Figure S1. Σ angular distortion as a function of reference γ_{HS}.
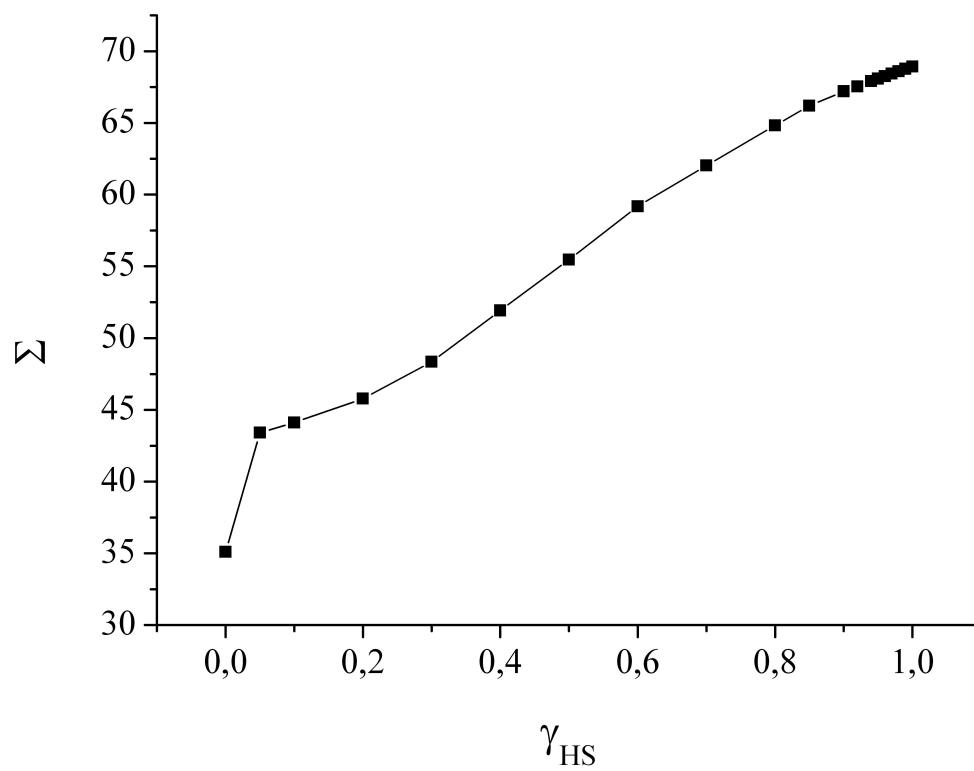
Table S1. Agreement indice R1 for the structural refinement of the simulated data.

γ_{HS}	R1 (all data)
0.99	0.0058
0.98	0.0115
0.97	0.0172
0.96	0.023
0.95	0.0287
0.95 after LS extract.	0.0009
0.94	0.0345
0.92	0.046
0.90	0.0575
0.85	0.0855
0.80	0.1128
0.80 after LS extract.	0.0002
0.70	0.1626
0.60	0.2003
0.50	0.2169
0.40	0.2039
0.30	0.1684
0.20	0.1164
0.10	0.0601
0.05	0.0295