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 $^{13}$C$^\alpha$ and $^{13}$C$^\beta$ peaks with unusual chemical shifts. LACS takes advantage of the finding that, for a correctly referenced protein dataset, linear regression plots of $\Delta\delta^{13}$C$^\alpha_i$, $\Delta\delta^{13}$C$^\beta_i$, or $\Delta\delta^1$H$^\alpha_i$ vs. $(\Delta\delta^{13}$C$^\alpha_i - \Delta\delta^{13}$C$^\beta_i)$ 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 $^{13}$C$^\alpha$ and $^{13}$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:


Acquiring the Technology

Available from: http://www.bija.nmrfam.wisc.edu/MANI-LACS/

Other Acknowledgements

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