

List of Publications - Joel L. Sussman – Feb 2019

Articles in Refereed Journals

1. Seeman, N.C., Sussman, J.L., Berman, H.M. & Kim, S.-H. (1971) "Nucleic acid conformation: crystal structure of a naturally occurring dinucleoside phosphate (UpA)" *Nature New Biol.* **233**, 90-92.
2. Sussman, J.L., Seeman, N.C., Kim, S.-H. & Berman, H.M. (1972) "The crystal structure of a naturally occurring dinucleotide phosphate Uridylyl 3',5'-adenosine phosphate. Models for RNA chain folding" *J Mol Biol* **66**, 403-421.
3. Sussman, J.L., Barzilay, I., Keren-Zur, M. & Lapidot, Y. (1973) "Correlation of the differences in conformation between 2'-5' and 3'-5' dinucleoside monophosphates with their behaviour on a Sephadex LH-20 column" *Biochim. Biophys. Acta* **308**, 189-197.
4. Barzilay, I., Sussman, J.L. & Lapidot, Y. (1973) "Further studies on the chromatographic behaviour of dinucleoside monophosphates" *J. Chromatogr.* **79**, 130-146.
5. Sussman, J.L. & Wodak, S.J. (1973) "The crystal structure of fulvine: a pyrrolizidine alkaloid" *Acta Cryst.* **B29**, 2918-2926.
6. Kim, S.-H., Suddath, F.L., Quigley, G.J., McPherson, A., Sussman, J.L., Wang, A.H.J., Seeman, N.C. & Rich, A. (1974) "Three-dimensional tertiary structure of yeast phenylalanine transfer RNA" *Science* **185**, 435-439.
7. Kim, S.-H., Sussman, J.L., Suddath, F.L., Quigley, G.J., McPherson, A., Wang, A.H.J., Seeman, N.C. & Rich, A. (1974) "The general structure of transfer RNA molecules" *Proc. Natl. Acad. Sci. USA* **71**, 4970-4974.
8. Quigley, G.J., Wang, A.H.J., Seeman, N.C., Suddath, F.L., Rich, A., Sussman, J.L. & Kim, S.-H. (1975) "Hydrogen bonding in yeast phenylalanine transfer RNA" *Proc. Natl. Acad. Sci. USA* **72**, 4866-4870.
9. Sussman, J.L. & Kim, S.-H. (1976) "Idealized atomic coordinates of yeast phenylalanine transfer RNA" *Biochem. Biophys. Res. Commun.* **68**, 89-96.
10. Kim, S.-H. & Sussman, J.L. (1976) " π turn is a conformational pattern in RNA loop and bends" *Nature* **260**, 645-646.
11. Sussman, J.L. & Kim, S.-H. (1976) "Three-dimensional structure of a transfer RNA in two crystal forms" *Science* **192**, 853-858.
12. Church, G.M., Sussman, J.L. & Kim, S.-H. (1977) "Secondary structural complementarity between DNA and proteins" *Proc. Natl. Acad. Sci. USA* **74**, 1458-1462.
13. Robillard, G.T., Tarr, C.E., Vosman, F. & Sussman, J.L. (1977) "An NMR approach to tRNA tertiary structure in solution" *Biophys. Chem.* **6**, 291-298.
14. Sussman, J.L., Holbrook, S.R., Church, G.M. & Kim, S.-H. (1977) "A structure-factor least squares refinement procedure for macromolecular structures using constrained and restrained parameters" *Acta Cryst.* **A33**, 800-804.
15. Holbrook, S.R., Sussman, J.L., Warrant, R.W., Church, G.M. & Kim, S.-H. (1977) "RNA-ligand interactions: (I) magnesium binding sites in yeast tRNA^{Phe}" *Nucl. Acids Res.* **4**, 2811-2820.
16. Kim, S.H. & Sussman, J.L. (1977) "Transfer RNA: structure-function correlation". in *Horizons in Biochemistry and Biophysics*, (Quagliariello, Palmieri & Singer, eds.), Addison-Wesley Publ. Co., Reading, MA, vol. 8, pp. 159-199.

17. Sussman, J.L. & Trifonov, E.N. (1978) "Possibility of nonkinked packing of DNA in chromatin" *Proc. Natl. Acad. Sci. USA* **75**, 103-107.
18. Sussman, J.L., Holbrook, S.R., Warrant, R.W., Church, G.M. & Kim, S.-H. (1978) "Crystal structure of yeast phenylalanine transfer RNA. I. crystallographic refinement" *J Mol Biol* **123**, 607-630.
19. Holbrook, S.R., Sussman, J.L., Warrant, R.W. & Kim, S.-H. (1978) "Crystal structure of yeast phenylalanine transfer RNA. II Structural features and functional implications" *J Mol Biol* **123**, 631-660.
20. Shoham, M., Sussman, J.L., Yonath, A., Moulton, J., Traub, W. & Kalb, A.J. (1978) "The effect of binding of metal ions on the three-dimensional structure of demetallized concanavalin A" *FEBS Lett.* **95**, 54-56.
21. Schevitz, R.W., Podjarny, A.D., Krishnamachari, N., Hughes, J.J., Sigler, P.B. & Sussman, J.L. (1979) "Crystal structure of eukaryotic initiator tRNA" *Nature* **278**, 188-190.
22. Shoham, M., Yonath, A., Sussman, J.L., Moulton, J., Traub, W. & Kalb, A.J. (1979) "The crystal structure of demetallized concanavalin A: the metal-binding region" *J Mol Biol* **131**, 137-155.
23. Sussman, J.L., Zipori, P., Harel, M., Yonath, A. & Werber, M.M. (1979) "Preliminary X-ray diffraction studies on 2 Fe-Ferredoxin from *Halobacterium* of the Dead Sea" *J Mol Biol* **134**, 375-377.
24. Trifonov, E.N. & Sussman, J.L. (1980) "The pitch of chromatin DNA is reflected in its nucleotide sequence" *Proc. Natl. Acad. Sci. USA* **77**, 3816-3820.
25. Nussinov, R., Sussman, J.L. & Trifonov, E.N. (1980) "MS2 RNA has a potential to form an unusually large number of stable hairpins" *J. Theor. Biol.* **85**, 481-486.
26. Holbrook, S.R., Sussman, J.L. & Kim, S.-H. (1981) "Absence of correlation between base-pair sequence and RNA conformation" *Science* **212**, 1275-1277.
27. Wain-Hobson, S., Nussinov, R., Brown, R.J. & Sussman, J.L. (1981) "Preferential codon usage in genes" *Gene* **13**, 355-364.
28. Olson, W.K. & Sussman, J.L. (1982) "How flexible is the furanose ring? 1. a comparison of experimental and theoretical studies" *J. Am. Chem. Soc.* **104**, 270-278.
29. Traub, W. & Sussman, J.L. (1982) "Adenine-guanine base pairing in ribosomal RNA" *Nucl. Acids Res.* **10**, 2701-2708.
30. Herzberg, O. & Sussman, J.L. (1983) "Protein model building by the use of a constrained-restrained least-squares procedure" *J. Appl. Cryst.* **16**, 144-150.
31. Bandel, G. & Sussman, J.L. (1983) "PLORTEP: a computer program to translate PLUTO instructions into those of ORTEP" *J. Appl. Cryst.* **16**, 650-651.
32. Sussman, J.L. & Podjarny, A.D. (1983) "The use of a constrained-restrained least-squares procedure for the low-resolution refinement of a macromolecule, yeast tRNA^{Met}" *Acta Cryst.* **B39**, 495-505.
33. Murata, M., Richardson, J.S. & Sussman, J.L. (1985) "Simultaneous comparison of three protein sequences" *Proc. Natl. Acad. Sci. USA* **82**, 3073-3077.
34. Sussman, J.L. (1985) "Constrained-restrained least-squares (CORELS) refinement of proteins and nucleic acids". in *Diffraction Methods for Biological Macromolecules*, (Wyckoff, H. W., Hirs, C. H. W. & Timasheff, S. N., eds.), Academic Press, New York, vol. 115, pp. 271-303.

35. Werber, M.M., Sussman, J.L. & Eisenberg, H. (1986) "Molecular basis for the special properties of proteins and enzymes from *Halobacterium marismortui*" *FEMS Microbiology Reviews* **39**, 129-135.
36. Saper, M.A., Eldar, H., Mizuuchi, K., Nickol, J., Appella, E. & Sussman, J.L. (1986) "Crystallization of a DNA tridecamer d(C-G-C-A-G-A-A-T-T-C-G-C-G)" *J Mol Biol* **188**, 111-113.
37. Harel, D., Unger, R. & Sussman, J.L. (1986) "Beauty is in the genes of the beholder" *TIBS* **11**, 155-156.
38. Yagil, G. & Sussman, J.L. (1986) "Structural models for non-helical DNA" *EMBO J.* **5**, 1719-1725.
39. Roy, S., Weinstein, S., Borah, B., Nickol, J., Appella, E., Sussman, J.L., Miller, M., Shindo, H. & Cohen, J.S. (1986) "Mechanism of oligonucleotide loop formation in solution" *Biochemistry* **25**, 7417-7423.
40. Unger, R., Harel, D. & Sussman, J.L. (1986) "DNAMAT - An efficient graphic matrix sequence homology algorithm and its application to structural analysis" *Comp. Appl. Biosci.* **2**, 283-289.
41. Miller, M., Wlodawer, A., Appella, E. & Sussman, J.L. (1987) "Crystallization of a DNA duplex 15-mer containing unpaired bases: d(CGCGAAATTTACGCG)" *J Mol Biol* **195**, 967-968.
42. Miller, M., Kirchoff, W., Schwarz, F., Appella, E., Chiu, Y.H., Cohen, J.S. & Sussman, J.L. (1987) "Conformational transitions of synthetic DNA sequences with inserted bases, related to the dodecamer d(CGCGAATTCGCG)" *Nucl. Acids Res.* **15**, 3877-3890.
43. Holland, D., Zilberstein, A., Zamir, A. & Sussman, J.L. (1987) "A quantitative approach to sequence comparisons of nitrogenase MoFe protein α - and β -subunits including the newly sequenced *nifK* Gene from *Klebsiella pneumoniae*." *Biochem. J.* **247**, 277-285.
44. Abad-Zapatero, C., Griffith, J.P., Sussman, J.L. & Rossmann, M.G. (1987) "Refined crystal structure of Dogfish M₄ apo-lactate dehydrogenase" *J Mol Biol* **198**, 445-467.
45. Harel, M., Shoham, M., Frolow, F., Eisenberg, H., Mevarech, M., Yonath, A. & Sussman, J.L. (1988) "Crystallization of halophilic malate dehydrogenase from *Halobacterium marismortui*" *J Mol Biol* **200**, 609-610.
46. Hirshberg, M., Sharon, R. & Sussman, J.L. (1988) "A kinked model for the solution structure of DNA tridecamers with inserted adenosines: energy minimization and molecular dynamics" *J. Biomol. Struct. Dyn.* **5**, 965-979.
47. Joshua-Tor, L., Rabinovich, D., Hope, H., Frolow, F., Appella, E. & Sussman, J.L. (1988) "The three-dimensional structure of a DNA duplex containing looped out bases" *Nature* **334**, 82-84.
48. Miller, M., Harrison, R.W., Wlodawer, A., Appella, E. & Sussman, J.L. (1988) "Crystal structure of 15-mer DNA duplex containing unpaired bases" *Nature* **334**, 85-86.
49. Sussman, J.L., Harel, M., Frolow, F., Varon, L., Toker, L., Futerman, A.H. & Silman, I. (1988) "Purification and crystallization of a dimeric form of acetylcholinesterase from *Torpedo californica* subsequent to solubilization with phosphatidylinositol-specific phospholipase C" *J Mol Biol* **203**, 821-823.
50. Wagner, U.G., Werber, M.M., Beck, Y., Hartman, J.R., Frolow, F. & Sussman, J.L. (1989) "Characterization of crystals of genetically engineered human manganese superoxide dismutase" *J Mol Biol* **206**, 787-788.
51. Unger, R., Harel, D., Wherland, S. & Sussman, J.L. (1989) "A 3D building blocks approach to analyzing and predicting structure of proteins" *Proteins: Struct. Funct. Genetics* **5**, 355-373.

52. Hope, H., Frolow, F. & Sussman, J.L. (1989) "Macromolecular X-ray data collection on a rotating anode diffractometer" *The Rigaku Journal (Japanese)* **20**, 20-27.
53. Unger, R., Harel, D., Wherland, S. & Sussman, J.L. (1990) "Analysis of the dihedral angles distribution - the doublets distribution determines polypeptides conformations" *Biopolymers* **30**, 499-508.
54. Livnah, O. & Sussman, J.L. (1990) "Crystal forms of avidin". in *Avidin-Biotin Technology*, (Wilchek, M. & Bayer, E. A., eds.), Academic Press, New York, vol. 184, pp. 90-93.
55. Harel, M., Su, C.-T., Frolow, F., Silman, I. & Sussman, J.L. (1991) " γ -chymotrypsin is a complex of α -chymotrypsin with its own autolysis products" *Biochemistry* **30**, 5217-5225.
56. Sussman, J.L., Harel, M., Frolow, F., Oefner, C., Goldman, A., Toker, L. & Silman, I. (1991) "Atomic structure of acetylcholinesterase from *Torpedo californica*: a prototypic acetylcholine-binding protein" *Science* **253**, 872-879.
57. Harel, M., Su, C.T., Frolow, F., Ashani, Y., Silman, I. & Sussman, J.L. (1991) "Refined crystal structures of "aged" and "non-aged" organophosphoryl conjugates of γ -chymotrypsin" *J Mol Biol* **221**, 909-918.
58. Ollis, D.L., Cheah, E., Cygler, M., Dijkstra, B., Frolow, F., Franken, S.M., Harel, M., Remington, S.J., Silman, I., Schrag, J., Sussman, J.L., Verschueren, K.H.G. & Goldman, A. (1992) "The α/β hydrolase fold" *Protein Eng.* **5**, 197-211.
59. Joshua-Tor, L., Frolow, F., Appella, E., Hope, H., Rabinovich, D. & Sussman, J.L. (1992) "Three-dimensional structures of bulge-containing DNA fragments" *J Mol Biol* **225**, 397-431.
60. Shafferman, A., Kronman, C., Flashner, Y., Leitner, M., Grosfeld, H., Ordentlich, A., Gozes, Y., Cohen, S., Ariel, N., Barak, D., Harel, M., Silman, I., Sussman, J.L. & Velan, B. (1992) "Mutagenesis of human acetylcholinesterase. Identification of residues involved in catalytic activity and in polypeptide folding" *J. Biol. Chem.* **267**, 17640-17648.
61. Duval, N., Bon, S., Silman, I., Sussman, J.L. & Massoulié, J. (1992) "Site-directed mutagenesis of active-site-related residues in *Torpedo* acetylcholinesterase. Presence of a glutamic acid in the catalytic triad" *FEBS Lett.* **309**, 421-423.
62. Harel, M., Sussman, J.L., Krejci, E., Bon, S., Chanal, P., Massoulié, J. & Silman, I. (1992) "Conversion of acetylcholinesterase to butyrylcholinesterase: modeling and mutagenesis" *Proc. Natl. Acad. Sci. USA* **89**, 10827-10831.
63. Berman, H.M., Sussman, J.L., Joshua-Tor, L., Revich, G.G. & Ripley, L.S. (1992) "A structural model for sequence-specific proflavin-DNA interactions during *In vitro* frameshift mutagenesis" *J. Biomol. Struct. Dyn.* **10**, 317-331.
64. Sussman, J.L. & Silman, I. (1992) "Acetylcholinesterase: structure and use as a model for specific cation-protein interactions" *Curr. Opin. Struct. Biol.* **2**, 721-729.
65. Joshua-Tor, L. & Sussman, J.L. (1993) "The coming of age of DNA crystallography" *Curr. Opin. Struct. Biol.* **3**, 323-335.
66. Tan, R.C., Truong, T.N., McCammon, J.A. & Sussman, J.L. (1993) "Acetylcholinesterase: electrostatic steering increases the rate of ligand binding" *Biochemistry* **32**, 401-403.
67. Cygler, M., Schrag, J.D., Sussman, J.L., Harel, M., Silman, I., Gentry, M.K. & Doctor, B.P. (1993) "Relationship between sequence conservation and three-dimensional structure in a large family of esterases, lipases, and related proteins" *Protein Sci.* **2**, 366-382.

68. Reich, Z., Friedman, P., Scolnik, Y., Sussman, J.L. & Minsky, A. (1993) "On the metastability of left-handed DNA motifs" *Biochemistry* **32**, 2116-2119.
69. Wagner, U.G., Patridge, K.A., Ludwig, M.L., Stallings, W.C., Werber, M.M., Oefner, C., Frolow, F. & Sussman, J.L. (1993) "Comparison of the crystal structures of genetically engineered human manganese superoxide dismutase and manganese superoxide dismutase from *Thermus thermophilus*. Differences in dimer-dimer interaction" *Protein Sci.* **2**, 814-825.
70. Livnah, O., Bayer, E.A., Wilchek, M. & Sussman, J.L. (1993) "The three-dimensional structure of avidin and the avidin-biotin Complex" *Proc. Natl. Acad. Sci. USA* **90**, 5076-5080.
71. Ripoll, D.R., Faerman, C.H., Axelsen, P., Silman, I. & Sussman, J.L. (1993) "An electrostatic mechanism for substrate guidance down the aromatic gorge of acetylcholinesterase" *Proc. Natl. Acad. Sci. USA* **90**, 5128-5132.
72. Harel, M., Schalk, I., Ehret-Sabatier, L., Bouet, F., Goeldner, M., Hirth, C., Axelsen, P., Silman, I. & Sussman, J.L. (1993) "Quaternary ligand binding to aromatic residues in the active-site gorge of acetylcholinesterase" *Proc. Natl. Acad. Sci. USA* **90**, 9031-9035.
73. Livnah, O., Bayer, E.A., Wilchek, M. & Sussman, J.L. (1993) "The structure of the complex between avidin and the dye, 2-(4'-hydroxyazobenzene) benzoic acid (HABA)" *FEBS Lett.* **328**, 165-168.
74. Sussman, J.L., Harel, M. & Silman, I. (1993) "Three-dimensional structure of acetylcholinesterase and of its complexes with anticholinesterase drugs" *Chem. Biol. Interactions* **87**, 187-197.
75. Massoulié, J., Sussman, J.L., Bon, S. & Silman, I. (1993) "Structure and functions of acetylcholinesterase and butyrylcholinesterase" *Prog. Brain Res.* **98**, 139-146.
76. Unger, R. & Sussman, J.L. (1993) "The importance of short structural motifs in protein structure analysis" *J. Comput. Aided Mol. Des.* **7**, 457-472.
77. Gilson, M.K., Straatsma, T.P., McCammon, J.A., Ripoll, D.R., Faerman, C.H., Axelsen, P., Silman, I. & Sussman, J.L. (1994) "Open "back door" in a molecular dynamics simulation of acetylcholinesterase" *Science* **263**, 1276-1278.
78. Axelsen, P.H., Harel, M., Silman, I. & Sussman, J.L. (1994) "Structure and dynamics of the active site gorge of acetylcholinesterase: synergistic use of molecular dynamics simulation and X-ray crystallography" *Protein Sci.* **3**, 188-197.
79. Eichler, J., Anselmet, A., Sussman, J.L., Massoulié, J. & Silman, I. (1994) "Differential effects of "peripheral" site ligands on *Torpedo* and chicken acetylcholinesterase" *Mol. Pharmacol.* **45**, 335-340.
80. Silman, I., Harel, M., Axelsen, P., Raves, M. & Sussman, J.L. (1994) "Three-dimensional structures of acetylcholinesterase and of its complexes with anticholinesterase agents" *Biochemical Soc. Trans.* **22**, 745-749.
81. Kreimer, D.I., Dolginova, E.A., Raves, M., Sussman, J.L., Silman, I. & Weiner, L. (1994) "A metastable state of *Torpedo* acetylcholinesterase generated by modification with organomercurials" *Biochemistry* **33**, 14407-14418.
82. Peitsch, M.C., Stampf, D.R., Wells, T.N.C. & Sussman, J.L. (1995) "The Swiss 3D-Image collection and Brookhaven protein data bank browser on the World-Wide Web" *TIBS* **20**, 82-84.
83. Dym, O., Mevarech, M. & Sussman, J.L. (1995) "Structural features that stabilize Halophilic malate dehydrogenase from an Archaeobacterium" *Science* **267**, 1344-1346.
84. Stampf, D.R., Felder, C.E. & Sussman, J.L. (1995) "PDBBrowse - a graphics interface to the Brookhaven protein data bank" *Nature* **374**, 572-574.

85. Alon, R.N., Mirny, L., Sussman, J.L. & Gutnick, D.L. (1995) "Detection of α/β -hydrolase gold in the cell surface esterases of *Acinetobacter* species using an analysis of 3D profiles" *FEBS Lett.* **371**, 231-235.
86. Harel, M., Kleywegt, G.J., Ravelli, R.B.G., Silman, I. & Sussman, J.L. (1995) "Crystal structure of an acetylcholinesterase-fasciculin complex: interaction of a three-fingered toxin from snake venom with its target" *Structure* **3**, 1355-1366.
87. Wlodek, S.T., Antosiewicz, J., McCammon, J.A., Straatsma, T.P., Gilson, M.K., Briggs, J.M., Humblet, C. & Sussman, J.L. (1996) "Binding of tacrine and 6-chlorotacrine by acetylcholinesterase" *Biopolymers* **38**, 109-117.
88. Harel, M., Quinn, D.M., Nair, H.K., Silman, I. & Sussman, J.L. (1996) "The X-ray structure of a transition state analog complex reveals the molecular origins of the catalytic power and substrate specificity of acetylcholinesterase" *J. Am. Chem. Soc.* **118**, 2340-2346.
89. Frolow, F., Harel, M., Mevarech, M., Sussman, J. L. & Shoham, M. (1996) "Protein adaptation to a saturated salt environment: Insights from the crystal structure of a halophilic 2Fe-2S ferredoxin" *Nature Struct. Biol.* **3**, 451-457.
90. Porschke, D., Créminon, C., Cousin, X., Bon, C., Sussman, J.L. & Silman, I. (1996) "Electrooptical measurements demonstrate a large permanent dipole moment associated with acetylcholinesterase" *Biophys. J.* **70**, 1603-1608.
91. Baker, E.N., Blundell, T.L., Vijayan, M., Dodson, E., Dodson, G., Gilliland, G.I. & Sussman, J.L. (1996) "Crystallographic data deposition" *Nature* **379**, 202.
92. Baker, E.N., Blundell, T.L., Vijayan, M., Dodson, E., Gilliland, G.I. & Sussman, J.L. (1996) "Deposition of macromolecular data" *Acta Cryst.* **D52**, 609.
93. Baker, E.N., Blundell, T.L., Vijayan, M., Dodson, E., Dodson, G., Gilliland, G.I. & Sussman, J.L. (1996) "Archival journal requirements for data deposition" *Biophys. J.* **70**, 2994.
94. Faerman, C., Ripoll, D., Bon, S., Le Feuvre, Y., Morel, N., Massoulié, J., Sussman, J.L. & Silman, I. (1996) "Site-directed mutants designed to test back-door hypotheses of acetylcholinesterase function" *FEBS Lett.* **386**, 65-71.
95. Marchot, P., Ravelli, R.B.G., Raves, M.L., Bourne, Y., Vellom, D.C., Kanter, J., Camp, S., Sussman, J.L. & Taylor, P. (1996) "Soluble monomeric acetylcholinesterase from mouse: expression, purification, and crystallization in complex with fasciculin" *Protein Sci.* **5**, 672-679.
96. Peng, L., Silman, I., Sussman, J.L. & Goeldner, M. (1996) "Biochemical evaluation of photolabile precursors of choline and carbamoylcholine for potential time-resolved crystallographic studies on cholinesterases" *Biochemistry* **35**, 10854-10861.
97. Abola, E.E., Manning, N.O., Prilusky, J., Stampf, D.R. & Sussman, J.L. (1996) "The protein data bank: current status and future challenges" *J. Res. Natl. Inst. Stand. Technol.* **101**, 231-241.
98. Raves, M.L., Harel, M., Pang, Y.-P., Silman, I., Kozikowski, A.P. & Sussman, J.L. (1997) "3D structure of acetylcholinesterase complexed with the nootropic alkaloid, (-)-huperzine A" *Nature Struct. Biol.* **4**, 57-63.
99. Sussman, J.L. (1997) "Bridging the gap" *Nature Struct. Biol.* **4**, 517.
100. Felder, C.E., Botti, S.A., Lifson, S., Silman, I. & Sussman, J.L. (1997) "External and internal electrostatic potentials of cholinesterase models" *J. Molec. Graphics & Modelling* **15**, 318-327.

101. Bar-On, P., Millard, C.B., Enz, A., Sussman, J.L. & Silman, I. (1997) "Evidence that the anti-Alzheimer drug, ENA-713, inhibits acetylcholinesterase by more than one mechanism" *Neurosci. Lett. Supp.* **48**, S6-S7.
102. Botti, S.A., Felder, C., Sussman, J.L. & Silman, I. (1997) "The conjunction of a conserved electrostatic motif and a common cholinesterase fold defines a class of adhesion proteins" *Neurosci. Lett. Supp.* **48**, S11.
103. Botti, S.A., Felder, C., Lifson, S., Silman, I. & Sussman, J.L. (1997) "An integrated model for the molecular traffic through the active site of cholinesterases" *Neurosci. Lett. Supp.* **48**, S11.
104. Giles, K., Sussman, J.L. & Silman, I. (1997) "Human acetylcholinesterase I: in vitro assembly of subunits" *Neurosci. Lett. Supp.* **48**, S19.
105. Giles, K., Sussman, J.L. & Silman, I. (1997) "Human acetylcholinesterase II: in vivo expression and tissue distribution via EST analysis" *Neurosci. Lett. Supp.* **48**, S19-S29.
106. Abola, E.E., Sussman, J.L., Prilusky, J. & Manning, N.O. (1997) "Protein data bank archives of three-dimensional macromolecular structures". in *Methods in Enzymology*, (Carter, C. W. & Sweet, R. M., eds.), Academic Press, New York, vol. 277, pp. 556-571.
107. Sussman, J.L., Bernstein, F.C., Jiang, J., Libeson, M., Lin, D., Manning, N.O., McCarthy, J., Shea, R., Abola, E.E., Felder, C.E., Prilusky, J. & Ritter, O. (1998) "Protein data bank (PDB): a database of 3D structural information of biological macromolecules". in *The Encyclopedia of Computational Chemistry*, (Schleyer, P., et al., eds.), John Wiley & Sons Ltd., Chichester, vol. 3, pp. 2160-2168.
108. Ravelli, R.B.G., Raves, M.L., Ren, Z., Bourgeois, D., Roth, M., Kroon, J., Silman, I. & Sussman, J.L. (1998) "Static Laue diffraction studies on acetylcholinesterase" *Acta Cryst.* **D54**, 1359-1366.
109. Botti, S.A., Felder, C.E., Sussman, J.L. & Silman, I. (1998) "Electrotactins: a class of adhesion proteins with conserved electrostatic and structural motifs" *Protein Eng.* **11**, 415-420.
110. Sussman, J.L., Lin, D., Jiang, J., Manning, N.O., Prilusky, J., Ritter, O. & Abola, E.E. (1998) "Protein data bank (PDB): a database of 3D structural information of biological macromolecules" *Acta Cryst.* **D54**, 1078-1084.
111. Bar-On, P., Harel, M., Millard, C.B., Enz, A., Sussman, J.L. & Silman, I. (1998) "Kinetic and structural studies on the interaction of the anti-Alzheimer drug, ENA-713, with acetylcholinesterase" *Neurosci. Lett. Supp.* **51**, S4.
112. Millard, C.B., Koellner, G., Ordentlich, A., Shafferman, A., Silman, I. & Sussman, J.L. (1998) "Crystal structure of acetylcholinesterase from *Torpedo californica* inhibited with the nerve agent VX" *Neurosci. Lett. Supp.* **51**, S29.
113. Sussman, J.L. (1998) "Protein data bank deposits" *Science* **282**, 1991.
114. Kryger, G., Silman, I. & Sussman, J.L. (1998) "Three-dimensional structure of a complex of E2020 with acetylcholinesterase from *Torpedo californica*" *J. Physiol. (Paris)* **92**, 191-194.
115. Bar-On, P., Harel, M., Millard, C.B., Enz, A., Sussman, J.L. & Silman, I. (1998) "Kinetic and structural studies on the interaction of the anti-Alzheimer drug, ENA-713, with *Torpedo californica* acetylcholinesterase" *J. Physiol. (Paris)* **92**, 406-407.
116. Botti, S.A., Felder, C., Sussman, J.L. & Silman, I. (1998) "Electrostatic homology modelling of a set of ChE-like neural adhesion proteins identifies a shared 'annular' motif with ChEs. Structural implications for a cell-recognition role of ChEs" *J. Physiol. (Paris)* **92**, 414-416.

117. Wlodawer, A., Davies, D., Petsko, G., Rossmann, M., Olson, A. & Sussman, J.L. Immediate release of crystallographic data: a proposal. *Science* (1998) **279**, 306-307.
118. Jiang, J., Abola, E. & Sussman, J.L. (1999) "Deposition of structure factors at the protein data bank" *Acta Cryst.* **D55**, 4.
119. Silman, I., Millard, C.B., Ordentlich, A., Greenblatt, H.M., Harel, M., Barak, D., Shafferman, A. & Sussman, J.L. (1999) "A preliminary comparison of structural models for catalytic intermediates of acetylcholinesterase" *Chem Biol Interactions* **119-120**, 43-52.
120. Kryger, G., Silman, I. & Sussman, J.L. (1999) "Structure of acetylcholinesterase complexed with E2020 (Aricept®): implications for the design of new anti-Alzheimer drugs" *Structure* **7**, 297-307.
121. Morel, N., Bon, S., Greenblatt, H., Wodak, S., Sussman, J., Massoulié, J. & Silman, I. (1999) "Effect of mutations in the peripheral anionic site on the stability of acetylcholinesterase" *Mol. Pharmacol.* **55**, 982-992.
122. Millard, C.B., Kryger, G., Ordentlich, A., Harel, M., Raves, M., Greenblatt, H.M., Segall, Y., Barak, D., Shafferman, A., Silman, I. & Sussman, J.L. (1999) "Crystal structure of "aged" phosphorylated *Torpedo* acetylcholinesterase: nerve agent reaction products at the atomic level" *Biochemistry* **38**, 7032-7039.
123. Sussman, J.L., Abola, E.E., Lin, D., Jiang, J., Manning, N.O. & Prilusky, J. (1999) "The protein data bank" *Genetica* **106**, 149-158.
124. Botti, S.A., Felder, C., Lifson, S., Sussman, J.L. & Silman, I. (1999) "A modular treatment of molecular traffic through the active site of cholinesterases" *Biophys. J.* **77**, 2430-2450.
125. Millard, C.B., Koellner, G., Ordentlich, A., Shafferman, A., Silman, I. & Sussman, J.L. (1999) "Reaction products of acetylcholinesterase and VX reveal a mobile histidine in the catalytic triad" *J. Am. Chem. Soc.* **121**, 9883-9884.
126. Greenblatt, H.M., Kryger, G., Lewis, T., Silman, I. & Sussman, J. (1999) "Structure of acetylcholinesterase complexed with (-)-galanthamine at 2.3Å resolution" *FEBS Lett.* **463**, 321-326.
127. Weik, M., Ravelli, R.B.G., Kryger, G., McSweeney, S., Raves, M., Harel, M., Gros, P., Silman, I., Kroon, J. & Sussman, J.L. (2000) "Specific chemical and structural damage to proteins produced by synchrotron radiation" *Proc. Natl. Acad. Sci. USA* **97**, 623-628.
128. Koellner, G., Kryger, G., Millard, C.B., Silman, I., Sussman, J.L. & Steiner, T. (2000) "Active-site gorge and buried water molecules in crystal structures of acetylcholinesterase from *Torpedo californica*" *J Mol Biol* **296**, 713-735.
129. Harel, M., Kryger, G., Rosenberry, T.L., Mallender, W.D., Lewis, T., Fletcher, R.J., Guss, J.M., Silman, I. & Sussman, J.L. (2000) "Three-dimensional structures of *Drosophila melanogaster* acetylcholinesterase and of its complexes with two potent inhibitors" *Protein Sci.* **9**, 1063-1072.
130. Kraut, D., Goff, H., Pai, R.K., Hosea, N.A., Silman, I., Sussman, J.L., Taylor, P. & Voet, J.G. (2000) "Inactivation studies of acetylcholinesterase with phenylmethanesulfonyl fluoride" *Mol. Pharmacol.* **57**, 1243-1248.
131. Lin, D., Manning, N.O., Jiang, J., Abola, E.E., Stampf, D., Prilusky, J. & Sussman, J.L. (2000) "AutoDep©: A web based system for deposition and validation of macromolecular structural information" *Acta Cryst.* **D56**, 828-841.
132. Greenblatt, H.M., Silman, I. & Sussman, J.L. (2000) "Structural studies on vertebrate and invertebrate acetylcholinesterases and their complexes with functional ligands" *Drug Develop. Res.* **50**, 573-583.

133. Lamzin, V., Perrakis, A., Bricogne, G., Jiang, J., Swaminathan, S. & Sussman, J.L. (2000) "Apotheosis, not apocalypse: methods in protein crystallography" *Acta Cryst.* **D56**, 1510-1511.
134. Kryger, G., Harel, M., Giles, K., Toker, L., Velan, B., Lazar, A., Kronman, C., Barak, D., Ariel, N., Shafferman, A., Silman, I. & Sussman, J.L. (2000) "Structures of recombinant native and E202Q mutant human acetylcholinesterase complexed with the snake-venom toxin fasciculin-II" *Acta Cryst.* **D56**, 1385-1394.
135. Abola, E.E., Bairoch, A., Barker, W.C., Beck, S., Benson, D.A., Berman, H., Cantor, C., Doubet, S., Hubbard, T.J.P., Jones, T.A., Kleywegt, G.J., Kolaskar, A.S., Van Kuik, A., Lesk, A.M., Mewes, H.-W., Neuhaus, D., Pfeiffer, F., TenEyck, L.F., Simpson, R.J., Stoesser, G., Sussman, J.L., Tateno, Y., Tsugita, A., Ulrich, E.L. & Vliegthart, J.F.G. (2000) "Quality control in databanks for molecular biology" *BioEssays* **22**, 1024-1034.
136. Zhu, W.-L., Tan, X.-J., Puah, C.M., Gu, J.-D., Jiang, H.-L., Chen, K.-X., Felder, C., Silman, I. & Sussman, J.L. (2000) "How does ammonium interact with aromatic groups? A density functional theory (DFT/B3LYP) investigation" *J. Phys. Chem. A* **104**, 9573-9580.
137. Bar-On, P., Harel, M., Millard, C.B., Enz, A., Sussman, J.L. & Silman, I. (2000) "Kinetic and structural studies on the interaction of cholinesterases with the anti-Alzheimer drug, ENA-713" *Neurosci. Lett.* **Supp.** **55**, S6.
138. Weik, M., Kryger, G., Schreurs, A.M., Bouma, B., Silman, I., Sussman, J.L., Gros, P. & Kroon, J. (2001) "Solvent behaviour in flash-cooled protein crystals at cryogenic temperatures" *Acta Cryst.* **D57**, 566-573.
139. Felder, C., Jiang, H.-L., Zhu, W.-L., Chen, K.-X., Silman, I., Botti, S.A. & Sussman, J.L. (2001) "Quantum/classical mechanical comparison of cation- π interactions between tetramethylammonium and benzene" *J. Phys. Chem. A* **105**, 1326-1333.
140. Liu, T., Gu, J.-D., Tan, X.-J., Zhu, W.-L., Luo, X.-M., Li, Q., Jiang, H.-L., Ji, R.-Y., Chen, K.-X., Silman, I. & Sussman, J.L. (2001) "Theoretical insight into the interactions of TMA-Benzene and TMA-Pyrrole with B3LYP density-functional theory (DFT) and ab initio second order Moller-Plesset perturbation theory (MP2) calculations" *J. Phys. Chem. A* **105**, 5431-5437.
141. Weik, M., Ravelli, R., Silman, I., Sussman, J.L., Gros, P. & Kroon, J. (2001) "Specific protein dynamics near the solvent glass transition assayed by radiation-induced structural changes" *Protein Sci.* **10**, 1953-1961.
142. Nicolas, A., Ferron, F., Toker, L., Sussman, J.L. & Silman, I. (2001) "Histochemical method for characterization of enzyme crystals: application to crystals of *Torpedo californica* acetylcholinesterase" *Acta Cryst.* **D57**, 1348-1350.
143. Doucet-Personeni, C., Bentley, P.D., Fletcher, R.J., Kinkaid, A., Kryger, G., Pirard, B., Taylor, A., Taylor, R., Taylor, J., Viner, R., Silman, I., Sussman, J.L., Greenblatt, H.M. & Lewis, T. (2001) "A structure-based design approach to the development of novel, reversible AChE inhibitors" *J. Med. Chem.* **44**, 3203-3215.
144. Tan, X.J., Zhu, W.L., Cui, M., Luo, X.M., Gu, J.D., Silman, I., Sussman, J.L., Jiang, H.L., Ji, R.Y. & Chen, K.X. (2001) "Noncovalent interaction or chemical bonding between alkaline earth cations and benzene? A quantum chemistry study with MP2 and density-functional theory methods" *Chem. Phys. Lett.* **349**, 113-122.
145. Harel, M., Kasher, R., Nicolas, A., Guss, J.M., Balass, M., Fridkin, M., Smit, A.B., Brejc, K., Sixma, T.K., Katchalski-Katzir, E., Sussman, J.L. & Fuchs, S. (2001) "The structure of the binding site of the acetylcholine receptor as visualized in the X-ray structure of a complex between α -bungarotoxin and a high affinity mimotope peptide" *Neuron* **32**, 265-275.
146. Sussman, J.L., Lin, D., Jiang, J., Manning, N.O., Prilusky, J. & Abola, E.E. (2001) "The protein data bank at Brookhaven". in *International Tables for Crystallography, Volume*

F. Crystallography of Biological Macromolecules, (Rossmann, M. G. & Arnold, E., eds.), Kluwer Academic Publishers, Dordrecht pp. Chap 24.1 (649-656).

147. Liu, T., Gu, J., Tan, X.-J., Zhu, W.-L., Luo, X.-M., Jiang, H.-L., Ji, R.-Y., Chen, K.-X., Silman, I. & Sussman, J.L. (2002) "The relationship between binding models of TMA with furan and imidazole and the molecular electrostatic potentials: DFT and MP2 computational studies" *J. Phys. Chem. A* **106**, 157-164.
148. Dvir, H., Wong, D.M., Harel, M., Barril, X., Orozco, M., Luque, F.J., Muñoz-Torrero, D., Camps, P., Rosenberry, T., L., Silman, I. & Sussman, J.L. (2002) "3D structure of *Torpedo californica* acetylcholinesterase complexed with Huprine X at 2.1 Å resolution: kinetic and molecular dynamic correlates" *Biochemistry* **41**, 2970-2981.
149. Bar-On, P., Millard, C.B., Harel, M., Dvir, H., Enz, A., Sussman, J.L. & Silman, I. (2002) "Kinetic and structural studies on the interaction of cholinesterases with the anti-Alzheimer drug rivastigmine" *Biochemistry* **41**, 3555-3564.
150. Koellner, G., Steiner, T., Millard, C.B., Silman, I. & Sussman, J.L. (2002) "A neutral molecule in a cation-binding site: specific binding of a PEG-SH to acetylcholinesterase from *Torpedo californica*" *J Mol Biol* **320**, 721-725.
151. Felder, C.E., Harel, M., Silman, I. & Sussman, J.L. (2002) "Structure of a complex of the potent and specific inhibitor BW284C51 with *Torpedo californica* acetylcholinesterase" *Acta Cryst.* **D58**, 1765-1771.
152. Dvir, H., Jiang, H.L., Wong, D.M., Harel, M., Chetrit, M., He, X.C., Tang, X.C., Silman, I., Bai, D.L. & Sussman, J.L. (2002) "X-ray structures of *Torpedo californica* acetylcholinesterase complexed with (+)-Huperzine A and (-)-Huperzine B: Structural evidence for an active site rearrangement" *Biochemistry* **41**, 10810-10818.
153. Weik, M., Bergès, J., Raves, M. L., Gros, P., McSweeney, S., Silman, I., Sussman, J. L., Houée-Levin, C. & Ravelli, R. B. G. (2002) Evidence for the formation of disulfide radicals in protein crystals upon X-ray irradiation. *J. Synchrotron Rad.* **9**, 342-346.
154. Luo, X., Feng, C., Tan, X.-J., Tan, C., Zhu, D., Shen, J., Huang, X., Liu, T., Chen, K., Jiang, H., Zhu, W., Puah, C. M., Dvir, H., Harel, M., Sussman, J. L. & Silman, I. (2002) Structural feature of AChE inhibitor Huperzine B in nature and in the binding site of AChE: Density functional theory study combined with IR determination. *J. Theor. Comp. Chem.* **1**, 81-92.
155. Wong, D.M., Greenblatt, H.M., Dvir, H., Carlier, P.R., Han, Y.-F., Pang, Y.-P., Silman, I. & Sussman, J.L. (2003) "Acetylcholinesterase complexed with bivalent ligands related to Huperzine A: experimental evidence for species-dependent protein-ligand complementarity" *J. Am. Chem. Soc.* **125**, 363-373.
156. Zeev-Ben-Mordehai, T., Silman, I. & Sussman, J.L. (2003) "Acetylcholinesterase in motion: Visualizing conformational changes in crystal structures by a morphing procedure" *Biopolymers* **68**, 395-406.
157. Premkumar, L., Bageshwara, U., Gokhmana, I., Zamir, A. & Sussman, J.L. (2003) "An Unusual Halotolerant α -type Carbonic Anhydrase from the Alga *Dunaliella salina* Functionally Expressed in *E. coli*" *Protein Expr. Purif.* **28**, 151-157.
158. Katchalski-Katzir, E., Kasher, R., Balass, M., Scherf, T., Harel, M., Fridkin, M., Sussman, J.L. & Fuchs, S. (2003) "Design and synthesis of peptides that bind α -bungarotoxin with high affinity and mimic the three-dimensional structure of the binding-site of acetylcholine receptor" *Biophys. Chem.* **100**, 293-305.
159. Premkumar, L., Greenblatt, H.M., Savchenkoa, T., Gokhmana, I., Zamir, A. & Sussman, J.L. (2003) "Identification, cDNA cloning, expression, crystallization and preliminary X-ray analysis of an exceptionally halotolerant carbonic anhydrase from *Dunaliella salina*" *Acta Cryst.* **D59**, 1084-1086.

160. Dvir, H., Harel, M., McCarthy, A.H., Toker, L., Silman, I., Futerman, A.H. & Sussman, J.L. (2003) "X-ray structure of human acid- β -glucosidase, the defective enzyme in Gaucher disease" *EMBO Rep.* **4**, 704-709.
161. Zeev-Ben-Mordehai, T., Rydberg, E.H., Solomon, A., Lilly Toker, L., Botti, S., Auld, V.J., Silman, I. & Sussman, J.L. (2003) "The intracellular domain of the drosophila cholinesterase-like neural adhesion protein, gliotactin, is natively unfolded" *Proteins* **53**, 758-767.
162. Fuchs, S., Kasher, R., Balass, M., Scherf, T., Harel, M., Fridkin, M., Sussman, J.L. & Katchalski-Katzir, E. (2003) "The binding site of acetylcholine receptor: From synthetic peptides to solution and crystal structure" *Ann. NY Acad. Sci.* **998**, 93-100.
163. Greenblatt, H.M., Dvir, H., Silman, I. & Sussman, J.L. (2003) "Acetylcholinesterase: a multifaceted target for structure-based drug design of anticholinesterase agents for the treatment of Alzheimer's disease" *J. Mol. Neurosci.* **20**, 369-384.
164. Xu, Y., Shen, J., Luo, X., Silman, I., Sussman, J.L., Chen, K. & Jiang, H. (2003) "How does Huperzine A enter and leave the binding gorge of acetylcholinesterase? Steered molecular dynamics simulations" *J. Am. Chem. Soc.* **125**, 11340-11349.
165. Pe'er, I., Felder, C.E., Man, O., Silman, I., Sussman, J.L. & Beckmann, J.S. (2004) "Proteomic signatures: amino acid and oligopeptide compositions differentiate between phyla" *Proteins* **54**, 20-40.
166. Futerman, A.H., Sussman, J.L., Horowitz, M., Silman, I. & Zimran, A. (2004) "New directions in the treatment of Gaucher disease" *Trends Pharm. Sci.* **25**, 147-151.
167. Bageshwara, U.K., Premkumar, L., Gokhmana, I., Savchenkoa, T., Sussman, J.L. & Zamir, A. (2004) "Natural protein engineering: a uniquely salt-tolerant, but not halophilic, alpha-type carbonic anhydrase from algae proliferating in low- to hyper-saline environments" *PEDS* **17**, 191-200.
168. Harel, M., Aharoni, A., Gaidukov, L., Brumshtein, B., Khersonsky, O., Yagur, S., Meged, R., Dvir, H., Ravelli, R.B.G., McCarthy, A., Toker, L., Silman, I., Sussman, J.L. & Tawfik, D.S. (2004) "3D-Structure, mechanism and evolution of serum paraoxonases – a family of detoxifying and anti-atherosclerotic enzymes" *Nat. Struct. Mol. Biol.* **11**, 412-419.
169. Zhang, S., Rich, A., Sussman, J.L. & Fersht, A.R. (2004) "Carl-Ivar Branden 1934-2004" *Nat. Struct. Mol. Biol.* **11**, 490-492.
170. Hasin, Y., Avidan, N., Bercovich, D., Korczyn, A.D., Silman, I., Beckmann, J.S. & Sussman, J.L. (2004) "A paradigm for single nucleotide polymorphism analysis: The case of the acetylcholinesterase gene" *Hum. Mutat.* **24**, 408-416.
171. Liu, T., Zhu, W., Gu, J., Shen, J., Luo, X., Chen, G., Pua, C.M., Silman, I., Chen, K., Sussman, J.L. & Jiang, H. (2004) "Additivity of Cation- π interactions: An ab initio computational study on π -cation- π sandwich complexes" *J. Phys. Chem. A* **108**, 9400-9405.
172. Dvir, H., Harel, M., Bon, S., Liu, W.-Q., Vidal, M., Garbay, C., Sussman, J.L., Massoulié, J. & Silman, I. (2004) "The synaptic acetylcholinesterase tetramer assembles around a polyproline-II helix" *EMBO J.* **23**, 4394-4405.
173. Greenblatt, H.M., Guillou, C., Guénard, D., Argaman, A., Botti, S., Badet, B., Thal, C., Silman, I. & Sussman, J.L. (2004) "The complex of a bivalent derivative of Galanthamine with *Torpedo* acetylcholinesterase displays drastic deformation of the active-site gorge: Implications for structure-based drug design" *J. Am. Chem. Soc.* **126**, 15405-15411.
174. Harel, M., Aharoni, A., Gaidukov, L., Brumshtein, B., Khersonsky, O., Meged, R., Dvir, H., Ravelli, R.B., McCarthy, A., Toker, L., Silman, I., Sussman, J.L. & Tawfik, D.S. (2004) "Corrigendum: Structure and evolution of the serum paraoxonase family of detoxifying and anti-atherosclerotic enzymes" *Nat. Struct. Mol. Biol.* **11**, 1253.

175. Jaakola, V.-P., Prilusky, J., Sussman, J.L. & Goldman, A. (2005) "G protein-coupled receptors show unusual patterns of intrinsic unfolding" *PEDS* **18**, 103-110.
176. Premkumar, L., Greenblatt, H.M., Bagashwar, U., Savchenkoa, T., Gokhmana, I., Sussman, J.L. & Zamir, A. (2005) "3D structure of a halotolerant algal carbonic anhydrase predicts halotolerance of a mammalian homolog" *Proc. Natl. Acad. Sci. USA* **102**, 7493-7498.
177. Harel, M., Hyatt, J.L., Brumshtein, B., Morton, C.L., Yoon, K.J., Wadkins, R.M., Silman, I., Sussman, J.L. & Potter, P.M. (2005) "The Crystal Structure of the Complex of the Anticancer Prodrug 7-Ethyl-10-[4-(1-piperidino)-1-piperidino]-carbonyloxycamptothecin (CPT-11) with *Torpedo californica* Acetylcholinesterase Provides a Molecular Explanation for Its Cholinergic Action" *Mol Pharmacol* **67**, 1874-1881.
178. Silman, I. & Sussman, J.L. (2005) "Acetylcholinesterase: 'Classical' and 'Non-Classical' Functions and Pharmacology" *Curr. Opin. Pharmacol.* **5**, 293-302.
179. Premkumar, L., Sawkar, A.R., Boldin-Adamsky, S., Toker, L., Silman, I., Kelly, J., Futerman, A.H. & Sussman, J.L. (2005) "X-Ray Structure of Human Acid- β -Glucosidase Covalently-Bound to Conduritol- β -Epoxide: Implications for Gaucher Disease" *J Biol Chem* **280**, 23815-23819.
180. Prilusky, J., Oueillet, E., Ulryck, N., Pajon, A., Bernauer, J., Krimm, I., Quevillon-Cheruel, S., Leulliot, N., Graille, M., Liger, D., Trésaugues, L., Sussman, J.L., Janin, J., van Tilbeurgh, H. & Poupon, A. (2005) "HalX: an open-source LIMS (Laboratory Information Management System) for small- to large-scale laboratories" *Acta Cryst.* **D61**, 671-678.
181. Hasin, Y., Avidan, N., Bercovich, D., Korczyn, A.D., Silman, I., Beckmann, J.S. & Sussman, J.L. (2005) "Analysis of genetic polymorphisms in acetylcholinesterase as reflected in different populations" *Curr. Alzheimer Res.* **2**, 207-218.
182. Haviv H, Wong, D.M., Greenblatt, H.M., Carlier, P.R., Pang, Y.-P., Silman, I., Sussman, J.L. (2005) "Crystal packing mediates enantioselective ligand recognition at the peripheral site of acetylcholinesterase" *J. Am. Chem. Soc.* **127**, 11029-11036.
183. Prilusky, J., Felder, C.E., Zeev-Ben-Mordehai, T., Rydberg, E., Man, O., Beckmann, J.S., Silman, I. & Sussman, J.L. (2005) "FoldIndex© predicts whether a given protein is intrinsically disordered" *Bioinformatics* **21**, 3435-3438.
184. Albeck, S., Burstein, Y., Dym, O., Jacobovitch, Y., Levi, N., Meged, R., Michael, Y., Peleg, Y., Prilusky, J., Schreiber, G., Silman, I., Unger, T. & Sussman, J.L. (2005) "3D structure determination of proteins related to human health in their functional context at the Israel Structural Proteomics Center (ISPC)" *Acta Cryst.* **D61**, 1364-1372.
185. Newman, J., Egan D., Walter T.S., Meged R., Berry, I., Ben Jelloul, M., Sussman, J.L., Stuart, D.I. & Perrakis, A. (2005) "Towards rationalization of crystallization screening for small- to medium-sized academic laboratories: the PACT/JCSG+ strategy" *Acta Cryst.* **D61**, 1426-1431.
186. Niu, C. Y., Xu, Y. C., Xu, Y., Luo, X. M., Duan, W. H., Silman, I., Sussman, J. L., Zhu, W. L., Chen, K. X., Shen, J. H. & Jiang, H. L. (2005) "Dynamic mechanism of E2020 binding to acetylcholinesterase: A steered Dynamic mechanism of E2020 binding to acetylcholinesterase: A steered molecular dynamics simulation" *J. Phys. Chem. B* **109**, 23730-23738.
187. Harel, M., Hyatt, J.L., Brumshtein, B., Morton, C.L., Wadkins, R.M., Silman, I., Sussman, J.L. & Potter, P.M. (2005) "The 3D structure of the anticancer prodrug CPT-11 with *Torpedo californica* acetylcholinesterase rationalizes its inhibitory action on AChE and its hydrolysis by butyrylcholinesterase and carboxylesterase" *Chem. Biol. Interact.* **157-158**, 153-157.

188. Hyatt, J.L., Tsurkan, L., Morton, C.L., Yoon, K.J., Harel, M., Brumshtein, B., Silman, I., Sussman, J.L., Wadkins, R.M. & Potter, P.M. (2005) Inhibition of acetylcholinesterase by the anticancer prodrug CPT-11. *Chem. Biol. Interactions*. **157-158**, 247-252.
189. Sussman, J. L. & Silman, I. (2006) "Shedding UV Light on the Phase Problem" *Structure (Camb)* **14**, 629-630.
190. Colletier, J.-P., Fournier, D., Greenblatt, H., Stojan, J., Sussman, J.L., Zaccai, G., Silman, I. & Weik, M. (2006) "Structural insights into substrate traffic and inhibition in acetylcholinesterase" *EMBO J.* **25**, 2746-2756.
191. Rydberg, E. H., Brumshtein, B., Greenblatt, H. M., Wong, D. M., Shaya, D., Williams, L. D., Carlier, P. R., Pang, Y.-P., Silman, I. & Sussman, J. L. (2006) "Complexes of alkylene-linked tacrine dimers with *Torpedo californica* acetylcholinesterase: Binding of bis(5)-tacrine produces a dramatic rearrangement in the active-site gorge" *J. Med. Chem.* **49**, 5491-5500.
192. Aricescu, A.R., Assenberg, R., Bill, R.M., Busso, D., Chang, V.T., Davis, S.J., Dubrovsky, A., Gustafsson, L., Hedfalk, K., Heinemann, U., Jones, I.M., Ksiazek, D., Lang, C., Maskos, K., Messerschmidt, A., Macieira, S., Peleg, Y., Perrakis, A., Poterszman, A., Schneider, G., Sixma, T.K., Sussman, J.L., Sutton, G., Tarboureich, N., Zeev-Ben-Mordehai, T. & Jones, E.Y. (2006) "Eukaryotic expression: developments for structural proteomics" *Acta Cryst.* **D62**, 1114-1124.
193. Berry, I.M., Dym, O., Esnouf, R.M., Harlos, K., Meged, R., Perrakis, A., Sussman, J.L., Walter, T.S., Wilson, J. & Messerschmidt, A. (2006) "SPINE high-throughput crystallization, crystal imaging and recognition techniques: current state, performance analysis, new technologies and future aspects" (2006) *Acta Cryst.* **D62**, 1137-1149.
194. Albeck, S., Alzari, P., Andreini, C., Banci, L., Berry, I.M., Bertini, I., Cambillau, C., Canard, B., Carter, L., Cohen, S.X., Diprose, J.M., Dym, O., Esnouf, R.M., Felder, C., Ferron, F., Guillemot, F., Hamer, R., Ben Jelloul, M., Laskowski, R.A., Laurent, T., Longhi, S., Lopez, R., Luchinat, C., Malet, H., Mochel, T., Morris, R.J., Moulinier, L., Oinn, T., Pajon, A., Peleg, Y., Perrakis, A., Poch, O., Prilusky, J., Rachedi, A., Ripp, R., Rosato, A., Silman, I., Stuart, D.I., Sussman, J.L., Thierry, J.C., Thompson, J.D., Thornton, J.M., Unger, T., Vaughan, B., Vranken, W., Watson, J.D., Whamond, G. & Henrick, K. (2006) "SPINE bioinformatics and data-management aspects of high-throughput structural biology" *Acta Cryst.* **D62**, 1184-1195.
195. Banci, L., Bertini, I., Cusack, S., de Jong, R.N., Heinemann, U., Jones, E.Y., Kozielski, F., Maskos, K., Messerschmidt, A., Owens, R., Perrakis, A., Poterszman, A., Schneider, G., Siebold, C., Silman, I., Sixma, T., Stewart-Jones, G., Sussman, J.L., Thierry, J.C. & Moras, D. (2006) "First steps towards effective methods in exploiting high-throughput technologies for the determination of human protein structures of high biomedical value" *Acta Cryst.* **D62**, 1208-1217.
196. Romier, C., Ben Jelloul, M., Albeck, S., Buchwald, G., Busso, D., Celie, P.H., Christodoulou, E., De Marco, V., van Gerwen, S., Knipscheer, P., Lebbink, J.H., Notenboom, V., Poterszman, A., Rochel, N., Cohen, S.X., Unger, T., Sussman, J.L., Moras, D., Sixma, T.K. & Perrakis, A. (2006) "Co-expression of protein complexes in prokaryotic and eukaryotic hosts: experimental procedures, database tracking and case studies" *Acta Cryst.* **D62**, 1232-1242.
197. Esnouf, R.M., Hamer, R., Sussman, J.L., Silman, I., Trudgian, D., Yang, Z.R. & Prilusky, J. (2006) "Honing the in silico toolkit for detecting protein disorder" *Acta Cryst.* **D62**, 1260-1266.
198. Peleg, Y., Albeck, A., Burstein, Y., Dym, O., Jacobovitch, Y., Levy, N., Meged, R., Michael, Y., Prilusky, J., Schreiber, G., Silman, I., Unger, T. & Sussman, J.L. (2006) "Protein expression for structural studies" *Microb. Cell Fact.* **5(Suppl 1)**, 1-2.
199. Brumshtein, B., Wormald, M., Silman, I., Futerman, A.H., & Sussman, J.L. (2006) Structural comparison of differentially glycosylated forms of acid- β -glucosidase" *Acta Cryst.* **D62**, 1458-1465.

200. Banci, L., Baumeister, W., Enfedaque, J., Heinemann, U., Schneider, G., Silman, I. & Sussman, J.L. (2007) "Structural proteomics: from the molecule to the system" *Nat. Struct. Mol. Biol.* **14**, 3-4.
201. Yokoyama, S., Terwilliger, T.C., Kuramitsu, S., Moras, D. & Sussman, J.L. (2007) "RIKEN aids international structural genomics efforts" *Nature* **445**, 21.
202. Haviv, H., Wong, D.M., Silman, I. & Sussman, J.L. (2007) "Bivalent ligands derived from Huperzine A as acetylcholinesterase Inhibitors" *Curr. Top. Med. Chem.* **7**, 375-387.
203. Hodis, E., Schreiber, G., Rother, K. & Sussman, J.L. (2007) "eMovie: A storyboard-based tool for making molecular movies" *TIBS* **32**, 199-204.
204. Felder, C.E., Prilusky, J., Silman, I. & Sussman, J.L. (2007) "A server and database for dipole moments of proteins" *Nucl. Acids Res.* **35**, W512-521.
205. Shaaltiel, Y., Bartfeld, D., Hashmueli, S., Baum, G., Brill-Almon, E., Galili, G., Dym, O., Boldin-Adamsky, S., Silman, I., Sussman, J.L., Sussman, J.L., Futerman, A.H. & Aviezer, D. (2007) "Production of active and structurally homologous recombinant human glucocerebrosidase in a plant cell system, as a novel enzyme therapy in Gaucher's disease" *Plant Biotech.* **5**, 579-590.
206. Brumshtein, B., Greenblatt, H.M., Butters, T.D., Shaaltiel, Y., Aviezer, D., Silman, I., Futerman, A.H., and Sussman, J.L. (2007) "Crystal structures of complexes of n-butyl- and n-nonyl-deoxyojirimycin bound to acid β -glucosidase: Insights into the mechanism of chemical chaperone action in gaucher disease" *J Biol Chem* **282**, 29052-29058.
207. Harel, M., Brumshtein, B., Meged, R., Dvir, H., Ravelli, R.B.G., McCarthy, A., Toker, L., Silman, I. & Sussman, J.L. (2007) "3-D Structure of serum paraoxonase 1 sheds light on its activity, stability, solubility and crystallizability" *Arch. Ind. Hyg. Toxicol.* **58**, 347-353.
208. Colletier, J.P., Royant, A., Specht, A., Sanson, B., Nachon, F., Masson, P., Zaccai, G., Sussman, J.L., Goeldner, M., Silman, I., Bourgeois, D. & Weik, M. (2007) "Use of a 'Caged' analog to study traffic of choline within acetylcholinesterase by kinetic crystallography" *Acta Cryst* **D63**, 1115-1128.
209. Banci, L., Baumeister, W., Heinemann, U., Schneider, G., Silman, I., Stuart, D.I., & Sussman, J.L. (2007) "An idea whose time has come" *Genome Biology* **8**, 408.
210. Gräslund, S., Arrowsmith, C.H., Bray, J., Gileadi, O., Hui, R., Knapp, S., Ming, J., Nordlund, P., Oppermann, U., dhe-Paganon, S., Park, H.-w., Savchenko, A., Weigelt, J., Yee, A., Edwards, A.M., Vincentelli, R., Cambillau, C., Kim, R., Kim, S.-H., Rao, Z., Shi, Y., Terwilliger, T.C., Kim, C.-Y., Hung, L.-W., Waldo, G.S., Peleg, Y., Albeck, S., Unger, T., Dym, O., Prilusky, J., Sussman, J.L., Lesley, S.A., Knuth, M.W., Klock, H., Wilson, I.A., Joachimiak, A., Collart, F., Dementieva, I., Donnelly, M.I., Eschenfeldt, W.H., Kim, Y., Stols, L., Wu, R., Zhou, M., Burley, S.K., Almo, S.C., Bonanno, J.B., Fiser, A., Swaminathan, S., Studier, F.W., Sali, A., Chance, M.R., Emtage, J.S., Sauder, J.M., Thompson, D., Bain, K., Luz, J., Gheyi, T., Zhang, F., Atwell, S., Acton, T.B., Xiao, R., Zhao, L., Ma, L.C., Hunt, J.F., Tong, L., Cunningham, K., Inouye, M., Anderson, S., Janjua, H., Shastry, R., Gunsalus, K., Ho, C.K., Wang, D., Wang, H., Jiang, M., Montelione, G.T., Schütz, A., Heinemann, U., Yokoyama, S., Stuart, D.I., Owens, R.J. & Daenk, S. (2008) "Production and purification" *Nat Methods*, **5**, 135-146.
211. Tsvetkov, P., Asher, G., Paz, A., Reuven, N., Sussman, J.L., Silman, I. & Shaul, Y. (2008) "Operational definition of intrinsically unstructured protein sequences based on susceptibility to the 20S proteasome" *Proteins* **70**, 1357-1366
212. Tompa, P., Prilusky, J., Silman, I. & Sussman, J.L. (2008) "Structural disorder serves as a weak signal for intracellular protein degradation" *Proteins* **71**, 903-909.
213. Manicka, S., Peleg, Y., Unger, T., Albeck, S., Dym, O., Greenblatt, H.M., Bourenkov, G., Lamzin, V., Krishnaswamy, S. & Sussman, J.L. (2008). "Crystal structure of YagE, a putative DHDPS-like protein from Escherichia coli K12" *Proteins* **71**, 2102-2108.

214. Xu, Y., Colletier, J.P., Jiang, H., Silman, I., Sussman, J.L. & Weik, M. (2008). "Induced-fit or pre-existing equilibrium dynamics? Lessons from protein crystallography and MD simulations on acetylcholinesterase" *Protein Sci* **17**, 601-605.
215. Silman, I. & Sussman, J.L. (2008). "Acetylcholinesterase: How is structure related to function?" *Chem Biol Interact* **175**, 3-10.
216. Meged, R., Dym, O. & Sussman, J.L. (2008). "High-Throughput pH optimization of protein crystallization" *Methods Mol Biol* **426**, 411-418.
217. Paz, A., Zeev-Ben-Mordehai, T., Lundqvist, M., Sherman, E., Mylonas, E., Weiner, L., Haran, G., Svergun, D.I., Mulder, F.A.A., Sussman, J.L. & Silman, I. (2008). "Biophysical characterization of the unstructured cytoplasmic domain of the human neuronal adhesion protein Neuroligin 3" *Biophys J* **95**, 1928-1944.
218. Harel, M., Sonoda, L.K., Silman, I., Sussman, J.L. & Rosenberry, T.L. (2008). "Crystal structure of thioflavin T bound to the peripheral site of *Torpedo californica* acetylcholinesterase reveals how thioflavin T acts as a sensitive fluorescent reporter of ligand binding to the acylation site" *J Am Chem Soc* **130**, 7856-7861.
219. Colletier, J.-P., Bourgeois, D., Sanson, B., Fournier, D., Sussman, J.L., Silman, I. & Weik, M. (2008). "Shoot-and-Trap: Use of specific X-ray damage to study structural protein dynamics by temperature-controlled cryo-crystallography" *Proc Natl Acad Sci USA* **105**, 11742-11747.
220. Xu, Y., Colletier, J.-P., Weik, M., Jiang, H., Moulton, J., Silman, I. & Sussman, J.L. (2008). "Flexibility of Aromatic Residues in the Active-Site Gorge of Acetylcholinesterase: X-ray versus Molecular Dynamics" *Biophys J* **95**, 2500-2511.
221. Brumshtein, B., Greenblatt, H.M., Futerman, A.H., Silman, I. & Sussman, J.L. (2008). "Control of the rate of evaporation in protein crystallization by the 'microbatch under oil' method" *J Appl Cryst* **41**, 969-971.
222. Hodis, E., Prilusky, J., Martz, E., Silman, I., Moulton, J. & Sussman, J.L. (2008). "Proteopedia – a scientific 'wiki' bridging the rift between 3D structure and function of biomacromolecules" *Genome Biol* **9**, R121.
223. Kacher, Y., Brumshtein, B., Boldin-Adamsky, S., Toker, L., Shainskaya, A., Silman, I., Sussman, J.L. & Futerman, A.H. (2008). "Acid- β -glucosidase: insights from structural analysis and relevance to Gaucher disease therapy" *Biological Chemistry* **389**, 1361-1369.
224. Dunker, A.K., Silman, I., Uversky, V.N. & Sussman, J.L. (2008). "Function and structure of inherently disordered proteins" *Curr Opin Struct Biol* **18**, 756-764.
225. Zeev-Ben-Mordehai, T., Paz, A., Peleg, Y., Toker, L., Wolf, S.G., Rydberg, E.H., Sussman, J.L. & Silman, I. (2009). "Amalgam, an axon guidance *Drosophila* adhesion protein belonging to the immunoglobulin superfamily: Over-expression, purification and biophysical characterization" *Protein Expr Purif* **63**, 147-157.
226. Hodis, E. & Sussman, J.L. (2009). "An encyclopedic effort to make 3D structures easier to understand" *TIBS* **34**, 100-101.
227. Paz, A., Xie, Q., Greenblatt, H.M., Fu, W., Tang, Y., Silman, I., Qiu, Z. & Sussman, J.L. (2009). "The Crystal Structure of a Complex of Acetylcholinesterase with a Bis-(-)-normeptazinol Derivative Reveals Disruption of the Catalytic Triad" *J Med Chem* **52**, 2543-2549.
228. Brumshtein, B., Aguilar-Moncayo, M., Garcia-Moreno, M.I., Ortiz Mellet, C., Garcia Fernandez, J.M., Silman, I., Shaaltiel, Y., Aviezer, D., Sussman, J.L. & Futerman, A.H. (2009). "6-Amino-6-deoxy-5,6-di-N-(N'-octyliminomethylidene)nojirimycin: Synthesis, Biological Evaluation, and Crystal Structure in Complex with Acid β -Glucosidase" *ChemBioChem* **10**, 1480-1485.

229. Khersonsky, O., Rosenblat, M., Toker, L., Yacobson, S., Hugenmatter, A., Silman, I., Sussman, J.L., Aviram, M. & Tawfik, D.S. (2009). "Directed evolution of serum paraoxonase PON3 by family shuffling and ancestor/consensus mutagenesis, and its biochemical characterization" *Biochemistry* **48**, 6644-6654.
230. Sharabi, O., Peleg, Y., Mashiach, E., Vardy, E., Ashani, Y., Silman, I., Sussman, J.L. & Shifman, J.M. (2009). "Design, expression and characterization of mutants of fasciculin optimized for interaction with its target, acetylcholinesterase" *PEDS* **22**, 641-648.
231. Noivirt-Brik, O., Prilusky, J. & Sussman, J.L. (2009). "Assessment of disorder predictions in CASP8" *Proteins: Structure, Function and Bioinformatics* **77**, 210-216.
232. Ben-David, M., Noivirt-Brik, O., Paz, A., Prilusky, J., Sussman, J.L. & Levy, Y. (2009). "Assessment of CASP8 structure predictions for template free targets" *Proteins: Structure, Function and Bioinformatics* **77**, 50-65.
233. Zeev-Ben-Mordehai, T., Mylonas, E., Paz, A., Peleg, Y., Toker, L., Silman, I., Svergun, D.I. & Sussman, J.L. (2009). "The quaternary structure of amalgam, a *Drosophila* neuronal adhesion protein, explains its dual adhesion properties" *Biophys J* **97**, 2316-2326.
234. Sanson, B., Nachon, F., Colletier, J.-P., Froment, M.-T., Toker, L., Greenblatt, H., Sussman, J.L., Ashani, Y., Masson, P., Silman, I. & Weik, M. (2009). "Crystallographic snapshots of nonaged and aged conjugates of soman with acetylcholinesterase, and of a ternary complex of the aged conjugate with Pralidoxime" *J Med Chem* **52**, 7593-7603.
235. Brumshtein, B., Salinas, P., Peterson, B., Chan, V., Silman, I., Sussman, J.L., Savickas, P.J., Robinson, G.S. & Futerman, A.H. (2010). "Characterization of gene-activated human acid- β -glucosidase: Crystal structure, glycan composition, and internalization into macrophages" *Glycobiology* **20**, 24-32.
236. Ashani, Y., Leader, H., Gupta, R. D., Goldsmith, M., Silman, I., Sussman, J. L. & Tawfik, D. S. (2010). "Stereo-specific synthesis of analogs of nerve agents and their utilization for selection and characterization of Paraoxonase (PON1) catalytic scavengers" *Chem. Biol. Interactions* **187**, 362-369.
237. Dvir, H., Silman, I., Harel, M., Rosenberry, T.L. & Sussman, J.L. (2010). "Acetylcholinesterase: From 3D structure to function" *Chem. Biol. Interactions* **187**, 10-22.
238. Hodis, E., Prilusky, J. & Sussman, J.L. (2010). "Proteopedia: A collaborative, virtual 3D web-resource for protein and biomolecule structure and function" *Biochem Mol Biol Educ* **38**, 341-342.
239. Albeck, S., Nordlund, P. & Sussman, J.L. (2010). "New trends in protein expression" *J Struct Biol* **172**, 1-2.
240. Offman, M.N., Krol, M., Silman, I., Sussman, J.L. & Futerman, A.H. (2010). "Molecular Basis of Defective Glucosylceramidase Activity in the Most Common Gaucher Disease Mutant N370s" *J Biol Chem* **285**, 42105-42114.
241. Xu, Y., Colletier, J.-P., Weik, M., Qin, G., Jiang, H., Silman, I. & Sussman, J.L. (2010). "Long Route or Shortcut? A Molecular Dynamics Study of Traffic of Thiocholine within the Active-Site Gorge of Acetylcholinesterase" *Biophys J* **99**, 4003-4011.
242. Gupta, R.D., Goldsmith, M., Ashani, Y., Simo, Y., Mullokandov, G., Bar, H., Ben-David, M., Leader, H., Margalit, R., Silman, I., Sussman, J.L. & Tawfik, D.S. (2011). "Directed evolution of hydrolases for prevention of G-type nerve agent intoxication" *Nat Chem Biol* **7**, 120-125.
243. Li, M.-J., Greenblatt, H.M., Dym, O., Albeck, S., Pais, A., Gunanathan, C., Milstein, D., Degani, H. & Sussman, J.L. (2011). "Structure of estradiol metal chelate and estrogen receptor complex: The basis for designing a new class of selective estrogen receptor modulators" *J Med Chem* **54**, 3575-3580.

244. Brumshtein, B., Aguilar-Moncayo, M., Benito, J.M., Garcia Fernandez, J.M., Silman, I., Shaaltiel, Y., Aviezer, D., Sussman, J.L., Futerman, A.H. & Ortiz Mellet, C. (2011). "Cyclodextrin-mediated crystallization of acid beta-glucosidase in complex with amphiphilic bicyclic nojirimycin analogues" *Org Biomol Chem* **9**, 4160-4167.
245. Busso, D., Peleg, Y., Heidebrecht, T., Romier, C., Jacobovitch, Y., Dantes, A., Salim, L., Troesch, E., Schuetz, A., Heinemann, U., Folkers, G.E., Geerlof, A., Wilmanns, M., Polewacz, A., Quedenau, C., Busow, K., Adamson, R., Blagova, E., Walton, J., Cartwright, J.L., Bird, L.E., Owens, R.J., Berrow, N.S., Wilson, K.S., Sussman, J.L., Perrakis, A. & Celie, P.H. (2011). "Expression of protein complexes using multiple *Escherichia coli* protein co-expression systems: A benchmarking study" *J Struct Biol* **175**, 159-170.
246. Prilusky, J., Hodis, E., Canner, D., Decatur, W.A., Oberholser, K., Martz, E., Berchansky, A., Harel, M. & Sussman, J.L. (2011). "Proteopedia: a status report on the collaborative, 3D web-encyclopedia of proteins and other biomolecules" *J Struct Biol* **175**, 244-252.
247. Perrakis, A., Daenke, S., Stuart, D.I. & Sussman, J.L. (2011). "From SPINE to SPINE-2 complexes and beyond" *J Struct Biol* **175**, 105.
248. Sanson, B., Colletier, J.P., Xu, Y., Therese Lang, P., Jiang, H., Silman, I., Sussman, J.L. & Weik, M. (2011). "Backdoor opening mechanism in acetylcholinesterase based on X-ray crystallography and MD simulations" *Protein Sci* **20**, 1114-1118.
249. Suskiewicz, M.J., Sussman, J.L., Silman, I. & Shaul, Y. (2011). "Context-dependent resistance to proteolysis of intrinsically disordered proteins" *Protein Sci* **20**, 1285-1297.
250. Offman, M.N., Krol, M., Rost, B., Silman, I., Sussman, J.L. & Futerman, A.H. (2011). "Comparison of a molecular dynamics model with the X-ray structure of the N370S acid- β -glucosidase mutant that causes Gaucher disease" *PEDS* **24**, 773-775.
251. Ashani, Y., Goldsmith, M., Leader, H., Silman, I., Sussman, J.L. & Tawfik, D.S. (2011). "In vitro detoxification of cyclosarin in human blood pre-incubated ex-vivo with recombinant serum paraoxonase" *Toxicol Lett* **206**, 24-28.
252. Xu, Y, Li, M, Greenblatt, H.M., Chen, W., Paz, A., Dym, O., Peleg, Y., Chen, T., Shen, X, He, J., Jiang, H., Silman, I. & Sussman, J.L. (2012). "Flexibility of the Flap in the Active Site of Bac1 as Revealed by Crystal Structures and Molecular Dynamics Simulations." *Acta Cryst D Biol Cryst* **D68**, 13-25.
253. Greenblatt, H.M., Otto, T.C., Cerasoli, D.M. & Sussman, J.L. (2012). "Structure of Recombinant Human Carboxylesterase 1 Isolated from Whole Cabbage Looper Larvae." *Acta Crystallograph Section F Structural Biology Crystal Communication* **F68**, 269-272.
254. Khare, S. D., Kipnis, Y., Greisen, P. J., Takeuchi, R., Ashani, Y., Goldsmith, M., Song, Y., Gallaher, J. L., Silman, I., Leader, H., Sussman, J. L., Stoddard, B. L., Tawfik, D. S. & Baker, D. (2012). "Computational redesign of a mononuclear zinc metalloenzyme for organophosphate hydrolysis." *Nat Chem Biol*, **8**, 294-300.
255. Wood, K., Paz, A., Dijkstra, K., Scheek, R. M., Otten, R., Silman, I., Sussman, J. L. & Mulder, F. A. (2012). "Backbone and side chain NMR assignments for the intrinsically disordered cytoplasmic domain of human neuroligin-3." *Biomol NMR Assign*, **6**, 15-18.
256. Acheampong, M. G., Dueno, D. E., Glover, B. K., Henry, A.A., Mata, R., VanBrakle, M.L., Westblade, L. F., Sussman, J.L. & Granberry, A. L. (2012) "Acetylcholinesterase: Substrate Traffic and Inhibition." *Biochem Mol Biol Educ*, **40**, 144.
257. Goldsmith, M, Ashani, Y., Simo, Y., Ben-David, M., Leader, H., Silman, I., Sussman, J.L. & Tawfik, D.S. (2012). "Evolved stereoselective hydrolases for broad-spectrum G-type nerve agent detoxification." *Chem & Biol* **19**, 456-466.
258. Ben-David, M., Elias, M., Filippi, J.-J., Duñach, E., Silman, I., Sussman, J. L. & Tawfik, D. S. (2012). "Catalytic versatility and backups in enzyme active sites: The case of serum paraoxonase 1." *J Mol Biol* **418**, 181-196.

259. Paz, A., Roth, E., Ashani, Y., Xu, Y., Shnyrov, V.L., Sussman, J.L., Silman, I. & Weiner, L. (2012). "Structural and functional characterization of the interaction of the photosensitizing probe methylene blue with *Torpedo californica* acetylcholinesterase" *Prot Sci* **21**, 1138-1152.
260. Ben-David, M., Wieczorek, G., Elias, M., Silman, I., Sussman, J. L. & Tawfik, D. S. (2013). "Catalytic Metal Ion Rearrangements Underline Promiscuity and Evolvability of a Metalloenzyme. *JMB* **425**, 1028-1038.
261. Silman, I., Roth, E., Paz, A., Triquigneaux, M. M., Ehrenshaft, M., Xu, Y., Shnyrov, V. L., Sussman, J. L., Deterding, L. J., Ashani, Y., Mason, R. P. & Weiner, L. (2013) "The specific interaction of the photosensitizer methylene blue with acetylcholinesterase provides a model system for studying the molecular consequences of photodynamic therapy" *Chem Biol Interact* **203**, 63-66.
262. Hanson, R. M., Prilusky, J., Renjian, Z., Nakane, T. & Sussman, J. L. (2013). "JSmol and the Next-Generation Web-Based Representation of 3D Molecular Structure as Applied to Proteopedia" *Israel J Chem* **53**, 207-216.
263. Prilusky, J. & Sussman, J. L. (2013). Guest Editorial: Databases and Bioinformatics Tools. *Israel J Chem* **53**, 143-143.
264. Dunker, A. K., Babu, M. M., Barbar, E., Blackledge, M., Bondos, S.E., Dosztányi, Z., Dyson, H.J., Forman-Kay, J., Fuxreiter, M., Gsponer, J., Han, K.-H., Jones, D.T., Longhi, S., Metallo, S. J., Nishikawa, K., Nussinov, R., Obradovic, Z., Pappu, R. V., Rost, B., Selenko, P., Subramaniam, V., Sussman, J.L., Tompa, P. & Uversky, V.N. (2013) "What's in a name? Why these proteins are intrinsically disordered" *Intrinsically Disordered Proteins* **1**, e24157-24151 - e24157-24155.
265. Varadi, M., Kosol, S., Lebrun, P., Valentini, E., Blackledge, M., Dunker, A.K., Felli, I.C., Forman-Kay, J.D., Kriwacki, R.W., Pierattelli, R., Sussman, J.L., Svergun, D.I., Uversky, V.N., Vendruscolo, M., Wishart, D., Wright, P.E., Tompa, P. (2014) " pE-DB: a database of structural ensembles of intrinsically disordered and of unfolded proteins" *Nucleic Acids Res* **42**, D326-D335.
266. Worek, F., Seeger, T., Goldsmith, M., Ashani, Y., Leader, H., Sussman, J. L., Tawfik, D., Thiermann, H., Wille, T. (2014) "Efficacy of the rePON1 mutant IIG1 to prevent cyclosarin toxicity in vivo and to detoxify structurally different nerve agents in vitro" *Arch of Toxicol* **88**, 1257-66.
267. Worek, F., Seeger, T., Reiter, G., Goldsmith, M., Ashani, Y., Leader, H., Sussman, J.L., Aggarwal, N., Thiermann, H. & Tawfik, D. S. (2014) "Post-exposure treatment of VX poisoned guinea pigs with the engineered phosphotriesterase mutant C23: a proof-of-concept study" *Toxicol. Lett.* **231**, 45-54.
268. Ben-David, M., Sussman, J.L., Maxwell, C.I., Szeler, K., Kamerlin, S.C.L., Tawfik, D.S. (2015) "Catalytic Stimulation by Restrained Active-Site Floppiness - The Case of High Density Lipoprotein-Bound Serum Paraoxonase-1" *J Mol Biol* **427**, 1359-74.
269. Goldsmith, M., Eckstein, S., Ashani, Y., Greisen, P.J., Leader, H., Sussman, J.L., Aggarwal, N., Ovchinnikov, S., Tawfik, D. S., Baker, D., Thiermann, H., Worek, F. (2015) "Catalytic Efficiencies of Directly Evolved Phosphotriesterase Variants with Structurally Different Organophosphorus Compounds *In Vitro*" *Arch Toxicol.* **90**, 2711-2724.
270. Dym, O., Song, W., Felder, C., Roth, E., Shnyrov, V., Ashani, Y., Xu, Y., Joosten, R.P., Weiner, L., Sussman, J.L. & Silman, I. (2016) "The impact of crystallization conditions on drug design: a case study on the methylene blue/acetylcholinesterase complex" *Prot Sci* **25**, 1096-1114 (cover illustration)
271. Goldenzweig, A., Goldsmith, M., Hill, S.E., Gertman, O., Laurino, P., Ashani, Y., Dym, O., Unger, T., Albeck, S., Prilusky, J., Lieberman, R.L., Aharoni, A., Silman, I., Sussman, J.L., Tawfik, D.S., Fleishman, S.J. (2016) "Automated computational design of human enzymes for high bacterial expression and stability" *Mol Cell* **63**, 337-346.

272. Wille, T., Neumaier, K., Koller, M., Ehinger, C., Aggarwal, N., Ashani, Y., Goldsmith, M., Sussman, J.L., Tawfik, D.S., Thiermann, H. & Worek, F. (2016) "Single treatment of VX poisoned guinea pigs with the phosphotriesterase mutant C23AL: Intraosseous versus intravenous injection" *Toxicological Letters* **258**, 198-206.
273. Ashani, Y., Leader, H., Aggarwal, N., Silman, I., Worek, F., Sussman, J.L. & Goldsmith, M. (2016) "In vitro evaluation of the catalytic activity of paraoxonases and phosphotriesterases predicts the enzyme circulatory levels required for in vivo protection against organophosphate intoxications" *Chem. Biol. Interact.* **259**, 252-256.
274. Goldsmith, M., Aggarwal, N., Ashani, Y., Jubran, H., Greisen, P.J., Ovchinnikov, S., Leader, H., Baker, D., Sussman, J.L., Goldenzweig, A., Fleishman, S.J., Tawfik, D.S. (2017) "Overcoming an optimization plateau in the directed evolution of highly efficient nerve agent bioscavengers" *Protein Eng Des Sel* **30**, 333-345.
275. Xu, Y, Cheng, S., Sussman, J. L., Silman, I. & Jiang, H. (2017) "Computational Studies on Acetylcholinesterases" *Molecules* **22**, 1324.
276. Silman, I. & Sussman, J.L. (2017) "Recent developments in structural studies on acetylcholinesterase" *J. Neurochem.* **142 Suppl 2**, 19-25.
277. Faraggi, E., Dunker, A. K., Sussman, J. L. & Kloczkowski, A. (2018) Comparing NMR and X-ray protein structure: Lindemann-like parameters and NMR disorder. *J. Biomol. Struct. Dyn.* **36**, 2331-2341.
278. Zorbaz, T., Braiki, A., Marakovic, N., Renou, J., de la Mora, E., Macek Hrvat, N., Katalinic, M., Silman, I., Sussman, J. L., Mercey, G., Gomez, C., Mougeot, R., Perez, B., Baati, R., Nachon, F., Weik, M., Jean, L., Kovarik, Z. & Renard, P. Y. (2018) Potent 3-hydroxy-2-pyridine aldoxime reactivators of organophosphate-inhibited cholinesterases with predicted blood-brain barrier penetration. *Chemistry* **24**, 9675-9691.
279. Santoni, G., de Sousa, J., de la Mora, E., Dias, J., Jean, L., Sussman, J. L., Silman, I., Renard, P. Y., Brown, R. C. D., Weik, M., Baati, R. & Nachon, F. (2018) Structure-based optimization of non-quaternary reactivators of acetylcholinesterase inhibited by organophosphorus nerve agents. *J. Med. Chem.* **61**, 7630-7639.
280. Leung, M. R., Bezouwen, L. S., Schopfer, L. M., Sussman, J. L., Silman, I., Lockridge, O. & Zeev-Ben-Mordehai, T. (2018) Cryo-EM structure of the physiological butyrylcholinesterase tetramer reveals a dimer of dimers stabilized by a superhelical assembly. *Proc. Natl. Acad. Sci. USA* **115**, 13270-13275.
281. Lalut, J., Santoni, G., Karila, D., Lecoutey, C., Davis, A., Nachon, F., Silman, I., Sussman, J., Weik, M., Maurice, T., Dallemagne, P. & Rochais, C. (2018) Novel multitarget-directed ligands targeting acetylcholinesterase and sigma1 receptors as lead compounds for treatment of Alzheimer's disease: Synthesis, evaluation, and structural characterization of their complexes with acetylcholinesterase and metabolite analogues with putative Alzheimer's disease-modifying properties. *Eur J Med Chem* **162**, 234-248.
282. Boelens, R., Svergun, D., Ellenberg, J., Cusack, S., Walsh, M., Schwalbe, H., Perrakis, A., Sklenář, V., Garcia, J., Oschkinat, H., Thompson, A., Thunnissen, M., Koster, B., Leonard, G., Brutscher, B., Stuart, D., Nissen, P., Wacklin, H., Perczel, A., Archer, M., Wierenga, R., Spyroulias, G. & Sussman, J.K (2018) iNEXT: a European facility network to stimulate translational structural biology. *FEBS Lett.* **592**, 1909-1917.
283. Oukoloff, K., Coquelle, N., Bartolini, M., Naldi, M., Le Guevel, R., Bach, S., Josselin, B., Ruchaud, S., Catto, M., Pisani, L., Denora, N., Iacobazzi, R. M., Silman, I., Sussman, J. L., Buron, F., Colletier, J.-P., Ludovic, J., Routier, S. & Renard, P.-Y. (2018) Design, Biological Evaluation and X-ray Crystallography of Nanomolar Multifunctional Ligands Targeting Simultaneously Acetylcholinesterase (AChE) and Glycogen Synthase Kinase-3 (GSK-3). *Eur. J. Med. Chem.* (submitted).
284. Dighe, S. N., De la Mora, E., Chan, S., Srinivas, K., McColl, G., Miles, J. A., Kumar Veliyath, S., Sreenivas, B. Y., Nassar, Z. D., Silman, I., Sussman, J. L., Weik, M., McGeary, R. P., Parat, M.-O., Brazzolotto, X. & Ross, B. P. (2018) Rivastigmine and

Metabolite Analogues with Putative Alzheimer's Disease-Modifying Properties in a *C. elegans* model. *Royal Soc. Chem.* (submitted).

285. Chandar, N. B., Efremenko, I., Silman, I., Martin, J. M. L. & Sussman, J. L. (2019) Molecular Dynamics Simulations of the Interaction of Mouse and Torpedo Acetylcholinesterase with Covalent Inhibitors Explain Their Differential Reactivity: Implications for Drug Design. *bioRxiv*, 532754.

Books

1. Balaban, M., Sussman, J.L., Traub, W. & Yonath, A., Eds. (1981) "Structural Aspects of Recognition and Assembly in Biological Macromolecules - The Seventh Aharon Katzir-Katchalsky Conference", Balaban ISS, Rehovot & Philadelphia.
2. Read, R.J. & Sussman, J.L. Eds. (2007) "Evolving Methods for Macromolecular Crystallography, Proceedings of the NATO Advanced Study Institute on Evolving Methods for Macromolecular Crystallography: The Structural Path to the Understanding of the Mechanism of Action of CBRN agents, Erice, Italy, 19-28 May 2005", Springer, Dordrecht.
3. Sussman, J. L. & Silman, I., Eds. (2008). "Structural Proteomics and its Impact on the Life Sciences" World Scientific Publishing Company (London)
4. Sussman, J.L & Spadon, P. Eds. (2009) "From Molecules to Medicines, Structure of Biological Macromolecules and Its Relevance in Combating New Diseases and Bioterrorism, Proceedings of the NATO Advanced Study Institute on Integrating Crystallography in the Fight Against Terrorism Erice, Italy 29 May-8 June 2008", Springer, Dordrecht.

Chapters in Books

1. Kim, S.-H., Suddath, F.L., Quigley, G.J., McPherson, A., Sussman, J.L., Wang, A.H.J., Seeman, N.C. & Rich, A. (1975) "The tertiary structure of yeast transfer RNA". in *Structure and Conformation of Nucleic Acids and Protein-Nucleic Acid Interaction*, (Sundaralingam, M. & Rao, S. T., eds.), University Park Press, Baltimore pp. 7-23.
2. Kim, S.-H., Sussman, J.L. & Church, G.M. (1975) "A model for a recognition scheme between double stranded DNA and proteins". in *Structure and Conformation of Nucleic Acids and Protein-Nucleic Acid Interaction*, (Sundaralingam, M. & Rao, S. T., eds.), University Park Press, Baltimore pp. 571-575.
3. Sussman, J.L. & Kim, S.H. (1976) "A preliminary refinement of yeast tRNA^{Phe} at 3Å resolution". in *Environmental Effects on Molecular Structure and Properties*, (Pullman, B., eds.), D. Reidel Publishing Co., Dordrecht, vol. 8, pp. 535-545.
4. Trifonov, E. & Sussman, J.L. (1979) "Smooth bending of DNA in chromatin". in *Molecular mechanisms of biological recognition*, (Balaban, M., eds.), Elsevier/North-Holland: Biomedical Press, pp. 227-232.
5. Sussman, J.L., Podjarny, A.D., Schevitz, R.W. & Sigler, P.B. (1981) "A preliminary comparison of the three-dimensional structures of yeast initiator tRNA^{Met} and tRNA^{Phe}". in *Structural Aspects of Recognition and Assembly in Biological Macromolecules - The Seventh Aharon Katzir-Katchalsky Conference*, (Balaban, M., Sussman, J.L., Traub, W., Yonath, A., eds.), Balaban ISS, Rehovot and Philadelphia pp. 597-614.
6. Sigler, P.B., Schevitz, R.W., Gross, G.M., Kaplansky, R.A., Podjarny, A.D. & Sussman, J.L. (1981) "The molecular basis for the role of initiator tRNA in eukaryotic protein

- synthesis inferred from the crystal structure of yeast tRNA^{Met}. in *Structural Aspects of Recognition and Assembly in Biological Macromolecules - The Seventh Aharon Katzir-Katchalsky Conference*, (Balaban, M., Sussman, J.L., Traub, W., Yonath, A., eds.), Balaban ISS, Rehovot and Philadelphia pp. 631-643.
7. Sussman, J.L. (1981) "The use of CORELS for the refinement of biological macromolecules". in *Refinement of Protein Structures - Proceedings of the Daresbury Study Weekend*, (Machin, P. A., Campbell, J. W. & Elder, M., eds.), Daresbury Laboratory, Daresbury pp. 13-23.
 8. Sussman, J.L. (1984) "Application of refinement constraints and restraints to proteins and nucleic acids". in *Methods and Applications in Crystallographic Computing*, (Hall, S. R. & Ashida, T., eds.), Clarendon Press, Oxford pp. 206-237.
 9. Sussman, J.L., Brown, J.H. & Shoham, M. (1986) "X-ray structural studies on a salt-loving Ferredoxin from *Halobacterium* of the Dead Sea.". in *Iron-Sulfur protein research*, (Matsubara, H., Katsube, Y. & Wada, K., eds.), Japan Scientific Societies Press, Tokyo pp. 69-82.
 10. Sussman, J.L., Joshua-Tor, L., Hirshberg, M., Saper, M.A., Frolow, F., Hope, H. & Appella, E. (1987) "A kinked model of a DNA tridecamer with an unpaired adenosine: energy minimization and X-ray structural studies". in *Molecular Structure: Chemical Reactivity and Biological Activity*, (Stezowski, J. J., Huan, J.-L. & Shao, M.-C., eds.), Oxford University Press, Oxford pp. 195-200.
 11. Hope, H., Frolow, F. & Sussman, J.L. (1987) "Macromolecular X-ray data collection on a rotating anode diffractometer" *The Rigaku Journal* **4**, 3-10.
 12. Sussman, J.L., Shoham, M. & Harel, M. (1989) "Protein adaptation to extreme salinity: the crystal structure of 2Fe-2S ferredoxin from *Halobacterium Marismortui*". in *Computer-Assisted Modeling of Receptor-Ligand Interactions. Theoretical Aspects and Applications to Drug Design*, (Rein, R. & Golombek, A., eds.), A.R. Liss, New York, vol. 289, pp. 171-187.
 13. Sussman, J.L., Harel, M., Frolow, F. & Silman, I. (1989) "X-ray crystallographic studies of acetylcholinesterase". in *1989 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Columbia, MD pp. 309-316.
 14. Baldwin, E.T., Sussman, J.L., St. Charles, R. & Wlodawer, A. (1991) "Molecular replacement structure solution of interleukin-8 using the NMR model". in *Techniques in Protein Chemistry II*, (Villafranka, J., ed.), Academic Press, New York pp. 347-356.
 15. Sussman, J.L., Harel, M., Frolow, F., Oefner, C., Toker, L. & Silman, I. (1991) "Structural studies on acetylcholinesterase from *Torpedo californica*". in *Cholinesterases: Structure, Function, Mechanism, Genetics and Cell Biology*, (Massoulié, J., et al., eds.), American Chemical Society, Washington, DC pp. 7-11.
 16. Sussman, J.L., Harel, M., Frolow, F., Goldman, A., Oefner, C., Toker, L. & Silman, I. (1991) "3-D structure of acetylcholinesterase from *Torpedo Californica*". in *1991 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD pp. 441-448.
 17. Sussman, J.L. (1991) "Introduction to macromolecular refinement". in *Crystallographic Computing*, (Moras, D., Podjarny, A. D. & Thierry, J. C., eds.), Oxford Univ. Press, New York, vol. 5, pp. 382-391.
 18. Sussman, J.L., Harel, M. & Silman, I. (1992) "3-D Structure of acetylcholinesterase and complexes of it with anticholinesterase agents". in *Membrane Proteins: Structures, Interactions and Models*, (Pullman, A., Jortner, J. & Pullman, B., eds.), Kluwer Academic Publishers, Dordrecht, Holland, vol. 25, pp. 161-175.
 19. Silman, I., Harel, M., Krejci, E., Bon, S., Chanal, P., Sussman, J.L. & Massoulié, J. (1992) "Modelling and mutagenesis of butyrylcholinesterase based on the X-ray structure of acetylcholinesterase". in *Membrane Proteins: Structures, Interactions and Models*,

- (Pullman, A., Jortner, J. & Pullman, B., eds.), Kluwer Academic Publishers, Dordrecht, Holland, vol. 25, pp. 177-184.
20. Sussman, J.L., Harel, M. & Silman, I. (1992) "Three dimensional structure of acetylcholinesterase". in *Multidisciplinary Approaches to Cholinesterase Functions*, (Shafferman, A. & Velan, B., eds.), Plenum Press, New York pp. 95-107.
 21. Cygler, M., Schrag, J.D., Sussman, J.L., Harel, M., Silman, I., Gentry, M.K. & Doctor, B.P. (1992) "Sequence alignment of esterases and lipases based on 3-D structure of two members of this family". in *Multidisciplinary Approaches to Cholinesterase Functions*, (Shafferman, A. & Velan, B., eds.), Plenum Press, New York pp. 109-116.
 22. Silman, I., Krejci, E., Duval, N., Bon, S., Chanal, P., Harel, M., Sussman, J.L. & Massoulié, J. (1992) "Site-directed mutagenesis of functional residues in *Torpedo* acetylcholinesterase". in *Multidisciplinary Approaches to Cholinesterase Functions*, (Shafferman, A. & Velan, B., eds.), Plenum Press, New York pp. 177-183.
 23. Harel, M., Silman, I. & Sussman, J.L. (1992) "A model of butyrylcholinesterase based on the X-ray structure of acetylcholinesterase indicates differences in specificity". in *Multidisciplinary Approaches to Cholinesterase Functions*, (Shafferman, A. & Velan, B., eds.), Plenum Press, New York pp. 189-194.
 24. Massoulié, J., Sussman, J.L., Doctor, B.P., Soreq, H., Velan, B., Cygler, M., Rotundo, R., Shafferman, A., Silman, I. & Taylor, P. (1992) "Recommendations for nomenclature in cholinesterases". in *Multidisciplinary Approaches to Cholinesterase Functions*, (Shafferman, A. & Velan, B., eds.), Plenum Press, New York pp. 285-288.
 25. Sadoff, J.C., Shafferman, A., Soreq, H., Sussman, J.L. & Silman, I. (1992) "Cloning, expression, production and X-ray crystallographic structure of acetylcholinesterase". in *Emerging Technologies: Life Science*, Borg Biomedical Services, The Woodlands, Texas.
 26. Gentry, M.K., Doctor, B.P., Cygler, M., Schrag, J.D., Sussman, J.L., Harel, M. & Silman, I. (1993) "3-D structure-based amino acid sequence alignment of esterases, lipases and related proteins". in *1993 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Baltimore, MD pp. 1127-1137.
 27. Sussman, J.L., Harel, M. & Silman, I. (1993) "3-D Structure of acetylcholinesterase and of its complexes with cholinergic ligands". in *1993 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Baltimore, MD. pp. 1139-1148.
 28. Silman, I., Harel, M., Eichler, J., Krejci, E., Anselmet, A., Chanal, P., Bon, S., Sussman, J.L. & Massoulié, J. (1993) "Structure-function relationships in acetylcholinesterase: modeling mutagenesis and comparative studies". in *1993 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Baltimore, MD. pp. 1149-1157.
 29. Silman, I., Harel, M., Eichler, J., Sussman, J.L., Anselmet, A. & Massoulié, J. (1994) "Structure-function relationships in the binding of reversible inhibitors in the active-site gorge of acetylcholinesterase". in *Alzheimer Disease: Therapeutic Strategies*, (Giacobini, E. & Becker, R., eds.), Birkhäuser, Boston pp. 88-92.
 30. Sussman, J.L., Harel, M., Raves, M., Quinn, D. & Silman, I. (1995) "3-D structure of acetylcholinesterase and complexes of it with Anticholinesterase agents". in *Modelling of Biomolecular Structures and Mechanisms*, (Pullman, A., Jortner, J. & Pullman, B., eds.), Kluwer Academic Publishers, Dordrecht, Holland, vol. 27, pp. 455-560.
 31. Ripoll, D.R., Faerman, C.H., Gillilan, R., Silman, I. & Sussman, J.L. (1995) "Electrostatic properties of human acetylcholinesterase". in *Enzymes of the Cholinesterase Family*, (Balasubramanian, A. L., Doctor, B. P., Taylor, P. & Quinn, D. M., eds.), Plenum Press, New York pp. 67-70.

32. Silman, I., Kreimer, D.I., Shin, I., Dolginova, E.A., Roth, E., Goldfarb, D., Szosenfogel, R., Raves, M., Sussman, J.L., Borochoy, N. & Weiner, L. (1995) "Studies on partially unfolded states of *Torpedo californica* acetylcholinesterase". in *Enzymes of the Cholinesterase Family*, (Balasubramanian, A. L., Doctor, B. P., Taylor, P. & Quinn, D. M., eds.), Plenum Press, New York pp. 77-82.
33. Sussman, J.L., Harel, M., Raves, M., Quinn, D.M., Nair, H.K. & Silman, I. (1995) "Structures of complexes of acetylcholinesterase with covalently and non-covalently bound inhibitors". in *Enzymes of the Cholinesterase Family*, (Balasubramanian, A. L., Doctor, B. P., Taylor, P. & Quinn, D. M., eds.), Plenum Press, New York pp. 59-65.
34. Sussman, J.L., Harel, M., Raves, M.L., Giles, K., Ravelli, R.B.G., Peng, L., Goeldner, M., Kleywegt, G.J., Quinn, D.M., Nair, H.K. & Silman, I. (1996) "Studies on the 3-D structure of *Torpedo* acetylcholinesterase". in *1996 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Baltimore, MD. pp. 13-22.
35. Sussman, J.L., Abola, E.E., Manning, N.O. & Prilusky, J. (1996) "The protein data bank: Current status and future challenges". in *Crystallographic Computing*, (Bourne, P. & Watenpugh, K. D., eds.), San Diego Supercomputer Center, San Diego, pp. 9-34.
36. Giles, K., Raves, M.L., Silman, I. & Sussman, J.L. (1997) "How three-fingered snake toxins recognize their targets: acetylcholinesterase-fasciculin, a case study". in *Theoretical and Computational Methods in Genome Research*, (Suhai, S., ed.), Plenum Press, New York pp. 303-315.
37. Sussman, J.L., Ritter, O. & Abola, E.E. (1997) "Protein data bank". in *Transactions ACA 1997*, (Berman, H. M. & Gilliland, G., eds.), American Crystallographic Association, Buffalo, NY, vol. 32, pp. 7-11.
38. Silman, I., Harel, M., Raves, M. & Sussman, J.L. (1997) "Crystallographic studies on complexes of acetylcholinesterase with the natural cholinesterase inhibitors fasciculin and Huperzine A". in *Progress in Alzheimers and Parkinsons Diseases*, (Fisher, A., Yoshida, M. & Flanin, I., eds.), Plenum Press, New York pp. 523-530.
39. Karlsson, E., Harvey, A.L., Cerveñansky, C., Kleywegt, G.J., Harel, M., Silman, I. & Sussman, J.L. (1998) "Fasciculins, Cholinesterase Inhibitors from Mamba Venoms". in *Enzymes from Snake Venoms*, (Bailey, G. S., eds.), Alaken, Inc., Fort Collins, pp. 633-688.
40. Silman, I. & Sussman, J.L. (1998) "Structural and functional studies on acetylcholinesterase: a perspective". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York pp. 25-33.
41. Botti, S.A., Felder, C., Lifson, S., Sussman, J.L. & Silman, I. (1998) "An integrated model for the molecular traffic through the active site of cholinesterases". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Quinn, D. M., Rotundo, R. L. & Taylor, P., eds.), Plenum, New York, vol. pp. 227-228.
42. Nicolas, A., Millard, C.B., Raves, M.L., Ravelli, R.B.G., Kroon, J., Silman, I. & Sussman, J.L. (1998) "Activity of *Torpedo californica* acetylcholinesterase in the crystalline state". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Quinn, D. M., Rotundo, R. L. & Taylor, P., eds.), Plenum, New York, vol. pp. 230-231.
43. Kryger, G., Giles, K., Harel, M., Toker, L., Velan, B., Lazar, A., Kronman, C., Barak, D., Ariel, N., Shafferman, A., Silman, I. & Sussman, J.L. (1998) "3D structure at 2.7Å resolution of native and E202Q mutant human acetylcholinesterase complexed with fasciculin-II". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York pp. 323-326.

44. Raves, M., Giles, K., Schrag, J.D., Schmid, M.F., Phillips, G.N., Chiu, W., Howard, A.J., Silman, I. & Sussman, J.L. (1998) "Quaternary structure of tetrameric acetylcholinesterase". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York pp. 351-356.
45. Kryger, G., Giles, K., Harel, M., Toker, L., Velan, B., Lazar, A., Kronman, C., Barak, D., Ariel, N., Shafferman, A., Silman, I. & Sussman, J.L. (1998) "3D structure of a complex of human acetylcholinesterase with fasciculin-II at 2.7Å resolution". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York, vol. pp. 370.
46. Greenblatt, H., Kryger, G., Harel, M., Lewis, T., Taylor, J., Silman, I. & Sussman, J.L. (1998) "Crystal structures of complexes of E2020-related compounds with *Torpedo* acetylcholinesterase". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York pp. 371.
47. Raves, M.L., Greenblatt, H.M., Kryger, G., Nicolas, A., Ravelli, R.B.G., Harel, M., Kroon, J., Silman, I. & Sussman, J.L. (1998) "Alternative crystal forms of *Torpedo californica* acetylcholinesterase". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Quinn, D. M., Rotundo, R. L. & Taylor, P., eds.), Plenum, New York, vol. pp. 372.
48. Bar-On, P., Harel, M., Millard, C., Enz, A., Sussman, J.L. & Silman, I. (1998) "Kinetic and X-ray crystallographic studies of the binding of ENA-713 to *Torpedo californica* acetylcholinesterase". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York, vol. pp. 373-374.
49. Millard, C., Kryger, G., Ordentlich, A., Harel, M., Raves, M., Greenblatt, H.M., Segall, Y., Barak, D., Shafferman, A., Silman, I. & Sussman, J.L. (1998) "Crystal structure of "aged" phosphorylated and phosphonylated *Torpedo californica* acetylcholinesterase: preliminary report". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York pp. 425-431.
50. Morel, N., Bon, S., Sussman, J.L., Massoulié, J. & Silman, I. (1998) "Surface residues near the peripheral site affect the stability of *Torpedo* Acetylcholinesterase". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Quinn, D. M., Rotundo, R. L. & Taylor, P., eds.), Plenum, New York, vol. pp. 435.
51. Giles, K., Ben-Yohanan, R., Velan, B., Shafferman, A., Sussman, J.L. & Silman, I. (1998) "Assembly of acetylcholinesterase subunits *in vitro*". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Quinn, D. M., Rotundo, R. L. & Taylor, P., eds.), Plenum, New York, vol. pp. 442-443.
52. Botti, S.A., Felder, C., Sussman, J.L. & Silman, I. (1998) "The conjunction of a conserved electrostatic motif and a common cholinesterase fold defines a class of adhesion proteins". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Quinn, D. M., Rotundo, R. L. & Taylor, P., eds.), Plenum, New York, vol. pp. 448-449.
53. Giles, K., Silman, I. & Sussman, J.L. (1998) "Expression and tissue distribution of cholinesterases via EST analysis". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Quinn, D. M., Rotundo, R. L. & Taylor, P., eds.), Plenum, New York, vol. pp. 450.

54. Millard, C., Kryger, G., Ordentlich, A., Harel, M., Raves, M., Greenblatt, H.M., Segall, Y., Barak, D., Shafferman, A., Silman, I. & Sussman, J.L. (1998) "Crystal structure of "aged" phosphorylated and phosphonylated *Torpedo californica* acetylcholinesterase: preliminary report". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York, vol. pp. 454-455
55. Kryger, G., Silman, I. & Sussman, J.L. (1998) "3D structure of a complex of the anti-Alzheimer drug, E2020, with acetylcholinesterase at 2.5Å resolution". in *Structure and Function of Cholinesterases and Related Proteins*, (Doctor, B. P., Taylor, P., Quinn, D. M., Rotundo, R. L. & Gentry, M. K., eds.), Plenum, New York pp. 469-475.
56. Millard, C., Kryger, G., Ordentlich, A., Harel, M., Raves, M., Greenblatt, H.M., Segall, Y., Barak, D., Shafferman, A., Silman, I. & Sussman, J.L. (1998) "Crystal structures of aged phosphorylated and phosphonylated *Torpedo californica* acetylcholinesterase: a preliminary report". in *1998 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Baltimore, MD. pp. 1-8.
57. Silman, I., Millard, C., Kryger, G., Ordentlich, A., Harel, M., Raves, M., Greenblatt, H.M., Segall, Y., Barak, D., Shafferman, A. & Sussman, J.L. (1998) "Structural models for the acylation and deacylation transition states of acetylcholinesterase: a preliminary comparison". in *1998 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research Institute of Chemical Defense, Baltimore, MD. pp. 1-10.
58. Bar-On, P., Harel, M., Millard, C.B., Enz, A., Sussman, J.L. & Silman, I. (1998) "Kinetic and structural studies on the interaction of the anti-Alzheimer drug, ENA-713, with *Torpedo californica* acetylcholinesterase". in *Xth International Symposium on Cholinergic Mechanisms - From Torpedo Electric Organ to Human Brain: Fundamental and Applied Aspects*, (Massoulié, J., ed.), Elsevier, Paris pp. 406-407.
59. Sussman, J.L., Abola, E.E., Lin, D., Jiang, J., Manning, N.O. & Prilusky, J. (1999) "The protein data bank: bridging the gap between the sequence and 3D structure world". in *Structural Biology and Functional Genomics*, (Bradbury, E. M. & Pongor, S., eds.), Kluwer Academic Publishers, Dordrecht, Boston, London pp. 251-264.
60. Silman, I. & Sussman, J.L. (2000) "Structural studies on acetylcholinesterase". in *Cholinesterases and Cholinesterase Inhibitors*, (Giacobini, E., ed.), Martin Dunitz, London pp. 9-25.
61. Sussman, J.L., Millard, C.B., Gillilan, R.E., Koellner, G., Kryger, G., Harel, H., Greenblatt, H.M., Ordentlich, A., Barak, D., Shafferman, A. & Silman, I. (2000) "Crystal structures of conjugates of AChE with nerve agents at atomic resolution". in *2000 U.S. Army Medical Defense Bioscience Review*, U.S. Army Medical Research and Material Command, Baltimore, MD. pp. 38-55.
62. Botti, S., Silman, I. & Sussman, J.L. (2001) "Structural genomics" in *Conformational Diseases - A Compendium, Based on the First International Workshop on Conformational Diseases*, (Solomon, B., Taraboulos, A. & Katchalski-Katzir, E., eds.), The Center for the Study of Emerging Diseases, Jerusalem, pp. 73-81.
63. Harel, D., Unger, R. & Sussman, J.L. (2003) "Beauty is in the genes of the beholder". in *DNA 50, The Secret of Life*, (Balaban, M., eds.), Faircount, London, vol. pp. 98-103.
64. Toutant, J.P., Massoulié, J., Fournier, D., Marty, J.L., Schmid, R., Pfeiffer, D., Selkirk, M., Sussman, J., Silman, I., Talesa, V., Wodak, S., Stojan, J., Magearu, V. (2004) "New Biosensors for Improved Detection of Environmental and Food Contamination by Anticholinesterase Pesticides" in *Cholinesterases in the Second Millennium: Biomolecular and Pathological Aspects*, (Inestrosa, N. & Campos, E.O, eds), P. Universidad Católica de Chile – FONDAP Biomedicina, Pucon, pp. 233-236.
65. Harel, M., Dvir, H., Bon, S., Liu, W.Q., Garbay, C., Sussman, J.L., Massoulié, J. & Silman, I. (2004). Crystal structure of the tetramerization domain of acetylcholinesterase at 2.3Å resolution. In *Cholinergic Mechanisms: Function and Dysfunction*, S. I., Soreq H, Anglister L, M. D., and F. A., eds. (London and New York, Taylor & Francis), pp. 183-186.

66. Srividhya, K.V., Rao, G.V., Raghavenderan, L., Mehta, P., Prilusky, J., Sankarnarayanan, M., Sussman, J.L. & Krishnaswamy, S. (2006) Database and comparative identification of prophages. in ICIC 2006, (Huang, D.-S., Li, K. & Irwin, G.W., eds) vol LNCIS 344 863-868, Springer-Verlag, Berlin, Heidelberg.
67. Premkumar L, Vokovitsky M, Gokhmana I, Sussman JL and Zamir A (2005) Molecular determinants of protein halotolerance: structural and functional studies of the extremely salt tolerant carbonic anhydrases from *Dunaliella salina*, in *Adaptation to life at high salt concentrations in Archaea, Bacteria, and Eukarya* (Gunde-Cimerman N, Oren A and Plemenitas A eds), Springer Science, The Netherlands.
68. Premkumar, L., Silman, I., Sussman, J. L. & Futerman, A. H. (2006) The X-ray structure of human acid- β -glucosidase: implications for second-generation enzyme replacement therapy. In *Gaucher disease* (Futerman, A. H. & Zimran, A., eds.), pp. 85-96. CRC Press, Boca Raton.
69. Man, O., Sussman, J.L. & Pilpel, Y. Examination of the tRNA Adaptation Index as a Predictor of Protein Expression Levels. in *Systems Biology and Regulatory Genomics: Joint Annual RECOMB 2005 Satellite Workshops on Systems Biology and on Regulatory Genomics, San Diego, CA, USA* (eds. Eskin, E., Ideker, T., Raphael, B. & Workman, D.) 107-118 (Springer Berlin / Heidelberg, 2007).
70. Read, R.J. & Sussman, J.L. "Preface" in *Evolving Methods for Macromolecular Crystallography; The Structural Path to the Understanding of the Mechanism of Action of CBRN agents* (eds. Read, R.J. & Sussman, J.L.) vii-viii (Springer, Dordrecht, 2007).
Read, R.J. & Sussman, J.L. "Preface" in *Evolving Methods for Macromolecular Crystallography; The Structural Path to the Understanding of the Mechanism of Action of CBRN agents* (eds. Read, R.J. & Sussman, J.L.) vii-viii (Springer, Dordrecht, 2007).
71. Sussman, J.L. & Silman, I. (2008). Preface. In *Structural Proteomics and its Impact on the Life Sciences*, J.L. Sussman, and I. Silman, eds. (London, World Scientific Publishing Company), pp. vi-vii.
72. Banci, L., Baumeister, W., Heinemann, U., Schneider, G., Silman, I. & Sussman, J.L. (2008). Structural Genomics and Structural Proteomics: A Global Perspective. In *Structural Proteomics and its Impact on the Life Sciences*, J.L. Sussman, and I. Silman, eds. (London, World Scientific Publishing Company), pp. 505-537.
73. Sussman, J.L. & Spadon, P. (2009). Preface. In *From Molecules to Medicines Structure of Biological Macromolecules and Its Relevance in Combating New Diseases and Bioterrorism*, J.L. Sussman, and P. Spadon, eds. (Dordrecht, Springer Netherlands), p. vii.
74. Hodis, E., J, P. & JL, S. (2009). Tools to make 3D structural data more comprehensible: eMovie & Proteopedia. In *From Molecules to Medicine - Structure of Biological Macromolecules and Its Relevance in Combating New Diseases and Bioterrorism*, S. JL, and P. Spadon, eds. (Dordrecht, Springer), pp. 169-182.
75. Sussman, J.L. & Silman, I. (2009). Structural studies on acetylcholinesterase and paraoxonase directed towards development of therapeutic biomolecules for the treatment of degenerative diseases and protection against chemical threat agents In *From Molecules to Medicines Structure of Biological Macromolecules and Its Relevance in Combating New Diseases and Bioterrorism*, J.L. Sussman, and P. Spadon, eds. (Dordrecht, Springer Netherlands), pp. 183-199.
76. Paz, A., Zeev-Ben-Mordehai, T., Sussman, J.L. & Silman, I. (2010). Purification of intrinsically disordered proteins. In *Instrumental Analysis of Intrinsically Disordered Proteins: Assessing Structure and Conformation*, V. Uversky, and S. Longhi, eds. (John Wiley & Sons, Inc), pp. 695-704.
77. Prilusky, J., Hodis, E. & Sussman, J.L. (2012). "Proteopedia: Exciting advances in the 3D encyclopedia of Biomolecular structure" In *Macromolecular Crystallography: Deciphering the Structure, Function and Dynamics of Biological Molecules*, M.A. Carrondo & P. Spadon, eds. (Dordrecht, Springer) pp. 149-162.

78. Offman, M. N., Silman, I., Sussman, J. L. & Futerman, A. H. (2013). Crystal structure of the enzyme acid β -glucosidase. In *Advances in Gaucher Disease: Basic and Clinical Perspectives*, pp. 124-138. Future Medicine Ltd.