

Supporting Information

Modeling Multiple Species of Nicotine and Deschloroepibatidine Interacting with $\alpha 4\beta 2$ Nicotinic Acetylcholine Receptor: From Microscopic Binding to Phenomenological Binding Affinity

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Supporting Information Available. Stereo version of Figures 2A and 2B; complete citations of references 10(a), 10(e), 34, 39, and 40. This material is available free of charge *via* the Internet at <http://pubs.acs.org>.

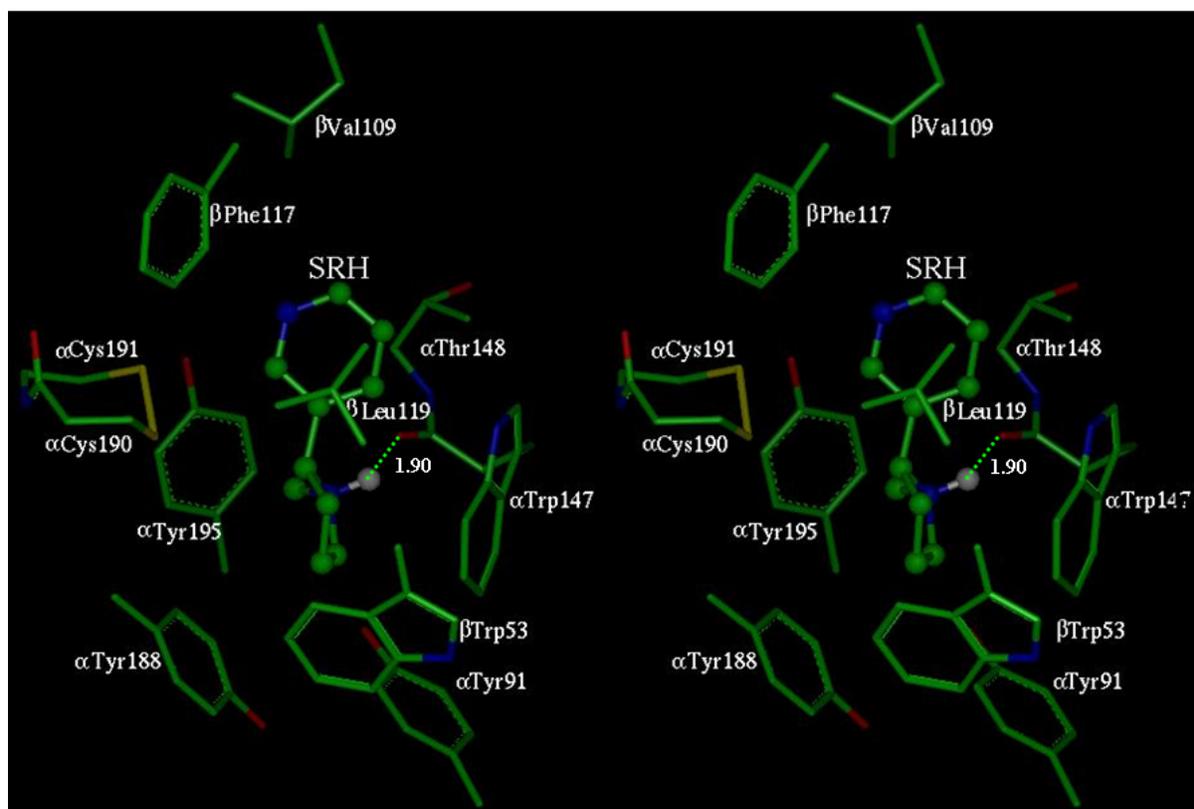


Figure S1. Stereo version of Figure 2A

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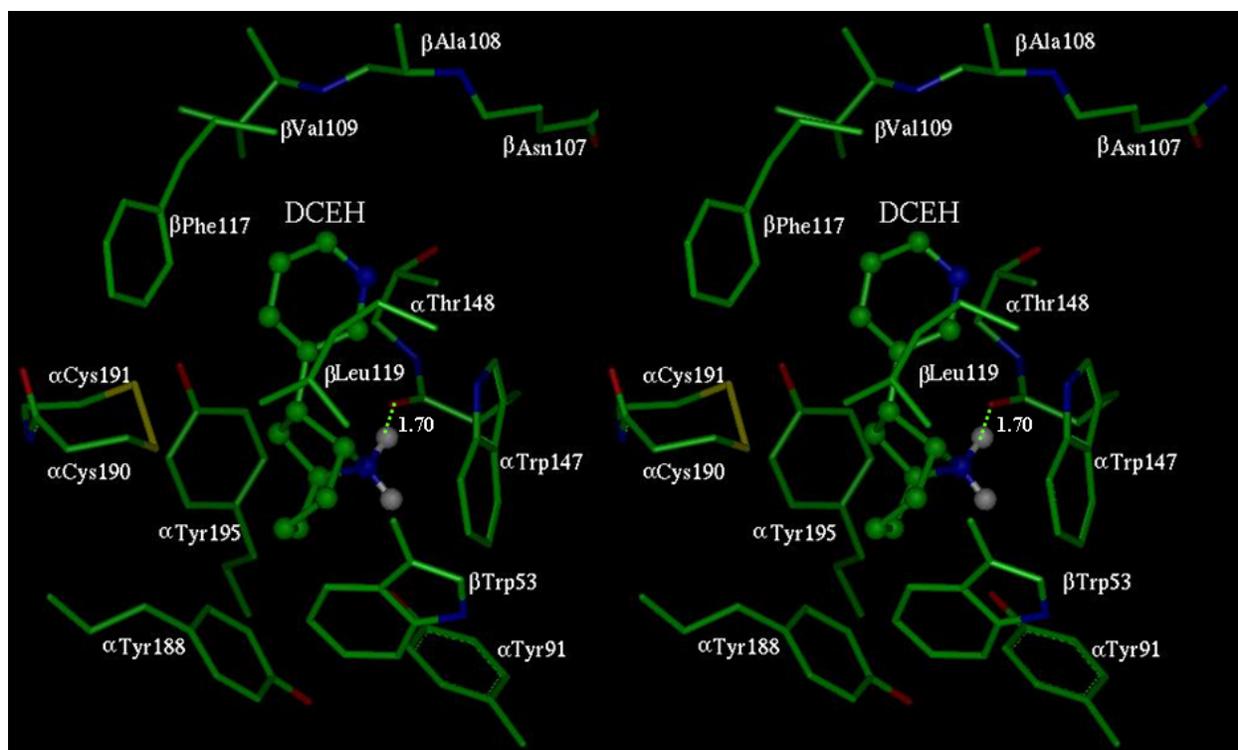


Figure S2. Stereo version of Figure 2B

Reference 10(a): (a) Briggs, C. A.; Anderson, D. J.; Brioni, J. D.; Buccafusco, J. J.; Buckley, M. J.; Campbell, J. E.; Decker, M. W.; Donnelly, R. D.; Elliott, R. L.; Gopalakrishnan, M.; Holladay, M. W.; Hui, Y. H.; Jackson, W. J.; Kim, D. J. B.; Marsh, K. C.; O'Neill, A.; Prendergast, M. A.; Ryther, K. B.; Sullivan, J. P.; Arneric, S. P. *Pharm. Biochem. Behav.* **1997**, *57*, 231-241.

Reference 10(e): Sullivan, J.P.; Donnelly-Roberts, D.; Briggs, C.A.; Anderson, D.J.; Gopalakrishnan, M.; Xue, I.C.; Plattoni-Kaplan, M.; Molinari, E.; Campbell, J.E.; McKenna, D.G.; Gunn, D.E.; Lin, N.H.; Ryther, K.B.; He, Y.; Holladay, M.W.; Wonnacott, S.; Williams, M.; Arneric, S.P. *J. Tharm. Exp. Therap.* **1997**, *283*, 235.

Reference 34: Case, D.A.; Pearlman, D.A.; Caldwell, J.W.; Cheatham III, T.E.; Wang, J.; Ross, W.S.; Simmerling, C.L.; Darden, T.A.; Merz, K.M.; Stanton, R.V.; Cheng, A.L.; Vincent, J.J.; Crowley, M.; Tsui, V.; Gohlke, H.; Radmer, R.J.; Duan, Y.; Pitera, J.; Massova, I.; Seibel, G.L.; Singh, U.C.; Weiner, P.K.; Kollman, P.A. *AMBER 7*, University of California, San Francisco, **2002**.

Reference 39: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.;

Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision A.1, Gaussian, Inc., Pittsburgh, PA, **2003**.

Reference 40: Schmidt, M. W.; Baldridge, K. K.; Boatz, J. A.; Elbert, S. T.; Gordon, M. S.; Jensen, J. H.; Koseki, S.; Matsunaga, N.; Nguyen, K. A.; Su, S. J.; Windus, T. L.; Dupuis, M.; Montgomery, J. A. *J. Comput. Chem.* **1993**, *14*, 1347.