Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Artificial neural networks for quantitative online NMR spectroscopy

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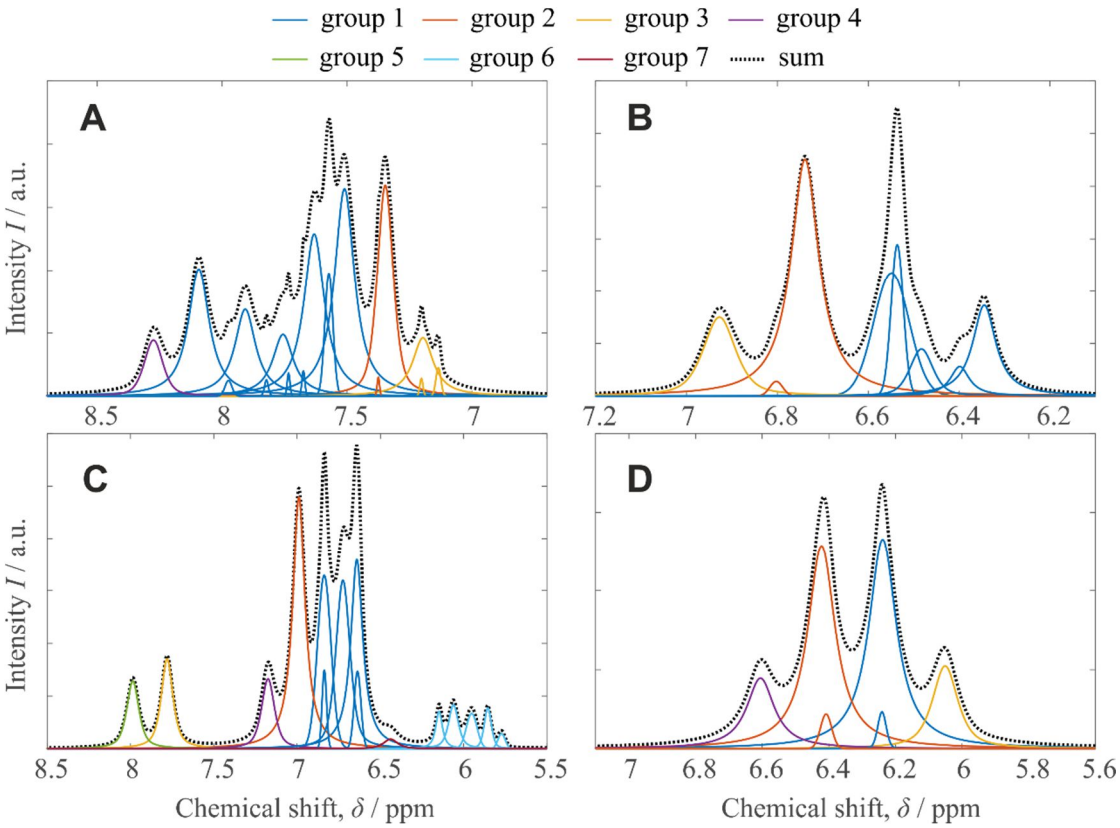

Fig. S1 Visualization of the peak groups for the pure component models which were created in PEAXACT 4 and grouped automatically using MATLAB. A: *o*-FNB; B: Li-toluidine; C: Li-MNDPA; and D: toluidine.

For further information see also Ref. [5] and [8]:

[5] Kern S, Wander L, Meyer K, Guhl S, Mukkula ARG, Holtkamp M, et al. Flexible automation with compact NMR spectroscopy for continuous production of pharmaceuticals. Anal Bioanal Chem. 2019; 411: 3037–3046.

[8] Kern S, Meyer K, Guhl S, Gräßer P, Paul A, King R, et al. Online low-field NMR spectroscopy for process control of an industrial lithiation reaction—automated data analysis. Anal Bioanal Chem. 2018; 410: 3349–3360.