

Supplement B. Docking results of the selected alkaloid compounds and metformin (as standard drug) against AMPK (PDB:4YEE).

Ligand	Docking Score (Kcal/Mol)	Interactions		
		H-Bond	Hydrophobic/Electrostatic/Other Pi-Cation/ Pi-anion/pi-alkyl/pi-sulfur/ pi-sigma interactions	Van Der Waals
Metformin	-4.8	Arg-82, Ser-138, Glu-139	Asp-136, Glu-139	His-109, Ser-84
Radicamine A	-6.6	Lys-102, Ser-93, Glu-89, Trp-133	Trp-99, Trp-133, Leu-146	Lys-88, Thr-101, Lys-126, Ser-144, Thr-148, Asn-150
Radicamine B	-6.4	Asn-150, Ser-93, Trp-99, Thr-101	Trp-99, Trp-133	Lys-88, Glu-89, Ser-100, Lys-102, Lys-126, Ser-144
Coptisine	-10.1	Lys-102	Trp-99, Trp-133, Leu-146, Trp-99	Glu-89, Thr-101, Lys-107, Phe-112, Lys-126, Ser-144, Thr-148, Asn-150
Vindoline	-7.6	Ile-115, Asp-117	Pro-72, Ile-103, Pro-78, Pro-104	Pro-72, Ser-74, Ile-106, Ile-115, Ala-114, Leu-116
Physostigmine	-7.3	Lys-102, Trp-99	Trp-133	Lys-88, Glu-89, Ser-100, Thr-101, Lys-126, Leu-146, Thr-148
Sanguinarine	-9.5	Lys-88	Trp-133, Trp-133	Glu-89, Trp-99, Lys-126, Thr-148, Ile-149
Harmane	-7.5	-	Trp-99, Trp-133, Lys-126	Gln-145, Leu-146, Ser-144, Thr-148
Jatrorrhizine	-8.8	Lys-88	Trp-99, Trp-133, Lys-126, Lys-107, Phe-112	Glu-89, Leu-146, Lys-102, Thr-148, Ser-144
Palmatine	-8.4	Asn-150	Trp-99, Trp-133, Lys-126	Gln-145, Leu-146, Thr-148, Ser-144
Pinoline	-6.7	-	Trp-99, Trp-133, Lys-126,	Asn-150, Leu-146, Thr-148, Ser-144
Cryptolepine	-8.4	Asn-150	Trp-99, Trp-133, -Lys-126	Gln-145, Leu-146, Ser-144, Thr-148
Galegine	-4.7	Ala-76, Asn-73, Pro-72	Pro-72, Pro-78, Alkyl-Ile-106	Asn-97, Asp-117, Gln-75, Ile-103, Ser-74, Thr-101
Groenlandicine	-9.4	Asn-150,	Trp-99, Trp-133, Lys-126	Glu-89, Leu-146, Lys-102, Lys-107, Ser-144, Thr-148
Magnoflorine	-8.8	Asn-150, Ser-144, Trp-99	Trp-133, Trp-99, Trp-133, Cys-126	Gln-124, Gln-145, Leu-146, Thr-148
Norharmane	-7.4	-	Trp-99, Trp-133, Leu-146, Lys-126	Asn-150, Ser-144, Thr-148
Vindoline	-6.8	Ser-100, Gly-87, Lys-88, Leu-105	Lys-107, Phe-112, Lys-107	Arg-77, Pro-78, Ile-106, Thr-101, Val-90, Glu-89
Berberine	-8.3	Asn-150, Lys-88, Glu-89	Trp-99, Lys-88, Lys-107	Phe-112, Trp-133, Thr-148, Ser-144, Leu-146
Catharathine	-7.9	Pro-72, Pro-104	Pro-72, -Ile103	Ile-115, Ala-114, Thr-101, Pro-72, Ser-74
Casurine 6-O- α -Glucoside	-6.4	Lys-107, Glu-89, Leu-105, Leu-105, Trp-99, Trp-133	Trp-99	Val-90, Phe-112, Lys-102, Lys-88, Ser-93, Thr-148, Leu-146, Thr-101, Ile-106, Ser-100
Epiberberine	-8.3	-	Trp-99, Trp-133, Leu-146, Lys-107	Ser-144, Asn-150, Thr-148, Lys-126, Lys-102, Glu-89, Lys-88
Capsaicin	-7.0	Lys102, Trp-99, Glu-89	Trp-133, Trp-99	Lys-126, Asn-150, Lys-88, Thr-101, Ser-100, Ser-93, Leu-146
Tecostanine	-5.8	Thr-148	Trp-138, Trp-99	Lys-126, Leu-146
Vasicine	-7.4	Asn-150	Trp-99, Trp-133, Lys-126	Leu-146, Gln-145, Ser-144, Gln-124, Thr-148
Tembetarine	-8.8	Lys-102, Asn-150	Glu-89, Trp-99.	Lys-88, Trp-133, Ser-100, Thr- 101, Ser-93,Ser -144, Thr-148, Lys-126, Leu-146
Lupinine	-5.4	-	Trp-133, Lys-126, Leu-146, Trp-99	Ser-144, Gln-145,Thr-148, Asn-150
Mahanimbine	-8.7	-	Trp-99, Trp-133, Leu-146, Lys-126	Ser-144, Gln-145, Thr-148
Piperumbellatm A	-8.7	Asn-150, Ser-144	Trp-99, Trp-133, Leu-146, Lys-126	Gln-146, Thr-148
Echinulin	-9.7	Leu-146	Trp-133, Trp-133, Lys-126, Lys-102, Trp-133, Leu-146	Lys-88, Ser-93, Ser-95, Thr-101, Gln-124, Ser-144, Gln-145, Thr-148
Vasicinol	-6.8	Asn-150, Thr-148,	Trp-99	Lys-126, Trp-133, Leu-146, Ser-144
Matrine	-7.6	Asn-150	Trp-99	Lys-126, Trp-133, Ser-144, Leu-146, Thr-148
Conophylline	-9.5	Lys-107, Ile-106, His-109, Thr-101	Val-155, Ile-153, Pro-104, Ile-106, Lys-107	Arg-77, Pro-78, Val-80, Lys-88, Glu-89, Ser-100, Lys-102, Leu-105, Ser-108, Phe-112, His-154, Lys-156