

CADD Center Publications

- 1) Yang, B., Wright, J., Eldefrawi, M.E., Poi, S., and MacKerell Jr., A.D., Conformational, aqueous solvation and pK<sub>a</sub> contributions to the binding of cocaine, WIN and a WIN vinyl analog. **Journal of the American Chemical Society**, 116:8722-8732, 1994.
- 2) Li, Y., MacKerell, Jr., A.D., Egorin, M.J., Ballesteros, M.F., Rosen, D.M., Wu, Y.-Y., Blamble, D.A. and Callery, P.S., Structure-Function Relationships of Polyamine Transport Inhibitors in L1210 Murine Leukemia Cells, **Cancer Investigation**, 57: 234-239, 1997.
- 3) Lieske, S., Yang, B., Eldefrawi, M.E. and MacKerell Jr., A.D., and Wright, J., (-)-3b-Substituted Ecgonine Methyl Esters as Inhibitors for Cocaine Binding and Dopamine Uptake., **Journal of Medicinal Chemistry**, 41: 864-876, 1998.
- 4) Chen, I.J., Neamati, N., Nicklaus, M.C., Orr, A., Anderson, L., Barchi, Jr., J.J., Kelley, J.A., Pommier, Y., and MacKerell, Jr. A.D., Identification of HIV-1 Integrase Inhibitors via Three-Dimensional Database Searching using ASV and HIV-1 Integrase as Targets., **Biororganic & Medicinal Chemistry**, 8: 2385-2389, 2000.
- 5) Chen, I.-J., Neamati, N. and MacKerell, Jr. A.D., Structure-Based Inhibitor Design Targeting HIV-1 Integrase., **Current Drug Targets - Infectious Disorders**, 2: 217-234, 2002.
- 6) Pan, Y., Huang, N., Cho, S. and A. D. MacKerell, Jr., Consideration of molecular weight during compound selection in virtual database screening., **Journal of Chemical Information and Computer Science**, 43: 267-272, 2003.
- 7) Chen, W., Wu, H., Bernard, D., Metcalf, M.D., Deschamps, J., Flippen-Anderson, J., MacKerell, Jr., A.D. and Coop, A., Rearrangement of 5-Trimethylsilylthebaine on Treatment with L-Selectride: An Efficient Synthesis of (+)-Bractazone, **Journal of Organic Chemistry**, 68: 1929-1932, 2003.
- 8) Bernard, D., A. Coop, A. and MacKerell, Jr., A.D. , 2D Conformationally Sampled Pharmacophore: A Novel Approach to Ligand Based Pharmacophore Development Applied to  $\delta$  Opioid Agonists and Antagonists, **Journal of the American Chemical Society**. 125: 3103-3107, 2003.
- 9) Rosen, G.M, Beselman, A., Tsai, P., Pou, S., Mailer, C. Ichikawa, K., Robinson, B.H., Nielsen, R., Halpern, H. and MacKerell, A.D. Jr., Influence of Structure on the EPR Spectrum of Spin Trapped Adducts of 5,5-Dimethyl-1-Pyrroline-N-Oxide, **Journal of Organic Chemistry**, 69: 1321-1330, 2004.

- 10) Macias, A., Hernandez, R.J., Mehta, A.K., MacKerell, A.D., Jr., Ticku, M.K. and Coop, A., 3-Chloropropanoic acid (UMB66): a ligand for the gamma-hydroxybutyric acid receptor lacking a 4-hydroxyl group, **Bioorganic & Medicinal Chemistry**, 12: 1643-1647, 2004.
- 11) Huang, N., Nagarsekar, A., Xia, G., Hayashi, J., MacKerell, A.D., Jr., Identification of Non-phosphate containing Small Molecular Weight Inhibitors of the Tyrosine Kinase p56 LCK SH2 Domain via In silico Screening against the pY+3 site. **Journal of Medicinal Chemistry**, 47: 3502-3511, 2004
- 12) MacKerell, A.D., Jr., Empirical Force Fields for Biological Macromolecules: Overview and Issues, **Journal of Computational Chemistry**, 25: 1584-1604, 2004
- 13) Markowitz, J., Chen, I., Gitti, R., Baldisseri, D. M., Pan, Y., Udan, R., Carrier, F., MacKerell, A. D., Jr., Weber, D. J., "Identification and Characterization of Small Molecule Inhibitors of the Calcium-Dependent S100B-p53 Tumor Suppressor Interaction," **Journal of Medicinal Chemistry**, 47; 5085-5093, 2004.
- 14) Wu, H., D. Bernard, W. Chen, G.D. Strahan, J.R. Deschamps, D.A. Parrish, J.W. Lewis, Al.D. MacKerell, Jr., and A. Coop, "Functionalization of the 6,14-bridge of the orvinols. 2. Preparation of 18- and 19-hydroxyl substituted thevinols and their treatment with benzyl bromide. Submitted to the **Journal of Organic Chemistry**, 70: 1907-1910, 2005
- 15) Boresch, S., Leitgeb, M., Beselman, A., MacKerell, A.D., Jr., "Unexpected relative aqueous solubilities of a phosphotyrosine analogue and two phosphonate derivatives" **Journal of the American Chemical Society**, 127; 4640-4648, 2005
- 16) H. Wu, L. N. Thatcher, D. Bernard, D. A. Parrish, J. R. Deschamps, K. C. Rice, A. D. MacKerell Jr., A. Coop: The Position of Coordination of the Lithium Ion Determines the Regioselectivity of Demethylations of 3,4-Dimethoxymorphinans with L-Selectride, **Organic Letters**, 7, 2531-2534, 2005
- 17) Bernard, D., Coop, A. and MacKerell, Jr., A.D. "Computer-Aided Drug Design: Structure-Activity Relationships of Delta Opioid Ligands." **Drug Design Reviews**, 2005, 2: 277-291.
- 18) Hancock, C.N., Macias, A. Lee, E.K., Yu, S.Y., MacKerell, Jr., A.D. and Shapiro, P. "Identification of novel extracellular signal-regulated kinase (ERK) docking domain inhibitors," **Journal of Medicinal Chemistry**, 2005, 48; 4586-4595.
- 19) Markowitz, J., MacKerell, A. D., Jr., Carrier, F., Charpentier, T.H., Weber, D. J. Design of Inhibitors of S100B," **Current Topics in Medicinal Chemistry**, 2005, 5: 1093-1108.

- 20) Bernard, D.; Coop, A.; MacKerell, A. D., Jr., "Conformationally Sampled Pharmacophore for Peptidic  $\mu$  Opioid Ligands,": **Journal of Medicinal Chemistry**, 2005, 48: 7773-7780.
- 21) Macias, A.T., Mia, M.Y., Xia, G., Hayashi, J. and MacKerell, Jr., A.D., "Lead Validation and SAR Development via Chemical Similarity Searching; Application to Compounds Targeting the pY+3 Site of the SH2 Domain of p56<sup>lck</sup>," **Journal of Chemical Information and Modeling**, 2005, 45: 1759-1766.
- 22) Hancock, C.N., Macias, A., MacKerell, Jr. A.D., and Shapiro, P., "Mitogen Activated Protein (MAP) Kinases: Development of ATP and Non-ATP Dependent Inhibitors," **Medicinal Chemistry**, 2006, 2, 213-222.
- 23) Chen, I.-J., Taneja, R., Yin, D., Seo, P.R., Young, D., MacKerell, Jr., A.D., and Polli, J.E., "Chemical Substituent Effect on Pyridine Permeability and Mechanistic Insights from Computational Molecular Descriptors" **Molecular Pharmaceutics**, 3:745-755, 2006.
- 24) Zhong, S., Macias, A.T., MacKerell, Jr., A.D. "Computational identification of the inhibitors of protein-protein interactions," **Current Topics in Medicinal Chemistry**, 7, 63-82, 2007.
- 25) Chen, F., Hancock, C.N., Macias, A.T., Joh, J., Still, K., Zhong, S., MacKerell, Jr., A.D. Shapiro, P.S., "Characterization of ATP independent ERK inhibitors identified through in silico analysis of the active ERK2 structure," **Bioorganic and Medicinal Chemistry Letters**, 16:6281-627, 2006.
- 26) Markowitz, J., MacKerell, Jr., A.D., and Weber, D.J. "A search for inhibitors of S100B, a member of the S100 family of calcium-binding proteins," **Mini-Reviews in Medicinal Chemistry**, 7: 609-616, 2007, PMID: 17584159.
- 27) Bernard, D., Coop, A. and MacKerell, Jr., A.D. "Quantitative Conformationally Sampled Pharmacophore for  $\mu$  Opioid Ligands: Reevaluation of Hydrophobic Moieties Essential for Biological Activity," **Journal of Medicinal Chemistry**, 50: 1799-1809, 2007.
- 28) Furci, L.M., Lopes, P., Eakanunkul, S., Zhong, S., MacKerell, A.D., Jr., Wilks, A., "Inhibition of the Bacterial Heme Oxygenases from *Pseudomonas aeruginosa* (pa-HO) and *Neisseria meningitidis* (nm-HO): A Novel Antimicrobial Target," **Journal of Medicinal Chemistry**, 50: 3804-3813, 2007.
- 29) Zhong, S. and MacKerell, Jr., A.D. "Binding Response: A Descriptor for Selecting Ligand Binding Site on Protein Surfaces," **Journal of Chemical Information and Modeling**, 47; 2303-2315, 2007, PMID: 17900106.
- 30) Chen X., Zhong S., Zhu, X., Dziegielewska, B., Ellenberger, T., Wilson, G.M, Bachman, K., MacKerell, Jr., A.D. and Tomkinson, A.E., "Rational Design of Human

DNA Ligase Inhibitors that Target Cellular DNA Replication and Repair,” **Cancer Research**, 68: 3169-3177, 2008, PMID: 18451142.

- 31) Yu, W.-M., Guvench, O., MacKerell, Jr., A.D., and Qu. C.-K. “Identification of small molecular weight inhibitors of SHP-2 tyrosine phosphatase via in silico screening combined with experimental assay.” **Journal of Medicinal Chemistry**, 51: 7396-7404, 2008. PMID: 19007293
- 32) Zhong, S. and MacKerell, Jr., A.D. “Pose Scaling: Geometrical Assessment of Ligand Binding Poses,” **Journal of Theoretical and Computational Chemistry**, 7: 833–852, 2008.
- 33) Acharya, C., Seo, P.R., Polli, J.E. MacKerell, Jr., A.D. “Computational Model for Predicting Chemical Substituent Effects on Passive Drug Permeability across Parallel Artificial Membranes” **Molecular Pharmaceutics**, 5, 818–828, 2008, DOI: 10.1021/mp800035h, PMID: 18710255
- 34) Zhong, S., Chen, X., Zhu, X., Dziegielewska, B., Bachman, K.E., Ellenberger, T., Ballin, J.D., Wilson, G.M., Tomkinson, A.E. and MacKerell, Jr., A.D., “Identification and Validation of Human DNA Ligase Inhibitors using Computer-Aided Drug Design,” **Journal of Medicinal Chemistry**, 51; 4553-4562, 2008, PMID: 18630893, DOI: 10.1021/jm8001668
- 35) Charpentier, T.H., Wilder, P.T., Liriano, M.A., Varney, K.M., Pozharski, E, MacKerell, Jr., A.D., Coop, A., Toth, E.A., Weber, D.J., “Divalent metal ion complexes of S100B in the absence and presence of pentamidine,” **Journal of Molecular Biology**, 382:56-73, 2008, PMID: 18602402
- 36) Chen, F., MacKerell, Jr., A.D., Luo, Y. and Shapiro, P. “Using *Caenorhabditis elegans* as a Model Organism for Evaluating Extracellular Signal-Regulated Kinase Docking Domain Inhibitors,” **Journal of Cell Communication and Signaling**, 2:81-92. 2008 PMID: 19105050
- 37) Matthews, M.M., Weber, D.J., Shapiro, P.S., Coop, A., and MacKerell, Jr., A.D. “Inhibition of protein-protein interactions with low molecular weight compounds.” **Current Trends in Medicinal Chemistry**, In Press, 2009
- 38) González, P.M., Acharya, C., MacKerell, Jr., A.D. and Polli, J.E., “Inhibition Requirements of the human Apical Sodium-dependent Bile acid Transporter (hASBT) using Aminopiperidine Conjugates of glutamyl-Bile Acids,” **Pharmaceutical Research**, 26: 1665-1678, 2009.
- 39) Guvench, O., and MacKerell, Jr., A.D. “Computational Fragment-Based Binding Site Identification by Ligand Competitive Saturation, **PLoS Computational Biology**, In Press, 2009.

- 40) K. Vanommeslaeghe, K., Hatcher, E., Acharya, C., Kundu, S., Zhong, S., Shim, J., Darian, E., Guvench, O., Lopes, P., Vorobyov, I., and MacKerell Jr., A.D. CHARMM General Force Field (CGenFF): A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields,” **Journal of Computational Chemistry**, In Press, 2009
- 41) Charpentier, T.H., Wilder, P.T., Liriano, M.A., Varney, K.M., Zhong, S., Coop, A., Pozharski, E., MacKerell, Jr., A.D., Toth, E.A., Weber, D.J. “Small Molecules Bound to Unique Sites in the Target Protein Binding Cleft of Calcium-Bound S100B As Characterized by Nuclear Magnetic Resonance and X-ray Crystallography,” **Biochemistry**, In Press, 2009, PMID: 19469484

### Patents

- 1) “Immunomodulatory Compounds.” Hayashi, J., MacKerell, Jr., A.D. U.S. Patent Number 7,521,463, April 2009.

### Patent Applications

- 1) “Immunomodulatory Compounds that target and inhibit the pY+3 binding site of tyrosine kinase p56 LCK SH2 domain” MacKerell, Jr., A.D. Hayashi, J., Nagarsekar, A., Macias, A., and Huang, N., U.S. Patent Application 10/582,640, International Patent Application PCT/US2003/39501 (pending)
- 2) “Immunomodulatory Compounds that target and inhibit the pY+3 binding site of tyrosine kinase p56 LCK SH2 domain” MacKerell, Jr., A.D. Hayashi, J., Filed August 2006.
- 3) “Inhibitors of the S100-p53 Protein-Protein Interaction and Method of Inhibiting Cancer Employing the Same,” Weber, D.J., Markowitz, J., Carrier, F. and MacKerell, Jr., A.D.,  
US. Patent Application 11/155,617  
International Patent Application PCT/US03/08678  
Australian Letters Patent #2003230705  
Japanese Patent Application Number: 2003-581715
- 4) “Inhibitors of Extracellular Signal-Regulated Kinase Docking Domains and Uses Thereof” Shapiro, P.S. and MacKerell, Jr., A.D., US Patent Application Number: 11/543,491, filed 10/5/06, International Patent Application PCT/US2006/011536, Publication # WO2006/105237
- 5) “Method for Treating Disease Due to Nonsense Mutation” Matsuga, R., Shiozuka, M., and MacKerell, Jr., A.D., U.S. Provisional Patent Application Serial #: 60/806,580, PCT/JP2007063436
- 6) Wilks, A., MacKerell, Jr., A.D., Lopes, P., and Furci, L., “Antimicrobial Heme Oxygenase Inhibitors and Methods of Use” UMB Docket No: AW-2007-003, PCT/US2007074233
- 7) Melnick, A.M, MacKerell, Jr., A.D. and Privé, G.G. “Small Molecule Inhibitors of BCL6” US Provisional Patent. Dkt. No. 96700/1127

- 8) "Small Molecule Inhibitors of LCK SH2 Domain Binding" MacKerell, Jr., A.D., Hayashi, J., Mia, Y., and Xia, G U. S. provisional patent application serial number 60/913,947, International Patent Application Number: PCT/US08/73498
- 9) "Compounds that Inhibit Human DNA Ligases and Methods of Treating Cancer" Tomkinson, A.E., Chen, X., MacKerell, Jr., A.D., Dziegieilewska, B., Zhong, S., Wilson, G., US Provisional Patent Application. International Patent Application Number: PCT/US08/59931,
- 10) "Identification of small molecular weight inhibitors of SHP-2 tyrosine phosphatase that is hyperactivated in childhood leukemia," Qu, C.-K., MacKerell, Jr., A.D., Yu, W.-M., Guvench, O., Provisional Patent, submitted Fall 2008, with Case Western Reserve University.
- 11) "Compositions and Methods for the Treatment of Diabetes" MacKerell, Jr., A.D. and Nikos G. Oikonomakos, N.G. (deceased), Provisional Patent, submitted Fall 2008.
- 12) "Method for binding site identification by molecular dynamics simulation (SILCS: Site Identification by Ligand Competitive Saturation)" MacKerell, Jr., A.D. and Olgun Guvench, Provisional Patent, submitted April 2009.