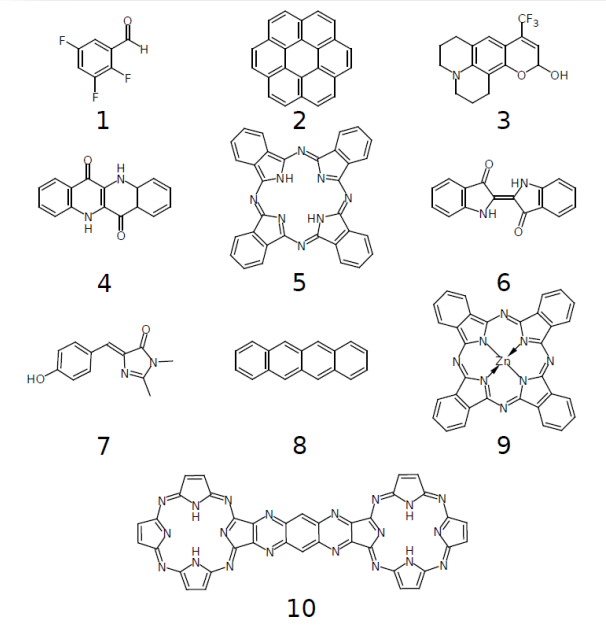
Implementation of Analytic Linear Response (LR) TDDFT Gradients in NWChem



Structures of organic dye molecules used for the calculation of absorption and emission maxima and Stokes shifts

Reference: D. W. Silverstein, N. Govind, H. J. J. van Dam, L. Jensen, J. Chem. Theory. Comput, 9 (12), 5490-5503 (2013), Publication Date (Web): November 6, 2013

Work was performed at Pacific Northwest National Laboratory and Penn State University

Scientific achievement

Development of a parallel implementation of analytical linear-response (LR) TDDFT gradients in NWChem

Significance and Impact

Excited state optimizations, dynamics, solvatochromatic studies (VEM), vibronic effects, excited state properties,

Research Details

- Parallel implementation of LR-TDDFT excited-state gradients in NWChem based on the Lagrangian approach of Furche & Ahlrichs
- Validation of the approach with calculations of the Stokes shifts for a range of organic dye molecules using a diverse set of exchange-correlation functionals (traditional, global hybrids and range-separated hybrids) and vibronic effects in one-photon absorption (OPA) and resonance Raman scattering (RRS)