

- of an active human immunodeficiency virus type 1 Nef/p21-activated kinase 2 complex. *J Virol* 79:12732-12741.
- [0187] 49. Danilczyk U G, Williams D B. 2001. The lectin chaperone calnexin utilizes polypeptide-based interactions to associate with many of its substrates in vivo. *J Biol Chem* 276:25532-25540.
- [0188] 50. Hahn M, Borisova S, Schrag J D, Tessier D C, Zapun A, Tom R, Kamen A A, Bergeron J J, Thomas D Y, Cygler M. 1998. Identification and crystallization of a protease-resistant core of calnexin that retains biological activity. *J Struct Biol* 123:260-264.
- [0189] 51. Soding J, Biegert A, Lupas A N. 2005. The HiiEIpred interactive server for protein homology detection and structure prediction. *Nucleic Acids Res* 33:W244-248.
- [0190] 52. Roy A, Kucukural A, Zhang Y. 2010. I-TASSER: a unified platform for automated protein structure and function prediction. *Nat Protoc* 5:725-738.
- [0191] 53. Pieper U, Webb B M, Dong G Q, Schneidman-Duhovny D, Fan H, Kim S J, Khuri N, Spill Y G, Weinkam P, Hammel M, Tainer J A, Nilges M, Sali A. 2014. ModBase, a database of annotated comparative protein structure models and associated resources. *Nucleic Acids Res* 42:D336-346.
- [0192] 54. Kelley L A, Sternberg M J. 2009. Protein structure prediction on the Web: a case study using the Phyre server. *Nat Protoc* 4:363-371.
- [0193] 55. Kallberg M, Wang H, Wang S, Peng J, Wang Z, Lu H, Xu J. 2012. Template-based protein structure modeling using the RaptorX web server. *Nat Protoc* 7:1511-1522.
- [0194] 56. Pawlowski M, Gajda M J, Matlak R, Bujnicki J M. 2008. MetaMQAP: a meta-server for the quality assessment of protein models. *BMC Bioinformatics* 9:403.
- [0195] 57. Berman H M, Westbrook J, Feng Z, Gilliland G, Bhat T N, Weissig H, Shindyalov I N, Bourne P E. 2000. The Protein Data Bank. *Nucleic Acids Res* 28:235-242.
- [0196] 58. The UniProt Consortium. 2014. UniProt: a hub for protein information. *Nucleic Acids Res* 43:D204-D212.
- [0197] 59. Fernandez-Fuentes N, Madrid-Aliste C J, Rai B K, Fajardo J E, Fiser A. 2007. M4T: a comparative protein structure modeling server. *Nucleic Acids Res* 35:W363-W368.
- [0198] 60. Biasini M, Bienert S, Waterhouse A, Arnold K, Studer G, Schmidt T, Kiefer F, Cassarino T G, Bertoni M, Bordoli L, Schwede T. 2014. SWISS-MODEL: modelling protein tertiary and quaternary structure using evolutionary information. *Nucleic Acids Res* 42:W252-W258.
- [0199] 61. Di Tommaso P, Moretti S, Xenarios I, Orobittg M, Montanyola A, Chang J M, Taly J F, Notredame C. 2011. T-Coffee: a web server for the multiple sequence alignment of protein and RNA sequences using structural information and homology extension. *Nucleic Acids Res* 39:W13-W17.
- [0200] 62. Kozakov D, Hall D R, Beglov D, Brenke R, Comeau S R, Shen Y, Li K, Zheng J, Vakili P, Paschalidis I C, Vajda S. 2010. Achieving reliability and high accuracy in automated protein docking: ClusPro, PIPER, SDU, and stability analysis in CAPRI rounds 13-19. *Proteins* 78:3124-3130.
- [0201] 63. Ritchie D W, Venkatraman V. 2010. Ultra-fast FFT protein docking on graphics processors. *Bioinformatics* 26:2398-2405.
- [0202] 64. Torchala M, Moal I H, Chaleil R A, Fernandez-Recio J, Bates P A. 2013. SwarmDock: a server for flexible protein-protein docking. *Bioinformatics* 29:807-809.
- [0203] 65. Pierce B G, Wiehe K, Hwang H, Kim B H, Vreven T, Weng Z. 2014. ZDOCK server: interactive docking prediction of protein-protein complexes and symmetric multimers. *Bioinformatics* 30:1771-1773.
- [0204] 66. Irwin J J, Shoichet B K. 2005. ZINC—a free database of commercially available compounds for virtual screening. *J Chem Info Model* 45:177-182.
- [0205] 67. Jubier-Maurin V, et al. 1999. Genetic Characterization of the nef Gene from Human Immunodeficiency Virus Type 1 Group M Strains Representing Genetic Subtypes A, B, C, E, F, G, and H. *AIDS Research and Human Retroviruses*. Volume 15, Number 1, pp. 23-32.
- We claim:
1. A method for restoring or preserving cholesterol efflux in a cell infected with Human Immunodeficiency Virus (HIV) comprising delivering to the cell an effective amount of a composition or formulation comprising a small molecule, wherein the small molecule prevents or decreases an interaction between a Negative Regulatory Factor (Nef) protein and a Calnexin protein.
  2. The method of claim 1, wherein the small molecule binds to at least one amino acid residue on the Nef protein, wherein the at least one amino acid residue is selected from the group consisting of a lysine at amino acid position 4, a serine at amino acid position 6, a lysine at amino acid position 7, and a tyrosine at amino acid position 124.
  3. The method of claim 1, wherein the small molecule binds to at least one amino acid residue on the Calnexin protein, wherein the at least one amino acid residue is selected from the group consisting of an aspartic acid at position 90, a glutamic acid at amino acid position 529, a glutamic acid at amino acid position 532, and a glutamic acid at amino acid position 533.
  4. The method of claim 1, wherein preventing or decreasing the interaction between the Nef protein and the Calnexin protein results in at least partial restoration of ATP-Binding Cassette A1 (ABCA1) activity.
  5. The method of claim 1, wherein the small molecule is a small molecule is selected from the group consisting of Formula (I), Formula (II), Formula (III) or an analog or derivative thereof:

