

Table S1. The structural files and the chain that were considered for molecular docking study

Protein	PDB ID	Short characterization of the structural file
<i>soil enzymes</i>		
dehydrogenases	1KEV, chains A, B, C, D	Crystallographic structure of <i>Clostridium beijerinckii</i> NADP-dependent alcohol dehydrogenase in complex with dihydro-nicotinamide-adenine-dinucleotide phosphate (NADP) at a resolution of 2.05 Å [48].
	3AUT chains A and B	Crystallographic structure of <i>Bacillus megaterium</i> glucose dehydrogenase 4 in complex with 1,4-dihydronicotinamide adenine dinucleotide at a resolution of 2.00 Å [49]. Only the B chain contains the ligand.
	3NT5 chains A and B	Crystallographic structure of <i>Bacillus subtilis</i> myo-inositol dehydrogenase in complex with nicotinamide-adenine-dinucleotide and inositol at a resolution of 2.90 Å [50].
	5GTL chains A, B, C, and D	Crystallographic structure of aldehyde dehydrogenase from <i>Bacillus cereus</i> in complex with dihydro-nicotinamide-adenine-dinucleotide phosphate at a resolution of 2.90 Å (not published yet).
urease	4AC7 chain C	The crystal structure of <i>Bacillus pasteurii</i> urease in complex with the inhibitor citrate at a resolution of 1.50 Å [51]. Only the C chain has been considered as it contains the catalytic domain of urease.
phosphatases	1H2F chain A	Crystallographic structure of the <i>Bacillus stearothermophilus</i> phosphatase PhoE in complex with trivanadate at a resolution of 2.00 Å [52].
	1QFX chains A and B	Crystallographic structure of the acid phosphatase from <i>Aspergillus niger</i> in complex with 2-acetamido-2-deoxy-beta-D-glucopyranose at a resolution of 2.40 Å [53].
	2YEQ chains A and B	Crystallographic structure of alkaline phosphatase from <i>Bacillus subtilis</i> in complex with 3,6,9,12,15,18,21,24-octaoxahexacosan-1-ol at a resolution of 1.98 Å and an active site containing iron and calcium [54].
<i>proteins that are important for assessing the effects of chemicals on the human health</i>		
alpha-1 acid glycoprotein	3KQ0 chain A	Crystallographic structure of human alpha1-acid glycoprotein in complex with (2R)-2,3-dihydroxypropyl acetate at a resolution of 1.80 Å [55].
human serum albumin	4Z69 chains A and I	Crystallographic structure of human serum albumin complexed with palmitic acid and diclofenac at a resolution of 2.19 Å [56].
cytochrome 1A2	2HI4 chain A	Crystallographic structure of human cytochrome 1A2 in complex with alpha-naphthoflavone at a resolution of 1.95 Å [57].
cytochrome 2C9	1OG5 chains A and B	Crystallographic structure of human cytochrome 2C9 in complex with S-warfarin at a resolution of 2.55 Å [58].
cytochrome 2C19	4GQS chains	Crystallographic structure of human cytochrome 2C19 in complex with (4-hydroxy-3,5-dimethylphenyl)(2-methyl-1-benzofuran-3-yl)methanone at a resolution of 2.87 Å [59].

	A, B, C and D	
cytochrome 2D6	4WNV chain A	Crystallographic structure of human cytochrome 2D6 in complex with quinine at a resolution of 2.35 Å [60].
cytochrome 3A4	1W0G chain A	Crystallographic structure of human cytochrome 2D6 in complex with metyrapone at a resolution of 2.35 Å [61].