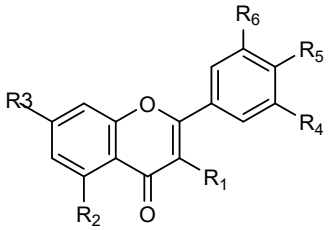
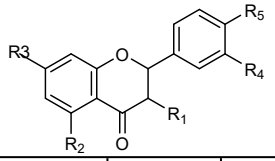
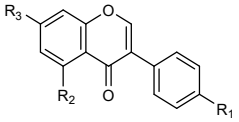
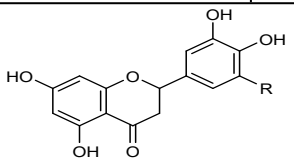
Electronic Supplementary Material (ESI) for RSC Advances.

Table S1: list of phytochemical constituents of Egyptian propolis selected for the xanthine oxidase inhibition *in-silico* screening.

Chemical class	structure						Compound name
Flavones & flavonols							
	R_1	**R_2**	**R_3**	**R_4**	**R_5**	**R_6**	
	H	OH	OH	H	H	H	Chrysin
	H	OH	OCH_3	H	H	H	Tectochrysin
	OH	OH	OH	H	H	H	Galangin
	OH	OCH_3	OH	H	H	H	Galangin-5-methylether
	OH	OH	OCH_3	H	H	H	Galangin-7-methylether (Izalpinin)
	H	OH	OH	OH	OH	H	Luteolin
	H	OH	OH	OCH_3	OH	H	Luteolin-3'-methylether
	H	OH	OH	H	OH	H	Apigenin
	H	OH	OH	H	OCH_3	H	Acacetin
	OH	OH	OH	OH	OH	H	Quercetin
	OCH_3	OH	OH	OH	OH	H	Quercetin-3-methylether
	OH	OH	OCH_3	OH	OH	H	Quercetin-7-methylether
	OH	OH	OCH_3	OCH_3	OH	H	Quercetin-7,3'-di methylether
	OCH_3	OH	OH	OCH_3	OH	H	Quercetin-3,3'-di methylether
	OH	OH	OH	OH	OH	OH	Myricetin
	H	OH	OCH_3	H	OH	H	Genkwanin
	H	H	OH	H	OCH_3	H	Formononetin
	OH	OH	OH	H	OH	H	Kaempferol
	OCH_3	OH	OH	H	OH	H	Kaempferol-3-methylether
	OH	OH	OH	OCH_3	OH	H	Isorhamnetin

Flavanones & flavanols						
	R_1	**R_2**	**R_3**	**R4**	**R5**	
	H	OH	OH	H	H	Pinocembrin
	H	OH	OCH_3	H	H	Pinostrobin
	OH	OH	OH	H	H	Pinobanksin
	$OCOCH_3$	OH	OH	H	H	Pinobanksin -3-*O*-acetate
	$OCOC_2H_5$	OH	OH	H	H	Pinobanksin-3-*O*-propianate
	$OCOC_3H_7$	OH	OH	H	H	Pinobanksin-3-*O*-butyrate
	$OCOC_4H_9$	OH	OH	H	H	Pinobanksin-3-*O*-pentanoate
	OH	OCH_3	OH	H	H	3,7-dihydroxy-5-methoxyflavanone
	H	OH	OH	H	OH	Naringenin
	H	OH	OH	H	OCH_3	Biochanin A
	H	H	OH	H	OH	Liquiritigenin
	OH	OH	OH	H	OH	Eriodictyol
	$OCOC_3H_7$	OH	OH	H	OH	5,7- Dihydroxy-3-butanoyloxyflavanone
	OH	OH	OH	H	OCH_3	Hesperetin
Isoflavonoids						
	R1	R2		R3		
	OH	OH		OH		Genistein
	OH	OH		OCH_3		Prunetin
	OCH_3	H		OH		Formonontin
Geranyl flavanones						Isonymphaeol B (Propolin F)

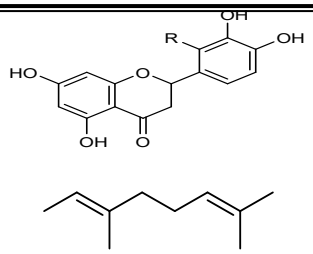
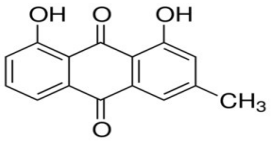
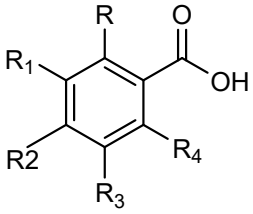
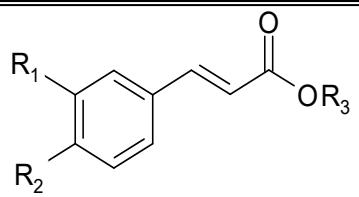
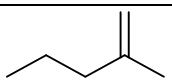
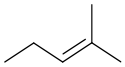
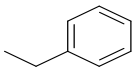
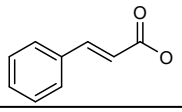
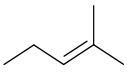
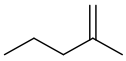
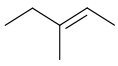
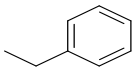
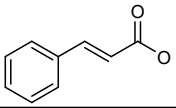
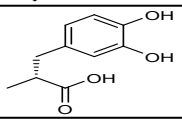
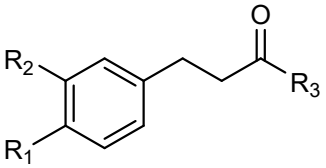
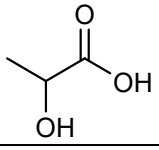
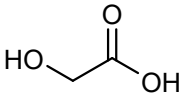
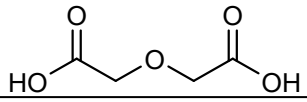
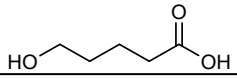
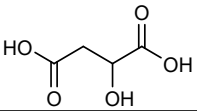
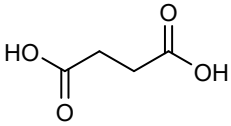
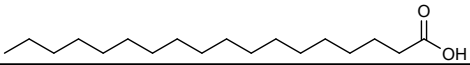
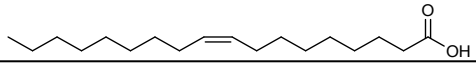
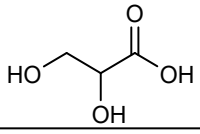
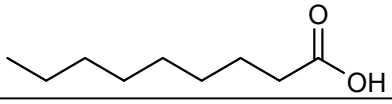
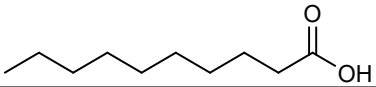
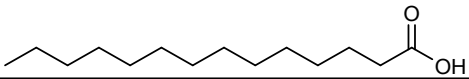
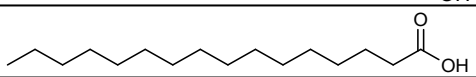
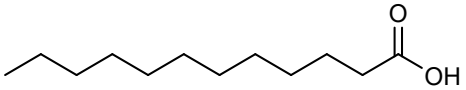
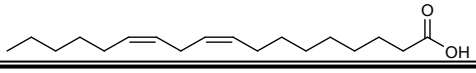
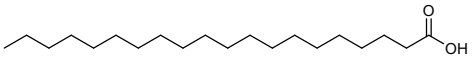
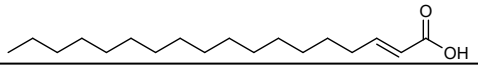
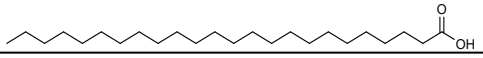
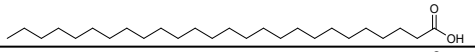
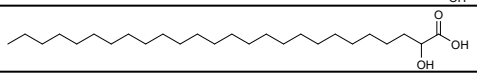
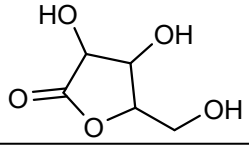
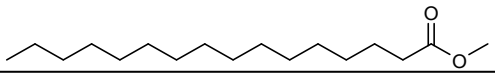
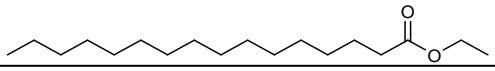
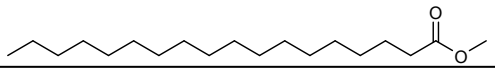
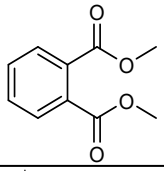
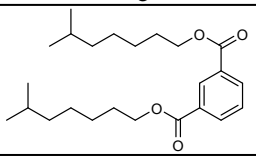
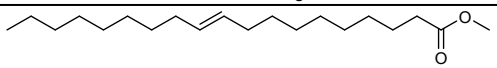
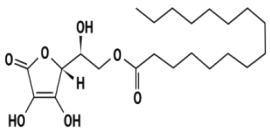
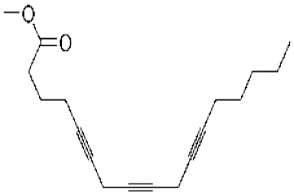
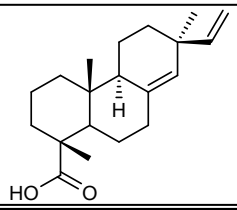
		Nymphaeol B (Propolin D)
Anthraquinones		Chrysophanic acid

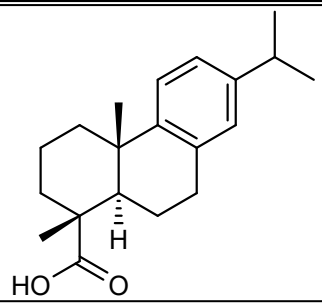
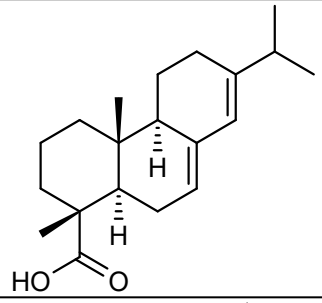
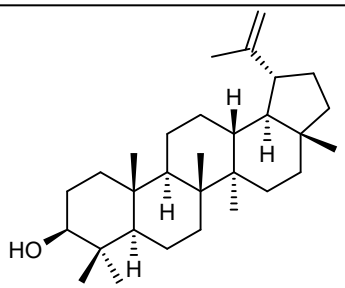
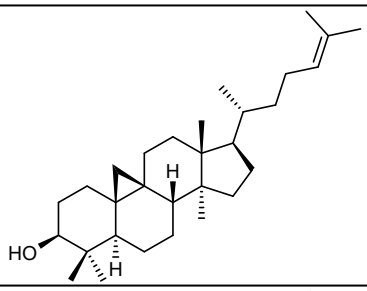
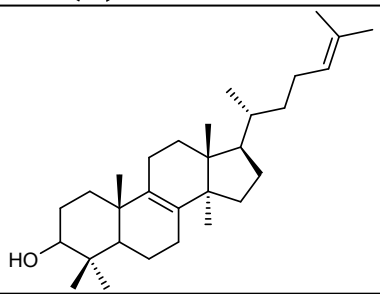
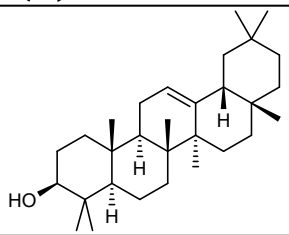
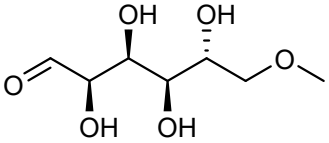
Table S1. (cont.)

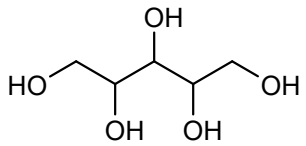
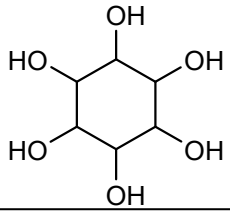
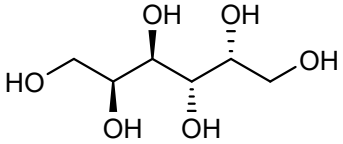
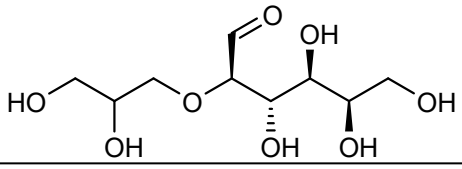
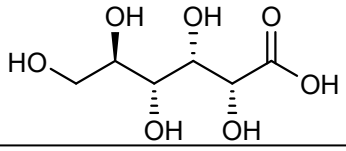
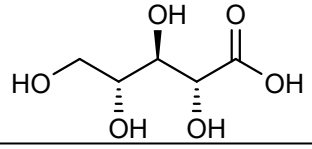
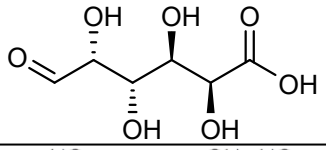
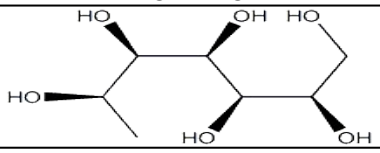
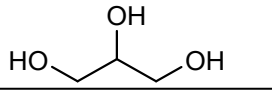
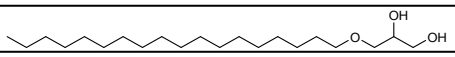
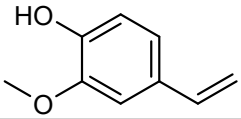
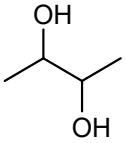
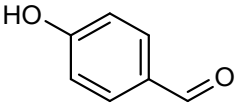
hydroxybenzoic acid derivatives					
	R	**R1**	**R2**	**R3**	**R4**
	H	H	H	H	H	Benzoic acid
	H	H	OH	H	H	P-Hydroxy benzoic acid
	H	OH	OH	H	OH	2, 3, 5-trihydroxybenzoic acid
	H	OH	OH	OH	H	Gallic acid
	H	OH	H	H	OH	Gentisic acid
	H	OH	OH	H	H	Protocatechuic acid
	H	H	H	H	OH	Salicylic acid
	H	H	OH	H	OH	4-Hydroxysalicylic acid
	OH	H	H	H	OH	6-Hydroxysalicylic acid
	OH	H	OH	H	OH	Phloroglucinic acid
	H	OCH3	OH	H	H	Vanillic acid

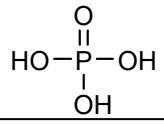
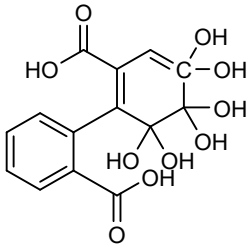
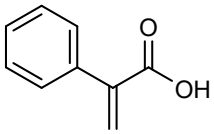
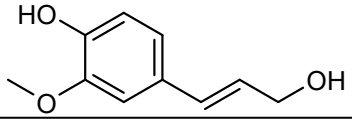
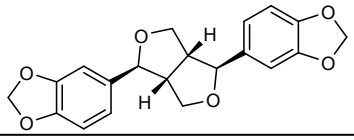
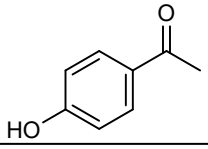
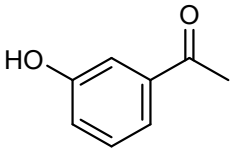
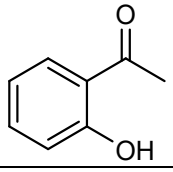
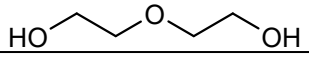
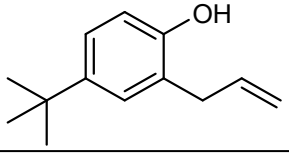
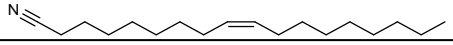
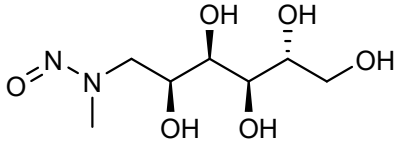
hydroxycinnamic acid derivatives and their esters			
	R1	**R2**	**R3**
	H	H	H
	OH	OH	H
	OCH_3	OCH_3	H
	OH	OCH_3	H
	OH	OCH_3	
	OH	OCH_3	H
	OH	OCH_3	
	H	OH	OH
	H	OH	OH
	H	OH	
	H	OH	
	OH	OH	
	OH	OH	
	OH	OH	
	OH	OH	
	OH	OH	Benzylcaffeate
	OH	OH	phenethylcaffeate
	OH	OH	
	OH	OH	
	OH	OH	
	OH	OH	
			Cinnamic acid
			Caffeic acid
			Dimethylcaffeic acid
			Ferulic acid
			3-Methyl 3-butenyl ferulate
			Isoferulic acid
			3-Methyl-2-butenyl isoferulate
			cis-*p*-Coumaric acid
			trans-*p*-Coumaric acid
			Benzyl-trans-coumarate
			Cinnamyl-trans-coumarate
			3-Methyl-2-butenylcaffeate
			3-Methyl-3-butenyl caffeate
			2-Methyl-2-butenylcaffeate
			Cinnamylcaffeate
			Rosmarinic acid
			Tetradecyl caffeate
			Tetradecenyl caffeate

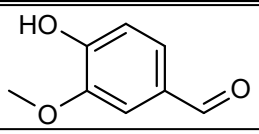
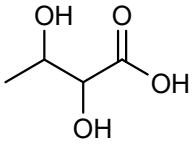
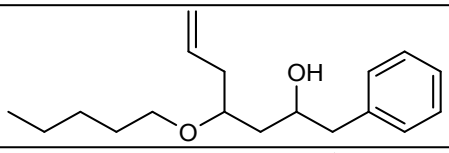
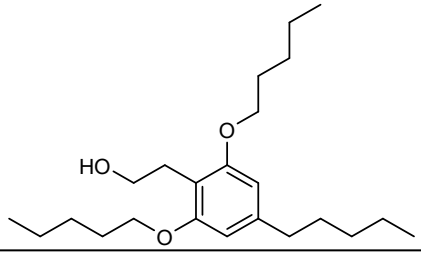
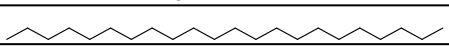
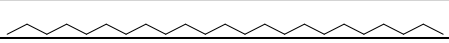
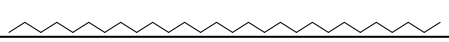
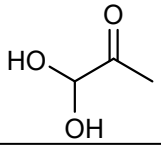
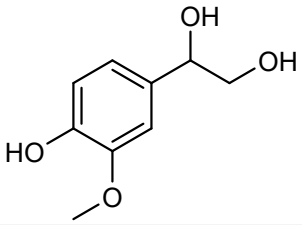
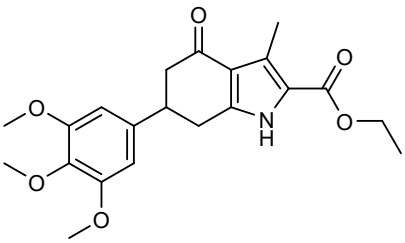
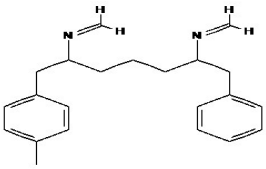
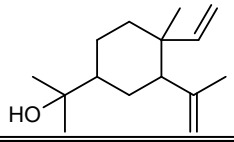
	OH	OH		Hexadecyl caffeate
				
	R1	R2	R3	
	OH	H	OH	Hydrocoumaric acid
	H	H	OH	Hydrocinnamic acid
	OH	OH	OH	Hydrocaffeic acid
Aliphatic acids and their esters				Lactic acid
				Glycolic acid
				Diglycolic acid
				5-Hydroxy-n-valeric acid
				Malic acid
				Succinic acid
				Stearic acid
				Oleic acid
				Glyceric acid
				Pelargonic acid
				Capric acid
				Myristic acid
				Palmitic acid
				lauric acid
				Linoleic acid

		Arachidic acid
		Octadecenoic acid
		Lignoceric acid
		Cerotic acid
		pyrrolidide
		Arabinonic acid
		Methyl palmitate
		Ethyl palmitate
		Stearic acid methyl ester
		Dimethyl phthalate
		Di-isooctyl phthalate
		Ethyloleate
		Ascorbyl palmitate
		5,8,11-Heptadecatriynoic acid methyl ester
Di and Triterpenes		Pimaric acid

		Dehydroabietic acid
		Abietic acid
		Lupeol
		Cycloartinol
		Lanosterol
		α-Amyrin
Sugars		Methylglucose

		Xylitol
		Inositol
		Galactitol
		2-O-Glycerylgalactose
		Gluconic acid
		Ribonic acid
		Galacturonic acid
		D-glycro-D-manno-Heptitol
Alcohols/ Phenols/ Aldehydes/others		Glycerol
		Glycerol octadecyl ether
		2-Methoxy-4-vinylphenol
		Butyraldehyde
		2,3- butandiol
		4 -Hydroxy-benzaldehyde

		Phosphoric acid
		Ellagic acid
		Atropic acid
		Coniferyl alcohol
		Sesamin
		P-Acetophenol
		m-Acetylphenol
		O-Acetylphenol
		Diethylene glycol
		4(t-Butyl)2(prop-2'enyl) phenol
		Oleanitrile
		Batilol
		Glucitole

		Vanillin
		4-deoxy-erythronic acid
		4-(pentyloxy)-1-phenylhept-6-en-2-ol
		2-(4-pentyl-2,6-bis(pentyloxy)phenyl)ethan-1-ol
		Docosane
		Tricosane
		Octacosane
		Dihydroxyacetone
		Vanylglycol
		1H-Indole-2-carboxylic acid, 3-methyl-4-oxo-6(3,4,5-trimethoxyphenyl)4,5,6,7-tetrahydro, ethyl ester
		1-Phenyl-7-p-tolyl-2,6-diisocyano-heptane
		2-(3-Isopropenyl-4-methyl-4-vinylcyclohexyl)-2-propanol

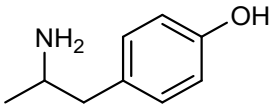
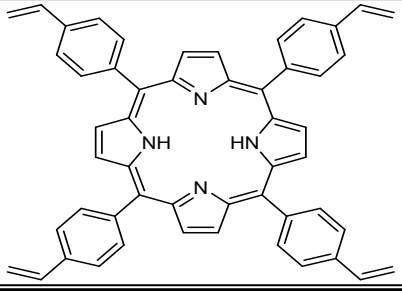
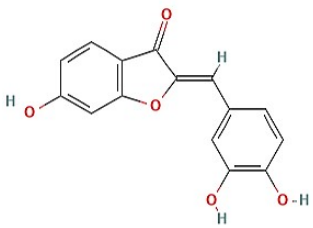
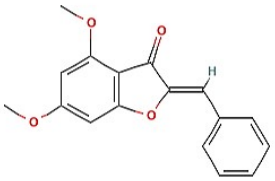
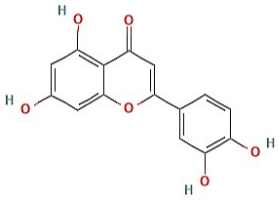
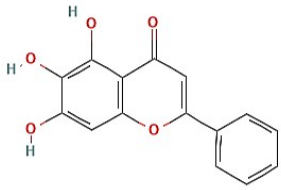
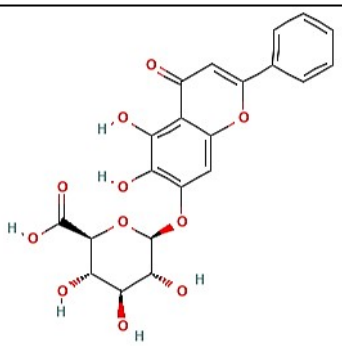
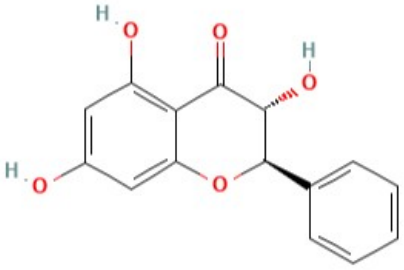
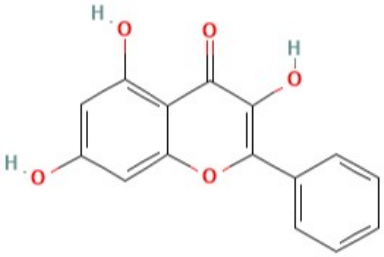
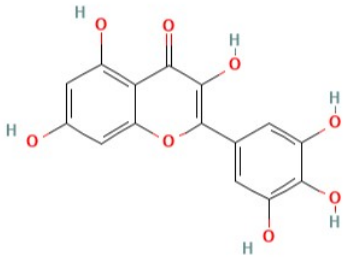
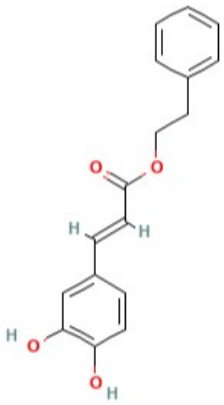
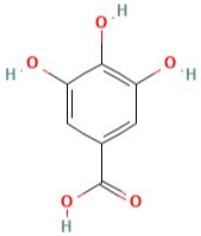
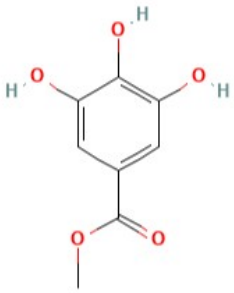
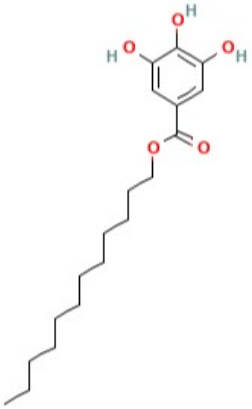
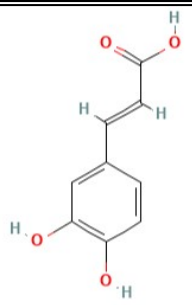
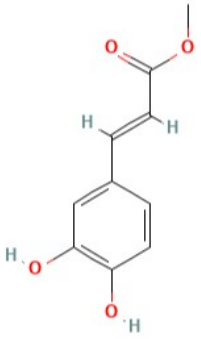
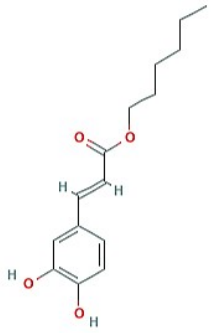
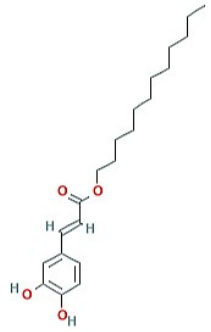
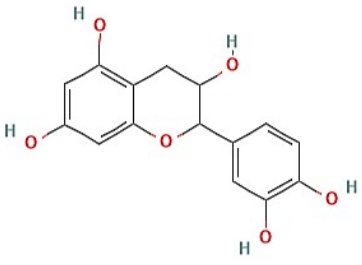
		4-(2-aminopropyl)phenol
		5,10,15,20-Tetrakis-(4-vinyl-phenyl)porphyrin

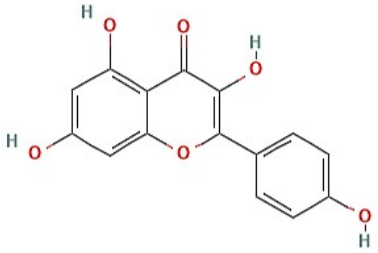
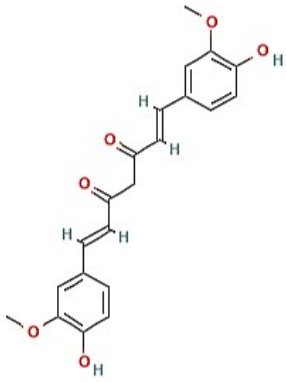
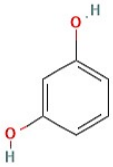
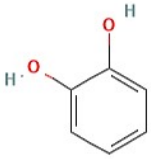
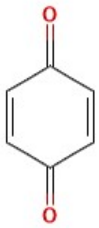
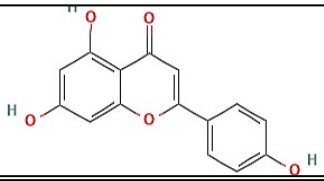
Table S2: Structural features and IC_{50} values of 30 compounds included in the validation set of docking process

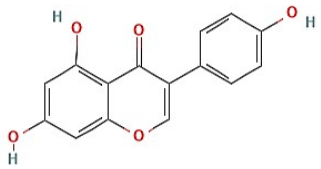
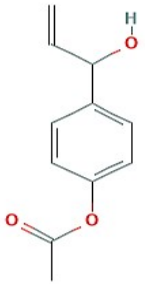
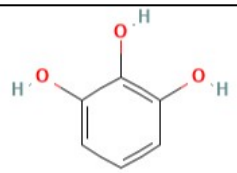
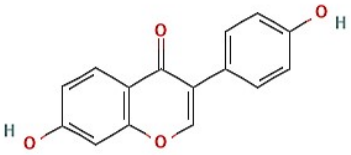
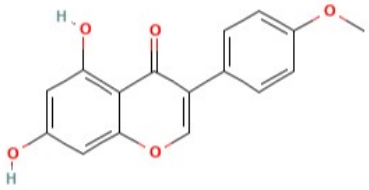
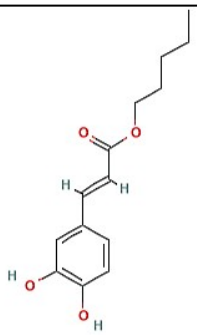
No	Name	IC_{50} (μM) (experimental)	Structure	Reference
1	Sulfuretin	3.10 ± 0.38		1

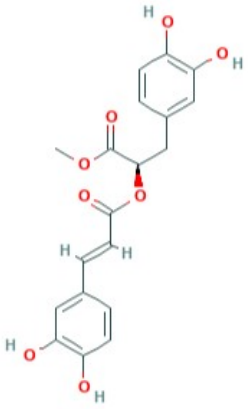
2	(2Z)-2-Benzylidenebenzofuran-3-(2H)-one	4.47 ± 0.21		1
3	Luteolin	4.79 ± 0.02		2
4	Baicalein	7.54 ± 0.06		3
5	Baicalin	1.23 ± 0.03		3
6	Pinobanksin	25.10 ± 0.14		4
7	Galangin	18.09± 0.12		4

8	Myricetin	2.17± 0.04		5
9	caffeic acid phenethyl ester	3.5±0.11		6
10	Gallic acid	200±0.32		7
11	Methyl gallate	212±0.4		7
12	Dodecyl gallate	49±0.21		7

13	Caffeic acid	204±1.2		7
14	Methyl caffeate	143 ± 13		7
15	Hexyl caffeate	19.0 ± 1.0		7
16	Decyl caffeate	10.0 ± 1.0		7
17	Catechin	22±1.28		8

18	Kaempferol	25±0.67		8
19	Curcumin	26±0.88		7
20	Resorcinol	55±0.4		8
21	Catechol	58±0.64		8
22	1,4-Benzoquinone	42±0.78		8
23	Apigenin	3.57 ± 0.03		9

24	genistein	1.73 ± 0.04		9
25	Hydroxychavicol	16.7±1.3		9
26	pyrogallol	36±0.36		8
27	Daidzein	3.16±0.1		9
28	Biochanin A	2.92±0.03		9
29	Pentyl caffeate	18.0 ± 0.9		7

30	Methyl rosmarinate	2.31±0.03		7

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