1 Supporting information

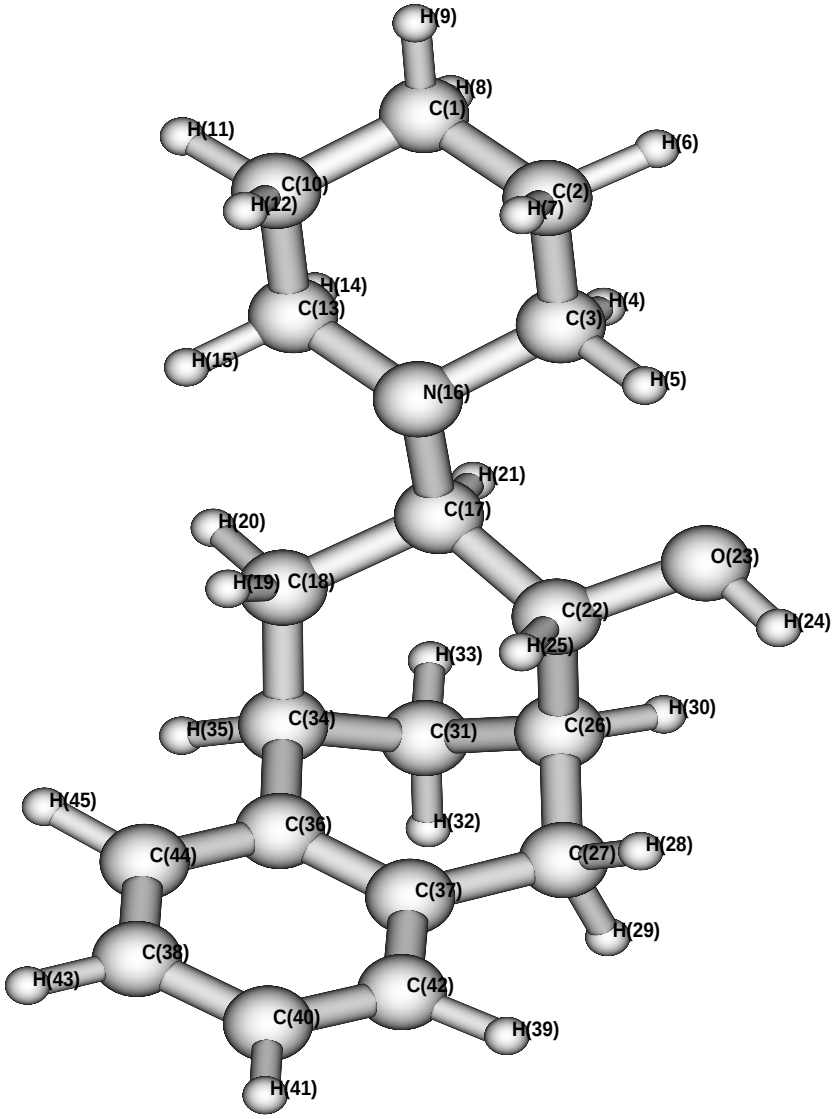

Figure 1 : Molecular structure and labeling

Table 1. RESP (from amber MD) and average D-RESP (from CPMD) charges for PMA in its different conformational states

Atom	RESP (Amber)	DRESP (Conf-1)	(conf-2)	(conf-3)
C1	-0.07865	-0.0186	-0.0162	-0.0168
C2	-0.07639	-0.0245	-0.0306	-0.0199
C3	0.16568	-0.0527	-0.0261	-0.0021
C10	-0.07686	-0.0279	-0.0274	-0.0193
C13	0.16787	-0.0286	-0.0429	-0.0017
N16	-0.72530	-0.2221	-0.1868	-0.0248
C17	0.20097	-0.0576	-0.0331	-0.0006
C18	-0.06724	-0.0381	-0.0454	-0.0168
C22	0.14810	-0.0031	-0.0040	-0.0102
O23	-0.60991	-0.2888	-0.3175	-0.3401
C26	-0.08243	-0.0026	-0.0063	0.0120
C27	-0.02274	0.0001	-0.0160	-0.0133
C31	-0.07091	-0.0217	-0.0075	-0.0398
C34	-0.01299	0.0172	0.0264	0.0152
C36	-0.06885	-0.0598	-0.0488	-0.0522
C37	-0.04496	-0.0397	-0.0378	-0.0364
C38	-0.13283	-0.0785	-0.0912	-0.0780
C40	-0.12958	-0.0867	-0.0945	-0.0905
C42	-0.13772	-0.1071	-0.0914	-0.0914
C44	-0.13011	-0.0963	-0.0888	-0.0902

Table 2. RESP and D-RESP charges for Hydrogen atoms

Atom	RESP (Amber)	DRESP (Conf-1)	(conf-2)	(conf-3)
H4	0.01240	-0.0087	0.0974	0.0004
H5	0.04506	0.0619	0.0491	0.0341
H6	0.03999	0.0710	0.0513	0.0084
H7	0.04985	-0.0138	-0.0260	0.0262
H8	0.03697	0.0294	0.0276	-0.0044
H9	0.03973	0.0230	0.0283	0.0153
H11	0.04028	0.0495	0.0670	0.0269
H12	0.05339	-0.0076	-0.0172	0.0009
H14	0.00661	0.0467	-0.0021	0.0255
H15	0.06469	0.0768	0.0618	0.0094
H19	0.04815	-0.0605	-0.0051	0.0658
H20	0.05313	0.1128	0.0249	0.0224
H21	0.04048	-0.0445	0.0068	-0.0404
H24	0.39879	0.2642	0.2213	0.2276
H25	0.03934	0.0687	0.0595	0.0081
H28	0.06740	0.1303	0.0735	0.0461
H29	0.04362	0.0446	0.0482	0.0613
H30	0.03876	-0.0432	-0.0499	0.0538
H32	0.04877	0.0357	0.0143	0.0148
H33	0.05166	0.0578	0.1051	-0.0161
H35	0.05287	0.0540	0.0545	0.0583
H39	0.12847	0.0603	0.0638	0.0663
H41	0.12822	0.0799	0.0742	0.0672
H43	0.12838	0.0699	0.0757	0.0755
H45	0.12783	0.0786	0.0808	0.0629

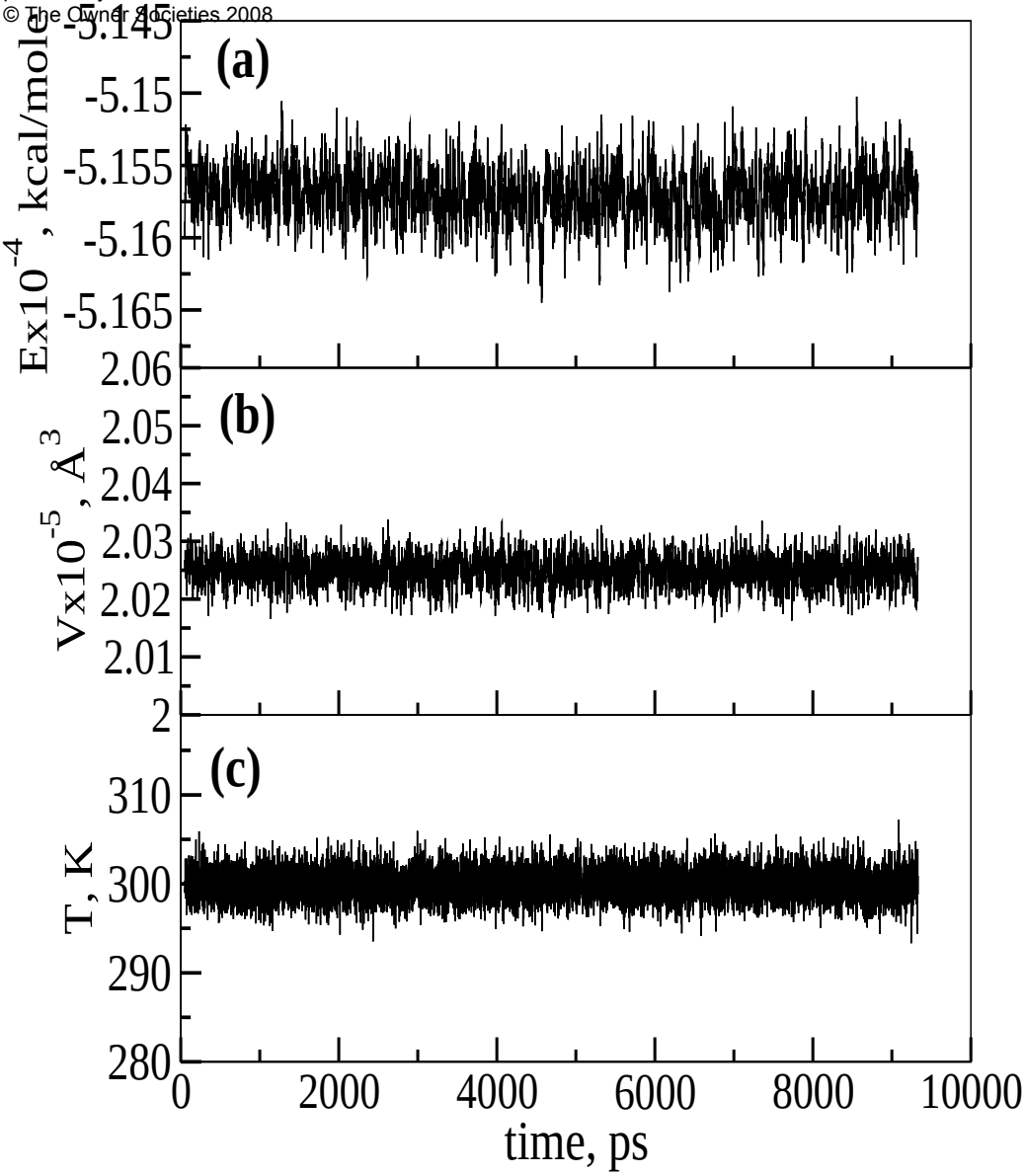

Figure 2 : Time evolution of *(a)* total energy, *(b)* volume and *(c)* temperature of the system during the molecular dynamics run.