

Table S1: Summary of Ethyl-1-cyclopropyl-2-methyl-5-[4H-1,2,4triazole-3-yl) methoxy]1-H-indole-3-carboxylate derivatives (**5a-5k**).

Aromatic aldehyde	Compound code	Temp (°C)	Time (h)	Solvent	Yield (%)	Melting point (°C)
Anisaldehyde	5a	25-30	22-24	Ethanol	78.90	179-181
4-clorobenzaldehyde	5b	25-30	22-24	Ethanol	65.78	167-169
2-hydroxy-5-nitrobenzaldehyde	5c	25-30	22-24	Ethanol	87.12	117-120
m-nitro benzaldehyde	5d	25-30	22-24	Ethanol	65.43	158-160
2,5-dimethoxybenzaldehyde	5e	25-30	22-24	Ethanol	88.22	180-184
2-4-dichlorobenzaldehyde	5f	25-30	22-24	Ethanol	59.04	187-190
6-methoxy-2-naphthol aldehyde	5g	25-30	22-24	Ethanol	73.34	180-186
Veretraldehyde	5h	25-30	22-24	Ethanol	81.45	140-143
Benzaldehyde	5i	25-30	22-24	Ethanol	51.49	152-156
4-hydroxybenzaldehyde	5j	25-30	22-24	Ethanol	81	156-165
Nitrovetraldehyde	5k	25-30	22-24	Ethanol	58.73	190-196

Table S2: Surflex Docking score (kcal/mol) of the compounds for α -glucosidase protein in the human intestine.

Compounds	C Score ^a	Crash Score ^b	Polar Score ^c	D Score ^d	PMF Score ^e	G Score ^f	Chem Score ^g
Casuarine-Enzyme complex	8.80	-1.49	7.35	-134.360	-143.989	-307.493	-29.806
5j	7.51	-2.22	7.89	-125.230	-135.620	-250.891	-29.120
5e	6.06	-2.17	1.02	-217.788	-129.181	-241.909	-30.941
5g	4.95	-2.68	0.26	-217.877	-136.638	-257.731	-31.403
5i	3.04	-1.18	0.09	-142.781	-89.668	-140.498	-20.357
5a	2.71	-0.82	0.15	-148.895	-60.397	-168.120	-18.391
5h	2.70	-0.87	1.14	-134.452	-41.400	-141.522	-18.510
5k	2.17	-2.28	0.60	-164.709	-131.261	-171.072	-25.954
5d	2.01	-1.62	0.14	-130.224	-81.294	-143.050	-15.273

^a CScore (Consensus Score) integrates a number of popular scoring functions for ranking the affinity of ligands bound to the active site of a receptor and reports the output of total score.

^b Crash-score revealing the inappropriate penetration into the binding site. Crash scores close to 0 are favorable. Negative numbers indicate penetration.

^c Polar indicating the contribution of the polar interactions to the total score. The polar score may be useful for excluding docking results that make no hydrogen bonds.

^d D-score for charge and van der Waals interactions between the protein and the ligand.

^e PMF-score indicating the Helmholtz free energies of interactions for protein-ligand atom pairs (Potential of Mean Force, PMF).

^f G-score showing hydrogen bonding, complex (ligand-protein), and internal (ligand-ligand) energies.

^g Chem-score points for H-bonding, lipophilic contact, and rotational entropy, along with an intercept term.