Structural Basis for Blue and Purple Fluorescence of Antibody-stilbene Complexes

Erik W. Debler[a], Gunnar F. Kaufmann[b], Angelo Di Bilio[c], Harry B. Gray[c], Richard A. Lerner[a,c], Kim D. Janda[c], Ian A. Wilson[a], [a]*Department of Molecular Biology and Skaggs Institute of Chemical Biology.* [b]*Department of Chemistry, The Scripps Research Institute, La Jolla, USA.* [c]*Beckman Institute, California Institute of Technology, Pasadena, USA.* E-mail: erik@scripps.edu

A panel of antibodies was generated against *trans*-stilbene[1] in order to explore the influence of protein environment on the excited electronic states of a chromophore. When irradiated by UV-light, stilbene readily undergoes photochemical *trans/cis*-isomerization and exhibits only weak fluorescence. In presence of these antibodies however, the electronically-excited stilbene affords strong fluorescence which is likely the result of precluding isomerization in the antibody pocket due to tight binding of the stilbene. Interestingly, antibody 19G2 exhibits the largest red-shift and a tenfold increase in fluorescence lifetime compared to the other purple-fluorescent antibodies.

Crystal structures of both blue (19G2) and purple (25C10) fluorescent antibodies in complex with stilbene have been determined to elucidate their different fluorescence properties and the mechanism of spectral tuning. In combination with biochemical and spectroscopic techniques, we are probing the unusually strong fluorescence of 19G2 compared to 25C10.

[1] Simeonov A., Matsushita M., Juban E.A., Thompson E.H., Hoffman T.Z., Beuscher A.E. 4th, Taylor M.J., Wirsching P., Rettig W., McCusker J.K., Stevens R.C., Millar D.P., Schultz P.G., Lerner R.A., Janda K.D. R.J., Liles D.C., *Science*, 2000, **290**, 307.

Keywords: antibody structure, protein dynamics, photophysics