

## Supplementary Material

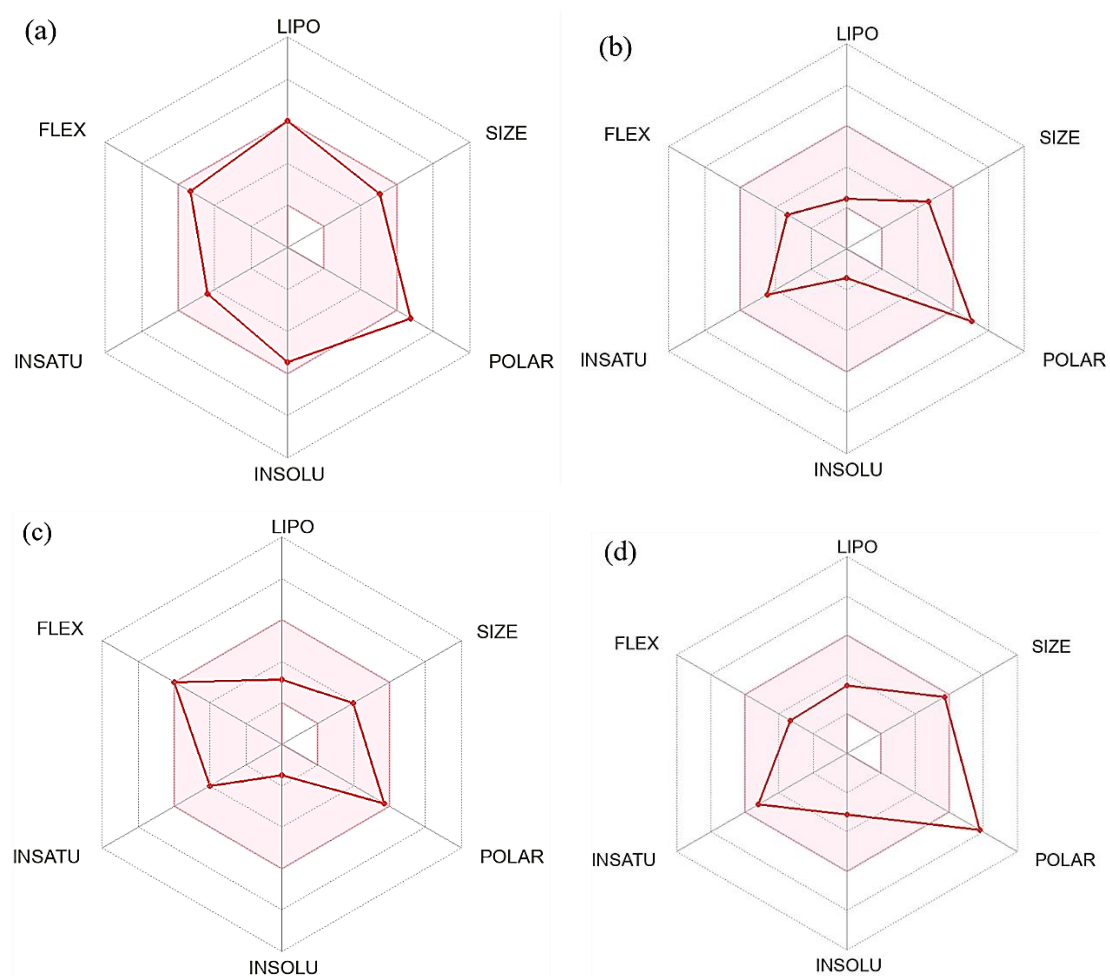


Figure S1. ADMET analyze of TCMIO5312, HMDB0012243, HMDB0014570, HMDB0037450.

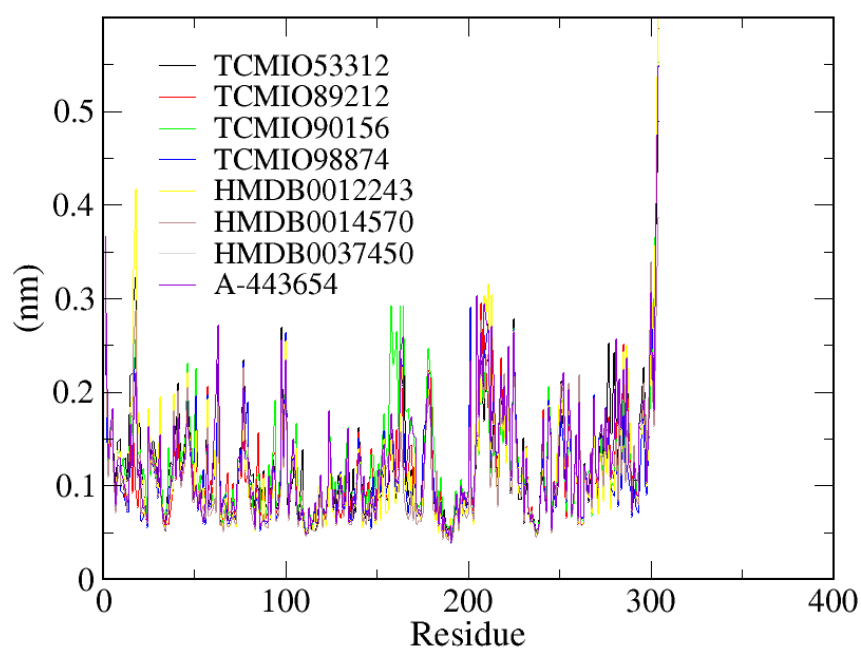


Figure S2. RMSF of AKT complexes:

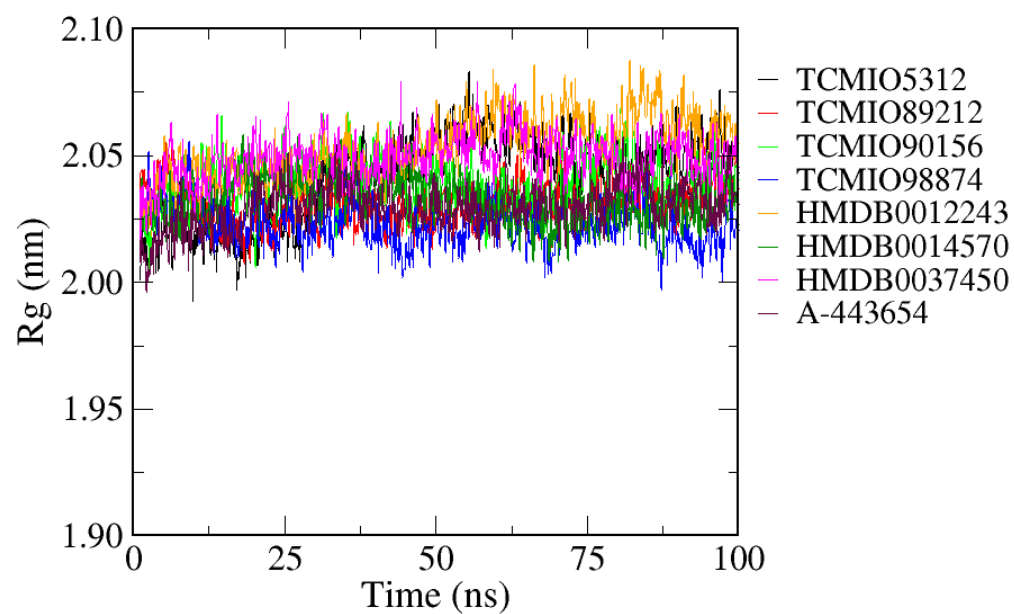
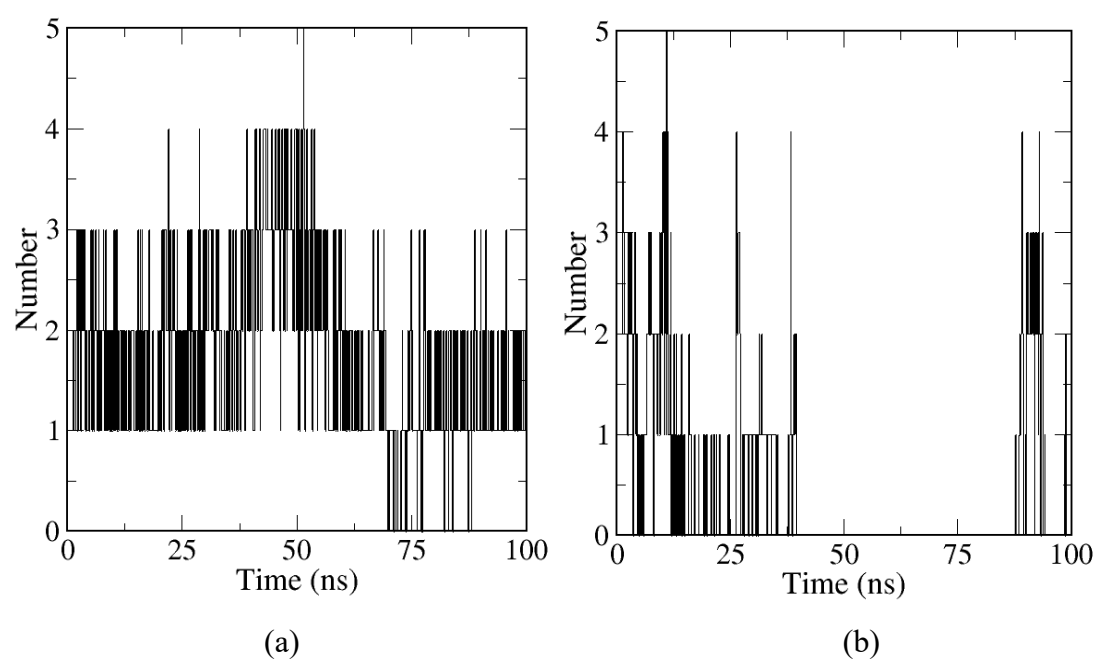


Figure S3. Rg of AKT complexes



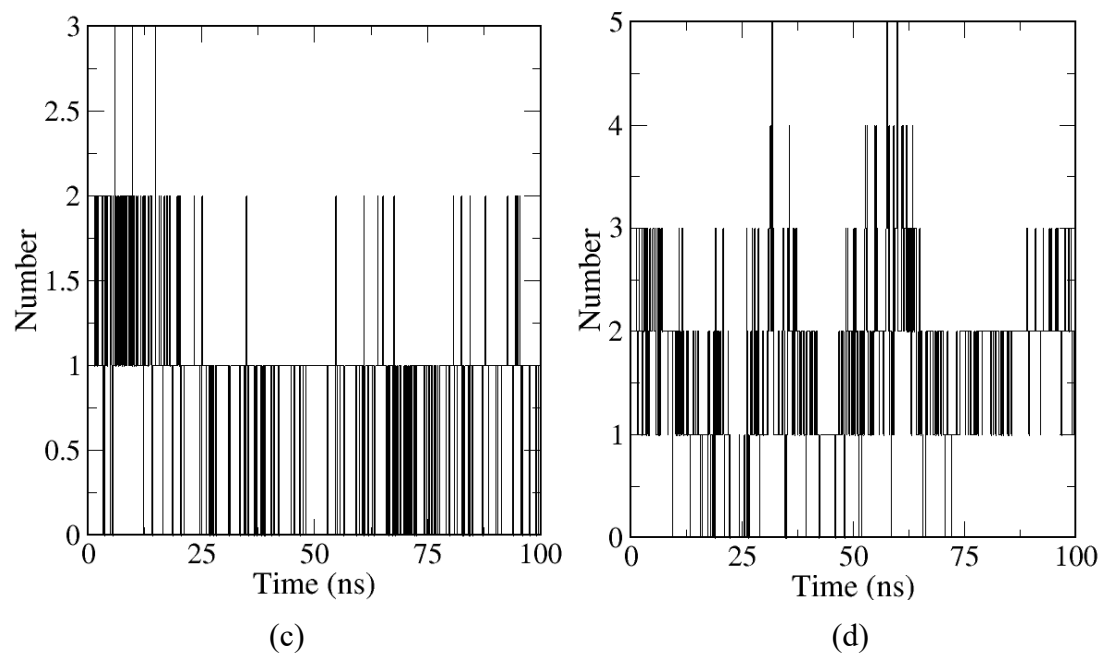
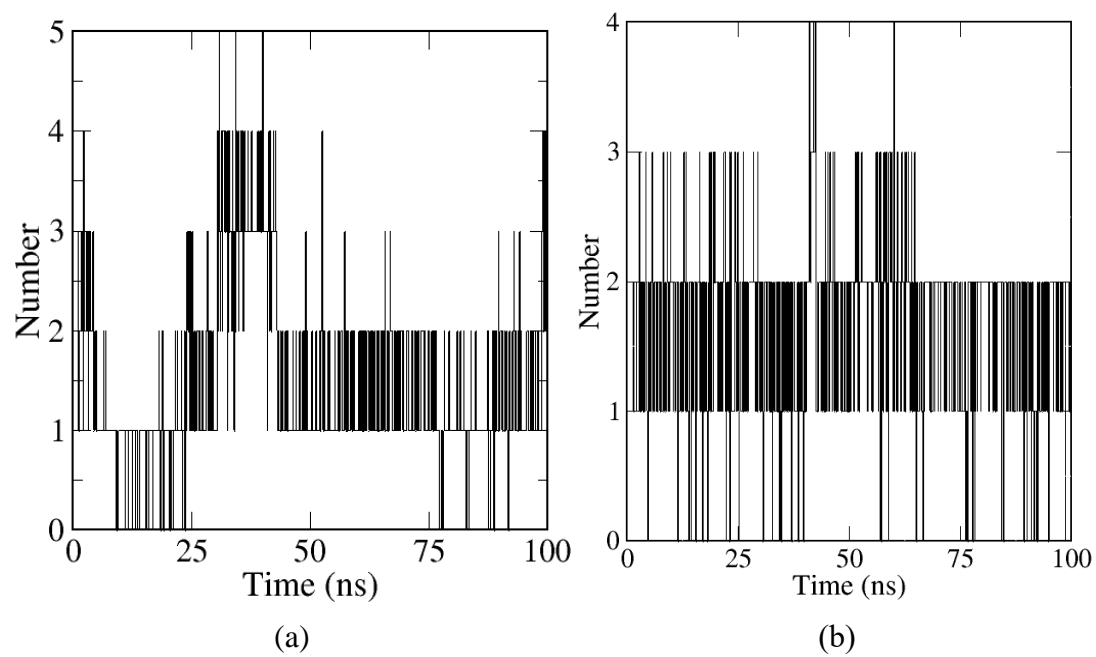
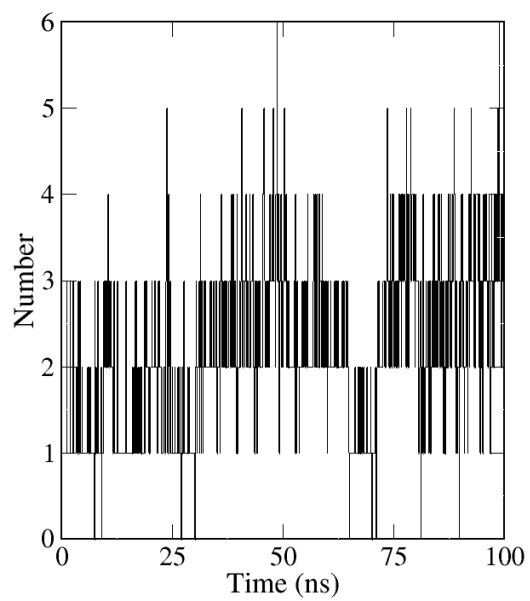
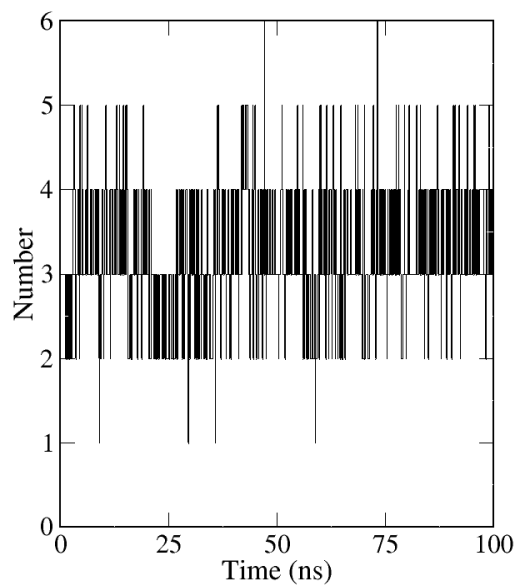


Figure S4. H-bond analyses of EGFR complexes (a) TCMIO5312, (b) HMDB0012243, (c) HMDB0037450, (d) HMDB0014570.

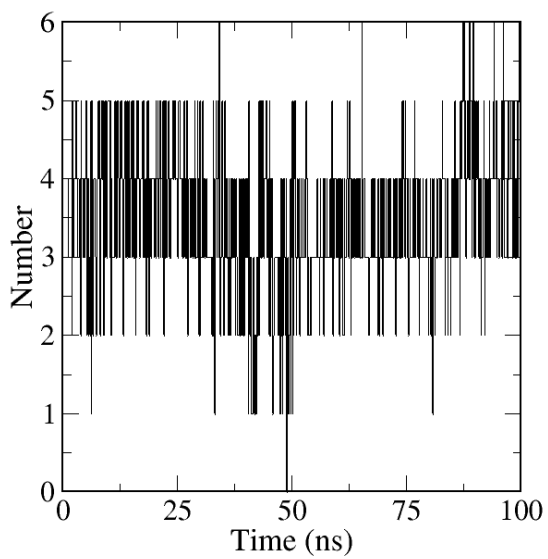




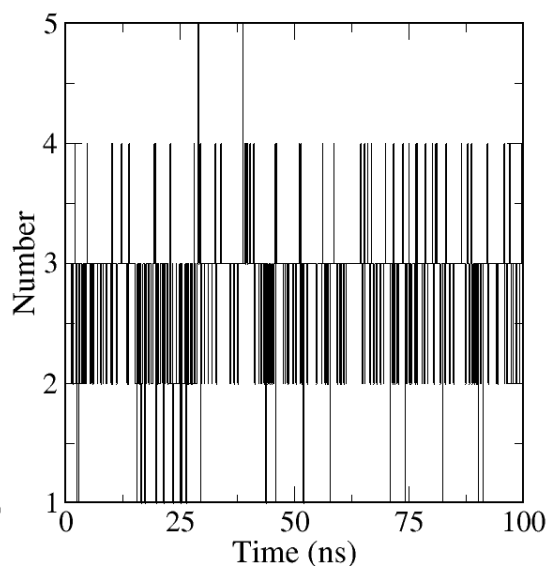
(c)



(d)



(e)



(f)

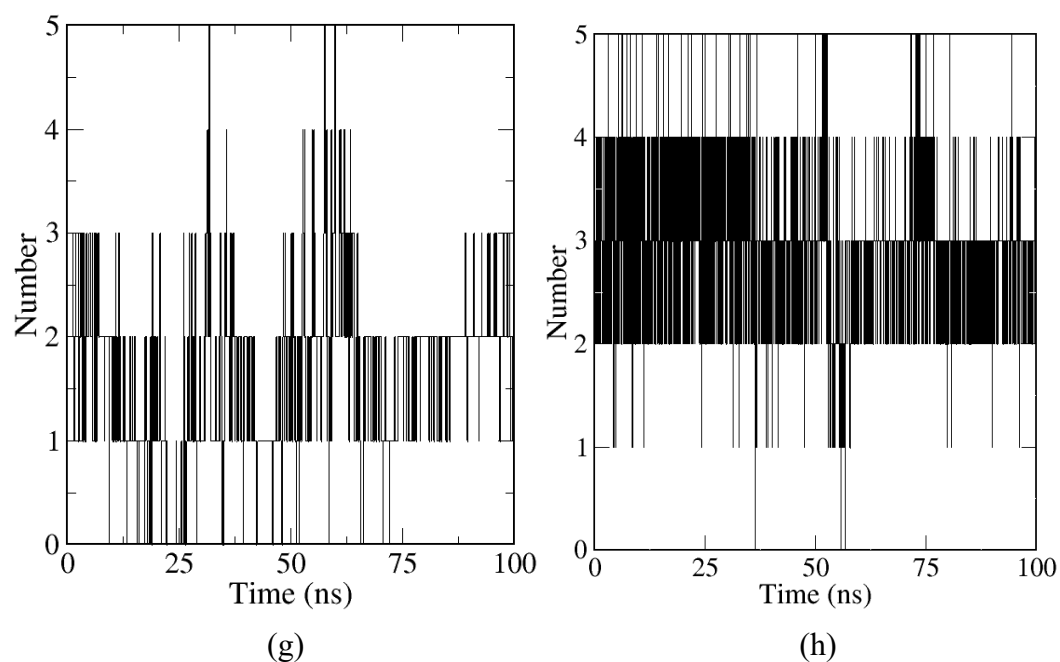
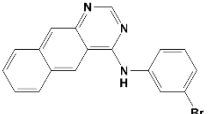
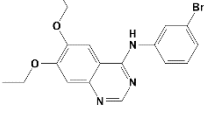
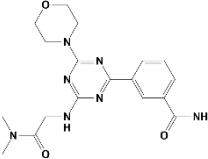
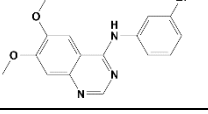
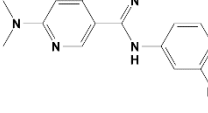
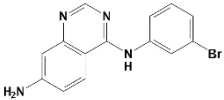
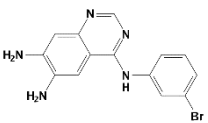
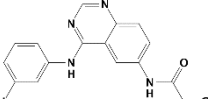
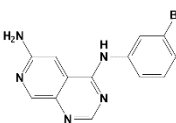
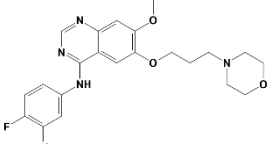
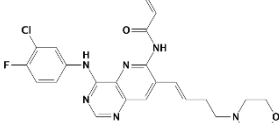
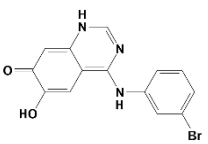
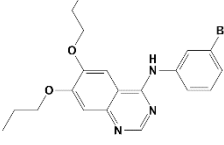
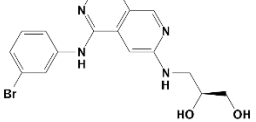
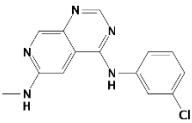
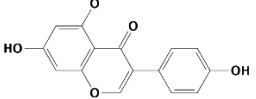
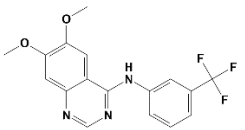
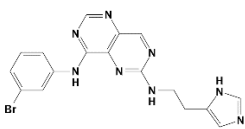
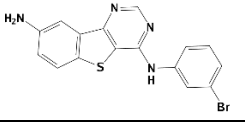
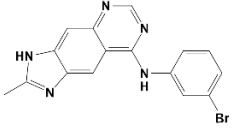


Figure S5. H-bond analyses of AKT complexes H-bond analyses of AKT complexes (a) TCMIO5312, (b) TCMIO89212, (c) TCMIO90156, (d) TCMIO98874, (e) HMDB0012243, (f) HMDB0037450, (g) HMDB0014570, (h) A-443654.

Table S1. The full list of the active ligands used

num	mol	Structure	IC50(um)
1	5328245		0.003
2	2857		0.006
3	122658923		0.007
4	4705		0.029
5	5328253		0.091

6	5328045		0.1
7	2426		0.12
8	10320940		0.12
9	5328258		0.13
10	123631		0.15
11	10528818		0.16
12	135402838		0.17
13	5328221		0.174
14	5328352		0.18
15	5328373		0.19
16	5280961		0.2

17	5328202		0.245
18	5328342		0.25
19	5328409		0.27
20	5328233		0.29