Supplementary material:

NMR-Spectroscopic Determination of Angles α and ζ in RNA from CH-Dipolar Coupling, P-CSA Cross-Correlated Relaxation

Christian Richter, Bernd Reif, Christian Griesinger, and Harald Schwalbe

Table S1: Derived torsion angle ζ in degrees as a function of the assumed values of the components of the ^{31}P-CSA tensors in ppm for the nucleotide U4. Under a, the literature values for the CSA tensors are given.

σ_{11}	σ_{22}	σ_{33}	ζ
a. -76.0	-16.0	103.0	100°
b. -68.4	-14.4	113.3	98°
c. -68.4	-14.4	92.7	97°
d. -68.4	-17.6	113.3	96°
e. -68.4	-17.6	92.7	95°
f. -83.6	-14.4	113.3	101°
g. -83.6	-14.4	92.7	104°
h. -83.6	-17.6	113.3	101°
i. -83.6	-17.6	92.7	103°

Figure S1: Graphical representation of the variation of the ε,ζ dependence of the cross-correlated relaxation rate $\Gamma^{DD,CSA}_{(C3'_i,H3'_i),(P_{i+1})}$ on the assumed values of the components of the ^{31}P-CSA tensors in ppm.

Figure S2: Graphical representation of the variation of the ε, ζ dependence of the cross-correlated relaxation rate $\Gamma^{DD,CSA}_{(C2'_i,H2'_i),(P_{i+1})}$ on the assumed values of the components of the ^{31}P-CSA tensors in ppm.

Figure S3: Graphical representation of the variation of the ε,ζ dependence of the cross-correlated relaxation rates assuming fast linear conformational averaging by ±10° around the preferred backbone conformation.

C3'H3'

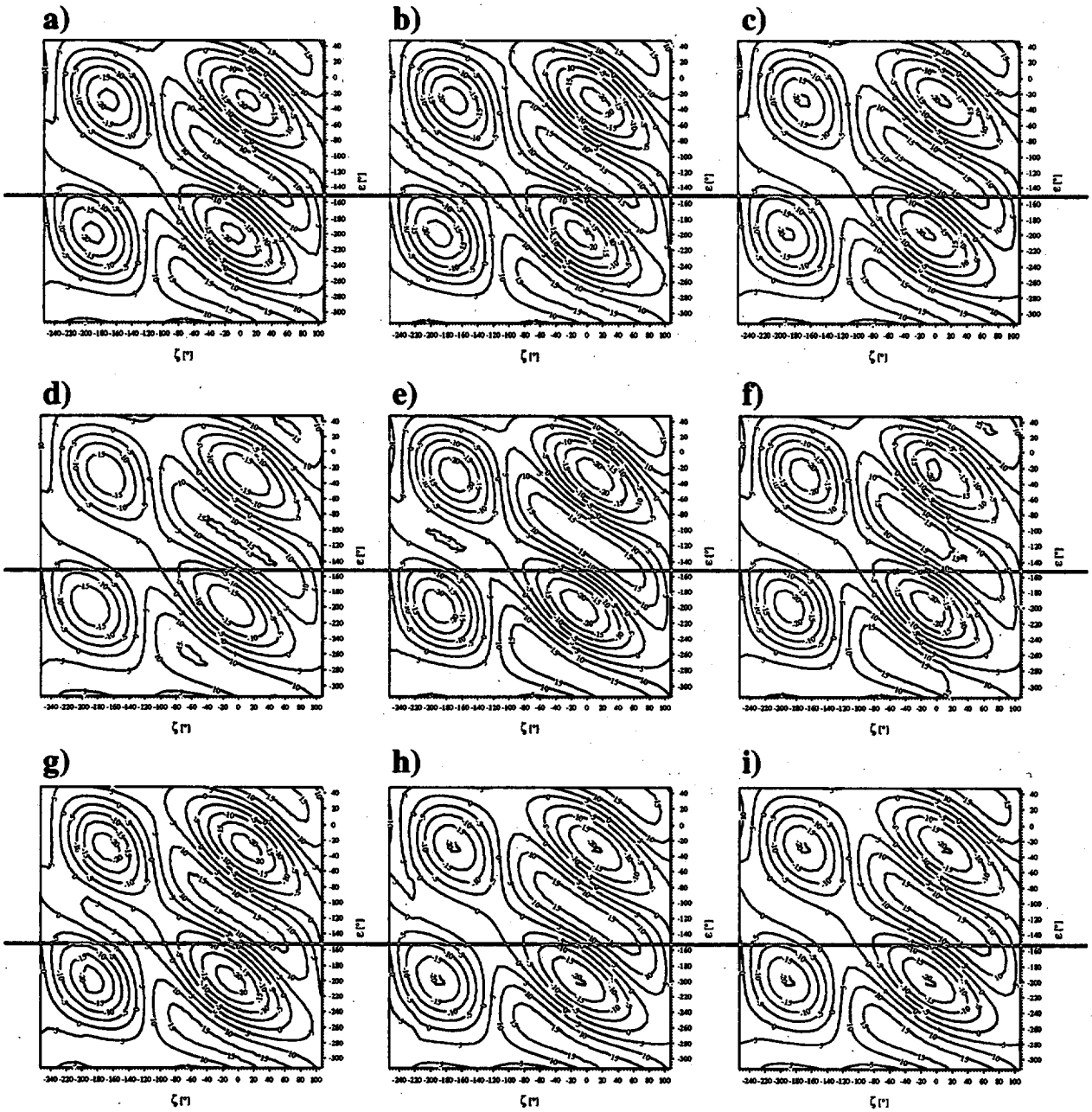

Figure S1

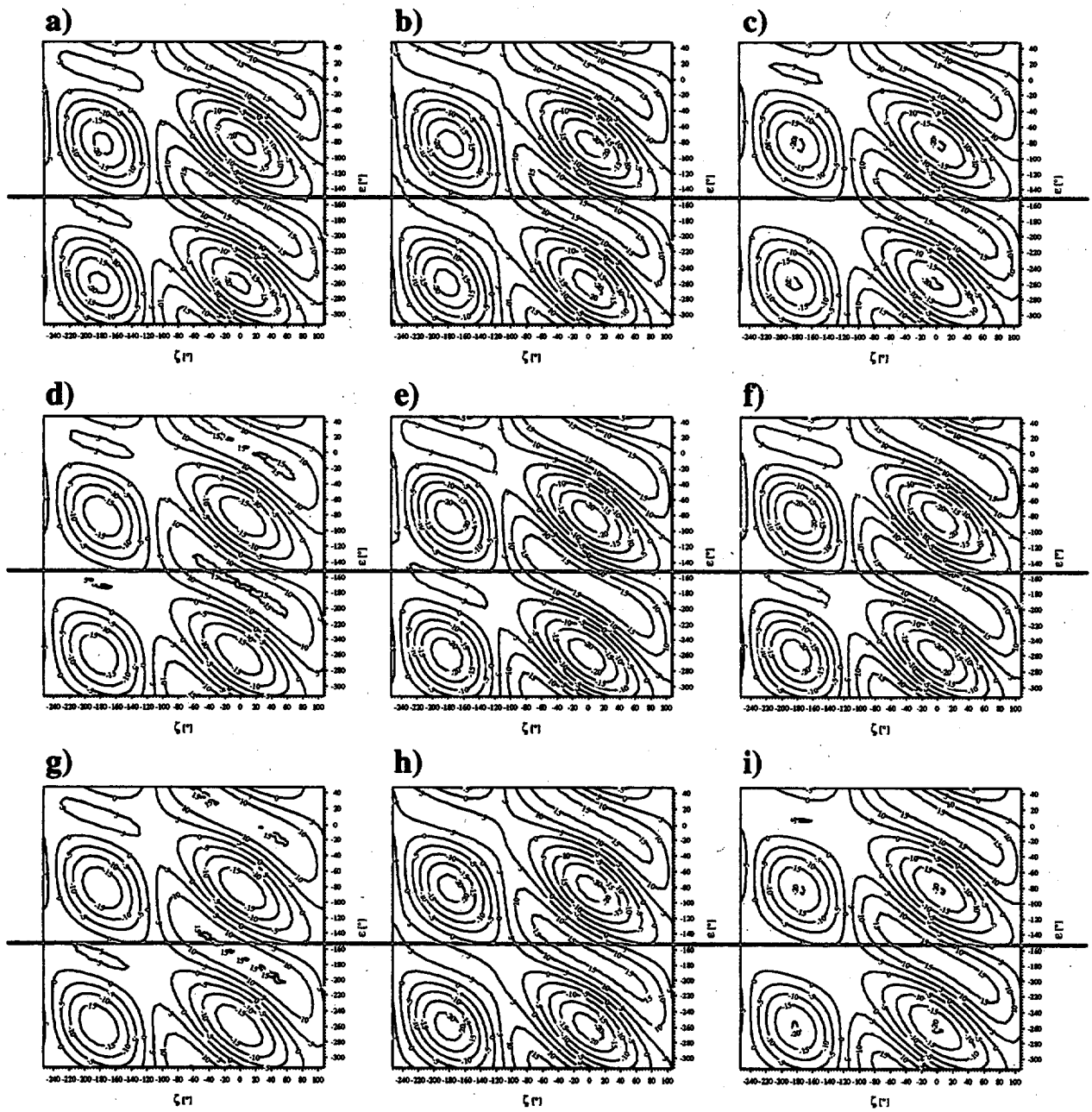

Figure S2

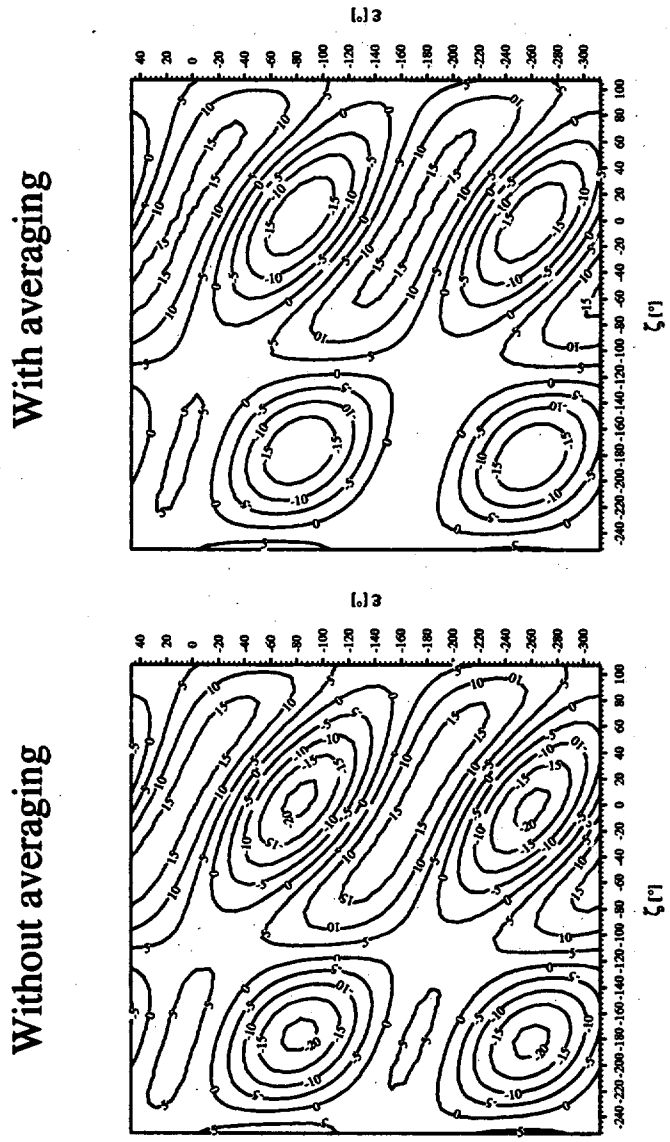

Figure S3