

Supplement A. Docking results of alkaloid compounds and epalrestat (as standard drug) against aldose reductase (PDB: 2R24).

Ligand	Docking Score (Kcal/Mol)	Interactions		
		H-Bond	Hydrophobic/Electrostatic/Other Pi-Cation/ Pi-anion/pi-alkyl/pi-sulfur/ pi-sigma interactions	Van Deer Waals
Epalrestat	-9.3	Trp-20, Tyr-48, His-110, Cys-298	Cys-80, Cys-298, Cys-303, Trp-219, Tyr-48, Trp-20, Trp-111, Leu-300	Val-47, Trp-79, Thr-113, Phe-115, Phe-122, Ala-299, Tyr-309
Radicamines A	-7.7	Trp-20, Lys-21, His-110, Ser-210, Ser-159, Gln-183	Cys-298, Tyr-209, Lys-77, His-110, Tyr-209	Trp-111, Pro-212, Ser-214, Pro-215, Asp-216, Asn-160, Ile-260, Thr-19, Gly-18, Lys-262
Radicamines B	-6.4	Trp-111, Ser-214, Tyr-48	Tyr-209, Cys-298	Gly-18, Thr-19, Trp-20, Lys-21, Asp-43, Lys-77, His-110, Ser-159, Gln-183, Ser-210, Ile-260, Lys-262
Coptisine	-10.9	Lys-21, Asn-160, Lys-77, Gln-183, Ser-159, Ser-210	Cys-298, Tyr-209, His-110, Tyr-209, Lys-262	Trp-20, Gly-18, Tyr-48, Trp-111, Leu-212, Pro-215, Ser-214, Ser-214, Asp-216, Pro-260, Ile-260, Pro-261
Vindoline	-7.6	Trp-20	Phe-122, Val-47, Trp-20	Lys-21, Tyr-48, Phe-121, Pro-218, Trp-219, Leu-300
Physostigmine	-7.7	His-110, Trp-111, Gln-183	Tyr-209, Cys-298, Trp-20	Val-47, Tyr-48, Lys-77, Trp-79, Phe-122, Asn-160, Trp-219, Leu-300
Sanguinarine	-8.8	Tyr-48, Gln-49, Cys-298, Val-47	Cys-298, Trp-20, Cys-298, Tyr-48	His-110, Trp-111, Phe-121, Phe-122, Trp-219
Harmame	-9.3	-	Cys-80, Cys-303, Trp-111, Phe-122, Leu-300, Cys-303, Cys-298	Ala-299, Phe-115, Thr-113, Trp-79, Trp-219, Tyr-306
Jatrorrhizine	-9.3	Trp-20	Trp-111, Cyc-80, Cyc-303, Trp-20, Trp-79, Phe-115, Phe-122, Val-47, Leu-300, Cys-303	Ala-299, Cys-298, Gln-49, Phe-311, Pro-218, Pro310, Thr-113, Trp-219, Tyr-48, Tyr-309
Palmatine	-8.0	-	Cys-80, Cys-303, Trp-111, Leu-300, Cys-303,	Ala-299, Cys-298, Phe-115, Phe-122, Thr-113, Trp-20, Trp-79, Trp-219, Tyr-3069
Pinoline	-8.5	Asp-43, Gln-183	Tyr-209, Tyr-209, Tyr-48, Trp-20,	Cys-298, Gly-18, His-110, Ile-260, Lys-21, Lys-262, Ser-210, Ser-214, Trp-111
Cryptolepine	-8.0	-	Cys-80, Cys-303, Trp-111, Leu-300, Leu-303	Ala-229, Cys-298, Phe-115, Phe-122, Pro-310, Thr-113, Trp-20, Trp-79, Trp-219, Tyr-309
Galegine	-5.8	-	Trp-111, Val-47, Cys-298, Trp-20, Tyr-48	Asp-43, Ile-260, Lys-77, Trp-111, Trp-219, Tyr-209
Groenlandicine	-9.7	-	Trp-20, Trp-111, Cys-80, Cys-303, Trp-79, Phe-115, Phe-122, Val-47	Ala-299, Cys-298, Phe-311, Pro-218, Pro-310, Thr-113, Trp-20, Trp-219, Tyr-48, Tyr-309
Magnoflorine	-7.8	Tyr-48	Leu-300, Trp-20, Leu-300, Val-47	Cys-298, Gln-49, Phe-122, Trp-79, Trp-111, Trp-219
Norharmame	-8.8	Thr-113	-Leu-300, Cys-80, Cys-303, Trp-111, Cys-303, -Leu-300, Cys-298	Ala-299, Phe-115, Phe-122, Trp-79, Trp-219, Tyr-309
Vindoline	-5.8	Gln-49	Leu-300, Phe-122, Trp-219, Pro-218	Pro-24, Phe-121, Tyr-48, Val-47, Trp-20, Lys-21
Berberine	-9.5	Trp-20	Cys-80, Cys-303, Trp111, Pro-310, Tyr-309, Leu-300	Pro-112, Thr-113, Phe-115, Trp-79, Phe-122, Val-47, Tyr-48, Trp-219, Cys-298, Ala-299, Phe-311
Catharathine	-7.9	-	Trp-219, Cys-298 Trp-20, His-110, Tyr-48, Leu-300	Trp-79, Trp-111, Phe-122, Val-17, Pro-218
Casurine 6-O- α -Glucoside	-6.7	Trp-20, Tyr-48, Ser-210, Ile-260	-	Val-297, Tyr-209, Lys-21, Pro-261, Pro-211, Lys-262, Gly-18, Thr-19, Cys-298, Lys-77, Trp-219, Val-47, Trp-79, Trp-111, His-110, Asn-160
Epiberberine	-8.2	-	Leu-300, Trp-111, Cys-303, Tyr-309, Val-47	Thr-113, Phe-115, Cys-80, Trp-79, Phe-122, Phe-121, Trp-20, Tyr-48, Trp-219, Cys-298, Ala-299, Phe-311
Capsaicin	-9.7	Tyr-48, His-110, Ser-210	Trp-20, Trp-111, Tyr-209, Cys-298, Leu-300, Cys-303, Cys-80, Trp-79, Phe-115, Phe-122	Lys-262, Gly-18, Thr-19, Ile-260, Lys-77, Asp-43, Gln-183, Trp-219, Tyr-309, Thr-113, Lys-21, Ser-214
Tecostanine	-6.0	His-110, Trp111	Val-47, Trp-20	Asn-160, Tyr-48, Trp-79, Phe-122, Trp-219, Leu-300, Cys-298
Vasicine	-8.1	Ala-299	Cys-80, Cys-303, Trp-111, Leu-300,	Thr-113, Phe-115, Trp-79, Phe-122, Trp-219, Cys-298, Tyr-309

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		H-Bond	Hydrophobic/Electrostatic/Other Pi-Cation/ Pi-anion/pi-alkyl/pi-sulfur/ pi-sigma interactions	Van Deer Waals
Tembetarine	-8.6	Leu-300	Trp-111, Leu-300, Cys-303, Trp-219, Phe-115,	Trp-20, His-110, Cys-80, Thr-113, Tyr-309, Phe-311, Ala-299, Cys-298
Lupinine	-5.8	-	Trp-111, Cys-298, Leu-300, Cys-303	Cys-80, Phe-115, Tyr-309, Ala-299, Trp-219, Trp-79, Phe-122
Mahanimbine	-11.5	-	Leu-300, Tyr-209, Cys-80, Cys-303, Cys-298, Trp-20, Trp-111	Tyr- 48, His-110, Asn-160, Phe-122, Trp-79, Phe-115, Thr-113, Tyr-309, Pro-310, Ala-299, Trp-219
Piperumbellatm A	-8.1	Cys-298, Trp-111	Trp-219, His110, Trp-111, Cys298, Cys-298, Leu-300	Ala-299, Phe-122, Val-47, Trp-79, Tyr-48
Echinulin	-11.3	-	Trp-111, Trp-219, Phe-122, Trp-219, Cys-298, Cys-80, Cys-303, Trp-79, Phe-115, Tyr-209, Leu-300	Tyr-309, Thr-113, Pro-218, Lys-21, Phe-121, Val-47, Tyr-48, Trp-20, Gln-49, Asn-160
Vasicinol	-8.1	His-110, Ser-210, Ser-159, Asp-43, Gln-183	Cys-298, Tyr-209	Gly-18, Trp-20, Lys-21, Tyr-48, Trp-111, Asn-160, Pro-211, Ile-260, Lys-262
Matrine	-7.3		Leu-300, Trp-20, Tyr-48, His-110	Val-47, Trp-79, Trp-111, Phe-122, Trp-219, Cys-298
Conophylline	-7.5	Ser-302	Phe-122, Trp-20	Gln-49, Val-47, Tyr-48, Trp-79, His-110, Trp-111, Phe-121, Trp-219, Pro-218, Leu-300