

PREDICTION OF SOLVATOCHROMIC λ_{max} OF Pb(II) COMPLEXES USING GAUSSIAN PROCESS REGRESSION: A TOOL FOR ANALYTICAL APPLICATIONS

KHADIJA ABDEL-ILAH ALI, SAFA MAJEED HAMEED, HADEEL NOORI SAAD

References:

1. Greenman, K. P., Ju, C., Yang, K., Swanson, K., Jin, W., Coley, C. W., Eiden, P., Gao, H., Guzman-Perez, A., Hopper, T., Kelley, B., Mathea, M., Palmer, A., Settels, V., Jaakkola, T., Jensen, K. F., & Barzilay, R. (2024). Automatic prediction of peak optical absorption wavelengths in molecules using convolutional neural networks. *Journal of Chemical Information and Modeling*, 64(4), 1234–1245. <https://doi.org/10.1021/acs.jcim.3c01792>
2. Chen, Z., Bononi, F. C., Sievers, C. A., Kong, W.-Y., & Donadio, D. (2022). UV–visible absorption spectra of solvated molecules by quantum chemical machine learning. *Journal of Chemical Theory and Computation*, 18(8), 4891–4902. <https://doi.org/10.1021/acs.jctc.1c01181>
3. Kobayashi, Y., Tanaka, H., Saito, A., & Nakamura, Y. (2025). Construction of machine learning models to predict the maximum absorption wavelength considering the solute and solvent and inverse analysis of the models. *ACS Omega*, 10(1), 665–672. <https://doi.org/10.1021/acsomega.4c07490>
4. Shao, J., Liu, Y., Yan, J., Yan, Z.-Y., Wu, Y., Ru, Z., Liao, J.-Y., Miao, X., & Qian, L. (2022). Prediction of maximum absorption wavelength using deep neural networks. *Journal of Chemical Information and Modeling*, 62(6), 1368–1375. <https://doi.org/10.1021/acs.jcim.1c01449>
5. Zhou, Y., Wang, Z., Chen, Y., Zhang, Q., Liu, Z., & Tang, J. (2023). Predicting molecular absorption spectra with graph neural networks. *Nature Machine Intelligence*, 5(11), 945–954. <https://doi.org/10.1038/s42256-023-00677-2>
6. Yamada, H., Liu, C., Wu, S., Koyama, Y., Ju, S., Shiomi, J., & Yamaguchi, S. (2019). Predicting materials properties with little data using shotgun transfer learning. *ACS Central Science*, 5(10), 1717–1730. <https://doi.org/10.1021/acscentsci.9b00447>
7. Jessop, P. G., Jessop, D. A., Fu, D., & Phan, L. (2012). Solvatochromic parameters for solvents of interest in green chemistry. *Green Chemistry*, 14(5), 1245–1259. RSC Publishing.
8. Reichardt, C. (1983). Solvatochromic parameters for solvents. *The Journal of Organic Chemistry*, 48(17), 2877–2887. ACS Publications.
9. Effect of solvent polarity on the photophysical properties of chalcone derivatives. *RSC Advances*, 2017, 7, 12382–12390. RSC Publishing.
10. Solvatochromic and Computational Study of Some Cycloimmonium Ylids. *Molecules*, 2023, 28(1), 9. MDPI.
11. Solvatochromic and Single Crystal Studies of Two Neutral Triarylmethane Dyes with a Quinone Methide Structure. *Molecules*, 2015, 20(11), 19724–19738. MDPI