

Supplementary material

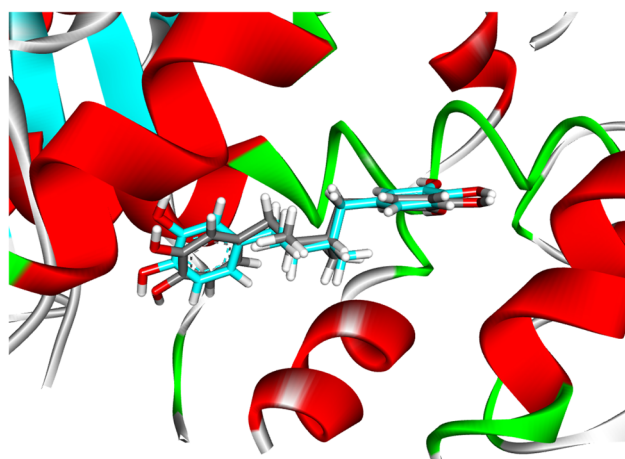


Figure S1: The root means square deviation between the original and docked poses of the cocrystal ligands of Lipoxxygenase enzyme (PDB: 6n2w) was 0.62 Å.

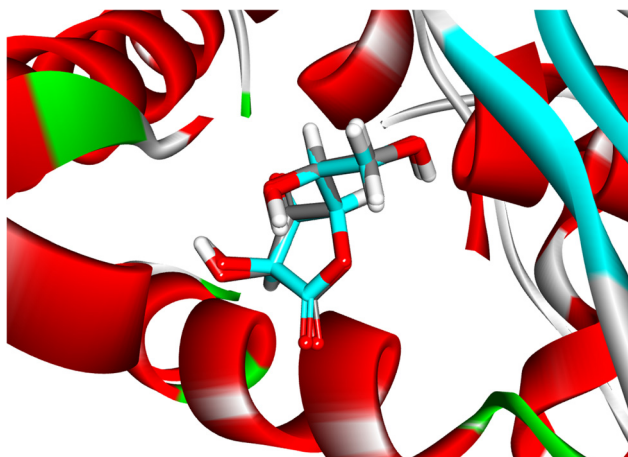


Figure S2: The root means square deviation between the original and docked poses of the cocrystal ligand (Ascorbic acid) of Peroxidase enzyme (PDB: 2x08) was 0.20 Å.

Table S1: Phenolic compounds previously reported and isolated from *Solanum nigrum* L

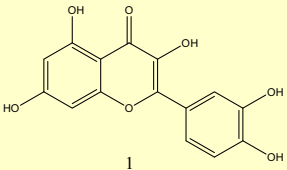
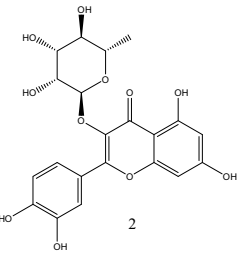
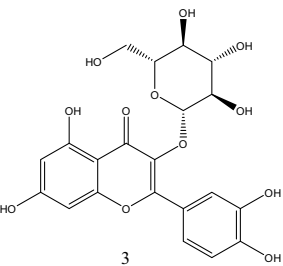
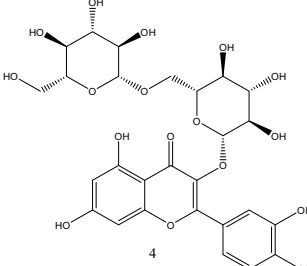
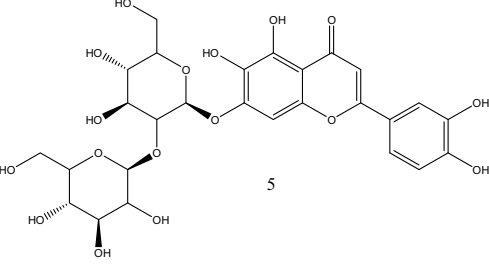
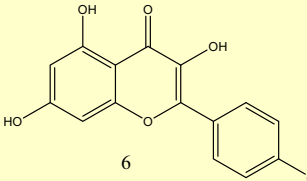
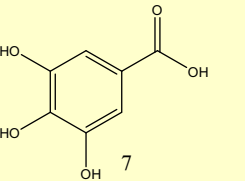
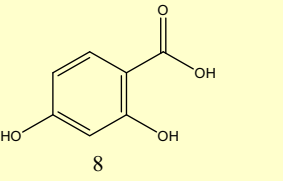
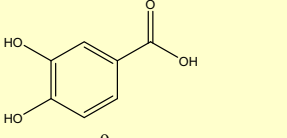
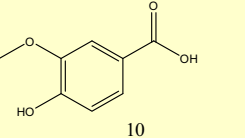
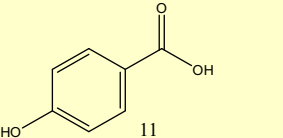
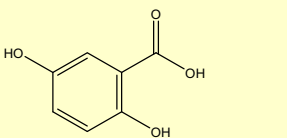
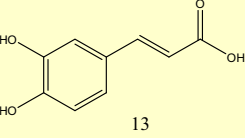
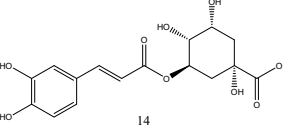
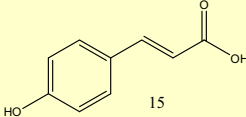
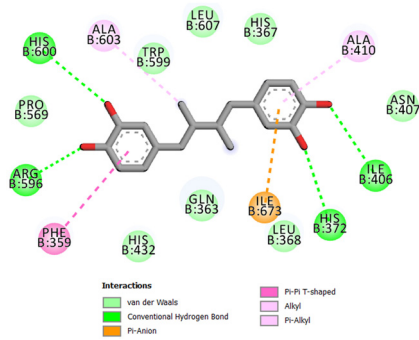
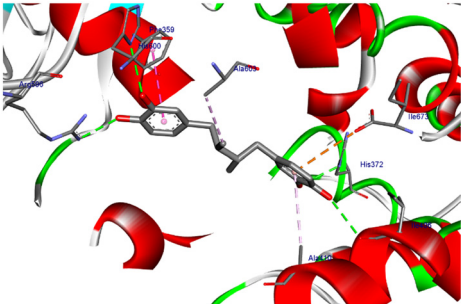
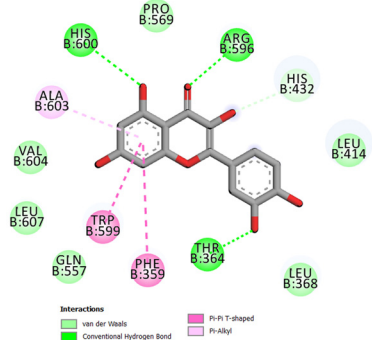
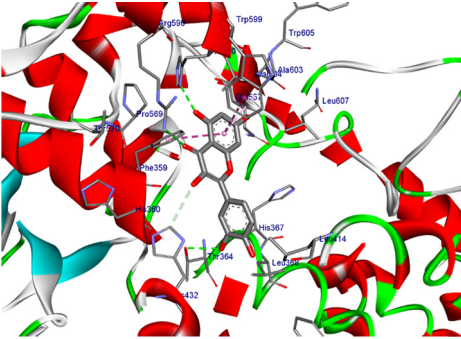
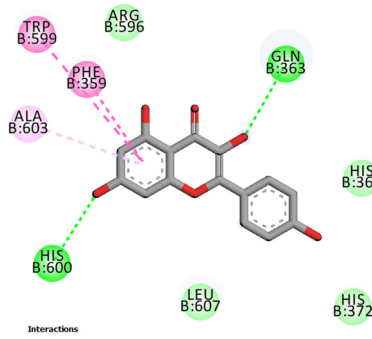
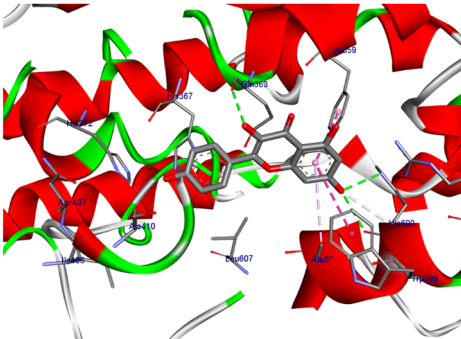
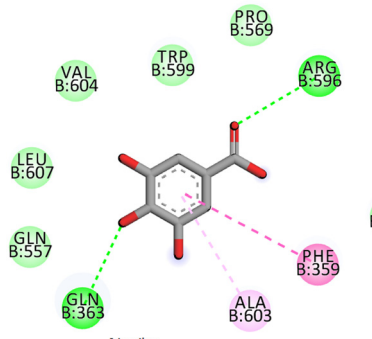
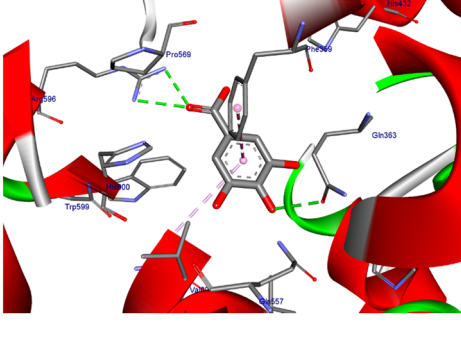
Quercetin 1  1	Quercitrin 2  2	Isoquercitrin 3  3
Quercetin-3-gentiobioside 4  4	6-Hydroxyluteolin 7-sophoroside 5  5	
Kaempferol 6  6	Gallic acid 7  7	2, 4-Dihydroxybenzoic acid 8  8
Protocatechuic acid 9  9	Vanillic acid 10  10	4-Hydroxybenzoic acid 11  11
2, 5-Dihydroxybenzoic acid (gentisic acid) 12  12	Caffeic acid 13  13	Chlorogenic acid 14  14
4-Hydroxycinnamic acid 15  15		

Table S2: Two- and three-dimensional protein/ligand interaction between the ten compounds and arachidonate-5-lipoxygenase (ALOX5, PDB:6n2w)

Com.No.	Lipoxygenase (6n2w)	
	2D	3D
Ligand		
Quercitrin		
Kaempferol		
Gallic acid		

(Continued)

Table S2: Continued

Com.No.	Lipoxygenase (6n2w)	
	2D	3D
2, 4-Dihydroxybenzoic acid	Interactions - van der Waals - Conventional Hydrogen Bond - Pi-Pi T-shaped - Pi-Alkyl	
Protocatechuic acid	Interactions - van der Waals - Conventional Hydrogen Bond - Pi-Pi T-shaped - Pi-Alkyl	
Vanillic acid	Interactions - van der Waals - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Pi T-shaped - Pi-Alkyl	
4-Hydroxybenzoic acid	Interactions - Conventional Hydrogen Bond - Pi-Pi T-shaped - Pi-Alkyl	

(Continued)

Table S2: Continued

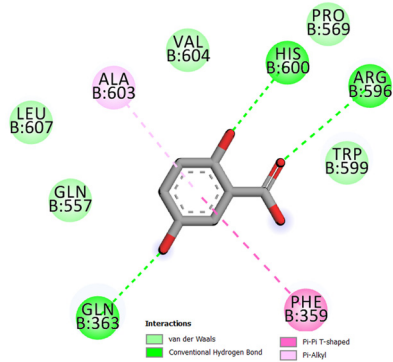
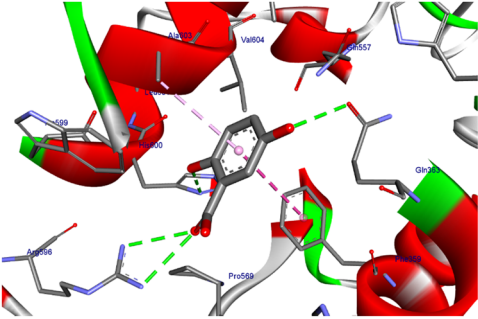
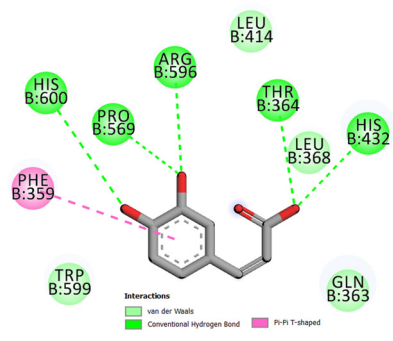
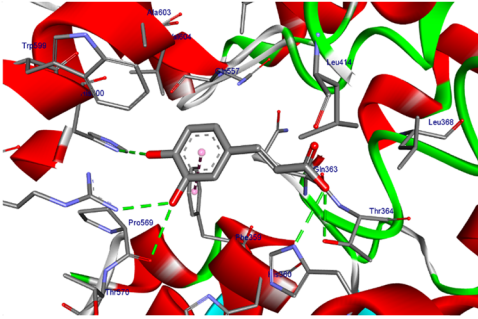
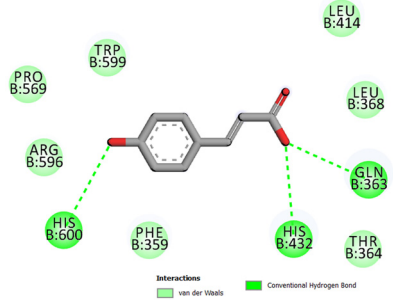
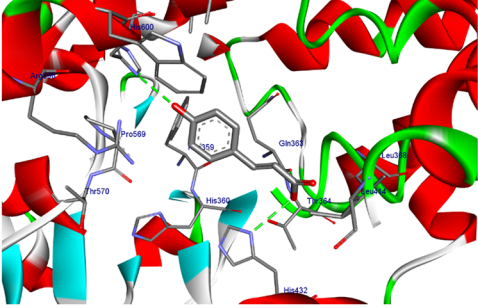
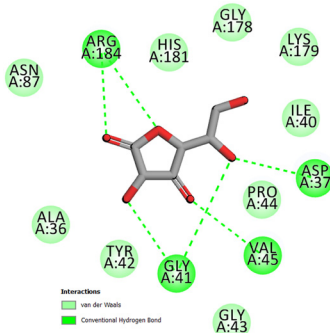
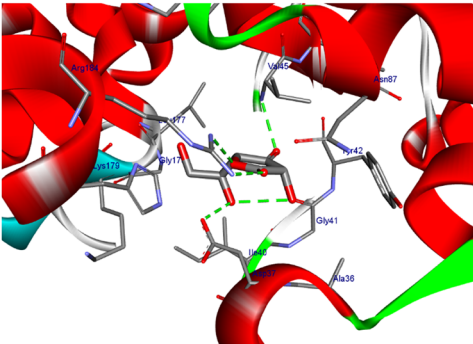
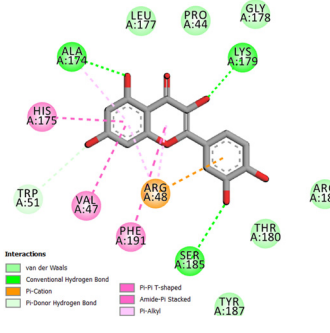
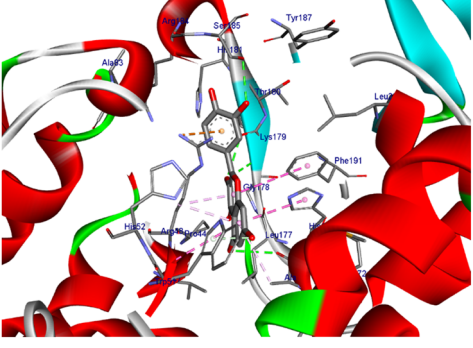
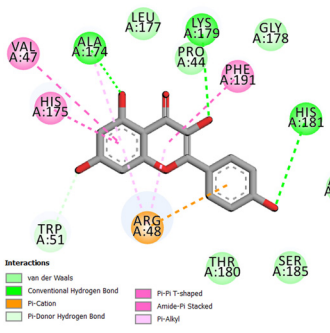
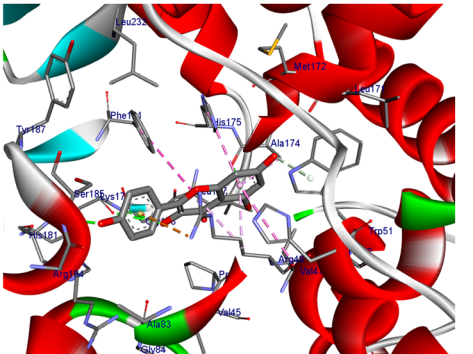
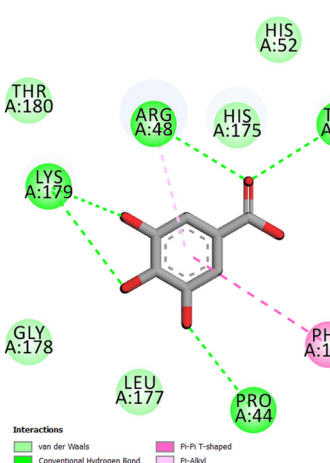
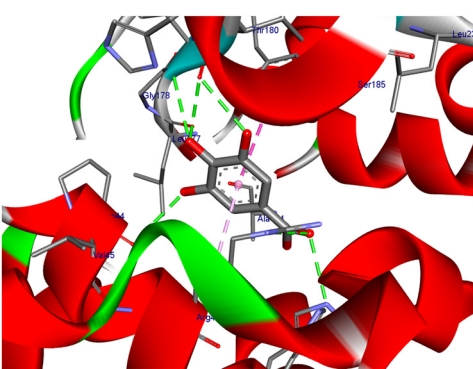
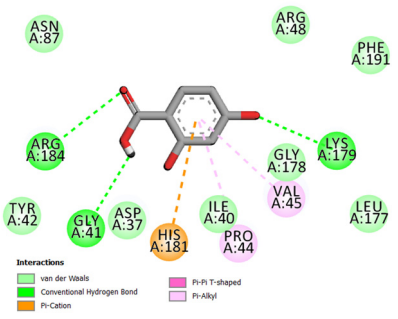
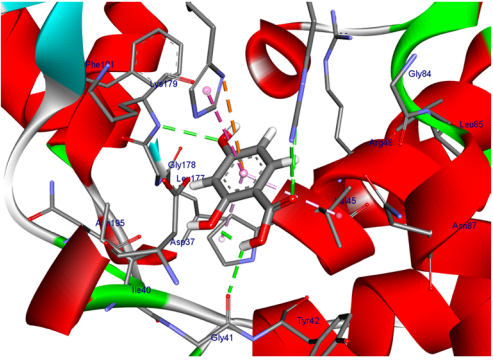
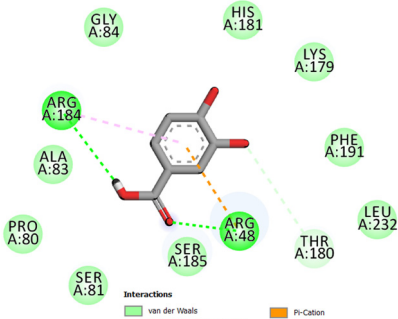
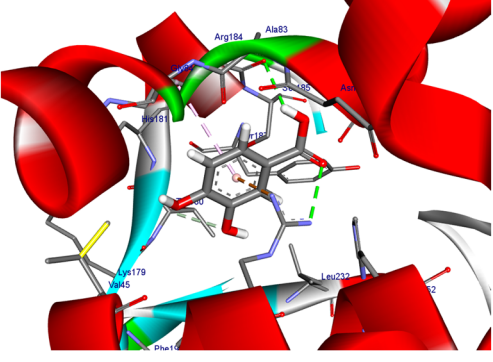
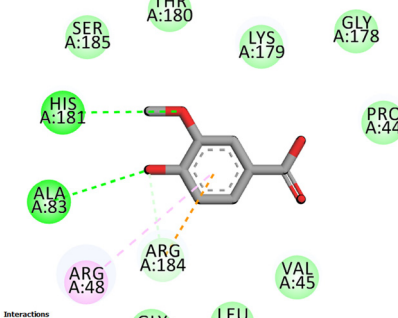
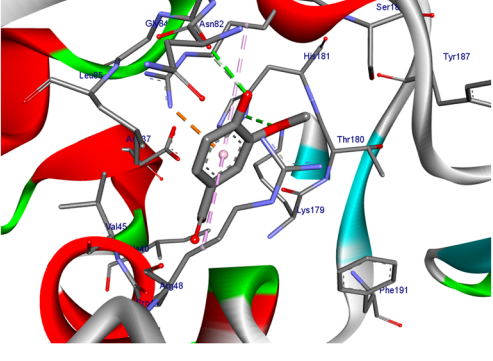
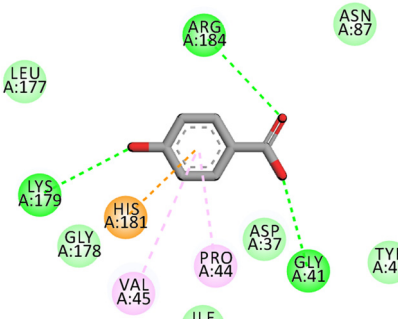
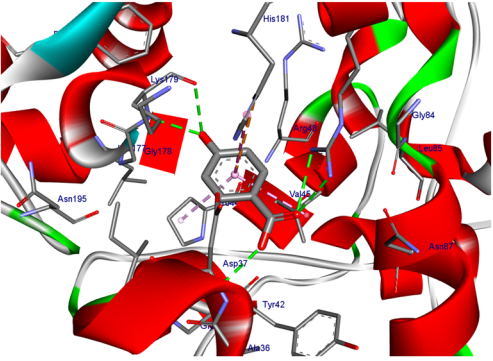
Com.No.	Lipoxygenase (6n2w)	
	2D	3D
2, 5-Dihydroxybenzoic acid (gentisic acid)		
Caffeic acid		
4-Hydroxycinnamic acid		

Table S3: Two- and three-dimensional protein/ligand interaction between the ten compounds Cytochrome c Peroxidase (PDB: 2x08)

Co.No.	Peroxidase (2x08)	
	2D	3D
Ascorbic acid		
Quercitrin		
Kaempferol		
Gallic acid		

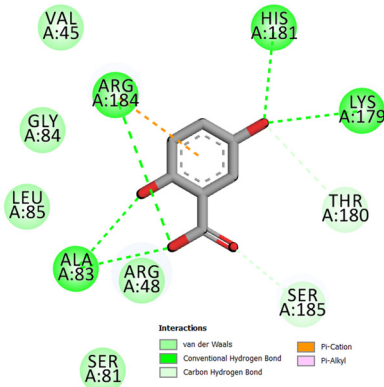
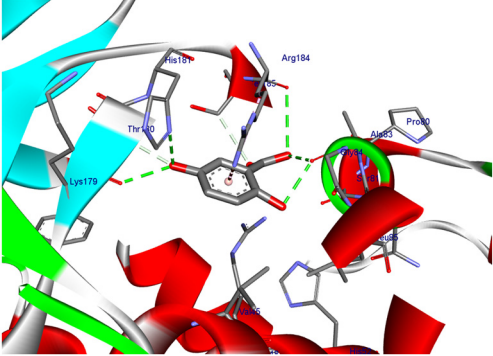
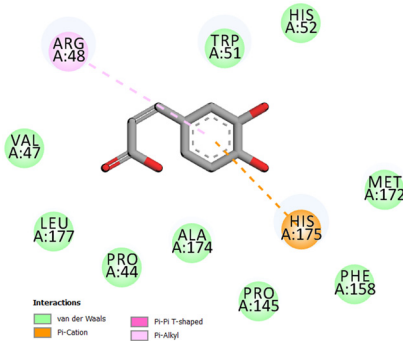
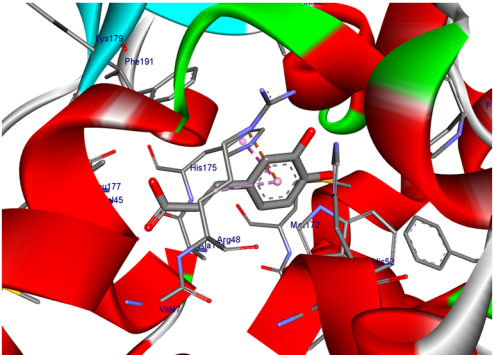
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Table S3: Continued

Co.No.	Peroxidase (2x08)	
	2D	3D
2, 4-Dihydroxybenzoic acid		
Protocatechuic acid		
Vanillic acid		
4-Hydroxybenzoic acid		

(Continued)

Table S3: Continued

Co.No.	Peroxidase (2x08)	
	2D	3D
2, 5-Dihydroxybenzoic acid (gentisic acid)		
Caffeic acid		
4-Hydroxycinnamic acid	