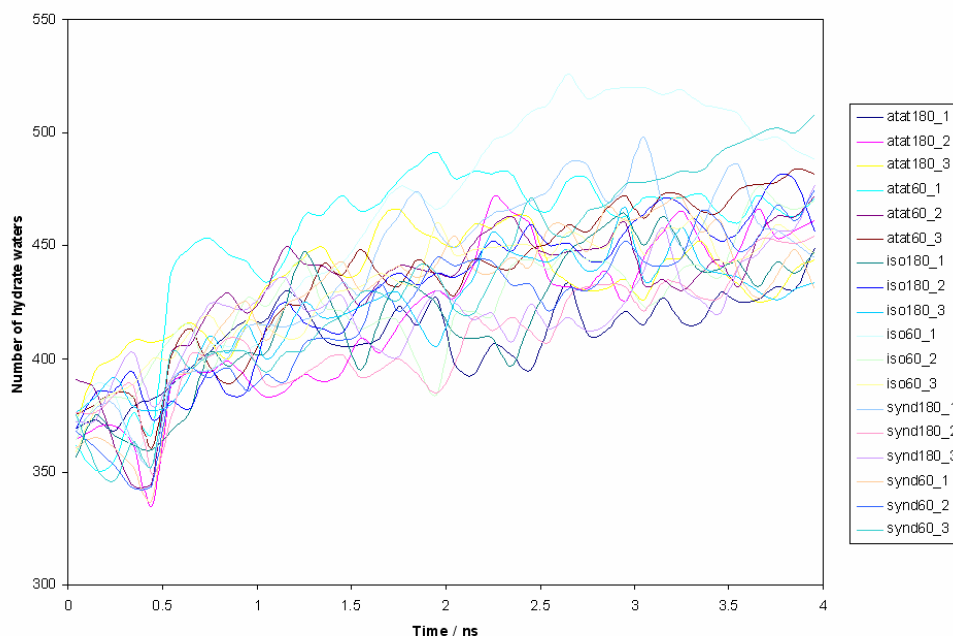


Supplementary information



Evolution of the number of hydrate waters for all inhibited systems.

Average number of hydrate waters for 2nd ns.

	atic180	atic60	isotatic180	istatic60	synd180	synd60	Uninhibited	
Insertion 1	416.5	466.7	422.2	448.2	437.5	432.1	351.8	395.1
Insertion 2	402.8	437.4	424.4	417.5	393.7	414.8	366.1	381.
Insertion 3	447.6	433.6	417.1	428.9	420.2	419.7	381.6	372
Average	422.3(23.0)	445.9(18.1)	421.2(3.7)	431.5(15.5)	417.1(22.1)	422.2(8.9)	374.7(14.9)	

Average number of hydrate waters for 3rd ns.

	atic180	atic60	isotatic180	istatic60	synd180	synd60	Uninhibited	
Insertion 1	408.7	474.8	429.7	505.5	470	450.9	377.6	379.1
Insertion 2	442.6	451.1	448.1	435.5	418.8	436.6	369.9	381.0703
Insertion 3	446.3	450.5	445	450.7	417.6	451.9	406.5	395.5
Average	432.5(20.7)	458.8(13.9)	440.9(9.9)	463.9(36.8)	435.5(29.9)	446.5(8.6)	384.9(13.5)	