detection systems and sample preparation, but also in terms of data elaboration and processing. The large number of variables collected during each analytical run provides a high level of information but requires appropriate strategies to exploit fully this potential. This review focuses on advances in comprehensive two-dimensional gas chromatography and analytical platforms combining two-dimensional gas chromatography with olfactometry, chemometrics, and quantitative assays for