

Electronic supplementary information

for

Lanthanide-induced shift reagents enable structural elucidation of natural products in inseparable complex mixtures - The case of elemenal from *Inula helenium* L. (Asteraceae)

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Fig. S1. Second order signal multiplicity of protons from the vinyl group of elemental at δ_H 5.83 (a) and 4.88-4.95 (b) in the experimental (red colored) and simulated spectra (blue colored).

WinDNMR software was used for this simulation.

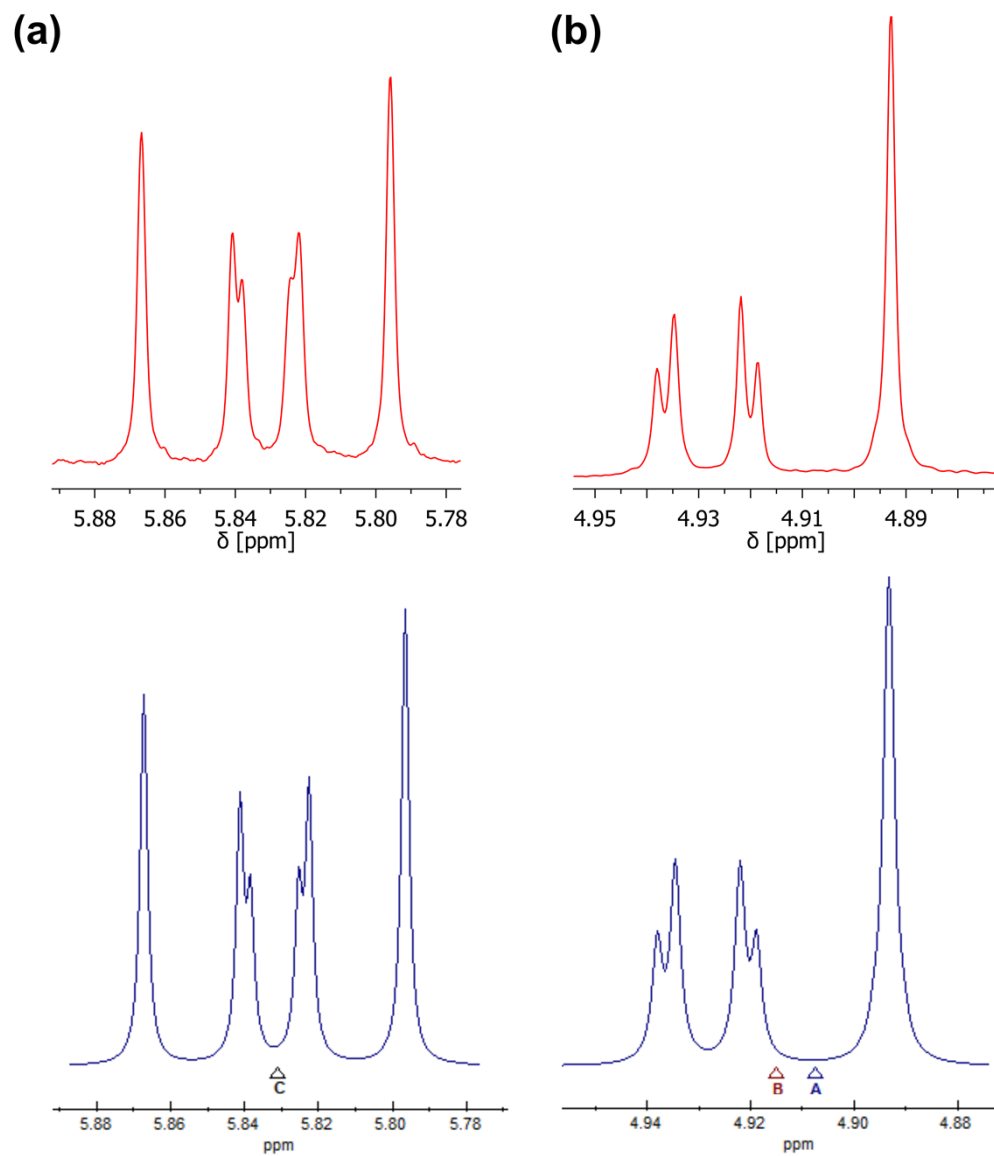


Fig S2. Fitting of the calculated (Δ_{cal}) to the observed (Δ_{Eu}) lanthanide-induced shift values for elemental-Eu(*fod*)₃ complex (H-12, H-13a and H-13b protons were excluded due to a significant share of the contact shift) for the position of europium at $r_o = 2.328 \text{ \AA}$, $\alpha_o = 120^\circ$ and $\beta_o = 180^\circ$.

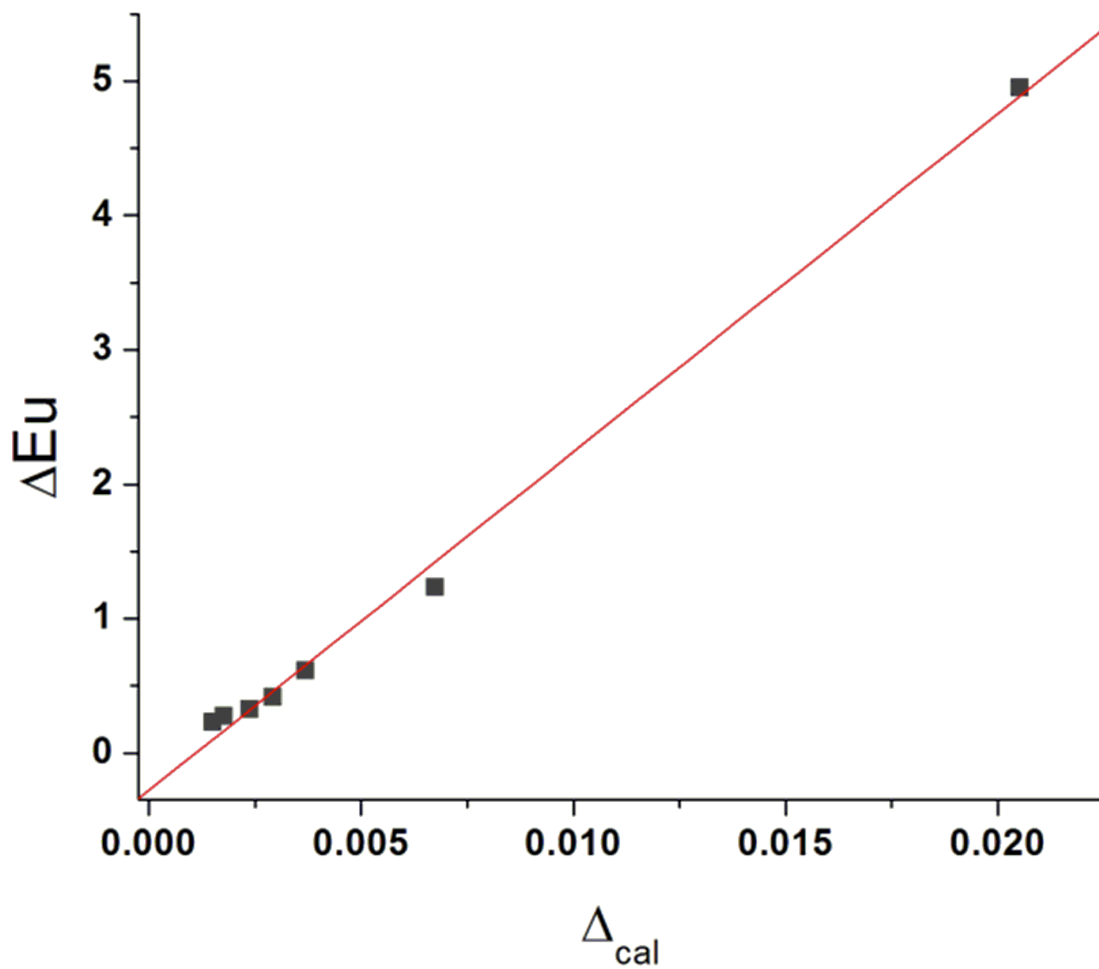


Fig. S3. The most likely conformation of elemental-Eu(fod)₃ complex (in a Cartesian coordinate system) obtained by the lanthanide probe method ($r_o = 2.328 \text{ \AA}$, $\alpha_o = 120^\circ$ and $\beta_o = 180^\circ$). The parameters required for the calculation of Δ_{cal} values according to the McConnell-Robertson equation are illustrated for proton H-13b; r_i is the distance between europium and this nucleus, and θ_i is the angle between the vector corresponding to r_i and the vector r_o representing the Eu–O bond.

