J-Coupling Constants for a Trialanine Peptide as a function of Dihedral Angles Calculated by

Density Functional Theory over the full Ramachandran Space.

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Supplementary Figures

Coupling involving ^{17}O

Numbering Scheme in figure S1

Figures S2-4 display the results of the calculations as functions of the dihedral angles   and   in

the format of Ramachandran plots. In each of these figures, the angle   is plotted vertically and

, horizontally, conforming to normal usage . The contours for the J's in Hz are labeled in the

legends.

[‡] University of Girona.
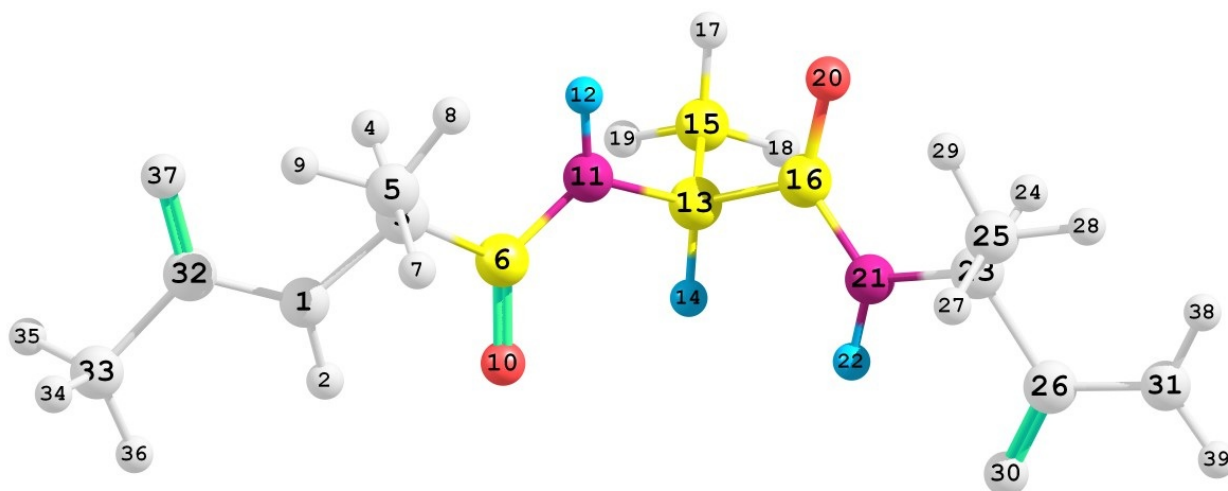[‡‡] City University of New York, visiting professor University of Girona, 2006..

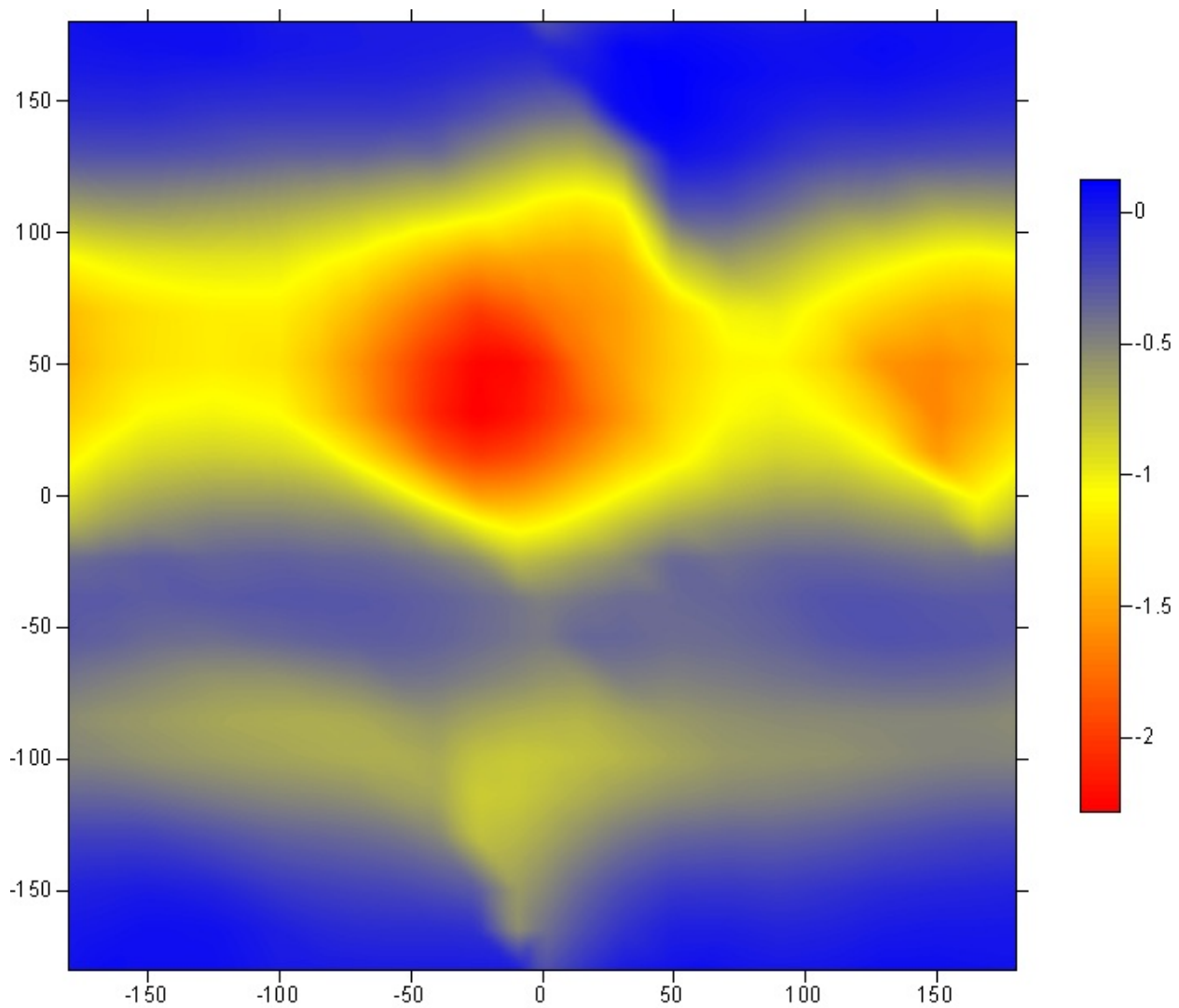Figure S1. Numbering scheme used for acetyl(ALA)$_3$NH$_2$. Colored atoms are those activated for the calculation of J's.
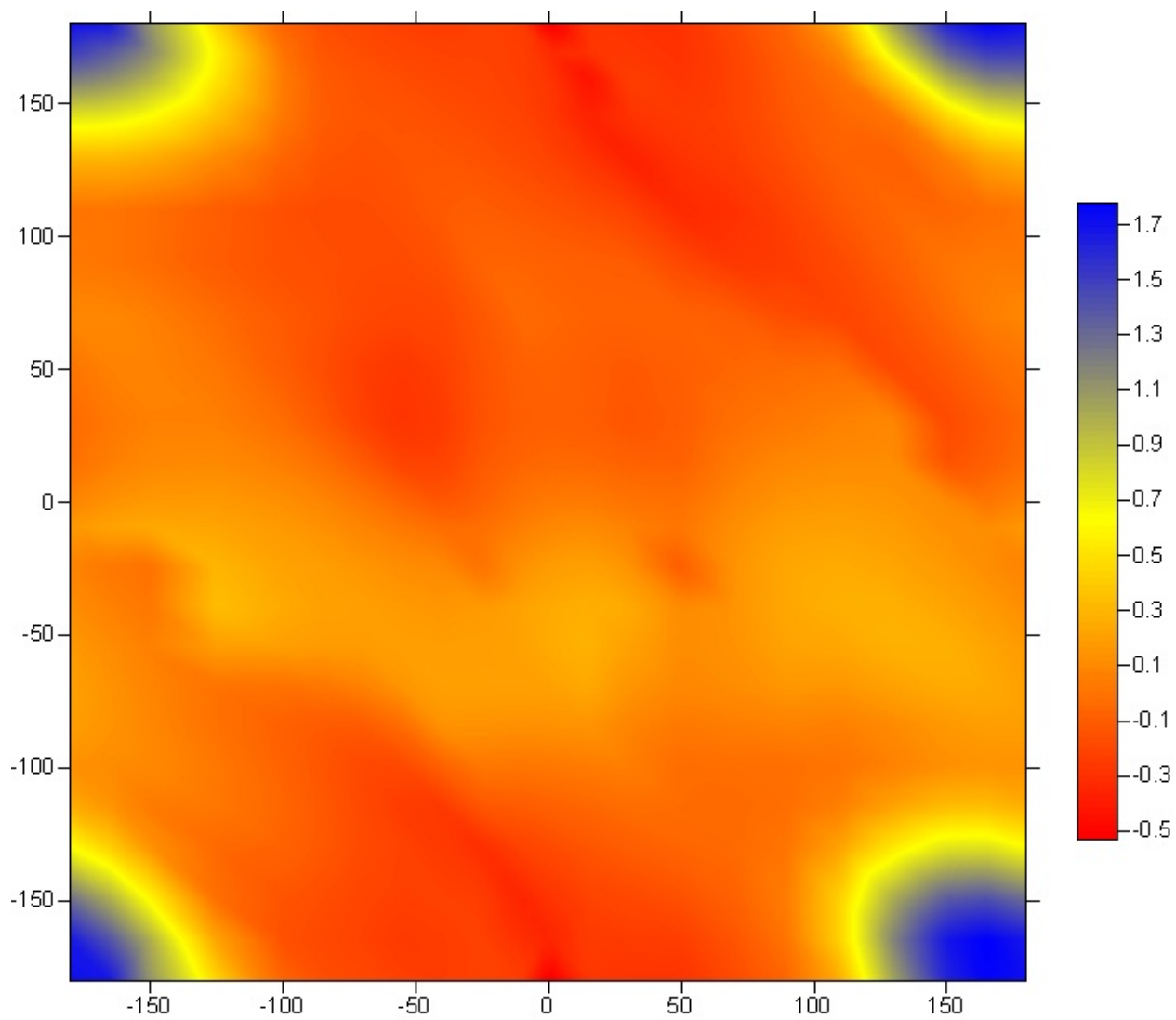
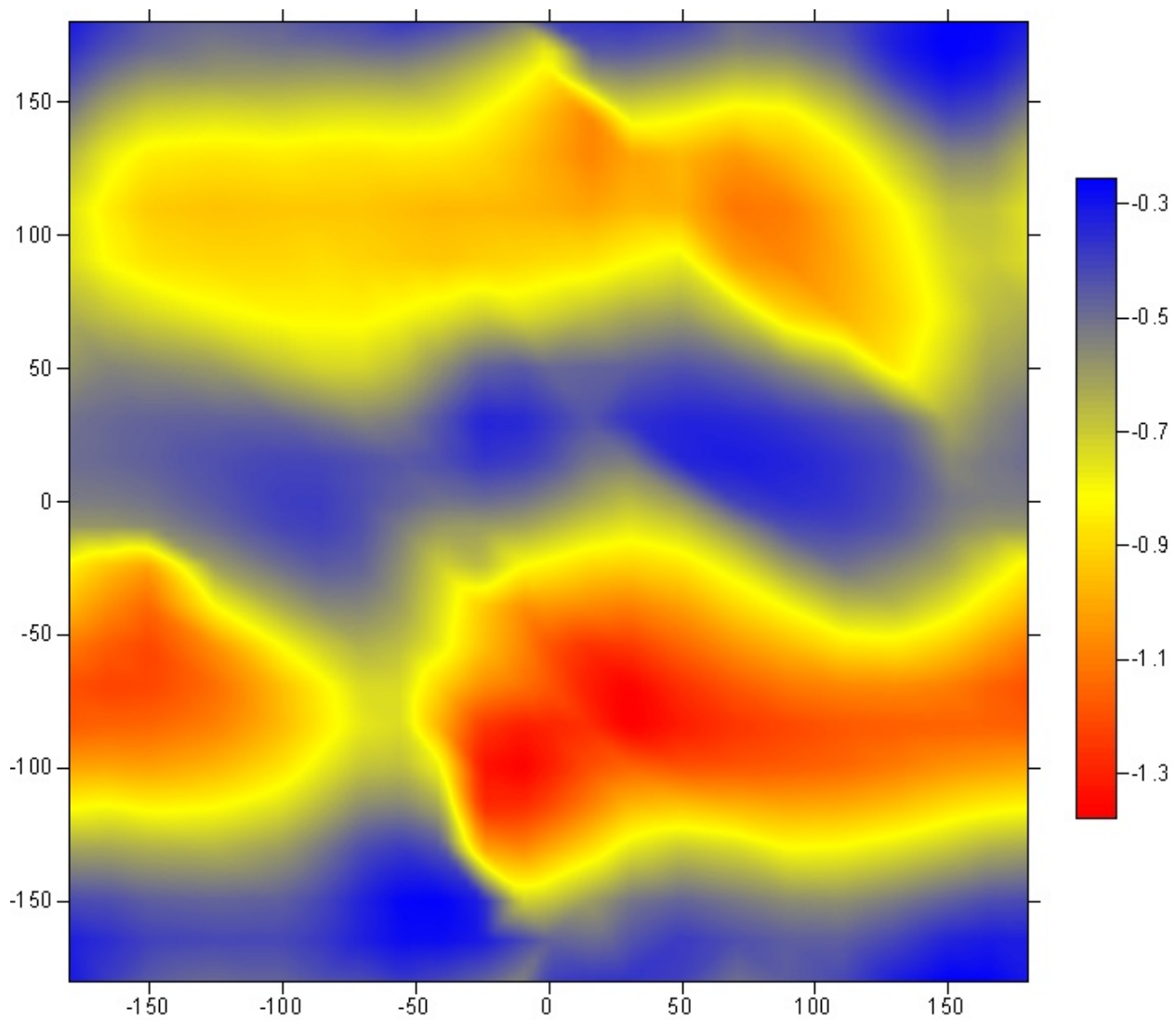Figure S2. ^3J (C$_{15}$-O$_{20}$)

Figure S3. $^3J(N_{11}\text{-}O_{20})$

Figure S4. $^3J\,(H_{14}\text{-}O_{20})$