NMR LIPIDS :
POPC:POPE Simulation with MacRog FF

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Simulation Conditions :

Composition	POPC:POPE 1:1
Force Field	MacRog
NaCl (M)	0
$CaCl_2$ (M)	0
Nb Lipids	128
Nb of water molecules	5120
Nb of additional cations	0
T (K)	300
t_{sim} (ns)	500
t_{anal} (ns)	300

Analysis results :

Carbon	Resname	Atom 1	Atom 2	OP mean	OP stdv	OP stem
Beta 1	POPC	C1	H1	-0.00819	0.09936	0.01242
Beta 2	POPC	C1	H2	-0.02655	0.10142	0.01268
Alpha 1	POPC	C5	H12	0.01280	0.10381	0.01298
Alpha 2	POPC	C5	H13	0.00980	0.09601	0.01200
Gamma 31	POPC	C6	H14	-0.25132	0.10020	0.01253
Gamma 32	POPC	C6	HH15	-0.10838	0.15037	0.01880
Gamma 2	POPC	C7	H16	-0.24582	0.11081	0.01385
Gamma 11	POPC	C10	H19	-0.21492	0.12737	0.01592
Gamma 12	POPC	C10	H20	0.01557	0.13587	0.01698
Beta 1	POPE	C1	H1	0.11158	0.16304	0.02038
Beta 2	POPE	C1	H2	0.03807	0.14162	0.01770
Alpha 1	POPE	C5	H12	0.12885	0.17664	0.02208

Alpha 2	POPE	C5	H13	0.02062	0.14898	0.01862
Gamma 31	POPE	C6	H14	-0.16533	0.15479	0.01935
Gamma 32	POPE	C6	HH15	-0.08152	0.17525	0.02191
Gamma 2	POPE	C7	H16	-0.10699	0.18972	0.02371
Gamma 11	POPE	C10	H19	-0.11238	0.18272	0.02284
Gamma 12	POPE	C10	H20	-0.00822	0.17325	0.02166