

	Energy of the complex	Energy of the binding pocket residues	Energy of the ligand	Nonbonding interaction energy
AEA binding pose 1_H7_HC				
Equilibrated <i>pose1(+1)</i> ^{a)}	-9234134.25	-8565637.49	-668429.97	-66.79
Equilibrated <i>pose3(+1)</i> ^{a)}	-10272217.71	-9603710.33	-668425.73	-81.65
Equilibrated <i>pose8(0)</i> ^{a)}	-9033473.83	-8364971.76	-668429.14	-72.93
AEA binding pose 1_H2/H3_HC				
Equilibrated <i>pose2(0)</i> ^{a),b)}	-10604884.22	-9936366.58	-668421.69	-95.95
Equilibrated <i>pose2'(0)</i> ^{a)}	-10313509.70	-9645002.27	-668430.73	-76.70
AEA binding pose 2_HC_a_H2/H3				
Equilibrated <i>pose4(+1)</i> ^{a)}	-9195744.65	-8527251.83	-668423.95	-68.87
Equilibrated <i>pose5(0)</i> ^{a)}	-10114011.17	-9445508.78	-668424.04	-78.36
Equilibrated <i>pose6(+1)</i> ^{a)}	-10044465.77	-9375972.62	-668422.09	-71.06
Equilibrated <i>pose7(+1)</i> ^{a)}	-9863215.22	-9194715.78	-668425.15	-74.29

^{a)}The value in the parenthesis shows the total charge of the system.

^{b)}The lipid tail, which was not involved in ligand interactions, was replaced by the methyl group.