Full List of SAMPL References

- [1] Monroe, J. I. and Shirts, M. R.: Converging free energies of binding in cucurbit[7]uril and octa-acid host–guest systems from SAMPL4 using expanded ensemble simulations. <u>J Comput Aided Mol Des</u>. 28(4): 401–415, March 2014.
- [2] Muddana, H. S., Yin, J., Sapra, N. V., Fenley, A. T., and Gilson, M. K.: Blind prediction of SAMPL4 cucurbit[7]uril binding affinities with the mining minima method. J Comput Aided Mol Des. 28(4): 463–474, February 2014.
- [3] Gallicchio, E., Chen, H., Chen, H., Fitzgerald, M., Gao, Y., He, P., Kalyanikar, M., Kao, C., Lu, B., Niu, Y., Pethe, M., Zhu, J., and Levy, R. M.: BEDAM binding free energy predictions for the SAMPL4 octa-acid host challenge. J Comput Aided Mol Des. 29(4): 315–325, March 2015.
- [4] Mikulskis, P., Cioloboc, D., Andrejić, M., Khare, S., Brorsson, J., Genheden, S., Mata, R. A., Söderhjelm, P., and Ryde, U.: Free-energy perturbation and quantum mechanical study of SAMPL4 octa-acid host–guest binding energies. J Comput Aided Mol Des. 28(4): 375–400, April 2014.
- [5] Hsiao, Y.-W. and Söderhjelm, P.: Prediction of SAMPL4 host–guest binding affinities using funnel metadynamics. J Comput Aided Mol Des. 28(4): 443–454, February 2014.
- [6] Bhakat, S. and Söderhjelm, P.: Resolving the problem of trapped water in binding cavities: Prediction of host-guest binding free energies in the SAMPL5 challenge by funnel metadynamics. <u>J Comput Aided Mol Des.</u> 2016.
- [7] Pal, R. K., Haider, K., Kaur, D., Flynn, W., Xia, J., Levy, R. M., Taran, T., Wickstrom, L., Kurtzman, T., and Gallicchio, E.: A combined treatment of hydration and dynamical effects for the modeling of host-guest binding thermodynamics: The SAMPL5 blinded challenge. Journal of Computer-Aided Molecular Design. 2016.
- [8] Yin, J., Henriksen, N. M., Slochower, D. R., and Gilson, M. K.: The SAMPL5 Host-Guest Challenge: Binding Free Energies and Enthalpies from Explicit Solvent Simulations. J Comput Aided Mol Des. 2016.
- [9] Bosisio, S., Mey, A. S. J. S., and Michel, J.: Blinded predictions of host-guest standard free energies of binding in the SAMPL5 challenge. J Comput Aided Mol Des. 2016.
- [10] Tofoleanu, F., Lee, J., Pickard IV., F. C., König, G., Huang, J., Baek, M., Seok, C., and Brooks, B. R.: Absolute binding free energy calculations for octa-acids and guests. J Comput Aided Mol Des. 2016.
- [11] Mobley, D. L., Wymer, K. L., Lim, N. M., and Guthrie, J. P.: Blind prediction of solvation free energies from the SAMPL4 challenge. J Comput Aided Mol Des. 28(3): 135–150, March 2014.
- [12] Muddana, H. S., Fenley, A. T., Mobley, D. L., and Gilson, M. K.: The SAMPL4 host–guest blind prediction challenge: An overview. J Comput Aided Mol Des. 28(4): 305–317, March 2014.
- [13] Sullivan, M. R., Sokkalingam, P., Nguyen, T., Donahue, J. P., and Gibb, B. C.: Binding of carboxylate and trimethylammonium salts to octa-acid and TEMOA deep-cavity cavitands. <u>J Comput Aided Mol Des.</u> pp 1–8, July 2016.
- [14] Deng, N., Forli, S., He, P., Perryman, A., Wickstrom, L., Vijayan, R. S. K., Tiefenbrunn, T., Stout, D., Gallicchio, E., Olson, A. J., and Levy, R. M.: Distinguishing Binders from False Positives by Free Energy Calculations: Fragment Screening Against the Flap Site of HIV Protease. <u>J. Phys. Chem. B.</u> 119(3): 976–988, January 2015.
- [15] Li, L., Dill, K. A., and Fennell, C. J.: Testing the semi-explicit assembly model of aqueous solvation in the SAMPL4 challenge. <u>J Comput Aided Mol Des.</u> 28(3): 259–264, January 2014.
- [16] Paranahewage, S. S., Gierhart, C. S., and Fennell, C. J.: Predicting water-to-cyclohexane partitioning of the SAMPL5 molecules using dielectric balancing of force fields. <u>J Comput Aided Mol Des.</u> pp 1–7, August 2016.
- [17] Klamt, A., Eckert, F., Reinisch, J., and Wichmann, K.: Prediction of cyclohexane-water distribution coefficients with COSMO-RS on the SAMPL5 data set. <u>J Comput Aided Mol Des.</u> pp 1–9, July 2016.

- [18] Tielker, N., Tomazic, D., Heil, J., Kloss, T., Ehrhart, S., Güssregen, S., Schmidt, K. F., and Kast, S. M.: The SAMPL5 challenge for embedded-cluster integral equation theory: Solvation free energies, aqueous pKa, and cyclohexane—water log D. J Comput Aided Mol Des. pp 1–10, August 2016.
- [19] König, G., Pickard, F. C., Huang, J., Simmonett, A. C., Tofoleanu, F., Lee, J., Dral, P. O., Prasad, S., Jones, M., Shao, Y., Thiel, W., and Brooks, B. R.: Calculating distribution coefficients based on multi-scale free energy simulations: An evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. J Comput Aided Mol Des. pp 1–18, August 2016.
- [20] Luchko, T., Blinov, N., Limon, G. C., Joyce, K. P., and Kovalenko, A.: SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling. <u>J Comput Aided Mol Des.</u> pp 1–13, September 2016.
- [21] Santos-Martins, D., Fernandes, P. A., and Ramos, M. J.: Calculation of distribution coefficients in the SAMPL5 challenge from atomic solvation parameters and surface areas. <u>J Comput Aided Mol Des.</u> pp 1–8, September 2016.
- [22] Perryman, A. L., Santiago, D. N., Forli, S., Santos-Martins, D., and Olson, A. J.: Virtual screening with AutoDock Vina and the common pharmacophore engine of a low diversity library of fragments and hits against the three allosteric sites of HIV integrase: Participation in the SAMPL4 protein–ligand binding challenge. <u>J.</u> Comput Aided Mol Des. 28(4): 429–441, February 2014.
- [23] König, G., Pickard, F. C., Mei, Y., and Brooks, B. R.: Predicting hydration free energies with a hybrid QM/MM approach: An evaluation of implicit and explicit solvation models in SAMPL4. <u>J Comput Aided Mol Des.</u> 28(3): 245–257, February 2014.
- [24] Voet, A. R. D., Kumar, A., Berenger, F., and Zhang, K. Y. J.: Combining in silico and in cerebro approaches for virtual screening and pose prediction in SAMPL4. J Comput Aided Mol Des. 28(4): 363–373, January 2014.
- [25] Park, H.: Extended solvent-contact model approach to SAMPL4 blind prediction challenge for hydration free energies. J Comput Aided Mol Des. 28(3): 175–186, February 2014.
- [26] Rustenburg, A. S., Dancer, J., Lin, B., Feng, J. A., Ortwine, D. F., Mobley, D. L., and Chodera, J. D.: Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge. <u>bioRxiv</u>. 063081 pp, July 2016.
- [27] Reinisch, J. and Klamt, A.: Prediction of free energies of hydration with COSMO-RS on the SAMPL4 data set. J Comput Aided Mol Des. 28(3): 169–173, January 2014.
- [28] Muddana, H. S., Sapra, N. V., Fenley, A. T., and Gilson, M. K.: The SAMPL4 hydration challenge: Evaluation of partial charge sets with explicit-water molecular dynamics simulations. <u>J Comput Aided Mol Des.</u> 28(3): 277–287, January 2014.
- [29] Manzoni, F. and Söderhjelm, P.: Prediction of hydration free energies for the SAMPL4 data set with the AMOEBA polarizable force field. J Comput Aided Mol Des. 28(3): 235–244, March 2014.
- [30] Sandberg, L.: Predicting hydration free energies with chemical accuracy: The SAMPL4 challenge. <u>J Comput Aided Mol Des.</u> 28(3): 211–219, February 2014.
- [31] Brini, E., Paranahewage, S. S., Fennell, C. J., and Dill, K. A.: Adapting the semi-explicit assembly solvation model for estimating water-cyclohexane partitioning with the SAMPL5 molecules. <u>J Comput Aided Mol Des.</u> pp 1–11, September 2016.
- [32] Kamath, G., Kurnikov, I., Fain, B., Leontyev, I., Illarionov, A., Butin, O., Olevanov, M., and Pereyaslavets, L.: Prediction of cyclohexane-water distribution coefficient for SAMPL5 drug-like compounds with the QMPFF3 and ARROW polarizable force fields. <u>J Comput Aided Mol Des</u>. pp 1–12, September 2016.
- [33] Diaz-Rodriguez, S., Bozada, S. M., Phifer, J. R., and Paluch, A. S.: Predicting cyclohexane/water distribution coefficients for the SAMPL5 challenge using MOSCED and the SMD solvation model. <u>J Comput Aided Mol Des.</u> pp 1–11, August 2016.

- [34] Kenney, I. M., Beckstein, O., and Iorga, B. I.: Prediction of cyclohexane-water distribution coefficients for the SAMPL5 data set using molecular dynamics simulations with the OPLS-AA force field. <u>J Comput Aided Mol Des.</u> pp 1–14, August 2016.
- [35] Caldararu, O., Olsson, M. A., Riplinger, C., Neese, F., and Ryde, U.: Binding free energies in the SAMPL5 octa-acid host–guest challenge calculated with DFT-D3 and CCSD(T). <u>J Comput Aided Mol Des.</u> pp 1–20, September 2016.
- [36] Genheden, S. and Essex, J. W.: All-atom/coarse-grained hybrid predictions of distribution coefficients in SAMPL5. J Comput Aided Mol Des. pp 1–8, July 2016.
- [37] Chung, K.-C. and Park, H.: Extended solvent-contact model approach to blind SAMPL5 prediction challenge for the distribution coefficients of drug-like molecules. J Comput Aided Mol Des. pp 1–15, July 2016.
- [38] Koziara, K. B., Stroet, M., Malde, A. K., and Mark, A. E.: Testing and validation of the Automated Topology Builder (ATB) version 2.0: Prediction of hydration free enthalpies. <u>J Comput Aided Mol Des</u>. 28(3): 221–233, January 2014.
- [39] Yin, J., Henriksen, N. M., Slochower, D. R., Shirts, M. R., Chiu, M. W., Mobley, D. L., and Gilson, M. K.: Overview of the SAMPL5 host–guest challenge: Are we doing better? <u>J Comput Aided Mol Des</u>. pp 1–19, September 2016.
- [40] Bannan, C. C., Burley, K. H., Chiu, M., Shirts, M. R., Gilson, M. K., and Mobley, D. L.: Blind prediction of cyclohexane–water distribution coefficients from the SAMPL5 challenge. <u>J Comput Aided Mol Des.</u> pp 1–18, September 2016.
- [41] Lee, J., Tofoleanu, F., Pickard, F. C., König, G., Huang, J., Damjanović, A., Baek, M., Seok, C., and Brooks, B. R.: Absolute binding free energy calculations of CBClip host–guest systems in the SAMPL5 blind challenge. J Comput Aided Mol Des. pp 1–15, September 2016.
- [42] Jones, M. R., Brooks, B. R., and Wilson, A. K.: Partition coefficients for the SAMPL5 challenge using transfer free energies. J Comput Aided Mol Des. pp 1–10, September 2016.
- [43] Pickard, F. C., König, G., Tofoleanu, F., Lee, J., Simmonett, A. C., Shao, Y., Ponder, J. W., and Brooks, B. R.: Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pKa corrections. <u>J</u> Comput Aided Mol Des. pp 1–14, September 2016.
- [44] Cao, L. and Isaacs, L.: Absolute and relative binding affinity of cucurbit[7]uril towards a series of cationic guests. Supramolecular Chemistry. 26(3-4): 251–258, March 2014.
- [45] Muddana, H. S. and Gilson, M. K.: Prediction of SAMPL3 host—guest binding affinities: Evaluating the accuracy of generalized force-fields. J Comput Aided Mol Des. 26(5): 517–525, January 2012.
- [46] Gibb, C. L. D. and Gibb, B. C.: Binding of cyclic carboxylates to octa-acid deep-cavity cavitand. <u>J Comput</u> Aided Mol Des. 28(4): 319–325, November 2013.
- [47] Klimovich, P. V. and Mobley, D. L.: Predicting hydration free energies using all-atom molecular dynamics simulations and multiple starting conformations. <u>Journal of Computer-Aided Molecular Design</u>. 24(4): 307–316, April 2010.
- [48] Mobley, D. L., Liu, S., Cerutti, D. S., Swope, W. C., and Rice, J. E.: Alchemical prediction of hydration free energies for SAMPL. <u>Journal of Computer-Aided Molecular Design</u>. 26(5): 551–562, PMC3583515, May 2012.
- [49] Muddana, H. S., Varnado, C. D., Bielawski, C. W., Urbach, A. R., Isaacs, L., Geballe, M. T., and Gilson, M. K.: Blind prediction of host–guest binding affinities: A new SAMPL3 challenge. <u>J Comput Aided Mol Des</u>. 26(5): 475–487, February 2012.
- [50] Skillman, A. G.: SAMPL3: Blinded prediction of host–guest binding affinities, hydration free energies, and trypsin inhibitors. <u>J Comput Aided Mol Des</u>. 26(5): 473–474, May 2012.
- [51] Newman, J., Dolezal, O., Fazio, V., Caradoc-Davies, T., and Peat, T. S.: The DINGO dataset: A comprehensive set of data for the SAMPL challenge. J Comput Aided Mol Des. 26(5): 497–503, December 2011.

- [52] Gallicchio, E., Deng, N., He, P., Wickstrom, L., Perryman, A. L., Santiago, D. N., Forli, S., Olson, A. J., and Levy, R. M.: Virtual screening of integrase inhibitors by large scale binding free energy calculations: The SAMPL4 challenge. J Comput Aided Mol Des. 28(4): 475–490, February 2014.
- [53] Klamt, A. and Diedenhofen, M.: Blind prediction test of free energies of hydration with COSMO-RS. <u>J Comput</u> Aided Mol Des. 24(4): 357–360, April 2010.
- [54] Fennell, C. J., Kehoe, C. W., and Dill, K. A.: Modeling aqueous solvation with semi-explicit assembly. <u>PNAS</u>. 108(8): 3234–3239, February 2011.
- [55] Ellingson, B. A., Skillman, A. G., and Nicholls, A.: Analysis of SM8 and Zap TK calculations and their geometric sensitivity. J Comput Aided Mol Des. 24(4): 335–342, April 2010.
- [56] Surpateanu, G. and Iorga, B. I.: Evaluation of docking performance in a blinded virtual screening of fragment-like trypsin inhibitors. J Comput Aided Mol Des. 26(5): 595–601, December 2011.
- [57] Purisima, E. O., Corbeil, C. R., and Sulea, T.: Rapid prediction of solvation free energy. 3. Application to the SAMPL2 challenge. J Comput Aided Mol Des. 24(4): 373–383, April 2010.
- [58] König, G. and Brooks, B. R.: Predicting binding affinities of host-guest systems in the SAMPL3 blind challenge: The performance of relative free energy calculations. <u>J Comput Aided Mol Des.</u> 26(5): 543–550, December 2011.
- [59] Kehoe, C. W., Fennell, C. J., and Dill, K. A.: Testing the semi-explicit assembly solvation model in the SAMPL3 community blind test. J Comput Aided Mol Des. 26(5): 563–568, December 2011.
- [60] Kumar, A. and Zhang, K. Y. J.: Computational fragment-based screening using RosettaLigand: The SAMPL3 challenge. J Comput Aided Mol Des. 26(5): 603–616, January 2012.
- [61] Meunier, A. and Truchon, J.-F.: Predictions of hydration free energies from continuum solvent with solute polarizable models: The SAMPL2 blind challenge. J Comput Aided Mol Des. 24(4): 361–372, March 2010.
- [62] Genheden, S., Martinez, A. I. C., Criddle, M. P., and Essex, J. W.: Extensive all-atom Monte Carlo sampling and QM/MM corrections in the SAMPL4 hydration free energy challenge. <u>J Comput Aided Mol Des</u>. 28(3): 187–200, February 2014.
- [63] Beckstein, O., Fourrier, A., and Iorga, B. I.: Prediction of hydration free energies for the SAMPL4 diverse set of compounds using molecular dynamics simulations with the OPLS-AA force field. <u>J Comput Aided Mol Des.</u> 28(3): 265–276, February 2014.
- [64] Coleman, R. G., Sterling, T., and Weiss, D. R.: SAMPL4 & DOCK3.7: Lessons for automated docking procedures. J Comput Aided Mol Des. 28(3): 201–209, February 2014.
- [65] Hogues, H., Sulea, T., and Purisima, E. O.: Exhaustive docking and solvated interaction energy scoring: Lessons learned from the SAMPL4 challenge. J Comput Aided Mol Des. 28(4): 417–427, January 2014.
- [66] Reinisch, J., Klamt, A., and Diedenhofen, M.: Prediction of free energies of hydration with COSMO-RS on the SAMPL3 data set. J Comput Aided Mol Des. 26(5): 669–673, May 2012.
- [67] Kulp, J. L., Blumenthal, S. N., Wang, Q., Bryan, R. L., and Guarnieri, F.: A fragment-based approach to the SAMPL3 Challenge. J Comput Aided Mol Des. 26(5): 583–594, January 2012.
- [68] Klamt, A. and Diedenhofen, M.: Some conclusions regarding the predictions of tautomeric equilibria in solution based on the SAMPL2 challenge. J Comput Aided Mol Des. 24(6-7): 621–625, April 2010.
- [69] Fu, J., Liu, Y., and Wu, J.: Fast prediction of hydration free energies for SAMPL4 blind test from a classical density functional theory. J Comput Aided Mol Des. 28(3): 299–304, March 2014.
- [70] Hamaguchi, N., Fusti-Molnar, L., and Wlodek, S.: Force-field and quantum-mechanical binding study of selected SAMPL3 host-guest complexes. J Comput Aided Mol Des. 26(5): 577–582, February 2012.
- [71] Colas, C. and Iorga, B. I.: Virtual screening of the SAMPL4 blinded HIV integrase inhibitors dataset. <u>J Comput</u> Aided Mol Des. 28(4): 455–462, January 2014.

- [72] Ellingson, B. A., Geballe, M. T., Wlodek, S., Bayly, C. I., Skillman, A. G., and Nicholls, A.: Efficient calculation of SAMPL4 hydration free energies using OMEGA, SZYBKI, QUACPAC, and Zap TK. <u>J Comput Aided Mol Des.</u> 28(3): 289–298, March 2014.
- [73] Sulea, T. and Purisima, E. O.: Predicting hydration free energies of polychlorinated aromatic compounds from the SAMPL-3 data set with FiSH and LIE models. <u>J Comput Aided Mol Des</u>. 26(5): 661–667, December 2011.
- [74] Geballe, M. T., Skillman, A. G., Nicholls, A., Guthrie, J. P., and Taylor, P. J.: The SAMPL2 blind prediction challenge: Introduction and overview. J Comput Aided Mol Des. 24(4): 259–279, May 2010.
- [75] Ribeiro, R. F., Marenich, A. V., Cramer, C. J., and Truhlar, D. G.: Prediction of SAMPL2 aqueous solvation free energies and tautomeric ratios using the SM8, SM8AD, and SMD solvation models. <u>J Comput Aided Mol Des</u>. 24(4): 317–333, April 2010.
- [76] Skillman, A. G., Geballe, M. T., and Nicholls, A.: SAMPL2 challenge: Prediction of solvation energies and tautomer ratios. J Comput Aided Mol Des. 24(4): 257–258, April 2010.
- [77] Gallicchio, E. and Levy, R. M.: Prediction of SAMPL3 host-guest affinities with the binding energy distribution analysis method (BEDAM). J Comput Aided Mol Des. 26(5): 505–516, February 2012.
- [78] Mikulskis, P., Genheden, S., Rydberg, P., Sandberg, L., Olsen, L., and Ryde, U.: Binding affinities in the SAMPL3 trypsin and host–guest blind tests estimated with the MM/PBSA and LIE methods. <u>J Comput Aided Mol Des.</u> 26(5): 527–541, December 2011.
- [79] Geballe, M. T. and Guthrie, J. P.: The SAMPL3 blind prediction challenge: Transfer energy overview. <u>J</u> Comput Aided Mol Des. 26(5): 489–496, April 2012.
- [80] Guthrie, J. P.: SAMPL4, a blind challenge for computational solvation free energies: The compounds considered. J Comput Aided Mol Des. 28(3): 151–168, April 2014.
- [81] Nicholls, A., Wlodek, S., and Grant, J. A.: SAMPL2 and continuum modeling. <u>J Comput Aided Mol Des</u>. 24(4): 293–306, April 2010.
- [82] Soteras, I., Orozco, M., and Luque, F. J.: Performance of the IEF-MST solvation continuum model in the SAMPL2 blind test prediction of hydration and tautomerization free energies. <u>J Comput Aided Mol Des.</u> 24(4): 281–291, March 2010.
- [83] Lawrenz, M., Wereszczynski, J., Ortiz-Sánchez, J. M., Nichols, S. E., and McCammon, J. A.: Thermodynamic integration to predict host-guest binding affinities. J Comput Aided Mol Des. 26(5): 569–576, February 2012.
- [84] Sulea, T., Hogues, H., and Purisima, E. O.: Exhaustive search and solvated interaction energy (SIE) for virtual screening and affinity prediction. J Comput Aided Mol Des. 26(5): 617–633, December 2011.
- [85] Beckstein, O. and Iorga, B. I.: Prediction of hydration free energies for aliphatic and aromatic chloro derivatives using molecular dynamics simulations with the OPLS-AA force field. <u>J Comput Aided Mol Des.</u> 26(5): 635–645, December 2011.
- [86] Benson, M. L., Faver, J. C., Ucisik, M. N., Dashti, D. S., Zheng, Z., and Merz, K. M.: Prediction of trypsin/molecular fragment binding affinities by free energy decomposition and empirical scores. <u>J Comput Aided Mol Des.</u> 26(5): 647–659, April 2012.
- [87] Kast, S. M., Heil, J., Güssregen, S., and Schmidt, K. F.: Prediction of tautomer ratios by embedded-cluster integral equation theory. J Comput Aided Mol Des. 24(4): 343–353, March 2010.
- [88] Mobley, D. L., Bayly, C. I., Cooper, M. D., and Dill, K. A.: Predictions of Hydration Free Energies from All-Atom Molecular Dynamics Simulations. J Phys Chem B. 113: 4533–4537, January 2009.
- [89] Newman, J., Fazio, V., Caradoc-Davies, T., Branson, K., and Peat, T. S.: Practical Aspects of the SAMPL Challenge: Providing an Extensive Experimental Data Set for the Modeling Community. <u>Journal of Biomolecular Screening</u>. 14(10): 1245, January 2009.

- [90] Klamt, A., Eckert, F., and Diedenhofen, M.: Prediction of the Free Energy of Hydration of a Challenging Set of Pesticide-Like Compounds†. J Phys Chem B. January 2009.
- [91] Guthrie, J. P.: A Blind Challenge for Computational Solvation Free Energies: Introduction and Overview. <u>J Phys Chem B</u>. 113(14): 4501–4507, January 2009.
- [92] Marenich, A. V., Cramer, C. J., and Truhlar, D. G.: Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies. <u>J. Phys. Chem. B.</u> 113(14): 4538–4543, April 2009.
- [93] Sulea, T., Wanapun, D., Dennis, S., and Purisima, E. O.: Prediction of SAMPL-1 Hydration Free Energies Using a Continuum Electrostatics-Dispersion Model. J. Phys. Chem. B. 113(14): 4511–4520, April 2009.
- [94] Nicholls, A., Wlodek, S., and Grant, J. A.: The SAMP1 Solvation Challenge: Further Lessons Regarding the Pitfalls of Parametrization. J. Phys. Chem. B. 113(14): 4521–4532, April 2009.
- [95] Nicholls, A., Mobley, D. L., Guthrie, J. P., Chodera, J. D., Bayly, C. I., Cooper, M. D., and Pande, V. S.: Predicting Small-Molecule Solvation Free Energies: An Informal Blind Test for Computational Chemistry. <u>J. Med. Chem.</u> 51(4): 769–779, February 2008.
- [96] Chamberlin, A. C., Cramer, C. J., and Truhlar, D. G.: Performance of SM8 on a Test To Predict Small-Molecule Solvation Free Energies. J. Phys. Chem. B. 112(29): 8651–8655, July 2008.

Bibliography and References Cited

- [97] Mobley, D. L. and Klimovich, P. V.: Perspective: Alchemical free energy calculations for drug discovery. <u>J.</u> Chem. Phys. 137(23): 230901, January 2012.
- [98] Christ, C. D. and Fox, T.: Accuracy Assessment and Automation of Free Energy Calculations for Drug Design. J. Chem. Inf. Model. 54(1): 108–120, January 2014.
- [99] Deng, N., Forli, S., He, P., Perryman, A., Wickstrom, L., Vijayan, R. S. K., Tiefenbrunn, T., Stout, D., Gallicchio, E., Olson, A. J., and Levy, R. M.: Distinguishing Binders from False Positives by Free Energy Calculations: Fragment Screening Against the Flap Site of HIV Protease. <u>J. Phys. Chem. B.</u> 119(3): 976–988, January 2015.
- [100] Sherborne, Bradley, : Opening the lid on FEP. J Comput Aided Mol Des. 2016.
- [101] Wang, L., Wu, Y., Deng, Y., Kim, B., Pierce, L., Krilov, G., Lupyan, D., Robinson, S., Dahlgren, M. K., Greenwood, J., Romero, D. L., Masse, C., Knight, J. L., Steinbrecher, T., Beuming, T., Damm, W., Harder, E., Sherman, W., Brewer, M., Wester, R., Murcko, M., Frye, L., Farid, R., Lin, T., Mobley, D. L., Jorgensen, W. L., Berne, B. J., Friesner, R. A., and Abel, R.: Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. J Am Chem Soc. 137(7): 2695–2703, February 2015.
- [102] Christ, C. D. Binding affinity prediction from molecular simulations: A new standard method in structure-based drug design?, May 2016.
- [103] Cui, G. Affinity Predictions with FEP+: A Different Perspective on Performance and Utility, May 2016.
- [104] Verras, A. Free Energy Perturbation at Merck: Benchmarking against Faster Methods, May 2016.
- [105] Schnieders, M. J., Baltrusaitis, J., Shi, Y., Chattree, G., Zheng, L., Yang, W., and Ren, P.: The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. <u>J. Chem.</u> Theory Comput. 8(5): 1721–1736, May 2012.
- [106] Park, J., Nessler, I., McClain, B., Macikenas, D., Baltrusaitis, J., and Schnieders, M. J.: Absolute Organic Crystal Thermodynamics: Growth of the Asymmetric Unit into a Crystal via Alchemy. <u>J. Chem. Theory</u> Comput. 10(7): 2781–2791, July 2014.
- [107] Liu, S., Cao, S., Hoang, K., Young, K. L., Paluch, A. S., and Mobley, D. L.: Using MD Simulations To Calculate How Solvents Modulate Solubility. <u>Journal of Chemical Theory and Computation</u>. 12(4): 1930– 1941, February 2016.
- [108] Leonis, G., Steinbrecher, T., and Papadopoulos, M. G.: A Contribution to the Drug Resistance Mechanism of Darunavir, Amprenavir, Indinavir, and Saquinavir Complexes with HIV-1 Protease Due to Flap Mutation I50V: A Systematic MM–PBSA and Thermodynamic Integration Study. <u>J. Chem. Inf. Model.</u> 53(8): 2141–2153, August 2013.
- [109] Lee, C. T., Comer, J., Herndon, C., Leung, N., Pavlova, A., Swift, R. V., Tung, C., Rowley, C. N., Amaro, R. E., Chipot, C., Wang, Y., and Gumbart, J. C.: Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. J. Chem. Inf. Model. 56(4): 721–733, April 2016.
- [110] Comer, J., Schulten, K., and Chipot, C.: Calculation of Lipid-Bilayer Permeabilities Using an Average Force. <u>J Chem. Theory Comput.</u> 10(2): 554–564, February 2014.
- [111] Liu, S., Wu, Y., Lin, T., Abel, R., Redmann, J. P., Summa, C. M., Jaber, V. R., Lim, N. M., and Mobley, D. L.: Lead optimization mapper: Automating free energy calculations for lead optimization. <u>J Comput Aided Mol Des.</u> 27(9): 755–770, September 2013.
- [112] Mikulskis, P., Genheden, S., and Ryde, U.: A Large-Scale Test of Free-Energy Simulation Estimates of Protein–Ligand Binding Affinities. J. Chem. Inf. Model. 54(10): 2794–2806, October 2014.
- [113] Homeyer, N., Stoll, F., Hillisch, A., and Gohlke, H.: Binding Free Energy Calculations for Lead Optimization: Assessment of Their Accuracy in an Industrial Drug Design Context. <u>J. Chem. Theory Comput.</u> 10(8): 3331–3344, August 2014.

- [114] Shirts, M. R., Mobley, D. L., and Brown, S. P. Free-energy calculations in structure-based drug design. In Merz, , Kenneth MJ., Ringe, D., and Reynolds, C. H. (Eds.): <u>Drug Design: Structure and Ligand-Based Approaches</u>. Cambridge University Press, January 2010.
- [115] Lim, N. M., Wang, L., Abel, R., and Mobley, D. L.: Sensitivity in binding free energies due to protein reorganization. Journal of Chemical Theory and Computation. July 2016.
- [116] Rocklin, G. J., Boyce, S. E., Fischer, M., Fish, I., Mobley, D. L., Shoichet, B. K., and Dill, K. A.: Blind Prediction of Charged Ligand Binding Affinities in a Model Binding Site. <u>J. Mol. Biol.</u> 425(22): 4569–4583, November 2013.
- [117] Nuzzo, R.: How scientists fool themselves –and how they can stop. Nature. 526(7572): 182–185, October 2015.
- [118] Mobley, D. L., Graves, A. P., Chodera, J. D., McReynolds, A. C., Shoichet, B. K., and Dill, K. A.: Predicting absolute ligand binding free energies to a simple model site. J. Mol. Biol. 371(4): 1118–1134, August 2007.
- [119] Boyce, S. E., Mobley, D. L., Rocklin, G. J., Graves, A. P., Dill, K. A., and Shoichet, B. K.: Predicting ligand binding affinity with alchemical free energy methods in a polar model binding site. <u>J. Mol. Biol.</u> 394(4): 747–763, December 2009.
- [120] Gathiaka, S., Liu, S., Chiu, M., Yang, H., Stuckey, J. A., Kang, Y. N., Delproposto, J., Dunbar, J. B., Carlson, H. A., Burley, S., Walters, W., Amaro, R. E., Feher, V., and Gilson, M. K.: D3R Grand Challenge 2015: Evaluation of Protein-Ligand Pose and Affinity Prediction. J Comput Aided Mol Des. 2016.
- [121] Nicholls, A., Mobley, D. L., Guthrie, J. P., Chodera, J. D., Bayly, C. I., Cooper, M. D., and Pande, V. S.: Predicting Small-Molecule Solvation Free Energies: An Informal Blind Test for Computational Chemistry. <u>J.</u> Med. Chem. 51(4): 769–779, February 2008.
- [122] Nicholls, A., Wlodek, S., and Grant, J. A.: The SAMP1 Solvation Challenge: Further Lessons Regarding the Pitfalls of Parametrization. J. Phys. Chem. B. 113(14): 4521–4532, April 2009.
- [123] Mobley, D. L., Bayly, C. I., Cooper, M. D., and Dill, K. A.: Predictions of Hydration Free Energies from All-Atom Molecular Dynamics Simulations. J Phys Chem B. 113: 4533–4537, January 2009.
- [124] Geballe, M. T., Skillman, A. G., Nicholls, A., Guthrie, J. P., and Taylor, P. J.: The SAMPL2 blind prediction challenge: Introduction and overview. J Comput Aided Mol Des. 24(4): 259–279, May 2010.
- [125] Geballe, M. T. and Guthrie, J. P.: The SAMPL3 blind prediction challenge: Transfer energy overview. <u>J</u> Comput Aided Mol Des. 26(5): 489–496, April 2012.
- [126] Mobley, D. L., Wymer, K. L., Lim, N. M., and Guthrie, J. P.: Blind prediction of solvation free energies from the SAMPL4 challenge. J Comput Aided Mol Des. 28(3): 135–150, March 2014.
- [127] Muddana, H. S., Fenley, A. T., Mobley, D. L., and Gilson, M. K.: The SAMPL4 host–guest blind prediction challenge: An overview. J Comput Aided Mol Des. 28(4): 305–317, March 2014.
- [128] Bannan, C. C., Burley, K. H., Chiu, M., Shirts, M. R., Gilson, M. K., and Mobley, D. L.: Blind prediction of cyclohexane—water distribution coefficients from the SAMPL5 challenge. <u>J Comput Aided Mol Des.</u> pp 1–18, September 2016.
- [129] Yin, J., Henriksen, N. M., Slochower, D. R., Shirts, M. R., Chiu, M. W., Mobley, D. L., and Gilson, M. K.: Overview of the SAMPL5 host–guest challenge: Are we doing better? <u>J Comput Aided Mol Des.</u> pp 1–19, September 2016.
- [130] Ignjatović, M. M., Caldararu, O., Dong, G., Muñoz-Gutierrez, C., Adasme-Carreño, F., and Ryde, U.: Binding-affinity predictions of HSP90 in the D3R Grand Challenge 2015 with docking, MM/GBSA, QM/MM, and free-energy simulations. J Comput Aided Mol Des. pp 1–24, August 2016.
- [131] Deng, N., Flynn, W. F., Xia, J., Vijayan, R. S. K., Zhang, B., He, P., Mentes, A., Gallicchio, E., and Levy, R. M.: Large scale free energy calculations for blind predictions of protein–ligand binding: The D3R Grand Challenge 2015. J Comput Aided Mol Des. pp 1–9, August 2016.

- [132] Sunseri, J., Ragoza, M., Collins, J., and Koes, D. R.: A D3R prospective evaluation of machine learning for protein-ligand scoring. J Comput Aided Mol Des. pp 1–11, September 2016.
- [133] Ellingson, B. A., Skillman, A. G., and Nicholls, A.: Analysis of SM8 and Zap TK calculations and their geometric sensitivity. J Comput Aided Mol Des. 24(4): 335–342, April 2010.
- [134] Ellingson, B. A., Geballe, M. T., Wlodek, S., Bayly, C. I., Skillman, A. G., and Nicholls, A.: Efficient calculation of SAMPL4 hydration free energies using OMEGA, SZYBKI, QUACPAC, and Zap TK. <u>J Comput Aided Mol Des.</u> 28(3): 289–298, March 2014.
- [135] Mobley, D. L., Liu, S., Cerutti, D. S., Swope, W. C., and Rice, J. E.: Alchemical prediction of hydration free energies for SAMPL. <u>Journal of Computer-Aided Molecular Design</u>. 26(5): 551–562, PMC3583515, May 2012.
- [136] Fennell, C. J., Wymer, K. L., and Mobley, D. L.: A Fixed-Charge Model for Alcohol Polarization in the Condensed Phase, and Its Role in Small Molecule Hydration. <u>J. Phys. Chem. B.</u> 118(24): 6438–6446, June 2014.
- [137] Paranahewage, S. S., Gierhart, C. S., and Fennell, C. J.: Predicting water-to-cyclohexane partitioning of the SAMPL5 molecules using dielectric balancing of force fields. <u>J Comput Aided Mol Des.</u> pp 1–7, August 2016.
- [138] Sulea, T. and Purisima, E. O.: Predicting hydration free energies of polychlorinated aromatic compounds from the SAMPL-3 data set with FiSH and LIE models. <u>J Comput Aided Mol Des</u>. 26(5): 661–667, December 2011.
- [139] Li, L., Dill, K. A., and Fennell, C. J.: Testing the semi-explicit assembly model of aqueous solvation in the SAMPL4 challenge. J Comput Aided Mol Des. 28(3): 259–264, January 2014.
- [140] Brini, E., Paranahewage, S. S., Fennell, C. J., and Dill, K. A.: Adapting the semi-explicit assembly solvation model for estimating water-cyclohexane partitioning with the SAMPL5 molecules. <u>J Comput Aided Mol Des.</u> pp 1–11, September 2016.
- [141] Klamt, A., Eckert, F., Reinisch, J., and Wichmann, K.: Prediction of cyclohexane-water distribution coefficients with COSMO-RS on the SAMPL5 data set. J Comput Aided Mol Des. pp 1–9, July 2016.
- [142] Mobley, D. L. and Gilson, M. K.: Predicting binding free energies: Frontiers and benchmarks. <u>bioRxiv</u>. 074625 pp, September 2016.
- [143] Muddana, H. S., Yin, J., Sapra, N. V., Fenley, A. T., and Gilson, M. K.: Blind prediction of SAMPL4 cucurbit[7]uril binding affinities with the mining minima method. <u>J Comput Aided Mol Des</u>. 28(4): 463–474, February 2014.
- [144] Yin, J., Henriksen, N. M., Slochower, D. R., and Gilson, M. K.: The SAMPL5 Host-Guest Challenge: Binding Free Energies and Enthalpies from Explicit Solvent Simulations. <u>J Comput Aided Mol Des</u>. 2016.
- [145] Muddana, H. S., Sapra, N. V., Fenley, A. T., and Gilson, M. K.: The SAMPL4 hydration challenge: Evaluation of partial charge sets with explicit-water molecular dynamics simulations. <u>J Comput Aided Mol Des</u>. 28(3): 277–287, January 2014.
- [146] Yin, J., Fenley, A. T., Henriksen, N. M., and Gilson, M. K.: Toward Improved Force-Field Accuracy through Sensitivity Analysis of Host-Guest Binding Thermodynamics. <u>The Journal of Physical Chemistry B</u>. 119(32): 10145–10155, August 2015.
- [147] Nielsen, J. E., Gunner, M. R., and García-Moreno E., B.: The pKa Cooperative: A collaborative effort to advance structure-based calculations of pKa values and electrostatic effects in proteins. <u>Proteins</u>. 79(12): 3249–3259, December 2011.
- [148] Janin, J.: Assessing predictions of protein–protein interaction: The CAPRI experiment. <u>Protein Science</u>. 14(2): 278–283, February 2005.
- [149] Moult, J., Fidelis, K., Kryshtafovych, A., Schwede, T., and Tramontano, A.: Critical assessment of methods of protein structure prediction (CASP) —round x. Proteins. 82: 1–6, February 2014.

- [150] Coleman, R. G., Sterling, T., and Weiss, D. R.: SAMPL4 & DOCK3.7: Lessons for automated docking procedures. J Comput Aided Mol Des. 28(3): 201–209, February 2014.
- [151] Reinisch, J., Klamt, A., and Diedenhofen, M.: Prediction of free energies of hydration with COSMO-RS on the SAMPL3 data set. J Comput Aided Mol Des. 26(5): 669–673, May 2012.
- [152] Beauchamp, K. A., Behr, J. M., Rustenburg, A. S., Bayly, C. I., Kroenlein, K., and Chodera, J. D.: Towards Automated Benchmarking of Atomistic Forcefields: Neat Liquid Densities and Static Dielectric Constants from the ThermoML Data Archive. <u>Journal of Physical Chemistry B</u>. 119(40): 12912–12920, September 2015.
- [153] Bannan, C. C., Calabró, G., Kyu, D. Y., and Mobley, D. L.: Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water. <u>Journal of Chemical Theory and Computation</u>. 12(8): 4015–4024, August 2016.
- [154] Wang, K., Chodera, J. D., Yang, Y., and Shirts, M. R.: Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics. <u>J Comput Aided Mol Des.</u> 27(12): 989–1007, December 2013.
- [155] Pickard, F. C., König, G., Tofoleanu, F., Lee, J., Simmonett, A. C., Shao, Y., Ponder, J. W., and Brooks, B. R.: Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pKa corrections. <u>J</u> Comput Aided Mol Des. pp 1–14, September 2016.
- [156] Rustenburg, A. S., Dancer, J., Lin, B., Feng, J. A., Ortwine, D. F., Mobley, D. L., and Chodera, J. D.: Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge. <u>bioRxiv</u>. 063081 pp, July 2016.
- [157] Bhatnagar, N., Kamath, G., and Potoff, J. J.: Prediction of 1-octanol–water and air–water partition coefficients for nitro-aromatic compounds from molecular dynamics simulations. <u>Physical Chemistry Chemical Physics</u>. 15(17): 6467, 2013.
- [158] Kollman, P. A.: Advances and continuing challenges in achieving realistic and predictive simulations of the properties of organic and biological molecules. <u>Accounts of Chemical Research</u>. 29(10): 461–469, 1996.
- [159] Muddana, H. S., Varnado, C. D., Bielawski, C. W., Urbach, A. R., Isaacs, L., Geballe, M. T., and Gilson, M. K.: Blind prediction of host–guest binding affinities: A new SAMPL3 challenge. <u>J Comput Aided Mol Des</u>. 26(5): 475–487, February 2012.
- [160] Bhakat, S. and Söderhjelm, P.: Resolving the problem of trapped water in binding cavities: Prediction of host-guest binding free energies in the SAMPL5 challenge by funnel metadynamics. <u>J Comput Aided Mol Des.</u> 2016.
- [161] Henriksen, N. M., Fenley, A. T., and Gilson, M. K.: Computational Calorimetry: High-Precision Calculation of Host–Guest Binding Thermodynamics. <u>Journal of Chemical Theory and Computation</u>. 11(9): 4377–4394, September 2015.
- [162] Ma, D., Glassenberg, R., Ghosh, S., Zavalij, P. Y., and Isaacs, L.: Acyclic cucurbituril congener binds to local anaesthetics. Supramolecular Chemistry. 24(5): 325–332, May 2012.
- [163] Cao, L. and Isaacs, L.: Absolute and relative binding affinity of cucurbit[7]uril towards a series of cationic guests. Supramolecular Chemistry. 26(3-4): 251–258, March 2014.
- [164] She, N., Moncelet, D., Gilberg, L., Lu, X., Sindelar, V., Briken, V., and Isaacs, L.: Glycoluril-Derived Molecular Clips are Potent and Selective Receptors for Cationic Dyes in Water. Chem. Eur. J. pp n/a–n/a, August 2016.
- [165] Cao, L., Šekutor, M., Zavalij, P. Y., Mlinarić-Majerski, K., Glaser, R., and Isaacs, L.: Cucurbit[7]uril-Guest Pair with an Attomolar Dissociation Constant. Angew. Chem. Int. Ed. 53(4): 988–993, January 2014.
- [166] Liu, S., Ruspic, C., Mukhopadhyay, P., Chakrabarti, S., Zavalij, P. Y., and Isaacs, L.: The Cucurbit[n]uril Family: Prime Components for Self-Sorting Systems. <u>Journal of the American Chemical Society</u>. 127(45): 15959–15967, November 2005.

- [167] Mock, W. L. and Shih, N. Y.: Structure and selectivity in host-guest complexes of cucurbituril. <u>The Journal of Organic Chemistry</u>. 51(23): 4440–4446, November 1986.
- [168] Assaf, K. I. and Nau, W. M.: Cucurbiturils: From synthesis to high-affinity binding and catalysis. Chem Soc Rev. 44(2): 394–418, January 2015.
- [169] Moghaddam, S., Yang, C., Rekharsky, M., Ko, Y. H., Kim, K., Inoue, Y., and Gilson, M. K.: New Ultrahigh Affinity Host-Guest Complexes of Cucurbit[7]uril with Bicyclo[2.2.2]octane and Adamantane Guests: Thermodynamic Analysis and Evaluation of M2 Affinity Calculations. <u>Journal of the American Chemical Society</u>. 133(10): 3570–3581, March 2011.
- [170] Shetty, D., Khedkar, J. K., Park, K. M., and Kim, K.: Can we beat the biotin–avidin pair?: cucurbit[7]uril-based ultrahigh affinity host–guest complexes and their applications. Chem. Soc. Rev. 44(23): 8747–8761, 2015.
- [171] Biedermann, F., Uzunova, V. D., Scherman, O. A., Nau, W. M., and De Simone, A.: Release of High-Energy Water as an Essential Driving Force for the High-Affinity Binding of Cucurbit[n]urils. <u>J. Am. Chem. Soc.</u> 134(37): 15318–15323, September 2012.
- [172] Isaacs, L.: Stimuli Responsive Systems Constructed Using Cucurbit[n]uril-Type Molecular Containers. <u>Acc.</u> Chem. Res. 47(7): 2052–2062, July 2014.
- [173] Vinciguerra, B., Zavalij, P. Y., and Isaacs, L.: Synthesis and Recognition Properties of Cucurbit[8]uril Derivatives. Org. Lett. 17(20): 5068–5071, October 2015.
- [174] Lucas, D., Minami, T., Iannuzzi, G., Cao, L., Wittenberg, J. B., Anzenbacher, P., and Isaacs, L.: Templated Synthesis of Glycoluril Hexamer and Monofunctionalized Cucurbit[6]uril Derivatives. J. Am. Chem. Soc. 133(44): 17966–17976, November 2011.
- [175] Ma, D., Zhang, B., Hoffmann, U., Sundrup, M. G., Eikermann, M., and Isaacs, L.: Acyclic Cucurbit[n]uril-Type Molecular Containers Bind Neuromuscular Blocking Agents In Vitro and Reverse Neuromuscular Block In Vivo. Angew. Chem. Int. Ed. 51(45): 11358–11362, November 2012.
- [176] Ma, D., Hettiarachchi, G., Nguyen, D., Zhang, B., Wittenberg, J. B., Zavalij, P. Y., Briken, V., and Isaacs, L.: Acyclic cucurbit[n]uril molecular containers enhance the solubility and bioactivity of poorly soluble pharmaceuticals. Nat Chem. 4(6): 503–510, June 2012.
- [177] Zhang, B. and Isaacs, L.: Acyclic Cucurbit[n]uril-type Molecular Containers: Influence of Aromatic Walls on their Function as Solubilizing Excipients for Insoluble Drugs. <u>J. Med. Chem.</u> 57(22): 9554–9563, November 2014.
- [178] Gilberg, L., Zhang, B., Zavalij, P. Y., Sindelar, V., and Isaacs, L.: Acyclic cucurbit[n]uril-type molecular containers: Influence of glycoluril oligomer length on their function as solubilizing agents. Org. Biomol. Chem. 13(13): 4041–4050, 2015.
- [179] Sigwalt, D., Moncelet, D., Falcinelli, S., Mandadapu, V., Zavalij, P. Y., Day, A., Briken, V., and Isaacs, L.: Acyclic Cucurbit[n]uril-Type Molecular Containers: Influence of Linker Length on Their Function as Solubilizing Agents. ChemMedChem. 11(9): 980–989, May 2016.
- [180] Zhang, B., Zavalij, P. Y., and Isaacs, L.: Acyclic CB[n]-type molecular containers: Effect of solubilizing group on their function as solubilizing excipients. <u>Org. Biomol. Chem.</u> 12(15): 2413–2422, 2014.
- [181] Ma, D., Zavalij, P. Y., and Isaacs, L.: Acyclic Cucurbit[n]uril Congeners Are High Affinity Hosts. <u>J. Org. Chem.</u> 75(14): 4786–4795, July 2010.
- [182] Ko, Y. H., Kim, E., Hwang, I., and Kim, K.: Supramolecular assemblies built with host-stabilized charge-transfer interactions. Chem. Commun. (13): 1305–1315, 2007.
- [183] Barrow, S. J., Kasera, S., Rowland, M. J., del Barrio, J., and Scherman, O. A.: Cucurbituril-Based Molecular Recognition. Chem. Rev. 115(22): 12320–12406, November 2015.
- [184] Urbach, A. R. and Ramalingam, V.: Molecular Recognition of Amino Acids, Peptides, and Proteins by Cucurbit[n]uril Receptors. <u>Isr. J. Chem.</u> 51(5-6): 664–678, May 2011.

- [185] Connors, K. A.: Binding Constants. New York, NY, John Wiley & Sons, 1987.
- [186] Masson, E., Ling, X., Joseph, R., Kyeremeh-Mensah, L., and Lu, X.: Cucurbituril chemistry: A tale of supramolecular success. RSC Adv. 2(4): 1213–1247, 2012.
- [187] Márquez, C., Hudgins, R. R., and Nau, W. M.: Mechanism of Host-Guest Complexation by Cucurbituril. <u>J. Am. Chem. Soc.</u> 126(18): 5806–5816, May 2004.
- [188] Biedermann, F., Nau, W. M., and Schneider, H.-J.: The Hydrophobic Effect Revisited—Studies with Supramolecular Complexes Imply High-Energy Water as a Noncovalent Driving Force. <u>Angew. Chem.</u> Int. Ed. 53(42): 11158–11171, October 2014.
- [189] 'il Saleh, N., Koner, A., and Nau, W.: Activation and Stabilization of Drugs by Supramolecular pKa Shifts: Drug-Delivery Applications Tailored for Cucurbiturils. Angewandte Chemie. 120(29): 5478–5481, July 2008.
- [190] Nau, W. M., Florea, M., and Assaf, K. I.: Deep Inside Cucurbiturils: Physical Properties and Volumes of their Inner Cavity Determine the Hydrophobic Driving Force for Host–Guest Complexation. <u>Isr. J. Chem.</u> 51(5-6): 559–577, May 2011.
- [191] Ghosh, I. and Nau, W. M.: The strategic use of supramolecular pKa shifts to enhance the bioavailability of drugs. Advanced Drug Delivery Reviews. 64(9): 764–783, June 2012.
- [192] Gibb, C. L. D. and Gibb, B. C.: Binding of cyclic carboxylates to octa-acid deep-cavity cavitand. <u>J Comput</u> Aided Mol Des. 28(4): 319–325, November 2013.
- [193] Sullivan, M. R., Sokkalingam, P., Nguyen, T., Donahue, J. P., and Gibb, B. C.: Binding of carboxylate and trimethylammonium salts to octa-acid and TEMOA deep-cavity cavitands. <u>J Comput Aided Mol Des.</u> pp 1–8, July 2016.
- [194] Carnegie, R. S., Gibb, C. L. D., and Gibb, B. C.: Anion Complexation and The Hofmeister Effect. <u>Angew.</u> Chem. 126(43): 11682–11684, October 2014.
- [195] Lin, Y.-L., Meng, Y., Jiang, W., and Roux, B.: Explaining why Gleevec is a specific and potent inhibitor of Abl kinase. Proc. Natl. Acad. Sci. 110(5): 1664–1669, January 2013.
- [196] Shan, Y., Seeliger, M. A., Eastwood, M. P., Frank, F., Xu, H., Jensen, M. O., Dror, R. O., Kuriyan, J., and Shaw, D. E.: A conserved protonation-dependent switch controls drug binding in the Abl kinase. PNAS. 106(1): 139–144, June 2009.
- [197] Szakács, Z., Béni, S., Varga, Z., Örfi, L., Kéri, G., and Noszál, B.: Acid-Base Profiling of Imatinib (Gleevec) and Its Fragments. Journal of Medicinal Chemistry. 48(1): 249–255, January 2005.
- [198] Grante, I., Actins, A., and Orola, L.: Protonation effects on the UV/Vis absorption spectra of imatinib: A theoretical and experimental study. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy. 129: 326–332, August 2014.
- [199] Hall, M. L., Jorgensen, W. L., and Whitehead, L.: Automated Ligand- and Structure-Based Protocol for *in Silico* Prediction of Human Serum Albumin Binding. <u>Journal of Chemical Information and Modeling</u>. 53(4): 907–922, April 2013.
- [200] Epps, D. E., Raub, T. J., Caiolfa, V., Chiari, A., and Zamai, M.: Determination of the Affinity of Drugs toward Serum Albumin by Measurement of the Quenching of the Intrinsic Tryptophan Fluorescence of the Protein. Journal of Pharmacy and Pharmacology. 51(1): 41–48, January 1999.
- [201] Bou-Abdallah, F., Sprague, S. E., Smith, B. M., and Giffune, T. R.: Binding thermodynamics of Diclofenac and Naproxen with human and bovine serum albumins: A calorimetric and spectroscopic study.
 The Journal of Chemical Thermodynamics">https://example.com/html/>
 The Journal of Chemical Thermodynamics. 103: 299–309, December 2016.
- [202] Merski, M., Fischer, M., Balius, T. E., Eidam, O., and Shoichet, B. K.: Homologous ligands accommodated by discrete conformations of a buried cavity. PNAS. 112(16): 5039–5044, April 2015.
- [203] Onufriev, A. V. and Alexov, E.: Protonation and pK changes in protein–ligand binding. Quarterly Reviews of Biophysics. 46(02): 181–209, May 2013.

- [204] Newman, J., Dolezal, O., Fazio, V., Caradoc-Davies, T., and Peat, T. S.: The DINGO dataset: A comprehensive set of data for the SAMPL challenge. <u>J Comput Aided Mol Des</u>. 26(5): 497–503, December 2011.
- [205] Rocklin, G. J., Mobley, D. L., Dill, K. A., and Hünenberger, P. H.: Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects. The Journal of Chemical Physics. 139(18): 184103, 2013.
- [206] Lin, Y.-L., Aleksandrov, A., Simonson, T., and Roux, B.: An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. J. Chem. Theory Comput. 10(7): 2690–2709, July 2014.
- [207] Reif, M. M. and Oostenbrink, C.: Net charge changes in the calculation of relative ligand-binding free energies via classical atomistic molecular dynamics simulation. <u>Journal of Computational Chemistry</u>. 35(3): 227–243, January 2014.
- [208] Fasano, M., Curry, S., Terreno, E., Galliano, M., Fanali, G., Narciso, P., Notari, S., and Ascenzi, P.: The extraordinary ligand binding properties of human serum albumin. <u>IUBMB Life (International Union of Biochemistry and Molecular Biology: Life)</u>. 57(12): 787–796, December 2005.
- [209] Elinder, M., Geitmann, M., Gossas, T., Kallblad, P., Winquist, J., Nordstrom, H., Hamalainen, M., and Danielson, U. H.: Experimental Validation of a Fragment Library for Lead Discovery Using SPR Biosensor Technology. Journal of Biomolecular Screening. 16(1): 15–25, January 2011.
- [210] Gilson, M., Given, J., Bush, B., and McCammon, J.: The statistical-thermodynamic basis for computation of binding affinities: A critical review. Biophysical Journal. 72(3): 1047–1069, March 1997.
- [211] Lexa, K. W., Dolghih, E., and Jacobson, M. P.: A Structure-Based Model for Predicting Serum Albumin Binding. PLoS ONE. 9(4): e93323, April 2014.
- [212] Evoli, S., Mobley, D., Guzzi, R., and Rizzuti, B.: Multiple binding modes of ibuprofen in human serum albumin identified by absolute binding free energy calculations. <u>bioRxiv</u>. 068502 pp, August 2016.
- [213] Martin, Y. C.: Let's not forget tautomers. <u>Journal of Computer-Aided Molecular Design</u>. 23(10): 693–704, October 2009.
- [214] Song, Y., Mao, J., and Gunner, M. R.: MCCE2: Improving protein pKa calculations with extensive side chain rotamer sampling. Journal of Computational Chemistry. pp NA–NA, 2009.
- [215] Latta, M., Knapp, M., Sarmientos, P., Bréfort, G., Becquart, J., Guerrier, L., Jung, G., and Mayaux, J.-F.: Synthesis and Purification of Mature Human Serum Albumin from E. Coli. <u>Bio/Technology</u>. 5(12): 1309–1314, December 1987.
- [216] Lang, B. E. and Cole, K. D.: Unfolding properties of recombinant human serum albumin products are due to bioprocessing steps. Biotechnology Progress. 31(1): 62–69, January 2015.
- [217] Reinhard, L., Mayerhofer, H., Geerlof, A., Mueller-Dieckmann, J., and Weiss, M. S.: Optimization of protein buffer cocktails using Thermofluor. <u>Acta Crystallographica Section F Structural Biology and Crystallization Communications</u>. 69(2): 209–214, February 2013.
- [218] Shirts, M. R., Klein, C., Swails, J. M., Yin, J., Gilson, M. K., Mobley, D. L., Case, D. A., and Shirts, M. R.: Lessons learned from comparing molecular dynamics englines on the SAMPL5 dataset. <u>J Comput Aided Mol Des.</u> 2016.
- [219] Monroe, J. I. and Shirts, M. R.: Converging free energies of binding in cucurbit[7]uril and octa-acid host–guest systems from SAMPL4 using expanded ensemble simulations. <u>J Comput Aided Mol Des</u>. 28(4): 401–415, March 2014.
- [220] Bosisio, S., Mey, A. S. J. S., and Michel, J.: Blinded predictions of host-guest standard free energies of binding in the SAMPL5 challenge. J Comput Aided Mol Des. 2016.
- [221] Mobley, D. L. and Guthrie, J. P.: FreeSolv: A database of experimental and calculated hydration free energies, with input files. J Comput Aided Mol Des. 28(7): 711–720, PMC4113415, June 2014.

[222] Liu, T., Lin, Y., Wen, X., Jorissen, R. N., and Gilson, M. K.: BindingDB: A web-accessible database of experimentally determined protein–ligand binding affinities. <u>Nucl. Acids Res.</u> 35(suppl 1): D198–D201, January 2007.