Potency and pharmacokinetics of broad spectrum and isoform specific p110γ and δ inhibitors in cancers

Supplementary tables

Ligand	G Score	Dock Score	Mol Dock Grid Score	Mol Dock Score	H-Bonds	Salt Bridges
ATP	-10.05	-8.7	-154.936	-160.147	Lys802 - O48 Ser806 - O35 Lys890 - O45	Lys802 - O42, O49 Lys890 - O42
GDC0941	-10.02	-7.51	-146.089	-14.6.305	Val882 -N42, N(H)41 Thr887- O56	--
AS252424	-8.39	-7.27	-132.326	-138.043	Lys833 - O36 Glu880 - O(H)33	Lys833 - N31
XL147	-8.53	-7.7	-134.554	-134.024	Lys833 - N30	--
TG100-115	-9.61	-9.61	-128.538	-124.486	Tyr867 - O42 Val882 - N41, N(H)44	--
CAY10505	-7.9	-7.81	-120.423	-120.607	Lys833 - O36 Tyr867 - O35	--
AS604850	-9.29	-7.82	-117.369	-117.963	Lys833 - O35 Tyr867 - O34	Lys833 - N27
Wortmannin	-3.24	-3.24	-116.247	-114.919	Ser806 - O41 Lys890 - O35	--
AS605240	-8.92	-7.45	-112.179	-112.704	Tyr867 - O33	Lys833 - N27
IPI145	-6.51	-6.49	-106.739	-108.091	Val882 - N42	--
LY294002	-8.57	-8.31	-91.1806	-91.3009	Glu-880 - O(H)37	--

Table 1: Molecular docking results of p110γ and its inhibitors. G score and dock score were obtained from Glide XP. Moldock grid score and Moldock score were obtained from Molegro virtual docker. Non covalent interactions between protein residues and ligand atoms are shown.

Ligand	G Score	Dock Score	Mol Dock Grid Score	Mol Dock Score	H-Bonds	Salt Bridges
ATP	-11.16	-9.81	-156.794	-145.19	Lys755 - O45, O47 Lys779 - O40 Val828 - N(H)36 Asp911 - O(H)37, O(H)52	Lys755 - O44 Lys779 - O44, O51
XL-147	-8.34	-8.17	-150.269	-152.429	Lys779 - O31	--
GDC0941	-9.87	-9.84	-149.007	-147.595	Val828 - N40	--
PIK294	-13.18	-13.18	-148.311	-148.288	Lys779 - O55 Glu826 - N(H)60 Val828 - N57 Asp911 - O(H)55	--
IC87114	-9.61	-9.61	-135.474	-136.461	Glu826 - N(H)48 Val828 - N45	--
CAL101	-8.87	-8.85	-134.853	-133.275	Glu826 - N(H)48 Val828 - N45	--
TG100-115	-6.67	-6.67	-122.283	-123.946	Lys779 - N40 Glu826 - O(H)41	--
Wortmannin	-5.24	-5.24	-121.948	-122.212	Asp836 - O49	--
IPI145	-7.15	-7.13	-119.024	-117.69	--	--
LY294002	-8.1	-7.5	-98.2315	-99.6422	Lys779 - O39	--

Table 2: Molecular docking results of p110δ and its inhibitors. G score and dock score were obtained from Glide XP. Moldock grid score and Moldock score were obtained from Molegro virtual docker. Non covalent interactions between protein residues and ligand atoms are shown.