

Supplement D. Docking results of the selected alkaloid compounds and glibenclamide (as standard drug) against protein tyrosine phosphatase 1B (PDB: 7LEO).

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
Glibenclamide	-7.0	Lys116, Gly-183, Ala-217, Gln-262, Ser-216, Gln-262	Tyr-46, Val-49, Ala-217	Arg-47, Asp-48, Lys-120, Asp-181, Phe-182, Cys-215, Ser-216, Gly-220, Arg-221, Thr-263, Gln-266
Radicamine A	-6.6	Gly-183, Ser-216, Gly-183, Glu-115:	Val-184	Asn-111, Lys-116, Lys-120, Trp-179, Phe-182, Cys-215, Ala-217, Gln-262, Thr-263, Asn-265, Gln-266
Radicamine B	-5.5	Lys-116, Gly-183, Gln-262, Glu-115	-	Asn-111, Lys-120, Asp-181, Phe-182, Val-184, Cys-215, Ser-216, Ala-217, Gly-220, Arg-221, Thr-263, Asp-265, Gln-266
Coptisine	-7.5	Ser-216, Asp-181, Gly-183	Arg-221, Cys-215, Arg-221	Asn-111, Glu-115, Lys-116, Lys-120, Phe-182, Val-184, Ala-217, Gly-220, Gln-262, Asp-265, Gln-266
Vindolinine	-6.3	Arg-24, Arg-24	Met-258	Tyr-20, Ala-27, Gly-259, Ile-219, Gln-262
Physostigmine	-6.3	Trp-179, Arg-221, Gln-266	Lys-116	Tyr-46, Lys-120, Asp-181 Phe-182, Gly-183, Ser-216, Ala-217, Gln-262, Thr-263
Sanguinarine	-7.5	Lys-120, Gly-183	Lys-116, Thr-263	Glu-115, Phe-182, Val-184, Ser-216, Arg-221, Asp-265, Gln-266
Harmane	-5.7	Ser-216	Arg-221, Cys-215, Lys-120, HArg-221	Ala-217, Asp-181, Gln-262, Gln-266, Glu-115, Gly-183, Gly-220, Lys-116, Phe-182, Thr-263,
Jatrorrhizine	-8.8	Lys-88	Trp-99, Trp-133, Lys-126, Lys-107, Trp-133, Phe-112	Arg-24, Gly-259, Ile-219, Val-49
Palmatine	-6.4	Try-46, Asp-265, Gln-262	Thr-263, Ala-217, Cys-215, Arg-221, Try-46	Gln-266, Gly-183, Gly-220, Lyus-116, Ser-216, Val-184
Pinoline	-5.2	Gln-262	Tyr-46, Tyr-46, Ala-217	Asn-111, Arg-221, Cys-215, Gly-220, Ile-219, Lys-120, Ser-216
Cryptolepine	-6.6	Gln-262	Tyr-46, Ala-217, Lys-120	Gln-145, Leu-146, Ser-144, Thr-148
Galegine	-4.6	Arg-221, Gln-266, Pro-180, Gly-183, Asp-181	Cys-215	Ala-217, Gln-262, Lys-116, Phe-182, Ser-216, Trp-179, Val-184
Groenlandicine	-6.8	Gln-262, Asp-29	Arg-254, Met-258, Met-258, Phe-52	Ala-27, Arg-24, Asp-48, Gly-259, Ile-219, Val-49
Magnoflorine	-6.8	Gly-183, Arg-221, Thr-263	Lys-116, Cys-215	Ala-217, Asn-111, Gln-262, Gln-266, Lys-120, Phe-182, Ser-261, Trp-179, Tyr-46
Norharmane	-5.6	Gln-262, Ser-216	Arg-221, Cys-215	Ala-217, Asn-111, Gln-266, Glu-115, Gly-220, Lys-116, Lys-120, Thr-263
Vindoline	-6.6	Ser-216, Ala217, Arg221, Gln-266, Gln262	Phe182	Gly-220, Asp-181, Gly-183, Cys-215, Ile-219, Gly-218, Glu-115, Lys-120, Lys-116, Tyr-46
Berberine	-6.1	Gly-183, Gln-262, Ser-216, Thr-263	Thr-263, Ala-217	Asp-265, Val-184, Gln-266, Trp-179, Arg-221
Catharathine	-6.8	Arg-22, Gln-266, Gly183	Lys-116, Cys-215, Ala-217	Thr-263, Trp-179, Gly-220, Asp-181, Ser-216, Glu-115, Lys-120, Gln-262
Casurine 6-O- α -glucoside	-6.7	Lys-116, Lys-120, Ala-217, Arg-221 Gln-266, Gln-262, Pro-180, Gly-183, Ser-216	-	Phe-182, Trp-179, Asp-181, Glu-115, Asn-111, Cys-215, Gly-220, Ile-219, Tyr-46, Thr-263
Epiberberine	-6.4		Arg-254, Met-258, -Arg-24, Ala-27	Ser-28, Gly-259, Ile-219, Gln-262, Thr-263, Tyr-20
Capsaicin	-5.4	Lys116, Arg221, Gly183, Gln262	Tyr-46	Asn-111, Ser-216, Ala-217, Gly-220, Gln-266, Pro-180, Trp-179, Asp-181, Thr-263, Lys-120, Glu-115
Tecostanine	-4.9	Gly-183, Pro-180, Arg-221	-	Trp-179, Gln-266, Thr-263, Gln-262, Ala-217, Ser-216, Lys-120, Lys-116, Asp-181, Phe-182
Vasicine	-6.2	Gln-266, Arg-221	Cys-215, Ala-217	Gln-262, Ser-216, Gly-220, Trp-179, Val-184, Gly-183, Phe-182, Asp-181, Lys-116

Supplement D. Docking results of the selected alkaloid compounds and glibenclamide (as standard drug) against protein tyrosine phosphatase 1B (PDB: 7LEO).

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
Tembetarine	-6.3	Gly183, Gly183, Tyr46, Gln262	Lys120, Tyr46	Tyr-46, Lys-116, Trp-179, Pro-180, Asp-181, Ser-216, Ala-217, Thr-263, Gln-266, Cys-215, Gly-220, Gln-262,
Lupinine	-5.1	-	Val-155, Leu-172, Lys-197	Asp-148, Lys-150, Tyr-153, Gln-157, Phe-174, Glu-200, ser201,
Mahanimbine	-7.2	Gln-262	Tyr-46, Tyr-46, Ala-217	Arg-47, Asp-48, Val-49, Lys-116, Lys-120, Asp-181, Arg-221, Glu-115, Ser-216, Cys-215, Thr-263, Gln-266
Piperumbellatm A	-6.9	Lys-120, Ser-216. Ala-217, Arg-221	Arg-221, -Cys-215, Tyr-46, Ala-217, -	Ile-219, Gly-218, Tyr-46, Gly-220, Gln-262, Gln-266, Trp-179, Gly-183, Phe182, Asp181, Lys-116
Echinulin	-7.2	Lys-116, Lys-120, Ser-216, Ala-217	Ala-217, Cys-215, Tyr-46	Va-l49, Asp-48, Glu-115, Asn-111, Asp-181, Phe-182, Trp-179, Gly-183, Gln266, Thr263
Vasicinol	-6.4	Ala-217, Arg-221 Gln-266, Tyr-46	Cys-215, Ala-217	Lys-116, Lys-120, Trp-179 Asp-181, Phe-182, Gly-183, Val-184, Ser-216, Gln-262, thr-263
Matrine	-7.0	Trp-179, Arg-221, Gln-266	Cys-215, Ala-217	Lys-116, Phe-182, Gly-183, 216, Gln -262,
Conophylline	-7.5	Lys-116, Arg-221, Arg221, Gln-266, Gly-183, Gln-262	Thr-263	Trp-16, Ala-17, Lys-120, Trp-179, Val-184, Ala-264