[2] George Apostolakis. The Concept of Probability in Safety Assessments of Technological Systems. *Science*, 250 (4986):1359–1364, 1990.

[3] Yarin Gal. Uncertainty in Deep Learning. *PhD thesis, Department of Engineering, University of Cambridge*, 2016.

[4] Corwin Hansch and Toshio Fujita. p-σ-π Analysis. A Method for the Correlation of Biological Activity and Chemical Structure. *Journal of the American Chemical Society*, 86(8):1616–1626, 1964.

[5] Alex Kendall and Yarin Gal. What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision? In *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017.

[6] Eyke Hüllermeier and Willem Waegeman. Aleatoric and Epistemic Uncertainty in Machine Learning: An Introduction to Concepts and Methods. *Machine Learning*, 110:457–506, 2021.

[7] Kevin Yang et al. Analyzing Learned Molecular Representations for Property Prediction. *Journal of Chemical Information and Modeling*, 59(8):3370–3388, 2019.

[8] Esther Heid, Charles J McGill, Florence H Vermeire, and William H Green. Characterizing Uncertainty in Machine Learning for Chemistry. *Journal of Chemical Information and Modeling*, 63(13):4012–4029, 2023.

[9] Fredrik K. Gustafsson, Martin Danelljan, and Thomas B. Schön. How Reliable is Your Regression Model's Uncertainty Under Real-World Distribution Shifts? *Transactions on Machine Learning Research*, 2023. ISSN 2835-8856. URL https://openreview.net/forum?id=WJt2Pc3qtI.

[10] Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra. Weight Uncertainty in Neural Network. In *International Conference on Machine Learning*, pages 1613–1622. PMLR, 2015.

[11] Robert P Sheridan. Three Useful Dimensions for Domain Applicability in QSAR Models Using Random Forest. *Journal of Chemical Information and Modeling*, 52(3):814–823, 2012.

[12] Yarin Gal and Zoubin Ghahramani. Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. In *International Conference on Machine Learning*, pages 1050–1059. PMLR, 2016.

[13] Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. Simple and Scalable Predictive Uncertainty Estimation Using Deep Ensembles. In *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017.

[14] Gabriele Scalia, Colin A Grambow, Barbara Pernici, Yi-Pei Li, and William H Green. Evaluating Scalable Uncertainty Estimation Methods for Deep Learning-Based Molecular Property Prediction. *Journal of Chemical Information and Modeling*, 60(6):2697–2717, 2020.

[15] Robert P Sheridan, Bradley P Feuston, Vladimir N Maiorov, and Simon K Kearsley. Similarity to Molecules in the Training Set is a Good Discriminator for Prediction Accuracy in QSAR. *Journal of Chemical Information and Computer Sciences*, 44(6):1912–1928, 2004.

[16] Francois Berenger and Yoshihiro Yamanishi. A Distance-Based Boolean Applicability Domain for Classification of High Throughput Screening Data. *Journal of Chemical Information and Modeling*, 59(1):463–476, 2018.

[17] Christopher M Bishop. Mixture Density Networks. *Technical Report. Aston University, Birmingham.*, 1994.

[18] David A Nix and Andreas S Weigend. Estimating the Mean and Variance of the Target Probability Distribution. In *Proceedings of 1994 IEEE International Conference on Neural Networks (ICNN'94)*, volume 1, pages 55–60. IEEE, 1994.

[19] Sungjoon Choi, Kyungjae Lee, Sungbin Lim, and Songhwai Oh. Uncertainty-Aware Learning from Demonstration Using Mixture Density Networks with Sampling-Free Variance Modeling. In *2018 IEEE International Conference on Robotics and Automation (ICRA)*, pages 6915–6922. IEEE, 2018.

[20] Alexander Amini, Wilko Schwarting, Ava Soleimany, and Daniela Rus. Deep Evidential Regression. In *Advances in Neural Information Processing Systems*, volume 33, pages 14927–14937. Curran Associates, Inc., 2020.

[21] Vladimir Vovk, Alexander Gammerman, and Glenn Shafer. *Algorithmic Learning in a Random World*, volume 29. Springer, 2005.

[22] Roger Koenker and Kevin F Hallock. Quantile Regression. *Journal of Economic Perspectives*, 15(4):143–156, 2001.

[23] Lior Hirschfeld, Kyle Swanson, Kevin Yang, Regina Barzilay, and Connor W Coley. Uncertainty Quantification Using Neural Networks for Molecular Property Prediction. *Journal of Chemical Information and Modeling*, 60(8): 3770–3780, 2020.