

## Appendix G: XpertAI citation evaluations

Reference	Citation	Is citation correct?	Supporting evidence
Case study 1: OMS			
Kökçam-Demir, U., Goldman, A., Esrafilı, L., Gharib, M., Morsali, A., Weingart, O., & Janiak, C. (2020). Coordinatively unsaturated metal sites (open metal sites) in metal–organic frameworks: design and applications. Chemical Society Reviews.	The documents discuss the importance of maintaining the structural integrity of MOFs while modifying metal ions to create OMS (Kökçam-Demir et al., 2020).	Yes	In MOF structures any change to the metal ions in the metal SBU must ensure the integrity of the network. Importantly, the MOF structure must not collapse, and their crystallinity and porosity should be preserved, that is, a labile terminal ligands should be removed without damage to the framework. The obtained not fully coordinated metal ions are termed open metal sites (OMS) or coordinatively unsaturated sites (CUS) or occasionally also open coordination sites (OCS).
Chung, Y. G., Haldoupis, E., Bucior, B. J., Haranczyk, M., Lee, S., Zhang, H., Vogiatzis, K. D., Milisavljevic, M., Ling, S., Camp, J. S., Slater, B., Siepmann, J. I., Sholl, D. S., & Snurr, R. Q. (2019). Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal–Organic Framework Database: CoRE MOF 2019. Journal of Chemical & Engineering Data.	The documents highlight the role of density in differentiating MOF structures and its impact on adsorption properties	No	
Zhou, W., Wu, H., & Yildirim, T. (2008). Enhanced H <sub>2</sub> Adsorption in Isostructural Metal-Organic Frameworks with Open	The documents discuss the influence of ionic radius on the binding strength of gases in MOFs, suggesting that	Yes	Our results suggest that the relative strength of interaction of M <sup>2+</sup> -H <sub>2</sub> may be empirically predicted by the ionic radius of the

Metal Sites: Strong Dependence of the Binding Strength on Metal Ions. Journal of the American Chemical Society.	cation size affects the coordination environment		cations in same coordination environment. This may provide a convenient guideline for the future development of MOFs with unsaturated metal sites.
Case study 2: PLD			
Chung, Y. G., Haldoupis, E., Bucior, B. J., Haranczyk, M., Lee, S., Zhang, H., Vogiatzis, K. D., Milisavljevic, M., Ling, S., Camp, J. S., Slater, B., Siepmann, J. I., Sholl, D. S., & Snurr, R. Q. (2019). Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal–Organic Framework Database: CoRE MOF 2019. *Journal of Chemical & Engineering Data*.	The documents discuss the importance of crystal density as a descriptor for MOF structures, which is related to the volume per atom. Variations in atomic packing, which are influenced by the volume per atom, can lead to different structures and pore sizes	No	In addition, important geometric properties such as the pore limiting diameter (PLD), largest cavity diameter (LCD), gravimetric and volumetric surface areas (GSA and VSA, respectively) will change upon removal of bound solvent molecules. Since these geometric properties are typically the first descriptor for selecting promising MOF candidates from a pool of MOF structures, it is important to assess the effect of bound solvent removal on the above-mentioned physical properties.
Haldoupis, E., Nair, S., & Sholl, D. S. (2010). Efficient Calculation of Diffusion Limitations in Metal Organic Framework Materials: A Tool for Identifying Materials for Kinetic Separations. *Journal of Physical Chemistry C*.	Haldoupis, E., Nair, S., & Sholl, D. S. (2010). Efficient Calculation of Diffusion Limitations in Metal Organic Framework Materials: A Tool for Identifying Materials for Kinetic Separations. *Journal of Physical Chemistry C*.	Yes	In this section, we pursue this concept by determining the Henry's constant for adsorption of spherical adsorbates and estimating the activation energy associated with net diffusion of the same adsorbates in a large number of MOFs.
Case study 3: TOX			
Alabugin, I. V., Kuhn, L., Medvedev, M. G., Krivoshchapov, N. V., Vil', V. A., Yaremenko, I. A.,	The document discusses the role of oxygen lone pairs in chemical reactivity, particularly in	Yes	Arguably, the most historically important stereoelectronic effect is the anomeric effect (AE), i.e.,

<p>Mehaffy, P., Yarie, M., Terent'ev, A. O., &amp; Zolfigol, M. A. (2021). Stereoelectronic power of oxygen in control of chemical reactivity: the anomeric effect is not alone.</p>	<p>anomeric systems where oxygen atoms interact with strong sigma-acceptors</p>		<p>the axial preference of acceptor groups at the anomeric position of sugars. Although AE is generally attributed to hyperconjugative interactions of s-acceptors with a lone pair at oxygen (negative hyperconjugation), recent literature reports suggested alternative explanations. In this context, it is timely to evaluate the fundamental connections between the AE and a broad variety of O-functional groups. Such connections illustrate the general role of hyperconjugation with oxygen lone pairs in reactivity.</p>
Case study 4: SOL			
<p>Ishikawa, M., &amp; Hashimoto, Y. (2011). Improvement in Aqueous Solubility in Small Molecule Drug Discovery Programs by Disruption of Molecular Planarity and Symmetry.</p>	<p>Additionally, disrupting molecular planarity and symmetry by eliminating aromaticity can enhance solubility</p>	<p>Yes</p>	<p>Improvement in Aqueous Solubility in Small Molecule Drug Discovery Programs by Disruption of Molecular Planarity and Symmetry</p>
<p>Walker, M. A. (2017). Improvement in aqueous solubility achieved via small molecular changes.</p>	<p>The presence of polar atoms like nitrogen or oxygen can alter solubility by affecting hydrogen bonding.</p>	<p>Yes</p>	<p>The General Solubility Equation (GSE, Eq. (1)) equates the solubility of a solid organic compound to its log P (hydrophobicity) and melting point (solid state stability). While the equation was developed as a predictive tool, it is useful for evaluating the relative contribution of hydrophobicity and solid state stability to solubility. Poorly soluble compounds, where the log P is larger than</p>

			<p>the melting point term, are said to display solvation limited solubility. Alternatively, when the melting point term dominates, the compounds are characterized as exhibiting solid state limited solubility. A recent analysis of poorly soluble drugs found that most suffer from solvation limited solubility. This is to be expected given the positive correlation between affinity and hydrophobicity mentioned above. Nonetheless, there are cases where high crystalline stability is the underlying factor. This can be the case for compounds which bind their targets via strong hydrogen bonds. The hydrogen bonding functionality can lead to strong intermolecular interactions in the crystalline state.</p>
Case study 5: UFL			
<p>Gharagheizi, F. (2009). Prediction of upper flammability limit percent of pure compounds from their molecular structures. *Journal of Hazardous Materials*.</p>	<p>The document by Gharagheizi (2009) discusses the use of information index descriptors like SIC0, which account for neighborhood symmetry, in predicting the upper flammability limit (UFL) of organic compounds. An increase in SIC0 correlates with an increase in UFL</p>	<p>Yes</p>	<p>"SIC0" is of information indices. These molecular descriptors are calculated as information content of molecules, based on the calculation of equivalence classes from the molecular graph. Among them, the indices of neighborhood symmetry take into account also neighbor degree and edge multiplicity. Increase in this descriptor increases the UFLP.</p>

Yuan, S., Jiao, Z., Quddus, N., Kwon, J. S., & Mashuga, C. V. (2019). Developing Quantitative Structure–Property Relationship Models To Predict the Upper Flammability Limit Using Machine Learning.	While the provided documents do not explicitly discuss the dipole moment's impact on UFL, it is well-known in the literature that dipole moments can influence molecular interactions and stability, which are critical for flammability	Yes	Table 1: Molecular Descriptors Used To Predict the UFL : structural information content index (neighborhood symmetry of 0-order), dipole moment
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