

Supporting Information

Calmodulin (CaM) Activates PI3K α by Targeting the “Soft” CaM-Binding Motifs in Both the nSH2 and cSH2 Domains of p85 α

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FIGURE S1. The initial structures for CaM-SH2 complexes.

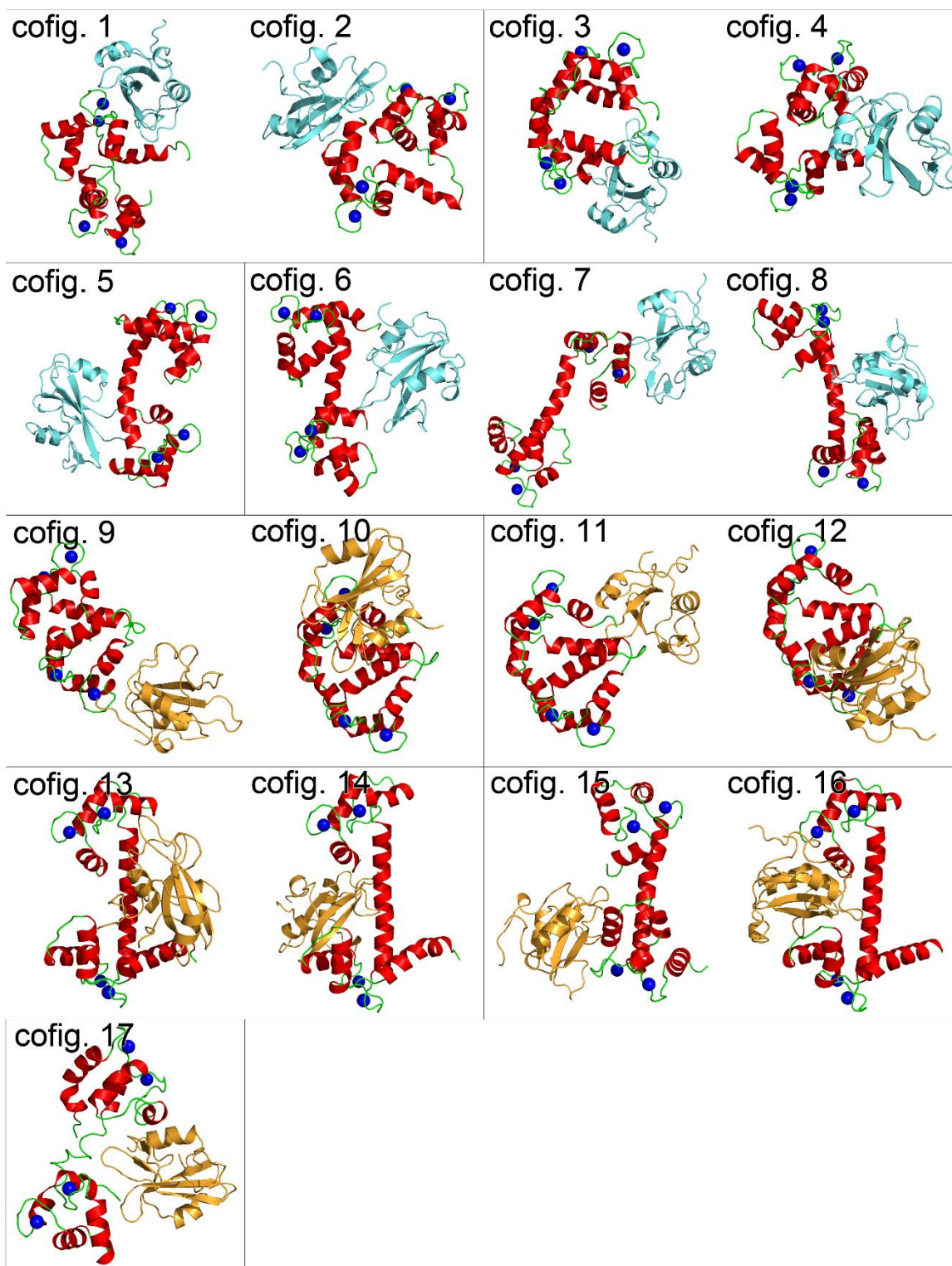


FIGURE S2. The initial structures for CaM-SH2^α complexes.

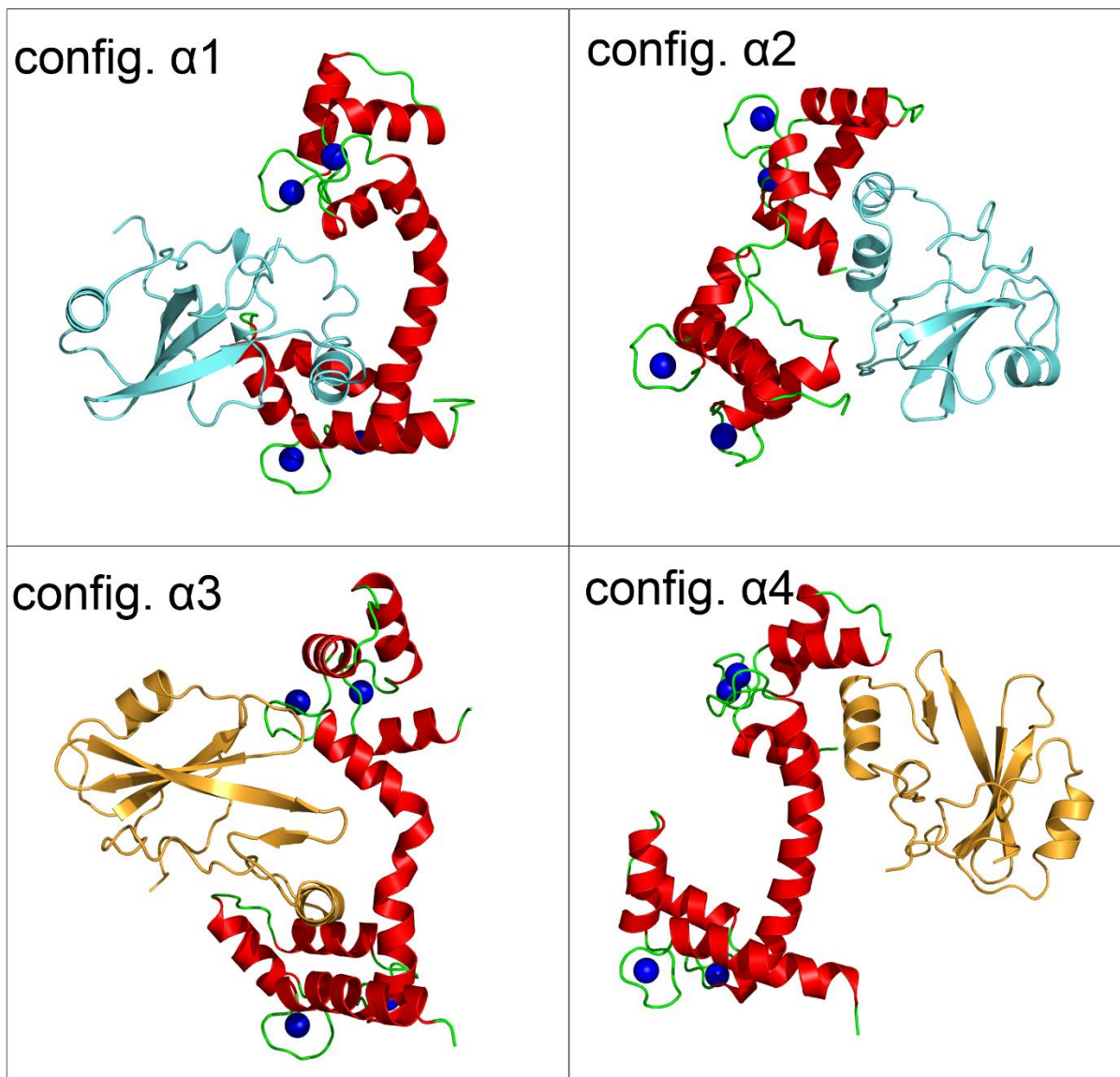


FIGURE 3. Scanning of CaM-binding motifs in (A) nSH2 and (B) cSH2 domains.

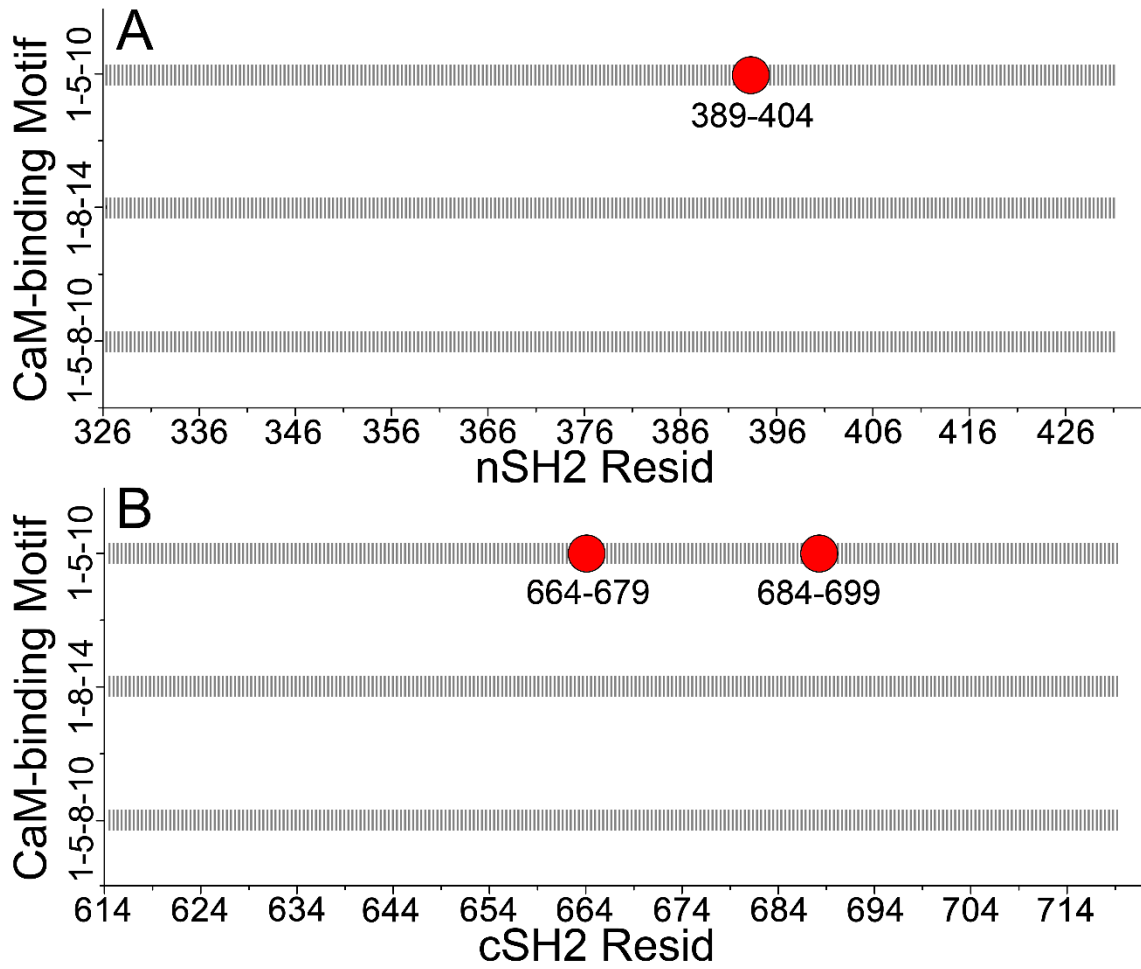


FIGURE S4. The final structures for CaM-SH2 complexes.

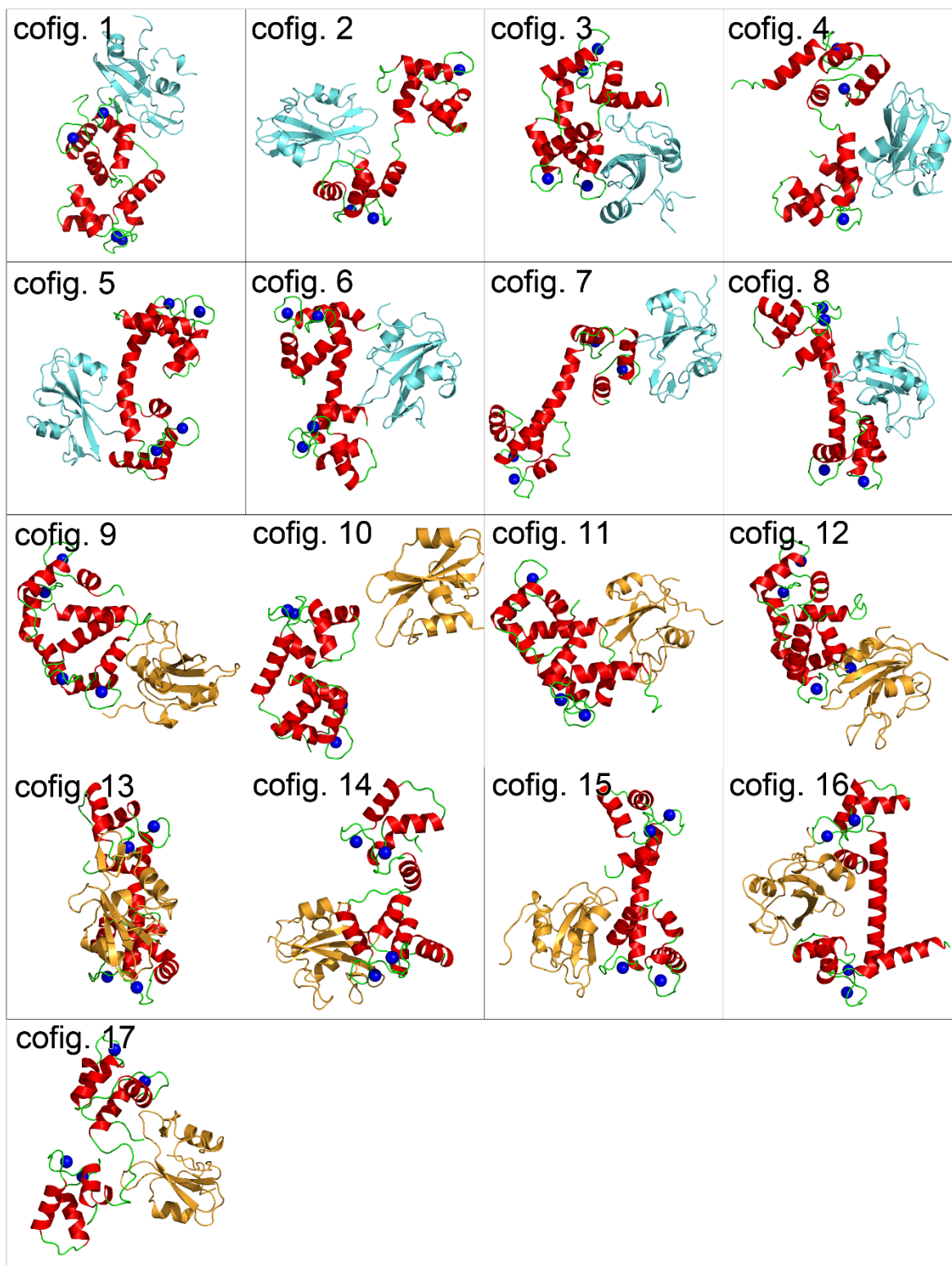


Table S1. Summary of simulation systems.

configurations	total number of atoms	number of waters	time
configuration 1	58865	18246	500ns
configuration 2	51648	15845	500ns
configuration 3	49310	15067	500ns
configuration 4	61503	19124	500ns
configuration 5	61671	19180	500ns
configuration 6	70183	22012	500ns
configuration 7	74220	23355	500ns
configuration 8	65537	20466	500ns
configuration 9	60199	18715	500ns
configuration 10	55470	17142	500ns
configuration 11	53875	16611	500ns
configuration 12	52041	16001	500ns
configuration 13	71768	22564	500ns
configuration 14	72512	22812	500ns
configuration 15	63712	19884	500ns
configuration 16	69688	21872	500ns
configuration 17	52805	16255	500ns
configuration α 1	59411	18428	500ns
configuration α 2	56627	17502	500ns
configuration α 3	54343	16767	500ns
configuration α 4	57226	17726	500ns