Shaping the Future of Obesity Treatment: *In Silico* Multi-Modeling of IP6K1 Inhibitors for Obesity and Metabolic Dysfunction

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Figure S1. Ramachandran plot of the generated homology model for IP6K1.

Figure S2. The docked poses of (A) the most active (**21**) and (B) the least active compound (**10**).

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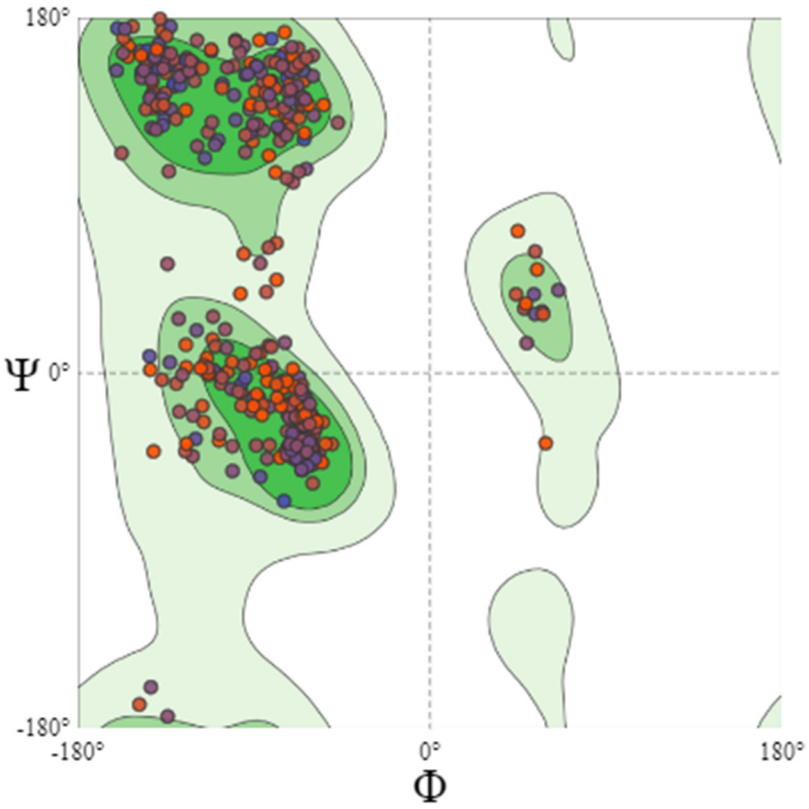
Figure S5. The Boiled-egg plot of three most potent compounds of the datasets (**15**, **20** and **21**)

Table S2. The ADMET properties of three most potent compounds of the datasets (**15**, **20** and **21**)



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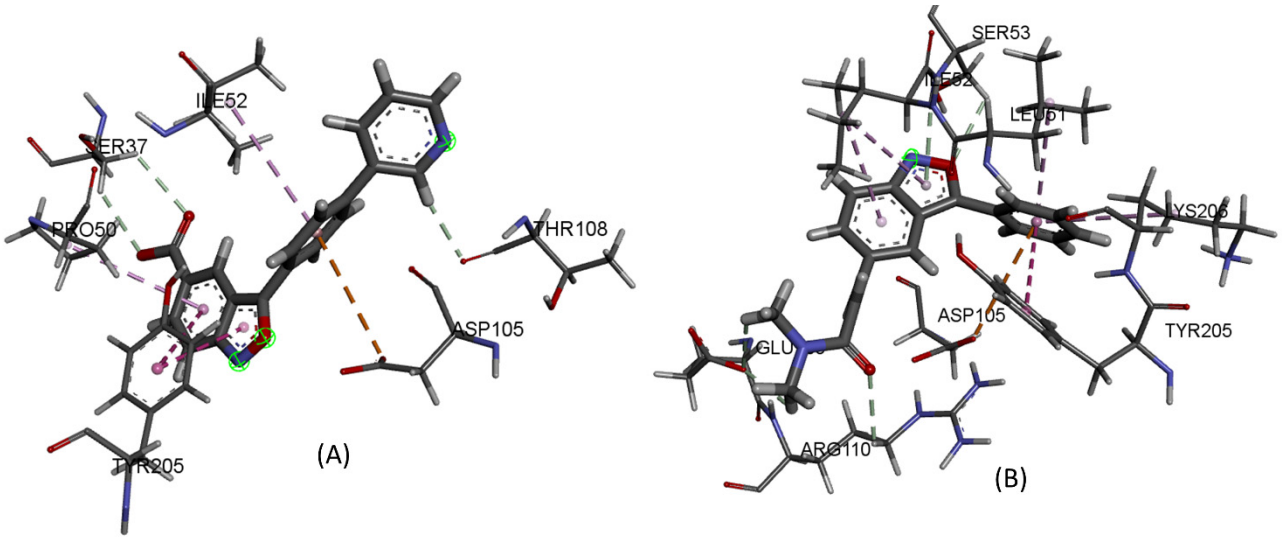

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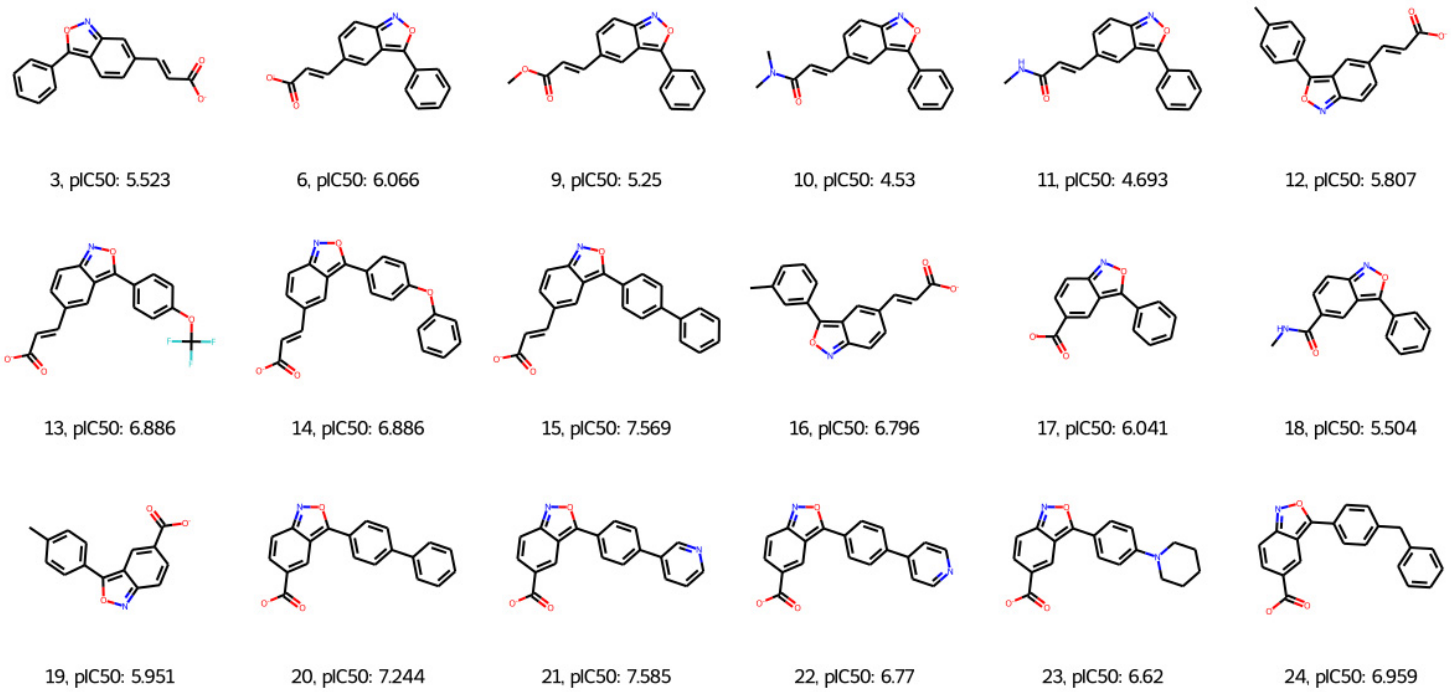


Figure S3. 2D structures of the dataset compounds (**3-24**)

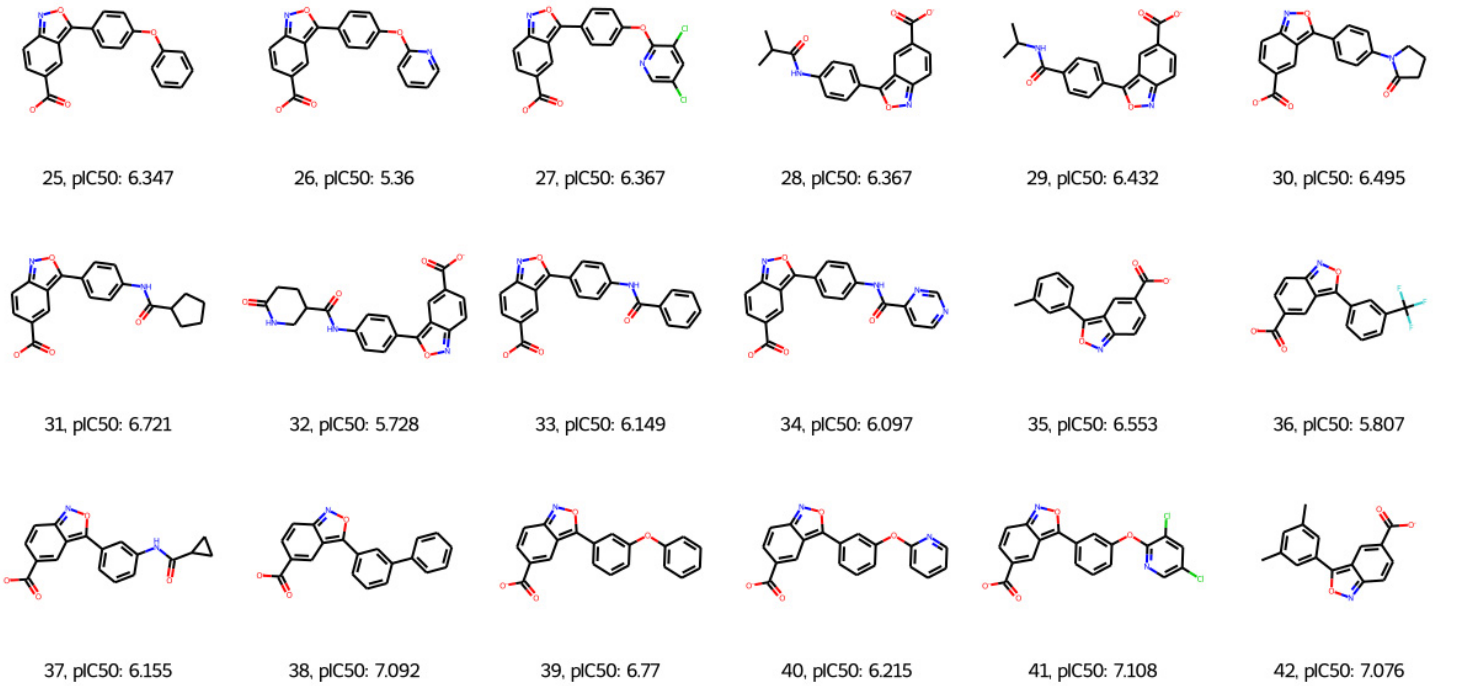
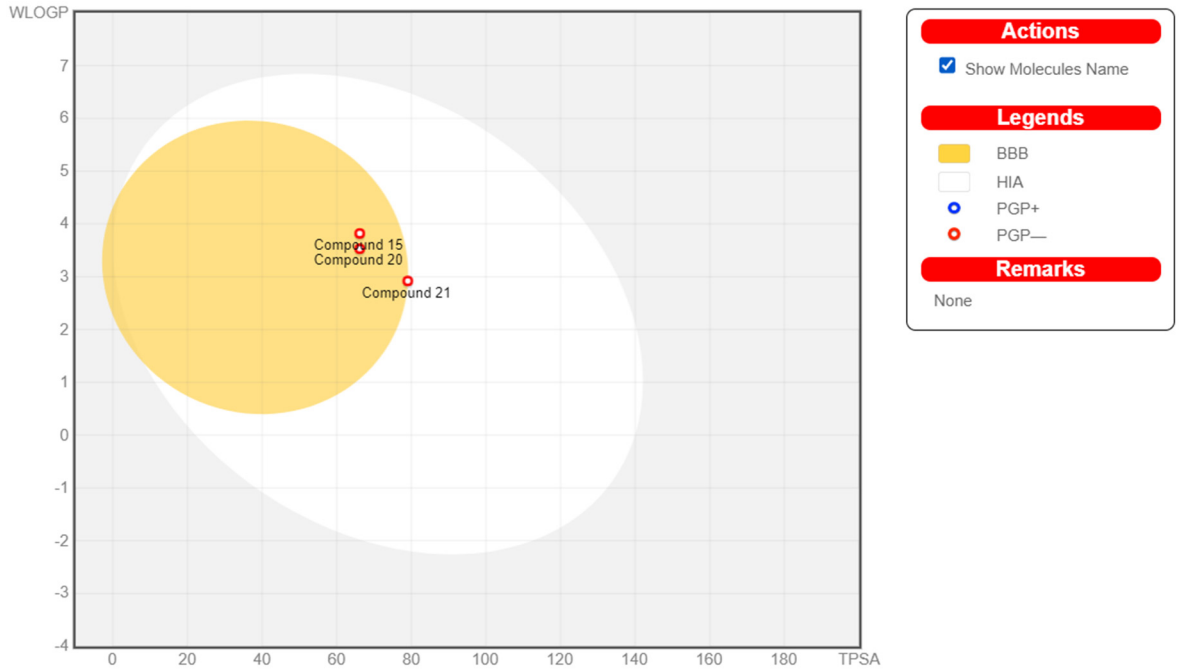


Figure S4. 2D structures of the dataset compounds (**25-42**)



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ADMET property	Compound 21	Compound 15	Compound 20
Ames mutagenesis	-	-	-
Acute Oral Toxicity (c)	III	III	III
Androgen receptor binding	+	+	+
Aromatase binding	+	+	+
Blood Brain Barrier	+	+	+
BRCP inhibitior	-	-	+
Biodegradation	-	-	-
BSEP inhibitior	+	+	+
Caco-2	-	-	-
Carcinogenicity (binary)	-	-	-
CYP1A2 inhibition	+	+	+
CYP2C19 inhibition	-	+	-

CYP2C8 inhibition	+	+	+
CYP2C9 inhibition	-	-	-
CYP2C9 substrate	-	-	-
CYP2D6 inhibition	-	-	-
CYP2D6 substrate	-	-	-
CYP3A4 inhibition	-	-	-
CYP3A4 substrate	-	-	-
CYP inhibitory promiscuity	-	+	-
Eye corrosion	-	-	-
Eye irritation	-	+	-
Estrogen receptor binding	+	+	+
Glucocorticoid receptor binding	+	+	+
Hepatotoxicity	+	+	+
Human Ether-a-go-go-Related Gene inhibition	-	+	-
Human Intestinal Absorption	+	+	+
Human oral bioavailability	+	+	+
MATE1 inhibitor	-	-	-
Mitochondrial toxicity	-	-	-
Micronuclear	+	+	+
Nephrotoxicity	-	-	+
Acute Oral Toxicity	2.382	1.712	2.283
OATP1B1 inhibitor	+	+	+
OATP1B3 inhibitor	+	+	+
OATP2B1 inhibitor	-	-	-
OCT1 inhibitor	-	-	-
OCT2 inhibitor	-	-	-
P-glycoprotein inhibitior	-	-	-
P-glycoprotein substrate	-	-	-
PPAR gamma	+	+	+
Plasma protein binding	0.895	0.961	1.001
Reproductive toxicity	+	+	+
Respiratory toxicity	+	+	+
Skin corrosion	-	-	-
Skin irritation	-	-	-
skin sensitisation	-	-	-
Subcellular localisation	Mitochondria	Plasma membrane	Mitochondria
Thyroid receptor binding	+	+	+
UGT catalysed	-	-	-
Water solubility	-3.862	-4.144	-3.864