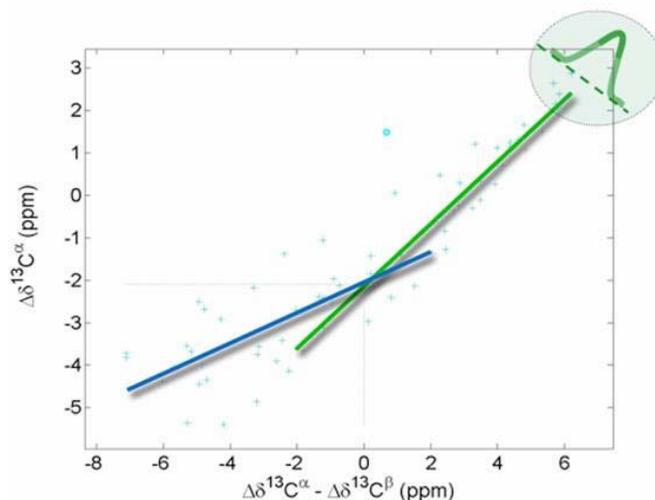


Center for Eukaryotic Structural Genomics

Technology Dissemination Report

CESG Tech Report No.	013
Title	LACS (Linear Analysis of Chemical Shifts)
Research Unit	NMR Spectroscopy
Authors	Wang, L., Eghbalnia, H.R., and Markley, J.L.
Primary Contact	markley@nmrfam.wisc.edu



Summary

LACS [1] provides the means for analyzing NMR data early on, prior to assignment or structure determination, to ascertain whether the ^{13}C chemical shifts are referenced properly and to identify $^{13}\text{C}^\alpha$ and $^{13}\text{C}^\beta$ peaks with unusual chemical shifts. LACS takes advantage of the finding that, for a correctly referenced protein dataset, linear regression plots of $\Delta\delta^{13}\text{C}^\alpha$, $\Delta\delta^{13}\text{C}^\beta$, or $\Delta\delta^1\text{H}^\alpha$ vs. $(\Delta\delta^{13}\text{C}^\alpha - \Delta\delta^{13}\text{C}^\beta)$ pass through the origin from two directions, the helix-to-coil and strand-to-coil directions. LACS is available from a webserver at: <http://bija.nmrfam.wisc.edu/MANI-LACS/> The BMRB uses LACS in screening chemical shift data sets being deposited and notifies depositors of possible problems with chemical shift referencing and the presence of outliers. The approach also has been used to derive unbiased $^{13}\text{C}^\alpha$ and $^{13}\text{C}^\beta$ chemical shift values for residues in random coil [2] and to determine nearest-neighbor effects on chemical shifts of residues in coil, helix, or strand [3].

Publications:

- [1] Wang, L., Eghbalnia, H.R., Bahrami, A., and Markley, J.L. (2005) Linear analysis of carbon-13 chemical shift differences and its application to the detection and correction of errors in referencing and spin system identifications. *J Biomol NMR* 32(1):13-22.
- [2] Wang, L., Eghbalnia, H.R., and Markley, J.L. (2006) Probabilistic approach to determining unbiased random-coil carbon-13 chemical shift values from the protein chemical shift database. *J Biomol NMR* 35(3):155-65.
- [3] Wang, L., Eghbalnia, H.R., Markley, J.L. (2007) Nearest-neighbor effects on C^α and C^β carbon-13 chemical shifts in proteins. *J Biomol NMR* 39(3):247-57.

Acquiring the Technology Available from: <http://www.bija.nmrfam.wisc.edu/MANI-LACS/>

Other Acknowledgements Partial support from NIH Grant P41 RR02301.

Center for Eukaryotic Structural Genomics (CESG), University of Wisconsin-Madison Biochemistry Department, 433 Babcock Drive, Madison, WI 53706-1549; phone: 608.263.2183; fax: 608.890.1942; email: cesginfo@biochem.wisc.edu; website: <http://www.uwstructuralgenomics.org>. This research funded by NIH / NIGMS Protein Structure Initiative grants U54 GM074901 and P50 GM064598.