

### Supplementary Data

This supplementary data is a part of paper entitled "Identification of Phosphatidylinositol 3-Kinase  $\delta$  (PI3K $\delta$ ) Inhibitor: Pharmacophore-based Virtual Screening and Molecular Dynamics Simulation".

**Table S1.** The hydrogen bonds summary

LASW1976				
Acceptor	Donor	Occupancy (%)	Distance	Angle
LIG@O4	LYS_779@HZ1: LYS_779@NZ	19.38	2.8321	154.2841
LIG@O11	TYR_813@HH: TYR_813@OH	19.00	2.8056	151.4145
LIG@O4	LYS_779@HZ2: LYS_779@NZ	18.96	2.8288	154.4780
LIG@O4	LYS_779@HZ3: LYS_779@NZ	17.17	2.8309	154.1194
ASP_787@OD1	LIG@H22: LIG@O11	12.75	2.7040	163.9481
LIG@O11	ASP_911@H: ASP_911@N	10.98	2.9121	147.4844
TYR_813@OH	LIG@H22: LIG@O11	10.77	2.8217	158.2042
ASP_787@OD2	LIG@H22: LIG@O11	9.10	2.7047	164.5774

  

Lig25/ZINC253496376				
Acceptor	Donor	Occupancy (%)	Distance (Å)	Angle
ASN_836@OD1	LIG@H10: LIG@N1	18.17	2.8508	161.7049
LIG@O2	ASN_836@HD21: ASN_836@ND2	12.58	2.8665	161.3705
ASP_897@OD1	LIG@H11: LIG@O1	6.14	2.705	157.9328
LIG@O4	LYS_779@HZ1: LYS_779@NZ	6.08	2.834	153.6269
LIG@O4	LYS_779@HZ3: LYS_779@NZ	4.59	2.8385	153.1854
LIG@O4	LYS_779@HZ2: LYS_779@NZ	4.29	2.8376	152.9561
LIG@O4	SER_754@HG: SER_754@OG	4.1	2.7551	160.871
ASP_897@OD2	LIG@H11: LIG@O1	2.55	2.6948	157.8535
ASP_753@O	LIG@H11: LIG@O1	1.21	2.7306	155.9408

  

Lig199/ZINC12638303				
Acceptor	Donor	Occupancy (%)	Distance (Å)	Angle
LIG@O3	ASP_911@H: ASP_911@N	29.37	2.8572	155.433
LIG@O	LYS_779@HZ2: LYS_779@NZ	17.73	2.8494	158.0609
LIG@O	LYS_779@HZ3: LYS_779@NZ	17.27	2.8509	158.3119
LIG@O	LYS_779@HZ1: LYS_779@NZ	17.03	2.8488	158.1917
LIG@O3	PHE_912@H: PHE_912@N	8.48	2.9122	161.5461
LIG@O3	TYR_813@HH: TYR_813@OH	0.56	2.8	157.2852

  

Lig449/ZINC85878047				
Acceptor	Donor	Occupancy (%)	Distance (Å)	Angle
LIG@N	SER_754@HG: SER_754@OG	12.56	2.8348	161.0314
LIG@O2	ASP_911@H: ASP_911@N	3.98	2.8956	149.7736
LIG@O5	ASN_836@HD21: ASN_836@ND2	3.61	2.8949	155.151
LIG@O2	TYR_813@HH: TYR_813@OH	0.94	2.7947	151.3205

## Lig554/ZINC253389510

Acceptor	Donor	Occupancy (%)	Distance (Å)	Angle
GLU_826@O	LIG@H49: LIG@O2	17.43	2.7683	149.2093
ASP_832@OD2	LIG@H49: LIG@O2	15.99	2.6771	164.9243
ASP_911@OD1	LIG@H54: LIG@O4	15.4	2.6663	163.5248
ASP_911@OD1	LIG@H73: LIG@O14	12.8	2.6889	160.5992
ASP_753@O	LIG@H75: LIG@O15	12.5	2.7488	152.2243
LIG@O2	VAL_828@H: VAL_828@N	11.6	2.9046	154.3873
ASP_911@OD2	LIG@H54: LIG@O4	8.32	2.6839	162.1231
ASP_911@OD2	LIG@H52: LIG@O3	7.74	2.7059	162.2474
ASP_911@OD1	LIG@H71: LIG@O13	7.47	2.7205	162.0516
ASP_832@OD1	LIG@H49: LIG@O2	5.3	2.6716	164.6396
LIG@O15	SER_754@HG: SER_754@OG	5.07	2.7794	162.2276
ASP_911@OD1	LIG@H52: LIG@O3	4.66	2.7094	162.4811
VAL_828@O	LIG@H49: LIG@O2	4.1	2.7805	158.1816
SER_749@O	LIG@H49: LIG@O2	4.02	2.7497	158.3409
ASP_753@O	LIG@H65: LIG@O11	3.98	2.729	158.5985
LIG@O6	LYS_779@HZ2: LYS_779@NZ	3.85	2.8663	155.1535
LIG@O11	ASP_753@H: ASP_753@N	3.84	2.9079	161.8676
LIG@O6	LYS_779@HZ3: LYS_779@NZ	3.73	2.8534	154.9095
ASP_753@OD2	LIG@H65: LIG@O11	3.05	2.7129	155.0601
ASP_753@OD2	LIG@H63: LIG@O10	2.93	2.6682	163.9365
ASP_911@OD2	LIG@H73: LIG@O14	2.8	2.7502	159.7989
LIG@O13	LYS_779@HZ1: LYS_779@NZ	2.57	2.8804	156.8394
LIG@O6	LYS_779@HZ1: LYS_779@NZ	2.46	2.8665	155.2725
ASP_897@OD1	LIG@H54: LIG@O4	1.74	2.6572	163.4485
ASP_753@OD1	LIG@H63: LIG@O10	1.58	2.6847	164.1326
ASP_753@OD1	LIG@H65: LIG@O11	1.46	2.7115	152.5103
ASP_753@O	LIG@H63: LIG@O10	1.41	2.7781	158.6556
ASP_897@OD2	LIG@H54: LIG@O4	1.11	2.6637	162.7398
LIG@O13	LYS_779@HZ3: LYS_779@NZ	1.05	2.8727	156.1291
ASP_911@OD2	LIG@H71: LIG@O13	1.03	2.6941	161.9972

## Lig682/ZINC98047241

Acceptor	Donor	Occupancy (%)	Distance (Å)	Angle
ASP_832@OD1	LIG@H1: LIG@O1	96.26	2.5762	160.8423
LIG@O	THR_751@HG1: THR_751@OG1	52.23	2.8151	160.591
ASP_832@OD2	LIG@H1: LIG@O1	2.89	2.5814	161.5876
LIG@O	THR_751@H: THR_751@N	2.22	2.9229	146.8994
LIG@O	ASN_836@HD22: ASN_836@ND2	1.35	2.8636	151.0019
LIG@F	TRP_760@HE1: TRP_760@NE1	1.35	2.8948	143.8625
LIG@O3	ASP_753@H: ASP_753@N	0.24	2.9288	157.3903