

Energy kJ/mol	Model N-N	Model C-C
Coul:Dimer	-20447	-20004
LJ:Dimer	-28249	-27472
Total Dimer	-48696	-45476
Coul:Dimer-Solv	-43159	-41751
LJ:Dimer-Solv	-5244	-4999
Total Dimer-Solv	-48403	-46750

Supporting Table S1. Energy decomposition of N-terminal (N-N) and C-terminal (C-C) models for A3G oligomerization.