Bak Conformational Changes Induced by Ligand Binding: Insight into BH3 Domain Binding and Bak Homo-Oligomerization

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Supplementary Information

Dataset S1. Average conformation of Noxa•Bak.

Dataset S2. Energy-minimized average conformation of Noxa•Bak.

Dataset S3. Bound-water–containing instantaneous conformation that is closest to the average conformation of Noxa•Bak.

Dataset S4. Average conformation of Bim•Bak from cluster 1 (19,500 out of 20,000 conformations).

Dataset S5. Energy-minimized average conformation of Bim•Bak from cluster 1 (19,500 out of 20,000 conformations).

Dataset S6. Bound-water–containing instantaneous conformation that is closest to the average conformation of Bim•Bak from cluster 1 (19,500 out of 20,000 conformations).

Dataset S7. Average conformation of Bim•Bak from cluster 2 (250 out of 20,000 conformations).

Dataset S8. Average conformation of Bim•Bak from cluster 3 (250 out of 20,000 conformations).

Table S1. Cluster Analysis of the First- and Second-Round Simulations of the Noxa•Bak Complex.

Cluster	No. of Conformers	E (kcal/mol)	Location of $Y89^{bak}$ inside or outside of the groove
First Round			
1	1221	-132	inside
2	46	-137	outside
3	802	-141	outside
4	1000	-118	inside
5	400	-111	inside
6	271	-154	outside
7	260	-126	inside
Second Round			
1	5100	-132	outside
2	100	-129	outside