1. Minino AM, Murphy SL, Xu J, Kochanek KD (2011) Deaths: final data for 2008. National vital statistics reports : from the Centers for Disease Control and Prevention, National Center for Health Statistics, National Vital Statistics System 59: 1-126.

2. Kaeberlein M, McVey M, Guarente L (1999) The SIR2/3/4 complex and SIR2 alone promote longevity in Saccharomyces cerevisiae by two different mechanisms. Genes & Development 13: 2570-2580.

3. Lin SJ, Defossez PA, Guarente L (2000) Requirement of NAD and SIR2 for life-span extension by calorie restriction in Saccharomyces cerevisiae. Science 289: 2126-2128.

4. Frye RA (1999) Characterization of five human cDNAs with homology to the yeast SIR2 gene: Sir2-like proteins (sirtuins) metabolize NAD and may have protein ADP-ribosyltransferase activity. Biochemical and Biophysical Research Communications 260: 273-279.

5. Frye RA (2000) Phylogenetic classification of prokaryotic and eukaryotic Sir2-like proteins. Biochemical and Biophysical Research Communications 273: 793-798.

6. Onyango P, Celic I, McCaffery JM, Boeke JD, Feinberg AP (2002) SIRT3, a human SIR2 homologue, is an NAD-dependent deacetylase localized to mitochondria. Proceedings of the National Academy of Sciences of the United States of America 99: 13653-13658.

7. Lombard DB, Alt FW, Cheng HL, Bunkenborg J, Streeper RS, et al. (2007) Mammalian sir2 homolog SIRT3 regulates global mitochondrial lysine acetylation. Molecular and Cellular Biology 27: 8807-8814.

8. Hallows WC, Lee S, Denu JM (2006) Sirtuins deacetylate and activate mammalian acetyl-CoA synthetases. Proceedings of the National Academy of Sciences of the United States of America 103: 10230-10235.

9. Schwer B, Bunkenborg J, Verdin RO, Andersen JS, Verdin E (2006) Reversible lysine acetylation controls the activity of the mitochondrial enzyme acetyl-CoA synthetase 2. Proceedings of the National Academy of Sciences of the United States of America 103: 10224-10229.

10. Hallows WC, Yu W, Smith BC, Devires MK, Ellinger JJ, et al. (2011) Sirt3 Promotes the Urea Cycle and Fatty Acid Oxidation during Dietary Restriction. Molecular Cell 41: 139-149.

11. Hirschey MD, Shimazu T, Goetzman E, Jing E, Schwer B, et al. (2010) SIRT3 regulates mitochondrial fatty-acid oxidation by reversible enzyme deacetylation. Nature 464: 121-U137.

12. Lu ZP, Bourdi M, Li JH, Aponte AM, Chen Y, et al. (2011) SIRT3-dependent deacetylation exacerbates acetaminophen hepatotoxicity. Embo Reports 12: 840-846.

13. Finley LWS, Carracedo A, Lee J, Souza A, Egia A, et al. (2011) SIRT3 Opposes Reprogramming of Cancer Cell Metabolism through HIF1 alpha Destabilization. Cancer Cell 19: 416-428.

14. Alhazzazi TY, Kamarajan P, Joo N, Huang JY, Verdin E, et al. (2011) Sirtuin-3 (SIRT3), a Novel Potential Therapeutic Target for Oral Cancer. Cancer 117: 1670-1678.

15. Kim HS, Patel K, Muldoon-Jacobs K, Bisht KS, Aykin-Burns N, et al. (2010) SIRT3 Is a Mitochondria-Localized Tumor Suppressor Required for Maintenance of Mitochondrial Integrity and Metabolism during Stress. Cancer Cell 17: 41-52.

16. Berger F, Ramirez-Hernandez MH, Ziegler M (2004) The new life of a centenarian: signalling functions of NAD(P). Trends in Biochemical Sciences 29: 111-118.

17. Chang ML, Yang J, Kem S, Klaidman L, Sugawara T, et al. (2002) Nicotinamide and ketamine reduce infarct volume and DNA fragmentation in rats after brain ischemia and reperfusion. Neuroscience Letters 322: 137-140.

18. Yang J, Klaidman LK, Adams JD (2002) Medicinal chemistry of nicotinamide in the treatment of ischemia and reperfusion. Mini reviews in medicinal chemistry 2: 125-134.

19. Yang J, Klaidman LK, Chang ML, Kem S, Sugawara T, et al. (2002) Nicotinamide therapy protects against both necrosis and apoptosis in a stroke model. Pharmacology Biochemistry and Behavior 73: 901-910.

20. Avalos JL, Boeke JD, Wolberger C (2004) Structural basis for the mechanism and regulation of Sir2 enzymes. Molecular Cell 13: 639-648.

21. Sauve AA, Moir RD, Schramm VL, Willis IM (2005) Chemical activation of Sir2-dependent silencing by relief of nicotinamide inhibition. Molecular Cell 17: 595-601.

22. Adams JD, Klaidman LK (2007) Sirtuins, nicotinamide and aging: A critical review. Letters in Drug Design & Discovery 4: 44-48.

23. Qin WP, Yang TL, Ho L, Zhao Z, Wang J, et al. (2006) Neuronal SIRT1 activation as a novel mechanism underlying the prevention of Alzheimer disease amyloid neuropathology by calorie restriction. Journal of Biological Chemistry 281: 21745-21754.

24. Wlodawer A, Vondrasek J (1998) Inhibitors of HIV-1 protease: A major success of structure-assisted drug design. Annual Review of Biophysics and Biomolecular Structure 27: 249-284.

25. Murcko M. (1992) Use of structural information in drug design Current Opinion in Structural Biology 2: 9.

26. Hou T, Wang J, Li Y, Wang W (2011) Assessing the performance of the molecular mechanics/Poisson Boltzmann surface area and molecular mechanics/generalized Born surface area methods. II. The accuracy of ranking poses generated from docking. J Comput Chem 32: 866-877.

27. Rastelli G, Rio AD, Degliesposti G, Sgobba M (2010) Fast and accurate predictions of binding free energies using MM-PBSA and MM-GBSA. Journal of Computational Chemistry 31: 797-810.

28. Guimarães CRW, Cardozo M (2008) MM-GB/SA Rescoring of Docking Poses in Structure-Based Lead Optimization. J Chem Inf Model.

29. Lyne PD, Lamb ML, Saeh JC (2006) Accurate Prediction of the Relative Potencies of Members of a Series of Kinase Inhibitors Using Molecular Docking and MM-GBSA Scoring. J Med Chem 49: 4805-4808.

30. Copeland RA (2005) Evaluation of enzyme inhibitors in drug discovery: a guide for medicinal chemists and pharmacologists. New Jersey: A John Wiley & Sons, Inc. 271 p.

31. Rye PT, Frick LE, Ozbal CC, Lamarr WA (2011) Advances in Label-Free Screening Approaches for Studying Sirtuin-Mediated Deacetylation. Journal of Biomolecular Screening 16: 1217-1226.

32. Jackson MD, Schmidt MT, Oppenheimer NJ, Denu JM (2003) Mechanism of nicotinamide inhibition and transglycosidation by Sir2 histone/protein deacetylases. Journal of Biological Chemistry 278: 50985-50998.

33. Sauve AA, Schramm VL (2003) Sir2 regulation by nicotinamide results from switching between base exchange and deacetylation chemistry. Biochemistry 42: 9249-9256.

34. Grubisha O, Smith BC, Denu JM (2005) Small molecule regulation of Sir2 protein deacetylases. Febs Journal 272: 4607-4616.

35. Avalos JL, Bever KM, Wolberger C (2005) Mechanism of Sirtuin Inhibition by Nicotinamide: Altering the NAD+ Cosubstrate Specificity of a Sir2 Enzyme. Molecular Cell 17: 855-868.

36. Avalos JL, Bever KM, Wolberger C (2005) Mechanism of sirtuin inhibition by nicotinamide: Altering the NAD(+) cosubstrate specificity of a Sir2 enzyme. Molecular Cell 17: 855-868.

37. North BJV, E. (2004) Sirtuins: Sir2-related NAD-dependent protein deacetylases. Genome Biology 5: 224.

38. Jin L, Wei WT, Jiang YB, Peng H, Cai JH, et al. (2009) Crystal Structures of Human SIRT3 Displaying Substrate-induced Conformational Changes. Journal of Biological Chemistry 284: 24394-24405.

39. Szczepankiewicz BG, Dai H, Koppetsch KJ, Qian DM, Jiang F, et al. (2012) Synthesis of Carba-NAD and the Structures of Its Ternary Complexes with SIRT3 and SIRT5. Journal of Organic Chemistry 77: 7319-7329.

40. Giralt A, Villarroya F (2012) SIRT3, a pivotal actor in mitochondrial functions: metabolism, cell death and aging. Biochemical Journal 444: 1-10.

41. Cen Y (2010) Sirtuins inhibitors: The approach to affinity and selectivity. Biochimica Et Biophysica Acta-Proteins and Proteomics 1804: 1635-1644.

42. Segel IH (1993) Enzyme Kinetics Behavior and analysis of rapid equilibrium and steady-state enzyme systems. USA: Wiley Classics Library. 957 p.

43. Cer RZ, Mudunuri U, Stephens R, Lebeda FJ (2009) IC50-to-K-i: a web-based tool for converting IC50 to K-i values for inhibitors of enzyme activity and ligand binding. Nucleic Acids Research 37: W441-W445.

44. Schuetz A, Min JR, Antoshenko T, Wang CL, Allali-Hassani A, et al. (2007) Structural basis of inhibition of the human NAD(+)-dependent deacetylase SIRT5 by suramin. Structure 15: 377-389.

45. Heltweg B, Gatbonton T, Schuler AD, Posakony J, Li HZ, et al. (2006) Antitumor activity of a small-molecule inhibitor of human silent information regulator 2 enzymes. Cancer Research 66: 4368-4377.

46. Schmidt MT, Smith BC, Jackson MD, Denu JM (2004) Coenzyme specificity of Sir2 protein deacetylases - Implications for physiological regulation. Journal of Biological Chemistry 279: 40122-40129.

47. Tervo AJ, Kyrylenko S, Niskanen P, Salminen A, Leppanen J, et al. (2004) An in silico approach to discovering novel inhibitors of human sirtuin type 2. Journal of Medicinal Chemistry 47: 6292-6298.

48. Anderson RM, Bitterman KJ, Wood JG, Medvedik O, Sinclair DA (2003) Nicotinamide and PNC1 govern lifespan extension by calorie restriction in Saccharomyces cerevisiae. Nature 423: 181-185.

49. Sauve AA (2010) Sirtuin chemical mechanisms. Biochimica Et Biophysica Acta-Proteins and Proteomics 1804: 1591-1603.

50. Sauve AA, Wolberger C, Schramm VL, Boeke JD (2006) The biochemistry of sirtuins. Annual Review of Biochemistry. pp. 435-465.

51. Bitterman KJ, Anderson RM, Cohen HY, Latorre-Esteves M, Sinclair DA (2002) Inhibition of silencing and accelerated aging by nicotinamide, a putative negative regulator of yeast Sir2 and human SIRT1. Journal of Biological Chemistry 277: 45099-45107.

52. Hoff KG, Avalos JL, Sens K, Wolberger C (2006) Insights into the sirtuin mechanism from ternary complexes containing NAD(+) and acetylated peptide. Structure 14: 1231-1240.

53. Henrich S, Feierberg I, Wang T, Blomberg N, Wade RC (2010) Comparative binding energy analysis for binding affinity and target selectivity prediction. Proteins-Structure Function and Bioinformatics 78: 135-153.

54. Szczepankiewicz BG, Dai H, Koppetsch KJ, Qian D, Jiang F, et al. (2012) Synthesis of carba-NAD and the structures of its ternary complexes with SIRT3 and SIRT5. J Org Chem 77: 7319-7329.

55. Chang JH, Kim HC, Hwang KY, Lee JW, Jackson SP, et al. (2002) Structural basis for the NAD-dependent deacetylase mechanism of Sir2. Journal of Biological Chemistry 277: 34489-34498.

56. Sherman W, Day T, Jacobson MP, Friesner RA, Farid R (2006) Novel procedure for modeling ligand/receptor induced fit effects. Journal of Medicinal Chemistry 49: 534-553.

57. Cen Y, Youn DY, Sauve AA (2011) Advances in Characterization of Human Sirtuin Isoforms: Chemistries, Targets and Therapeutic Applications. Current Medicinal Chemistry 18: 1919-1935.

58. Disch JS, Evindar G, Chiu CH, Blum CA, Dai H, et al. (2013) Discovery of Thieno[3,2-d]pyrimidine-6-carboxamides as Potent Inhibitors of SIRT1, SIRT2, and SIRT3. J Med Chem.

59. Jorgensen WL (2009) Efficient Drug Lead Discovery and Optimization. Accounts of Chemical Research 42: 724-733.

60. Chakrabarti R, Klibanov AM, Friesner RA (2005) Sequence optimization and designability of enzyme active sites. Proceedings of the National Academy of Sciences of the United States of America 102: 12035-12040.

61. Chakrabarti R, Klibanov AM, Friesner RA (2005) Computational prediction of native protein-ligand binding and enzyme active site sequences. Proceedings of the National Academy of Sciences of the United States of America 102: 10153-10158.

62. Hansson T, Aqvist J (1995) Estimation of binding free energies for HIV proteinase inhibitors by molecular dynamics simulations. Protein Engineering 8: 1137-1144.

63. Guimaraes CRW, Cardozo M (2008) MM-GB/SA rescoring of docking poses in structure-based lead optimization. Journal of Chemical Information and Modeling 48: 958-970.

64. Tounge BA, Reynolds CH (2003) Calculation of the binding affinity of beta-secretase inhibitors using the linear interaction energy method. Journal of Medicinal Chemistry 46: 2074-2082.

65. Aqvist J, Marelius J (2001) The linear interaction energy method for predicting ligand binding free energies. Combinatorial Chemistry & High Throughput Screening 4: 613-626.

66. Bollini M, Gallardo-Macias R, Spasov KA, Tirado-Rives J, Anderson KS, et al. (2013) Optimization of benzyloxazoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase to enhance Y181C potency. Bioorganic & Medicinal Chemistry Letters 23: 1110-1113.

67. Bradford MM (1976) RAPID AND SENSITIVE METHOD FOR QUANTITATION OF MICROGRAM QUANTITIES OF PROTEIN UTILIZING PRINCIPLE OF PROTEIN-DYE BINDING. Analytical Biochemistry 72: 248-254.

68. Rastelli G, Del Rio A, Degliesposti G, Sgobba M (2010) Fast and Accurate Predictions of Binding Free Energies Using MM-PBSA and MM-GBSA. Journal of Computational Chemistry 31: 797-810.

69. Goodsell DS, Morris GM, Olson AJ (1996) Automated docking of flexible ligands: Applications of AutoDock. Journal of Molecular Recognition 9: 1-5.

70. Moustakas DT, Lang PT, Pegg S, Pettersen E, Kuntz ID, et al. (2006) Development and validation of a modular, extensible docking program: DOCK 5. Journal of Computer-Aided Molecular Design 20: 601-619.

71. Kim R, Skolnick J (2008) Assessment of programs for ligand binding affinity prediction. Journal of Computational Chemistry 29: 1316-1331.

72. Friesner RA, Banks JL, Murphy RB, Halgren TA, Klicic JJ, et al. (2004) Glide: A new approach for rapid, accurate docking and scoring. 1. Method and assessment of docking accuracy. Journal of Medicinal Chemistry 47: 1739-1749.

73. Halgren TA, Murphy RB, Friesner RA, Beard HS, Frye LL, et al. (2004) Glide: A new approach for rapid, accurate docking and scoring. 2. Enrichment factors in database screening. Journal of Medicinal Chemistry 47: 1750-1759.

74. Smith BC, Denu JM (2006) Sirtuins caught in the act. Structure 14: 1207-1208.

75. Jacobson MP, Kaminski GA, Friesner RA, Rapp CS (2002) Force Field Validation Using Protein Side Chain Prediction. The Journal of Physical Chemistry B 106: 11673-11680.

76. Shelley JC, Cholleti A, Frye LL, Greenwood JR, Timlin MR, et al. (2007) Epik: a software program for pK (a) prediction and protonation state generation for drug-like molecules. Journal of Computer-Aided Molecular Design 21: 681-691.

77. Carlson HA, McCammon JA (2000) Accommodating protein flexibility in computational drug design. Mol Pharmacol 57: 213-218.

78. Schaffer L, Verkhivker GM (1998) Predicting structural effects in HIV-1 protease mutant complexes with flexible ligand docking and protein side-chain optimization. Proteins 33: 295-310.

79. Nabuurs SB, Wagener M, de Vlieg J (2007) A Flexible Approach to Induced Fit Docking. Journal of Medicinal Chemistry 50: 6507-6518.

80. Ghosh A, Rapp CS, Friesner RA (1998) Generalized born model based on a surface integral formulation. Journal of Physical Chemistry B 102: 10983-10990.

81. Li JN, Abel R, Zhu K, Cao YX, Zhao SW, et al. (2011) The VSGB 2.0 model: A next generation energy model for high resolution protein structure modeling. Proteins-Structure Function and Bioinformatics 79: 2794-2812.

Imai, S. and Yoshino, J. The importance of NAMPT/NAD/SIRT1 in the systemic regulation of metabolism and ageing. *Diabetes, Obesity & Metabolism* 15: 26-33, 2013.

Verdin E. Coupling of NAD metabolism, sirtuins and lifespan. *Nature Med.* 20: 25-26, 2014.

Mouchiroud L., Houtkooper R. H., Moullan N., Katsyuba E., Ryu D., Canto C., Mottis A., Jo Y-S., Viswanathan M., Schoonjans K., Guarente L. and Auwerx J. The NAD+/Sirtuin Pathway Modulates Longevity through Activation of Mitochondrial UPR and FOXO Signaling. *Cell* 154: 430-441, 2013.

Canto C., Houtkooper R. H., Pirinen E., Youn D. Y., Oosterveer M. H., Cen Y., Fernandez-Marcos P. J., Yamamoto H., Andreux P. A., Cettour-Rose P., Gademann K., Rinsch C., Schoonjans K., Sauve A. A. and Auwerx J. The NAD+ Precursor Nicotinamide Riboside Enhances Oxidative Metabolism and Protects against High-Fat Diet-Induced Obesity. *Cell Metabolism* 15 (6): 838-847, 2012.

Gomes A. P., Price N. L., Ling A. J., Moslehi J. J., Montgomery M. K., Rajman L., White J. P., Teodoro J. S., Wrann C. D., Hubbard B. P., Mercken E. M., Palmeira C. M., de Cabo R., Rolo A. P., Tumer N., Bell E. L., and Sinclair D. A. Declining NAD Induces a Pseudohypoxic State Disrupting Nuclear-Mitochondrial Communication during Aging. *Cell* 155: 1624-1638. 2013.

Massudi H., Grant R., Braidy N., Guest J., Farnswoth B., and Gullemin G.J. Age-associated changes in oxidative stress and NAD metabolism in human tissue. *PLOS One* 7 (7): e42357, 2012.

Ramsey K. M., Yoshino J., Brace C. S., Abrassart D., Kobayashi Y., Marcheva B., Hong H-K., Chong J. L., Buhr E. D., Lee, C., Takahashi J. S., Imai S-I. and Bass, J. Circadian Clock Feedback Cycle through NAMPT-Mediated NAD Biosynthesis. *Science* 324: 651-654, 2009.

Peek C. B., Affinati A. H., Ramsey K. M., Kuo H-Y., Yu W., Sena L. A., Ilkayeva O., Marcheva B., Kobayashi Y., Omura C., Levine D. C., Bacsik D. J., Gius D., Newgard C. B., Goetzman E., Chandel N. S., Denu J. M., Mrksich M. and Bass J. Circadian Clock NAD+ Cycle Drives Mitochondrial Oxidative Metabolism in Mice. *Science* 342: 1243417, 2013.

Forger D. B. and Peskin C. S. A detailed predictive model of the mammalian circadian clock. *Proc. Natl. Acad. Sci. USA* 100 (25): 14806-14811, 2003.

Guarente L. Sirtuins and the Warburg effect. *Nature Med.* 20: 24-25, 2014.

Finley L. W., Carracedo A., Lee J., Souza A., Egia A., Zhang J., Teruya-Feldstein J., Moreira P. I., Cardoso S. M., Clish C.B., Pandolfi P. P. and Haigis M. C. SIRT3 Opposes Reprogramming of Cancer Cell Metabolism through HIF-1-alpha Destabilization. *Cancer Cell* 19 (3): 416-428, 2011.

Feldman J. L., Josue B. and Denu J. M. Activation of the Protein Deacetylase SIRT6 by Long-chain Fatty Acids and Widespread Deacylation by Mammalian Sirtuins. *J. Biol. Chem.* 288 (43): 31350-21356, 2013.

Fischer F., Gertz M., Suenkel B., Lakshminarasimhan M., Schutkowski M., and Steegborn C. Sirt5 deacylation activities show differential sensitivities to nicotinamide inhibition. *PLOS One* 7 (9): e45098.

P. Hu, S Wang, and Y. Highly dissociative and concerted mechanism for the NAM cleavage reaction in Sir2Tm. JACS (2008) 130: 16721-16728.

A Liang, et al. Investigation of the catalytic mechanism of Sir2 enzyme with QM/MM approach: SN1 vs SN2? J Phys. Chem. (2010) 114: 11927-11933.

Y. Shi, Y. Zhou, S. Wang, and Y. Zhang. Sirtuin Deacetylation Mechanism and Catalytic Role of the Dynamic Cofactor Binding Loop. (2013) J Phy. Chem. 4: 491-495.

Jl Avalos, KM Bever, and C Wolberger. Mechanism of sirtuin inhibition by NAM: altering the NAD+ cosubstrate specificity of a Sir2 enzyme. Mol. Cell (2005) 17: 855-868.

Hoff, K. G., Avalos, J. L., Sens, K., and Wolberger, C. (2006) Insights into the sirtuin mechanism from ternary complexes containing NAD\_ and acetylated peptide. *Structure* 14, 1231–1240

Gambini J., Gomez-Cabrera MC, Borras C, Valles SL, Lopez Grueso R., Martinez-Bello VE, Herranz D., Pallardo FV, e t al. Free [NADH]/[NAD+] regulates sirtuin expression. Arch. Biochem. Biophys. 512: 24-9, 2011.

Guarente L. Calorie restriction and sirtuins revisited. *Genes & Development* 27: 2072-2085, 2013.

SIRT1 structure (may not be published yet)

Lei Jin, Heidi Galonek,1 Kristine Israelian,1 Wendy Choy,1 Michael Morrison,1, Yu Xia,2 Xiaohong Wang,2 Yihua Xu,2 Yuecheng Yang,2 Jesse J. Smith,1, Ethan Hoffmann,1 David P. Carney,1 Robert B. Perni,1 Michael R. Jirousek,1, Jean E. Bemis,1 Jill C. Milne,1 David A. Sinclair,1 and Christoph H. Westphal1,

Biochemical characterization, localization, and tissue distribution of the longer form of mouse SIRT3. *Protein Sci.* 18: 514-525, 2009.

Yang H., Yang T., Baur J. A., Perez E., Matsui T., Carmona J. J., Lamming D.W., Souza-Pinto N.C., Bohr V.A., Rosenzweig A., de Cabo R., Sauve A.A. and Sinclair, D.A. Nutrient-Sensitive Mitochondrial NAD+ Levels Dictate Cell Survival. *Cell* 130: 1095-1107, 2007

Lu, Q., Tan, Y., Luo, R., Molecular Dynamics of p53 DNA Binding Domain, J. Phys. Chem. 2007, 111:11538-11545

Walker, R.C, de Souza, M.M., Mercer, I.P., Gould, I.R., Klug, D.R., J. Phys. Chem. B., 2002, 106(44), 11658-11665

Pavelites, J.J., Gao, J.L., Bash, P.A., Mackerell, A.D., J. Comput. Chem. 1997, 18, 221

G.V. Papamokos,G. Tziatzos, D.G. Papageorgiou, S.D. Georgatos, A.S. Politou, E. Kaxiras, Biophysical Journal 102 (2012) 1926-1933.

Computation method references

1. Wang J, Cieplak P, Kollman P A. (2000) How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules? J Comput Chem 21: 1049–1074.

2. Hornak V, Abel R, Okur A (2006) Comparison of multiple Amber force fields and development of improved protein backbone parameters. PROTEINS Struct Funct Bioinforma 65: 712–725.

3. Lu Q, Tan Y, Luo R (2007) Molecular Dynamics Simulations of p53 DNA-Binding Domain. J Phys Chem B 111: 11538–11545.

4. Walker RC, de Souza MM, Mercer IP, Gould IR, Klug DR (2002) Large and Fast Relaxations inside a Protein:  Calculation and Measurement of Reorganization Energies in Alcohol Dehydrogenase. J Phys Chem B 106: 11658–11665.

5. Pavelites J, Gao J, Bash P, Mackerell JA (1997) A molecular mechanics force field for NAD+ NADH, and the pyrophosphate groups of nucleotides. J Comput Chem 18: 221–239.

6. Papamokos G V, Tziatzos G, Papageorgiou DG, Georgatos SD, Politou AS, et al. (2012) Structural role of RKS motifs in chromatin interactions: a molecular dynamics study of HP1 bound to a variably modified histone tail. Biophys J 102: 1926–1933.

7. Phillips JC, Braun R, Wang W, Gumbart J, Tajkhorshid E, et al. (2005) Scalable molecular dynamics with NAMD. J Comput Chem 26: 1781–1802.

8. Darden T, York D, Pedersen L (1993) Particle mesh Ewald: An N⋅ log (N) method for Ewald sums in large systems. J Chem Phys: 10089–10092.

9. Ryckaert J, Ciccotti G, Berendsen H (1977) Numerical integration of the cartesian equations of motion of a system with constraints: molecular dynamics of n-alkanes. J Comput Phys 23: 327–341.

10. Miller BR, McGee TD, Swails JM, Homeyer N, Gohlke H, et al. (2012) MMPBSA.py: An efficient program for end-state free energy calculations. J Chem Theory Comput 8: 3314–3321.

11. Onufriev A, Bashford D, Case D a (2004) Exploring protein native states and large-scale conformational changes with a modified generalized born model. Proteins 55: 383–394.

12. Weiser J, Shenkin PS, Still WC (1999) Approximate atomic surfaces from linear combinations of pairwise overlaps (LCPO). J Comput Chem 20: 217–230.

MM-PB(GB)SA binding affinity calculation references above?