Electronic Supplementary Material (ESI) for RSC Advances

Supporting information for "All-Atom molecular dynamics simulation of HPMA polymers" Glib Meleshko, Jiri Kulhavy, Alison Paul*, David J. Willock*, James A. Platts*

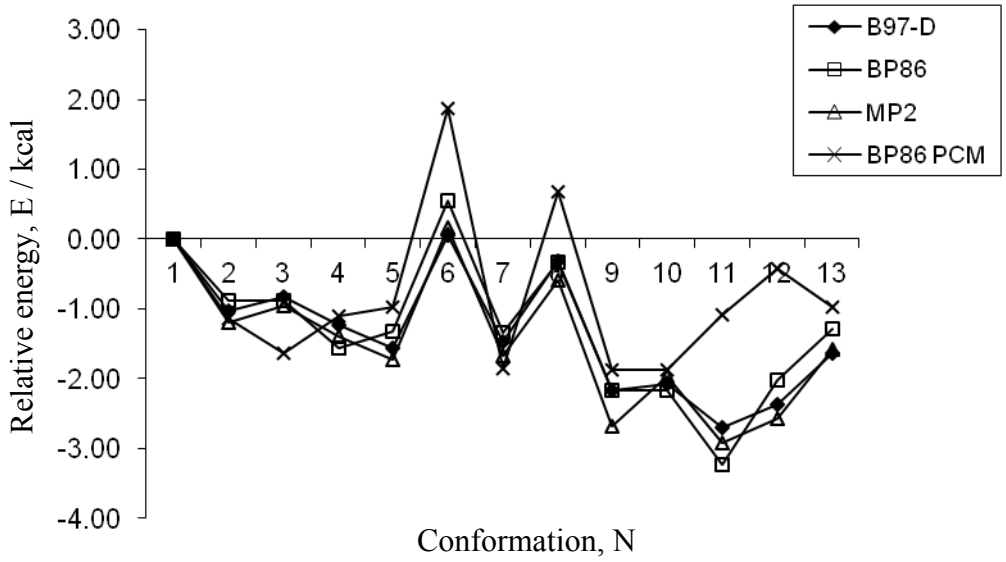
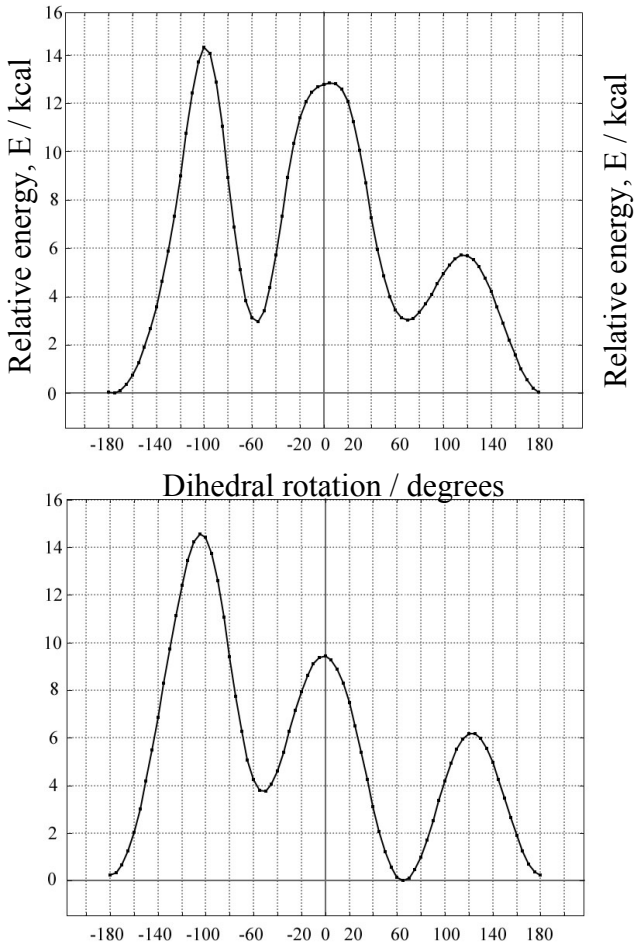


Figure S1. Results of total energies calculations for DFT and *ab-initio* methods



(a)

(b)

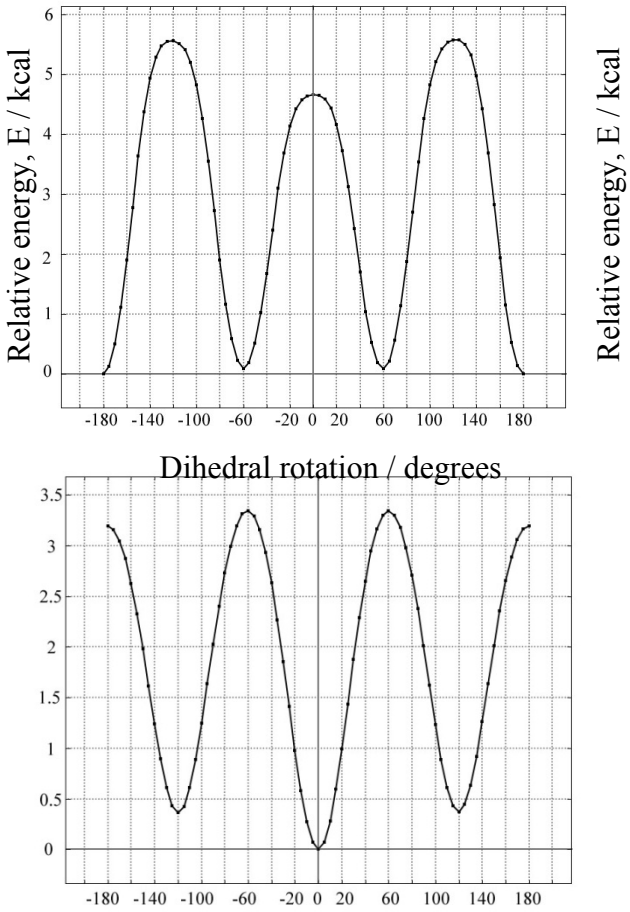


Figure S2. Dihedral energies plots of 1 C-C bond a – MMFF94, b – OPLS-aa, 2 C-C bond c – MMFF94, d – OPLS-aa

Table S1: Number of repeats used for averages in Table 1

Monomer	Average sampling
HPMA-20	6
	6
	5
HPMA-40	6
	4
	6
HPMA-60	3
	3
	4
HPMA-80	3
	5
	4
HPMA-100	3
	4
	3
HPMA-120	2
	3
	4
HPMA-140	3
	3
	3
HPMA-160	3
	3
	3
HPMA-180	2
	3
	3
HPMA-200	2
	2
	2
HPMA-220	2
	2
	2

HPMA-265	2
	2
	2