

**Table A.3.** Molecular docking results of compounds in BF binding to PI3K $\alpha$ , PI3K $\gamma$ , AKT1, and PDK1.

PI3K $\alpha$ (PDB ID: 6PYS)		PI3K $\gamma$ (PDB ID: 4ANV)		AKT1 (PDB ID: 7NH4)		PDK1 (PDB ID: 3QC4)	
No.	gscore	No.	gscore	No.	gscore	No.	gscore
YDZ122	-15.740	YDZ117	-13.680	YDZ117	-15.308	YDZ117	-13.662
YDZ121	-14.805	YDZ124	-12.051	YDZ102	-13.620	YDZ126	-12.844
YDZ126	-14.458	YDZ120	-11.979	YDZ121	-13.467	YDZ127	-12.352
YDZ117	-14.021	YDZ122	-11.238	YDZ38	-13.361	YDZ148	-11.237
YDZ120	-13.635	YDZ121	-10.669	YDZ119	-13.221	YDZ145	-10.976
YDZ119	-13.429	YDZ125	-10.43	YDZ126	-12.890	YDZ137	-10.577
YDZ127	-13.275	YDZ115	-10.259	YDZ103	-12.660	YDZ107	-10.293
YDZ125	-12.451	YDZ9	-10.133	YDZ120	-12.334	YDZ146	-10.211
YDZ114	-12.198	YDZ127	-9.967	YDZ65	-12.271	YDZ140	-10.16
YDZ118	-11.706	YDZ114	-9.692	YDZ9	-11.645	YDZ149	-9.534
YDZ115	-11.510	YDZ116	-9.583	YDZ58	-11.472	YDZ124	-8.653
YDZ124	-10.960	YDZ145	-9.529	YDZ52	-11.221	YDZ33	-8.595
YDZ149	-10.848	YDZ126	-9.479	YDZ54	-11.098	YDZ162	-8.525
YDZ9	-10.637	YDZ50	-9.470	YDZ50	-11.064	YDZ134	-8.515
YDZ46	-10.503	YDZ64	-9.341	YDZ122	-11.010	YDZ139	-8.433
YDZ116	-10.343	YDZ59	-9.304	YDZ145	-10.979	YDZ114	-8.376
YDZ150	-10.269	YDZ119	-9.279	YDZ118	-10.955	YDZ165	-8.354
YDZ72	-10.097	YDZ113	-9.231	YDZ63	-10.826	YDZ121	-8.231
YDZ11	-10.079	YDZ47	-9.113	YDZ49	-10.716	YDZ133	-8.056
YDZ107	-10.044	YDZ167	-9.109	YDZ107	-10.702	YDZ115	-8.002
YDZ87	-9.946	YDZ161	-9.073	YDZ60	-10.648	YDZ138	-7.934
YDZ103	-9.920	YDZ52	-9.061	YDZ64	-10.621	YDZ12	-7.909
YDZ37	-9.916	YDZ13	-8.953	YDZ127	-10.592	YDZ166	-7.906
YDZ141	-9.911	YDZ107	-8.948	YDZ37	-10.568	YDZ122	-7.872
YDZ35	-9.865	YDZ146	-8.884	YDZ55	-10.560	YDZ116	-7.871
YDZ34	-9.778	YDZ137	-8.882	YDZ87	-10.551	YDZ135	-7.871
YDZ33	-9.697	YDZ118	-8.876	YDZ32	-10.495	YDZ62	-7.808
YDZ63	-9.652	YDZ112	-8.849	YDZ147	-10.464	YDZ143	-7.764
YDZ32	-9.643	YDZ123	-8.816	YDZ57	-10.439	YDZ150	-7.662
YDZ113	-9.629	YDZ34	-8.780	YDZ148	-10.423	YDZ167	-7.642
YDZ36	-9.614	YDZ51	-8.725	YDZ46	-10.340	YDZ113	-7.627
YDZ146	-9.589	YDZ56	-8.703	YDZ101	-10.328	YDZ46	-7.618
YDZ10	-9.577	YDZ62	-8.686	YDZ149	-10.298	YDZ56	-7.578
YDZ12	-9.567	YDZ48	-8.684	YDZ150	-10.292	YDZ59	-7.547
YDZ65	-9.479	YDZ149	-8.608	YDZ33	-10.154	YDZ142	-7.542
YDZ145	-9.314	YDZ54	-8.546	YDZ124	-10.149	YDZ123	-7.500
YDZ144	-9.310	YDZ95	-8.512	YDZ12	-10.141	YDZ110	-7.453
YDZ51	-9.273	YDZ11	-8.492	YDZ36	-9.838	YDZ154	-7.375
YDZ148	-9.269	YDZ58	-8.487	YDZ115	-9.820	YDZ72	-7.275
YDZ64	-9.122	YDZ150	-8.434	YDZ146	-9.744	YDZ51	-7.256
YDZ86	-9.074	YDZ165	-8.378	YDZ10	-9.727	YDZ147	-7.191
YDZ143	-9.021	YDZ164	-8.374	YDZ137	-9.694	YDZ119	-7.170
YDZ13	-9.009	YDZ46	-8.290	YDZ53	-9.664	YDZ53	-7.121
YDZ49	-8.963	YDZ49	-8.290	YDZ56	-9.607	YDZ159	-7.088
YDZ54	-8.951	YDZ72	-8.253	YDZ62	-9.596	YDZ141	-7.048
YDZ112	-8.897	YDZ12	-8.167	YDZ13	-9.582	YDZ120	-7.022
YDZ56	-8.826	YDZ60	-8.164	YDZ47	-9.570	YDZ125	-7.019
YDZ57	-8.823	YDZ141	-8.133	YDZ86	-9.564	YDZ65	-6.953
YDZ142	-8.801	YDZ144	-8.084	YDZ142	-9.488	YDZ9	-6.942
YDZ123	-8.770	YDZ102	-8.075	YDZ35	-9.488	YDZ156	-6.876

YDZ38	-8.729	YDZ86	-7.978	YDZ3	-9.439	YDZ47	-6.852
YDZ55	-8.605	YDZ148	-7.972	YDZ59	-9.424	YDZ160	-6.836
YDZ60	-8.602	YDZ142	-7.970	YDZ141	-9.410	YDZ38	-6.806
YDZ62	-8.562	YDZ10	-7.963	YDZ61	-9.370	YDZ50	-6.745
YDZ94	-8.465	YDZ136	-7.962	YDZ51	-9.352	YDZ60	-6.643
YDZ52	-8.400	YDZ57	-7.962	YDZ93	-9.345	YDZ48	-6.626
YDZ50	-8.379	YDZ63	-7.952	YDZ11	-9.322	YDZ128	-6.615
YDZ167	-8.303	YDZ133	-7.917	YDZ114	-9.288	YDZ158	-6.612
YDZ101	-8.284	YDZ98	-7.884	YDZ144	-9.255	YDZ86	-6.487
YDZ95	-8.275	YDZ160	-7.865	YDZ34	-9.201	YDZ52	-6.480
YDZ136	-8.154	YDZ33	-7.696	YDZ125	-9.063	YDZ118	-6.477
YDZ147	-8.142	YDZ37	-7.601	YDZ143	-9.035	YDZ58	-6.414
YDZ134	-8.118	YDZ65	-7.592	YDZ134	-8.984	YDZ37	-6.397
YDZ137	-8.112	YDZ32	-7.567	YDZ105	-8.939	YDZ13	-6.382
YDZ93	-7.975	YDZ147	-7.403	YDZ140	-8.875	YDZ111	-6.337
YDZ161	-7.955	YDZ55	-7.402	YDZ72	-8.681	YDZ49	-6.314
YDZ53	-7.925	YDZ143	-7.391	YDZ133	-8.541	YDZ64	-6.313
YDZ48	-7.895	YDZ135	-7.287	YDZ48	-8.517	YDZ34	-6.310
YDZ58	-7.878	YDZ35	-7.266	YDZ116	-8.411	YDZ132	-6.293
YDZ138	-7.795	YDZ87	-7.198	YDZ104	-8.322	YDZ87	-6.277
YDZ47	-7.783	YDZ53	-7.161	YDZ42	-8.230	YDZ35	-6.154
YDZ59	-7.707	YDZ105	-7.143	YDZ98	-8.169	YDZ106	-6.106
YDZ133	-7.626	YDZ103	-7.140	YDZ94	-8.073	YDZ54	-6.079
YDZ164	-7.554	YDZ158	-7.113	YDZ162	-8.008	YDZ57	-6.071
YDZ160	-7.417	YDZ159	-7.098	YDZ167	-7.986	YDZ36	-6.040
YDZ140	-7.357	YDZ42	-7.034	YDZ113	-7.965	YDZ161	-6.039
YDZ162	-7.323	YDZ132	-7.025	YDZ136	-7.912	YDZ129	-6.011
YDZ92	-7.320	YDZ156	-6.923	YDZ2	-7.861		
YDZ139	-7.281	YDZ163	-6.922	YDZ139	-7.839		
YDZ17	-7.253	YDZ39	-6.853	YDZ8	-7.811		
YDZ44	-7.225	YDZ38	-6.786	YDZ96	-7.737		
YDZ27	-7.213	YDZ44	-6.688	YDZ123	-7.727		
YDZ132	-7.211	YDZ36	-6.681	YDZ97	-7.496		
YDZ26	-7.108	YDZ1	-6.573	YDZ22	-7.407		
YDZ105	-7.047	YDZ162	-6.525	YDZ95	-7.389		
YDZ158	-7.013	YDZ3	-6.461	YDZ71	-7.275		
YDZ83	-6.968	YDZ80	-6.445	YDZ41	-7.198		
YDZ163	-6.965	YDZ140	-6.382	YDZ112	-7.159		
YDZ96	-6.941	YDZ96	-6.208	YDZ92	-7.155		
YDZ156	-6.921	YDZ154	-6.186	YDZ138	-7.141		
YDZ102	-6.807	YDZ139	-6.015	YDZ70	-7.128		
YDZ4	-6.794	YDZ2	-6.001	YDZ20	-7.037		
YDZ165	-6.745			YDZ7	-6.918		
YDZ45	-6.705			YDZ17	-6.898		
YDZ159	-6.682			YDZ82	-6.887		
YDZ3	-6.682			YDZ79	-6.870		
YDZ97	-6.672			YDZ80	-6.853		
YDZ84	-6.610			YDZ135	-6.851		
YDZ21	-6.579			YDZ1	-6.830		
YDZ41	-6.562			YDZ74	-6.806		
YDZ130	-6.536			YDZ100	-6.784		
YDZ110	-6.472			YDZ81	-6.709		
YDZ166	-6.459			YDZ45	-6.698		

YDZ154	-6.456
YDZ98	-6.416
YDZ42	-6.363
YDZ5	-6.261
YDZ135	-6.259
YDZ22	-6.097
YDZ80	-6.057
YDZ66	-6.028
YDZ104	-6.020

YDZ111	-6.670
YDZ128	-6.664
YDZ66	-6.623
YDZ6	-6.597
YDZ129	-6.577
YDZ165	-6.445
YDZ84	-6.435
YDZ5	-6.340
YDZ21	-6.339
YDZ44	-6.255
YDZ164	-6.246
YDZ67	-6.230
YDZ27	-6.086
YDZ99	-6.063