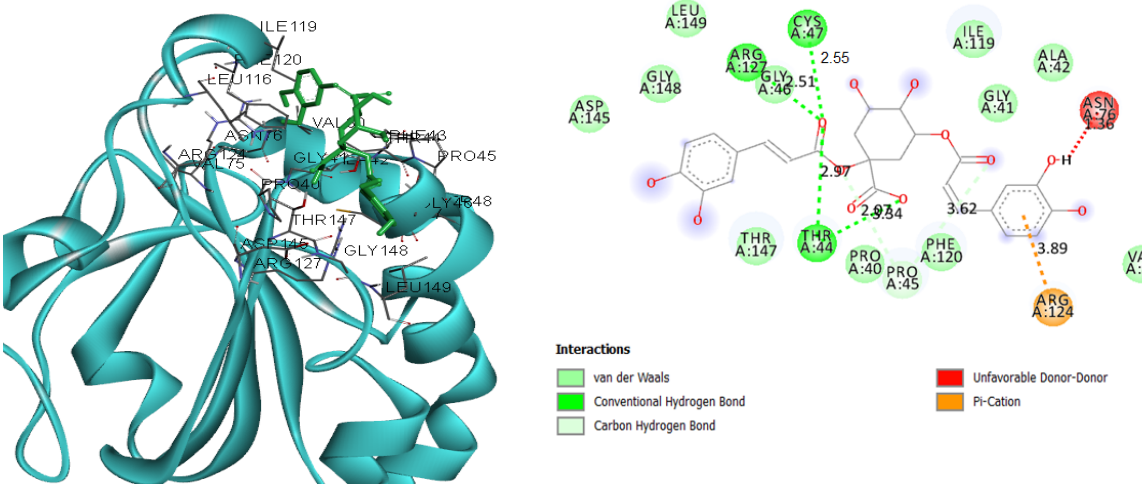
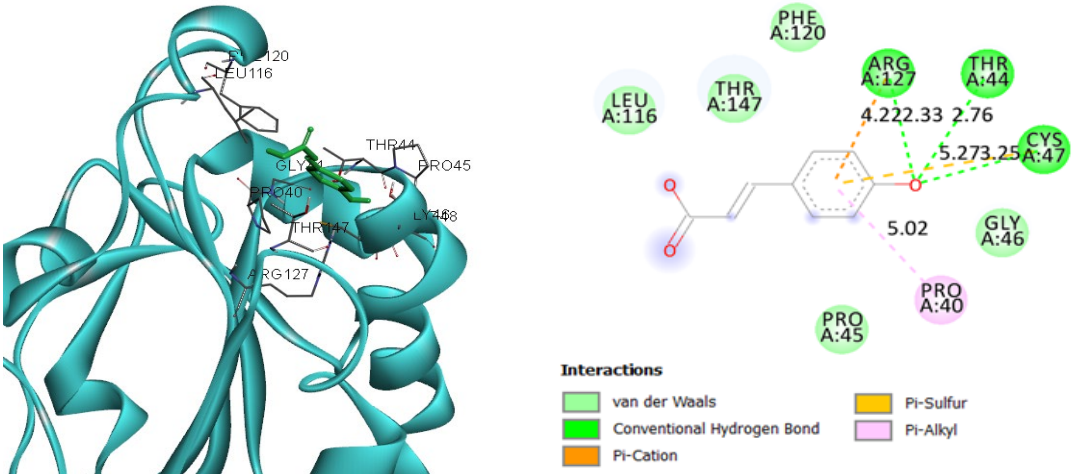
Table S1. Major phytochemicals with the lowest binding energies and their interaction residues with human peroxredoxin 5.

Compounds Receptor vs. Targets	Interaction type	Interacting Residues (1HD2)	Binding Energy (kcal/mol)
1,3-di-O-caffeoyquinic acid	van der Waals H bond C-H bond Unfavorable Donor-Donor Pi-Cation	Pro40, Gly41, Ala42, Gly46, Val80, Ile119, Phe120, Asp145, Thr147, Gly148, Leu149 Thr44 (2.07) (2.97), Cys47 (2.55), Arg127 (2.51) Pro45 (3.34) (3.62) Asn76 (1.36) Arg124 (3.83)	-6.6
p-Coumaric acid	van der Waals C-H bond Pi-Cation Pi-Sulfur Pi-Alkyl	Pro45, Gly46, Leu116, Phe120, Thr147 Thr44 (2.76), Cys47 (3.25), Arg127 (2.33) Arg127 (4.22) Cys47 (5.27) Pro40 (5.02)	-4.4
Trans-Ferulic acid	van der Waals H bond C-H bond Unfavorable Donor-Donor Pi-Cation Pi-Sulfur Pi-Alkyl	Thr44, Pro45, Leu116, Leu149, Phe120 Gly46 (2.37) (2.56), Cys47 (2.41) Thr147 (3.06) Arg127 (1.62) Arg127 (4.21) Arg127 (5.24) Pro40 (5.07)	-4.7
Naringin	van der Waals H bond C-H bond Unfavorable Acceptor-Acceptor Alkyl/Pi-Alkyl	Gly41, Thr44, Gly46, Leu149, Phe120, Arg127 Ala42 (1.97), Phe43 (2.57), Asn76 (2.15), Arg124 (2.11) (2.36), Thr147 (2.60) Phe43 (3.13) Phe43 (2.86) Pro45 (4.80), Val80 (3.98) (4.53), Ile119 (4.87)	-7.0
Rosmarinic acid	van der Waals H bond C-H bond Unfavorable Donor-Donor Pi-Cation Pi-Alkyl	Gly41, Ala42, Thr44, Pro45, Gly46, Val80, Leu116, Ile119, Phe120 Cys47 (2.76), Arg127 (2.37) Thr147 (3.01) Asn76 (1.11). Arg124 (4.15). Pro40 (5.27)	-6.6
Rutin	van der Waals H bond C-H bond Unfavorable Donor-Donor Pi-Sigma	Ala42, Phe43, Thr44, Pro45, Phe120, Val75, Val80. Asp77 (2.38), Arg124 (1.89). Asn76 (3.42). Asn122 (2.39). Ile119 (3.83).	-6.5
Salviolinic acid	van der Waals H bond	Pro40, Gly41, Ala42, Asn76, Val80, Ile119, Leu149.	-6.3

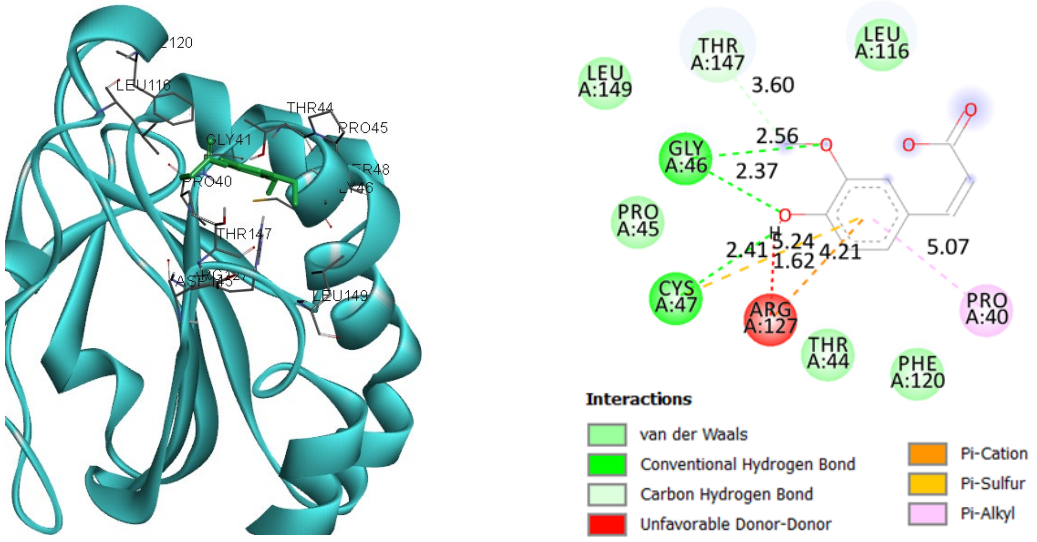
	Unfavorable Donor-Donor: Pi-Cation Pi-Pi T shaped	Phe43 (3.01), Thr44 (2.92), Gly46 (2.37), Cys47 (2.79), Thr147 (2.62). Arg127 (1.30). Arg124 (3.73). Phe120 (5.42). Pi-Alkyl: Po45 (5.43).	
4,5-di-O-caffeoyquinic acid	van der Waals H bond C-H bond Pi-Pi T shaped	Pro40, Gly41, Gly46, Cys47, Leu116, Leu112, Ile119, Arg127, Gly146, Thr147 Asp145 (2.57) (3.58) Pro45 (3.55), Thr44 (3.58) Phe120 (5.09)	-5.5
Apegenin-7-O-glucoside	van der Waals H bond Pi-Pi stacked Pi-Alkyl	Ala42, Thr44, Pro45, Val75, Ile119 Asp73 (2.76), Asn76 (2.43), Asn122 (2.06), Arg124 (2.56) (2.96). Phe120 (5.35), Phe43 (5.94) Val80 (5.39)	-6.5
Quercetrin (quercetin-3-O-rhamonoside)	van der Waals: H bond: Unfavorable Acceptor-Acceptor/Donor-Dnor Alkyl/Pi-Alkyl:	Gly41, Ala42, Thr44, Pro45, Ile119 Phe43 (3.04), Asn76 (2.48), Arg124 (2.54) Phe120 (2.70), Arg124 (5.36) Phe43 (4.61), Val80 (3.97)	-6.3
Cirsiliol	van der Waals H bond Unfavorable Donor-Donor Pi-Cation Pi-Pi T shaped Pi-Alkyl:	Gly41, Ala42, Phe43, Thr44, Pro45, Val80. Asn76 (1.95) (2.52). Arg124 (1.07). Arg124 (4.01). Phe120 (4.89). Ile119 (5.04)	-5.5



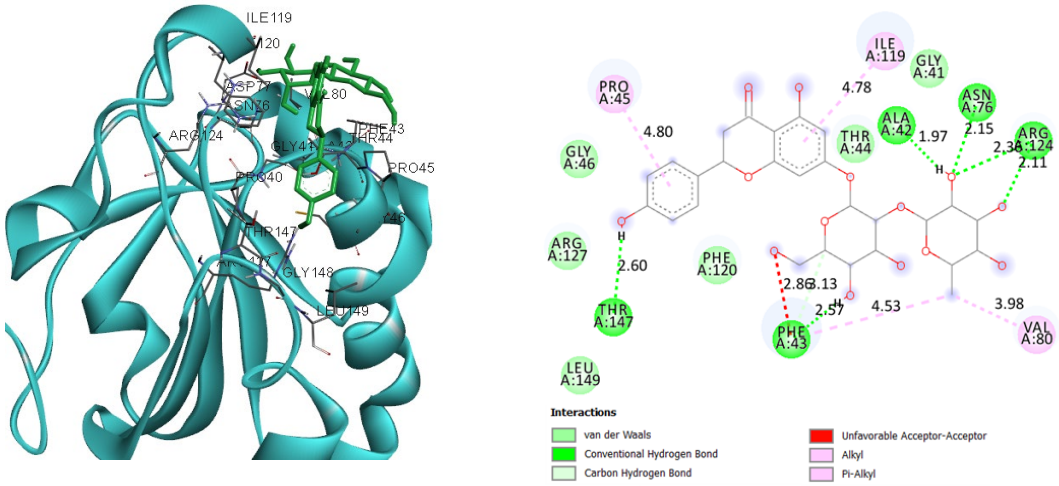
1,3-di-O-caffeoyquinic acid-1HD2



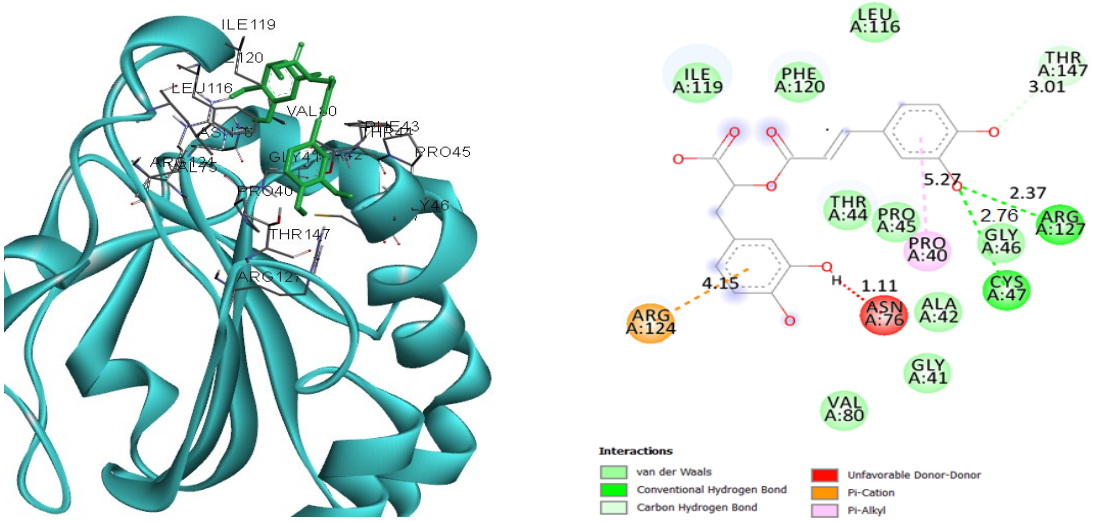
p-Coumaric acid-1HD2



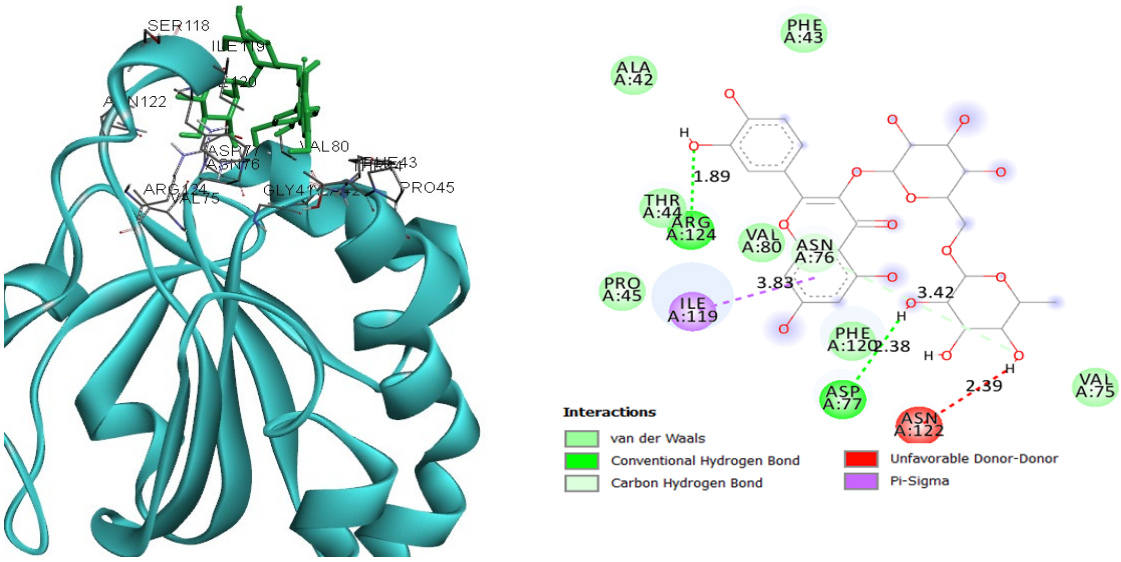
***Trans*-Ferulic acid-1HD2**



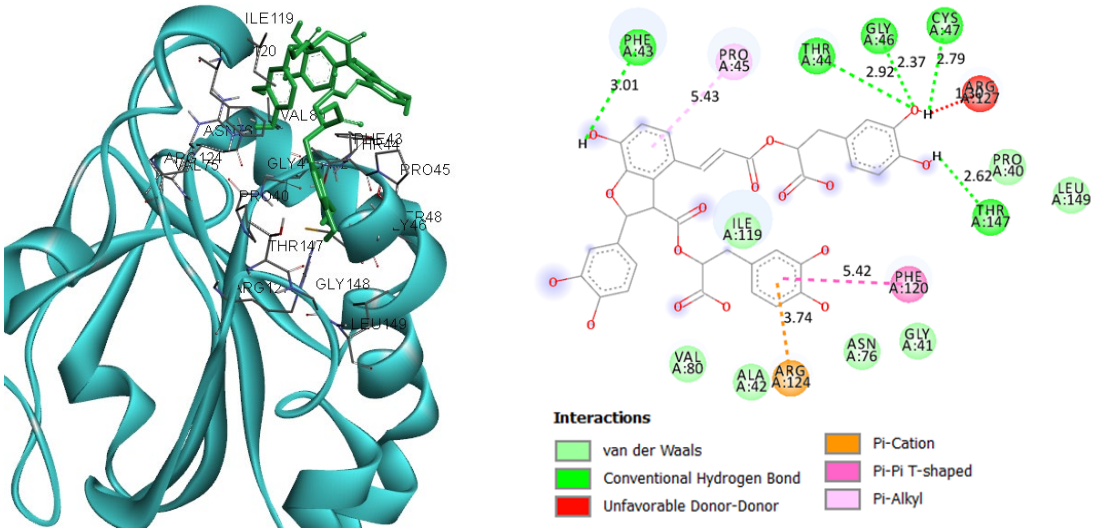
Naringin-1HD2



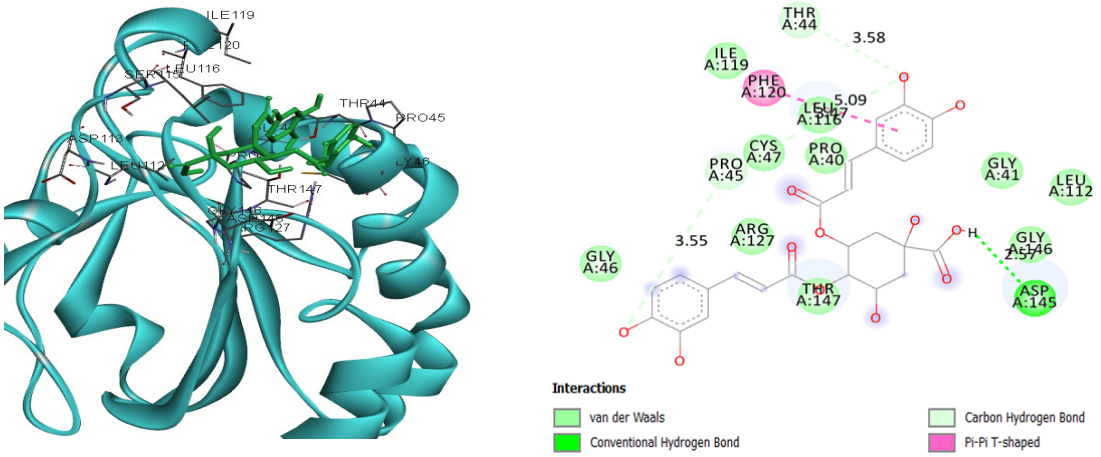
Rosmarinic acid-1HD2



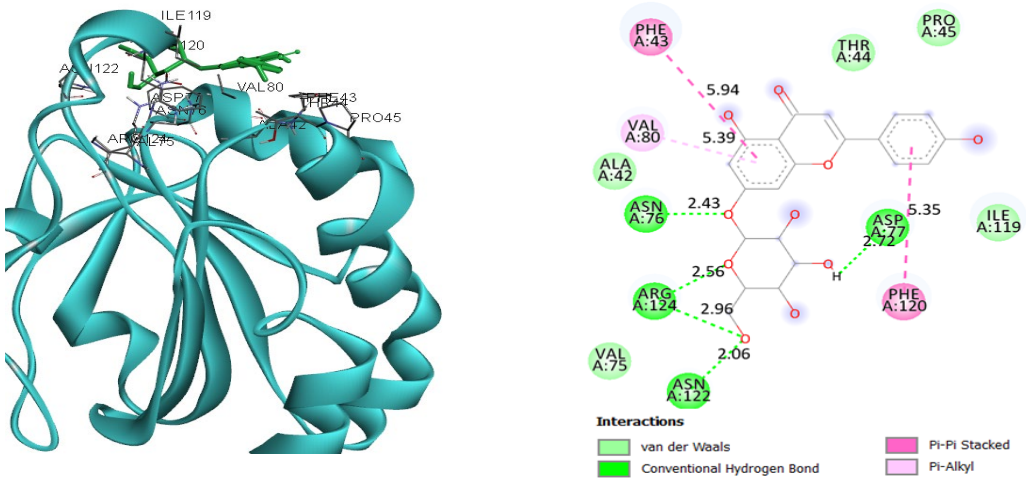
Rutin-1HD2



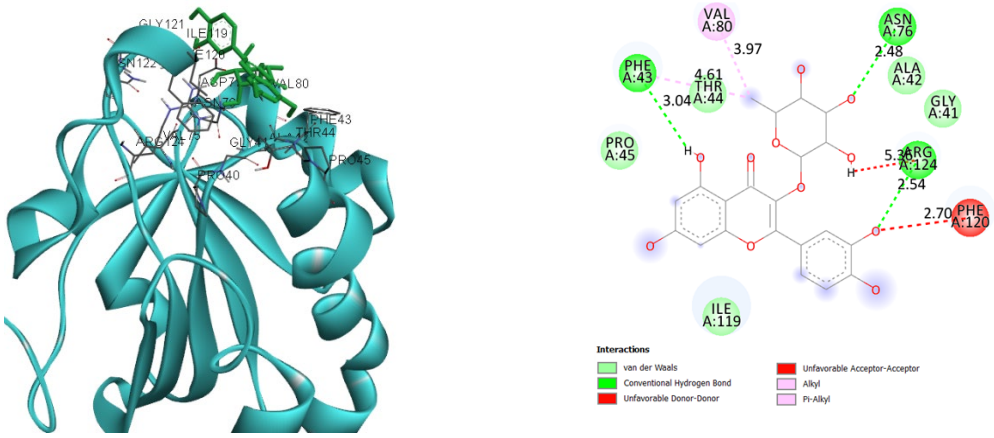
Salviolinic acid-1HD2



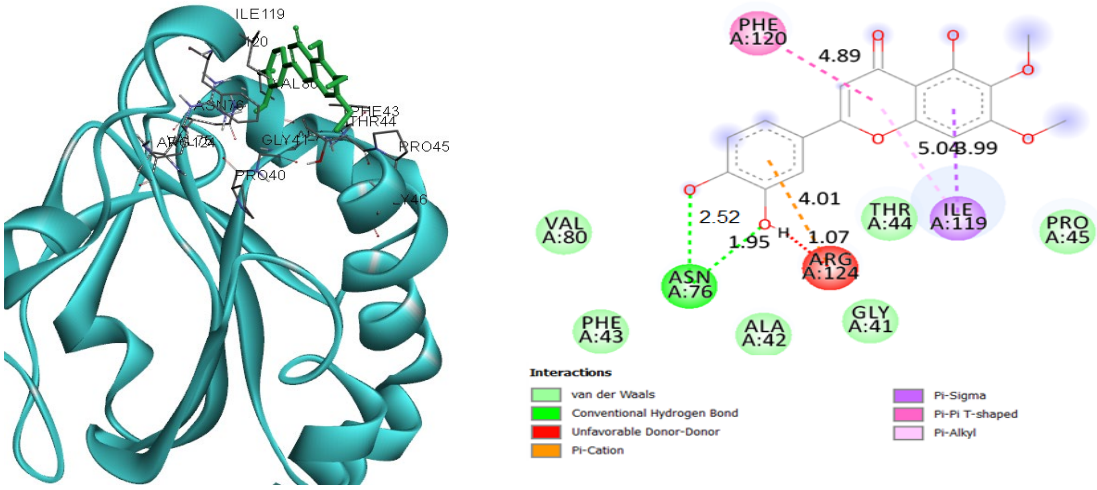
4,5-di-O-caffeoyquinic acid-1HD2



Apegenin-7-O-glucoside-1HD2



Quercetrin-1HD2



Cirsiliol-1HD2

Figure S1. Interactions of human Peroxiredoxin 5 receptor (PDB: 1HD2**)** with the selected major phytochemicals of *E. humile* Desf. ethyl extract with the lowest binding energies.

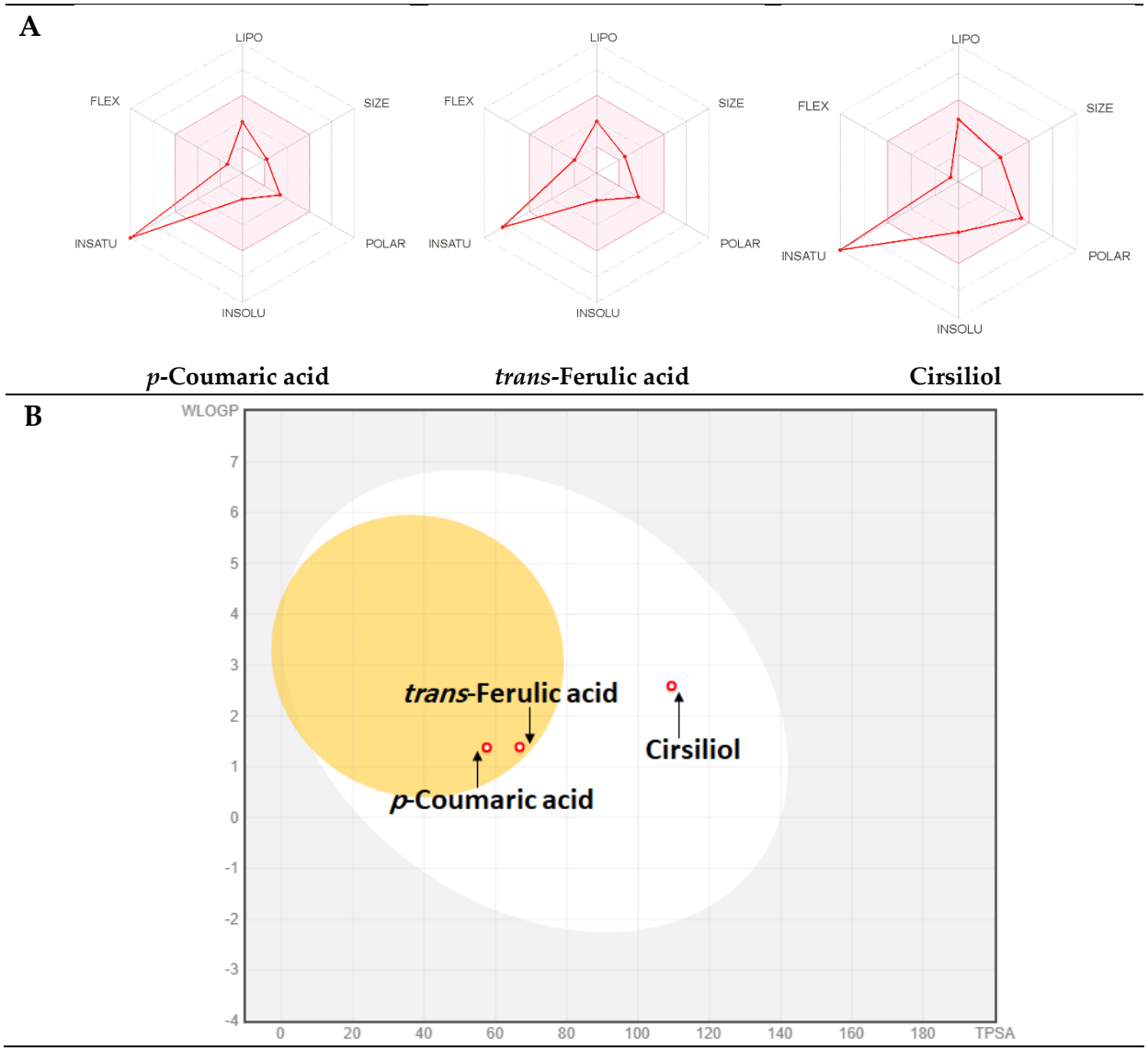


Figure S2. Bioavailability radar (**A**) and BOILED-Egg model (**B**) of the major constituents.