**Table S1**. Glossary and Abbreviation for Computational Chemistry Methods or Name of Programs (in Alphabetical Order) Listed in Figure 1.

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| **(A) Model Preparation** | |
| ***Structures*** |  |
| Avogadro | An open-source molecular editor and visualizer |
| GaussView | A commercial molecular editor and visualizer for Gaussian programs |
| ***Conformational Search*** |  |
| ABCluster | An open-source program using an artificial bee colony algorithm for cluster global optimization developed by Zhang and Dolg |
| CREST | An efficient, open-source and user-friendly program: Conformer-Rotamer Ensemble Sampling Tool developed by Grimme |
| MacroModel | A commercial and integrated program using molecular mechanics method |
| RDKit | An open-source cheminformatics program developed by Riniker and coworkers |
| Tinker | An open-source computational chemistry program using molecular mechanics methods developed by Ponder and coworkers |
| **(B) Computational Methods** | |
| ***Geometry Optimization & Frequency*** | |
| B3LYP | A 3-parameter hybrid functional with Becke exchange and 20% HF exchange combined with Lee-Yang-Parr correlation functionals |
| B3LYP-D3 | A 3-parameter hybrid functional with Becke exchange and 20% HF exchange combined with Lee-Yang-Parr correlation functionals as well as third-generation dispersion correction (developed by Grimme) |
| DFT | Density functional theory method (pioneered by Kohn and coworkers) |
| DFT-D3 | A third-generation dispersion correction method for DFT (developed by Grimme) |
| M06/M06-2X/M06-L | The 06 family of Minnesota functionals (developed by Truhlar) |
| MN15 | A global-hybrid meta-nonseparable gradient approximation exchange-correlation (developed by Truhlar) functional |
| PBE0 | A hybrid functional with Perdew-Burke-Ernzerhof exchange-correlation functional |
| PBE0-D3 | A hybrid functional with Perdew-Burke-Ernzerhof exchange-correlation functional combined with third-generation dispersion correction (developed by Grimme) |
| PWPB95 | A doubly hybrid meta-GGA functional based on the reparameterized Perdew-Wang exchange, Becke 95 (B95) correlation and spin-opposite scaled perturbation treatment to the second order (PT2) (developed by Grimme) |
| PWPB95-D3 | A doubly hybrid meta-GGA functional based on the reparameterized Perdew-Wang exchange, Becke 95 (B95) correlation and spin-opposite scaled perturbation treatment to the second order (PT2) combined with third-generation dispersion correction (developed by Grimme) |
| B97X-D | A range-separated hybrid functional based on Becke 97 functional including empirical dispersion correction (developed by Head-Gordon) |
| B97X-V | A range-separated hybrid functional based on Becke 97 functional including dispersion-corrected (VV10 non-local correlation) functional (developed by Head-Gordon) |
| XYG3 | A doubly hybrid functional based on the adiabatic connection formalism and Görling-Levy coupling constant perturbation expansion to the second order (PT2) (developed by Xu) |
| (RI) CCSD(T) | Coupled cluster with singles and doubles excitations augmented with perturbative triples correction method (combined with resolution-of-the-identity approximation method for the electron-electron interaction integrals) |
| DFTB(-D) | (Semi-empirical) density functional-based tight binding method (including dispersion correction) |
| GFN-xTB | (Semi-empirical) Geometry, Frequency, Noncovalent, eXtended Tight Binding method developed by Grimme |
| GFN1-xTB | (Semi-empirical) the first-generation GFN-xTB method developed by Grimme |
| GFN2-xTB | (Semi-empirical) the second-generation GFN-xTB method developed by Grimme |
| PM6 | (Semi-empirical) parametric method 6 (developed by Stewart) |
| ONIOM | Multi-scale method: our own n-layered integrated molecular orbital and molecular mechanics methods (developed by the Morokuma group) |
| QM/MM | Hybrid quantum mechanics/molecular mechanics methods (pioneered by Karplus, Levitt and Warshel) |
| ***Reaction Path*** | |
| IRC | Intrinsic reaction coordinate (developed by Fukui) |
| NEB | Nudged elastic band method |
| NEB-TS | Climbing-image NEB method followed by transition state (TS) optimization |
| G09/16 | Gaussian 09/16 (one of the popular commercial computational chemistry programs) |
| ORCA | One of the popular free computational chemistry programs developed by Neese and coworkers |
| **Implicit Solvent Models** | |
| COSMO | Conductor-like screening model (implicit solvent model developed by Klamt) |
| CPCM | Conductor-like polarizable continuum model (developed by Barone and Cossi) |
| PCM | Polarizable continuum model (implicit solvent model developed by Tomasi and coworkers) |
| SMD | Continuum solvation model based on solute electron density (implicit solvent model developed by Truhlar and Cramer) |
| **(C) Energy** | |
| ***Refinement*** |  |
| (RI) CCSD(T) | Coupled cluster with singles and doubles excitations augmented with perturbative triples correction method (combined with resolution-of-the-identity approximation method for the electron-electron interaction integrals) |
| DLPNO-CCSD(T) | Domain-based local pair natural orbital coupled cluster theory with single-, double-, and perturbative triple excitations method (developed by Neese) |
| LNO-CCSD(T) | Local natural orbital coupled cluster with single-, double-, and perturbative triple excitations method (developed by Kállay) |
| CCSD(T)-in-DFT-D3 | (Quantum-embedding) Wavefunction-in-DFT method by coupling CCSD(T) (as the wavefunction method) with DFT-D3 methods |
| Molpro | A commercial quantum chemistry program for advanced molecular electronic structure calculations (developed by Werner, Knowles and coworkers) |
| ONIOM(CCSD(T):DFT-D3) | Hybrid ONIOM method combining CCSD(T) and DFT-D3 methods |
| ***Corrections*** |  |
| Goodvibes | An open-source program to compute quasi-harmonic free energies from electronic structure calculations with different corrections (such as quasi-harmonic corrections to (Truhlar- or Grimme-type) entropy and Head-Gordon-type enthalpy; concentration correction) developed by the Paton Group |
| **(D) Analysis** | |
| ***Energy*** |  |
| DIA | Distortion/Interaction Analysis (activation-strain model) (developed by Houk and Bickelhaupt) |
| EDA | Energy decomposition analysis (pioneered by Morokuma) |
| LED | Local energy decomposition analysis (developed by Neese) |
| SAPT (F/I-SAPT) | Symmetry-adapted perturbation theory (or functional-group (F)/interaction (I)-SAPT) (developed by Jeziorski, Szalewicz and coworkers) |
| QTAIM-IQA | Quantum theory of atoms in molecules-interacting quantum atoms (developed by Blanco) |
| ***Steric*** | |
| SambVca | An open-source program or web tool for calculating buried volume as steric descriptor (developed by Cavallo) |
| Sterimol | Steric parameters (e.g., L, B1 and B5) (developed by Verloop) |
| wSterimol | An open-source program for computing Boltzmann-weighted sterimol parameters (developed by the Paton group) |
| ***Noncovalent Interactions*** | |
| dftb3 | An open-source program to compute classical dispersion energy correction developed by Grimme. It can also decompose dispersion energy into different groups (fragments) for dispersion decomposition analysis |
| IGM | Independent gradient model for revealing molecular interactions, including NCIs (developed by Hénon) |
| Multiwfn | An open-source program for electronic wavefunction analysis (developed by Lu) |
| NCIPLOT | An open-source program for revealing non-covalent interactions (NCIs) based on the reduced density gradient (developed by Yang, Contreras-García and coworkers) |
| QTAIM | Quantum theory of atoms in molecules for revealing features of bonding and NCIs (developed by Bader) |
| ***Electronic*** |  |
| ESP | Electrostatic potential |
| FMO | Frontier Molecular Orbital theory proposed by Fukui and coworkers |
| Fukui function | Fukui function was originally developed by Parr and coworkers and can be used to describe different chemical reactivity (electrophilic or nucleophilic attack) by computing electrophilicity and nucleophilicity index |
| NBO | Natural bond orbital (developed by Weinhold) |
|  | **(E) Isotope Effects** |
| Quiver | A program for computing isotope effects based on Bigeleisen-Mayer method and (Bell- or Wigner-type) tunneling correction method |
| SCT | Multi-dimensional small-curvature tunneling correction method (developed by Truhlar) |
| Polyrate | An open-source program for computing chemical reaction rates based on transition state theory (TST) or variational transition state theory (VTST) and various tunneling correction methods (developed by Truhlar) |
| TST | Transition state theory |
| VTST | Variational Transition state theory (developed by Truhlar) |
| **(F) Molecular Dynamics** | |
| MM | Molecular mechanics |
| Q2MM | Quantum-guided molecular mechanics method and its open-source program (developed by Norrby and Wiest groups) |
| EVB | Empirical valance bond method (developed by Warshel) |
| SE | Semi-empirical method |
| BOMD | Born-Oppenheimer molecular dynamics |
| Progdyn | An open-source program for quasiclassical and classical molecular dynamics simulations using Gaussian electronic structure program (developed by Singleton) |
| VENUS | An open-source chemical molecular dynamics program developed by the Hase group |
| **Machanistic Studies** | |
| KIEs | Kinetic isotope effects |
| EIEs | Equilibrium isotope effects |