Supplementary materials

https://doi.org/10.47093/3034-4700.2025.2.1.53-68-annex-c

Supplement C. Docking results of the selected alkaloid compounds and acarbose (as standard drug) against alpha glucosidase (PDB:8YIE).

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
Acarbose	-8.4	Trp-250, Asp-221, Glu-278, Asp-159, Glu-278		Ser-160, Val-161, Phe-162, Trp-158, Phe-185, Arg-219, Val-222, His-224, His-235, Asp-337, Arg-239, Gly-240, Pro-241, Ala-243, His 245, Asn-246, Met-249, Trp-280, Ile-417, Arg-428
Radicamine A	-8.7	Ala-450, Gln-72, Asp-448, Thr-419, Gly-38, Ala-36, Asp-448, Asp-186	Ala-449, Ala-450, Arg-73	Asn-37, Asp-39, Pro-71, His-75, Thr-187, Pro-416, Arg-442, Thr-453
Radicamine B	-5.5	Asn37, Gln-414	Arg-73, Pro-416, -Ala-449	Arg-31, Ala-36, Gly-38, Pro-71, Gln-72, Asp-186, Thr-187, Arg-442, Asp-448, Ala-450
Coptisine	-9.7	Arg-428, Asp-74	Glu-278, Trp-280, Val-222	Tyr-77, Val-161, Phe-162, Phe-185, Asp-221, His-224, Asp-337
Vindolinine	-8.1	Asn-246, Trp-250	Ala-243, Val-161	Asp-159, His-235, Arg-239, Gly240, Pro-241, Gly-244, His-245, Met-249
Physostigmine	-7.2	Arg-428, Asp-221, Asp-74	Glu-278, Trp-280, Phe-185, Phe-185, Val-222	Tyr-77, His-117, Phe-162, Gln-189, Arg-219, His 224, Asp-337
Sanguinarine	-9.3	Arg-428, Asp-74	Glu-278, Asp-337, Val-161, Val-222	Tyr-77, Phe-162, Phe-185, Asp-221, Hs-224, Trp-280, Ile-417
Harmane	-7.0	Ala-450	Asp-186, Arg-420, Arg-73, Ala-449, Ala-450	Arg-442, Asn-37, Asp-448, Gln-414, Gly-38, Pro-416, Thr-187, Thr-419, Thr-453
Jatrorrhizine	-8.0	Gly-244, Asp-159, Trp-250	Trp-280, His-224, Trp-250, Met-249, Val-161,	Ala-243, Asn-246, Asp-337, Glu-278, His-235, His-245, Phe-185, Val-222
Palmatine	-7.7	-	Glu-278, Asp-337, Phe-185, Try-77	Arg-428, Asp-74, Asp-221, Ile-417, Phe-162, Trp-280, Val-161, Val-222
Pinoline	-7.2	Thr-419, ARg-73, Asp-186	Asp-448, His-75, Arg-73, Ala-449	Ala-450, Arg-420, Arg-442, Asn-37, Asp-39, Gln-72, Gln-414, Gly-38, Pro-416, Thr-187, Thr-453
Cryptolepine	-8.2	Arg-442, Arg-73, Ala-449, Thr-419, Asn-37, Gly-38	Asp-186, Ala-449, Arg-73, Ala-449, Ala-450, Arg-73	Arg-420, Asp-448, Gln-72, Gln-414, His-75, Pro-416, Thr-187, Thr-453
Galegine	-4.9	Asp-159, Asn-246, Gly-238, Asp-159	His-245, Trp-250	Ala-243, Arg-239, Asn-157, Gly-240, Gly-244, His-235, Trp-158
Groenlandicine	-8.6	Arg-428, Asp-337, His-224	Glu-278, Asp-337, Trp-280, Phe-185, Ile-417, Phe-162	Arg-432, His-245, Val-161, Val-222
Magnoflorine	-8.4	Trp-280, Glu-278, Asp-337, His-224,	Trp-280, Val-222, Val-338, Phe-185, Val-161	Trp-250
Norharmane	-7.2	Thr-419, Ala-450	Asp-186, Asp-448, Ala-449, Arg-73, Ala-450	Arg-420, Arg-442, Asn-37, Asp-39, Gln-414, Gly-38, Pro-416, Thr-187, Thr-452
Vindoline	-7.4	His-245, Trp-250, Gly-244, Asp-159, Trp-280	Trp-250, His-235, -Val-161	Met-249
Berberine	-8.5	Asn-246, His-235	Trp-280, Met-249, Trp-280, Ala-243, Val-161	His-245, Gly-244, Pro-241, Gly-240, Arg-239, Gly-238, Asn-157, Trp-158, Asp-159, Trp-250
Catharathine	-7.2	Trp-250, His-224, Gly-244, Val-161		Trp-280, Phe-185, Val-222, Asn-246, Trp-158, His-235, Arg-239, Gly-238, Ala-243, Gly-240, Asp-159, Ser-160, His-245
Casurine 6-O-α-glucoside	-7.6	Gly-240, Asn-246, Trp-250, Ser-160, Gly-244, Asn-157, Gly-238		His-245, Trp-280, Met-249, Val-161, Trp-158, His-235, Gly-238, Ala-243, Arg-239, Asp-159, Pro-241
Epiberberine	-8.7	Thr-187	Arg-420, Asp-186, Pro-416, Ala-449, Ala-450, Ala-452	Arg-73, Arg-442, Thr-168, Gln-414, Thr-419, Thr-453
Capsaicin	-7.1	His-245, Trp-250	Trp-280, Phe-185, Tyr-77, His-224, Trp-250, Phe162, His-245	Asp-221, His-117, Gln-189, Asp-337, Val-161, Pro-282, Asn-246, Glu-275, Val-222, Arg-428, Asp-74
Tecostanine	-6.5	Thr-419, Gly-38, Asp415, Asp448	Pro-416, Ala-449	Asp-39, Thr-453, Ala-450, Thr-187, Arg-442, Ser-188, Asp-186, Arg-73, Gln-414, Asn-37, Asp-39
Vasicine	-6.8	Asp-448, Gln-414	Asp-186, Arg-420, Ala-449, Ala-450	Thr-453, Thr-419, Pro-416, Arg-73, Asn-37, Gly-38, Arg-442, Thr-187

Supplement C. Docking results of the selected alkaloid compounds and acarbose (as standard drug) against alpha glucosidase (PDB:8YIE).

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	- 8.0	Glu-278, Glu-278, Trp-250	Trp-280, His-224, Trp-250, Val-222, Phe-185	His-245, Gly-244, Trp-158 , Ser-160, Asp-159
Lupinine	-5.3	Gln-347, Asp-370	Pro-403, Trp-461	Val-342, Leu-371, Gly-374, Thr-343, Leu-406, Glu-404
Mahanimbine	- 8.9	Glu-278	Asp-337, Val-161, Tyr-77, Val-161, His-224, Trp-250	Asp-221, Asp-74, Arg-428, Phe-162, Phe-185, Ile417, Trp280, Val-222
Piperumbellatm A	- 8.5	Asp-337	Trp-280, Tyr-77, Phe-185, Glu-278, His-224	Val-222, Phe-185
Echinulin	- 8.9	Asp-337	Phe-185, Trp-250, Trp-280, Val-161, Val-222, Ile-417, Arg-428, -His-117, His-224	Asp-221, Val-338, Glu-278
Vasicinol	-6.9	Gln-414	Asp-186, Arg-420, Ala-449, Ala-450	Gly-38, Arg-73, Thr-187, Pro-416 Thr-419, Arg-442, Asp-448, Thr-453
Matrine	-7.3	Arg-428:	Trp-280	Asp-74, Val-161, Phe-185, Asp-221, Val-222, Asp-337, Ile-417
Conophylline	-9.5	His-245, Asn-246, Arg-313, Pro-241, Pro-282, His-224	His-224, Trp-280	Val-161, Asp-303, Gln-307, Pro-308, Val-306, Gly-244, Trp-250, Phe-185