The use of Singular Value Decomposition and Multiple Linear Regression to Analyze multi-component kinetic Spin-Trapping Data

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Signal averaging, the most commonly used method of noise reduction, is only appropriate when the signal is not changing as a function of time. However, this method is commonly used in spin-trapping studies where the signal is almost never static. Modern computers and EPR instruments allow the rapid collection, digitization and storage of EPR data, facilitating the use of more complex data analysis strategies. We have explored the use of principal component analysis (PCA) using the singular value decomposition algorithm with kinetic EPR spin trapping data. The systems explored are superoxide trapping using DMPO and DEPMPO, and radical trapping during the oxidation of formate and glutathione by peroxynitrite. Spectra are taken every 3 seconds with a sweep time of 2.56 s. The three dimensional data set (amplitude x time x field) are subject to principal component analysis. This technique has all the advantages of signal averaging in terms of signal-to-noise improvement, however, the kinetic information is retained. This allows, within a single experiment, full kinetic and spectral characterization of a system containing sub-micromolar radical concentration with a time resolution of 3 s. In addition, PCA, in combination with least squares multiple regression techniques allows statistical deconvolution of multiple spectra if pure (or simulated) spectra can be obtained. These and similar techniques make signal averaging an obsolete technique in EPR spin trapping studies.