

FIGURES

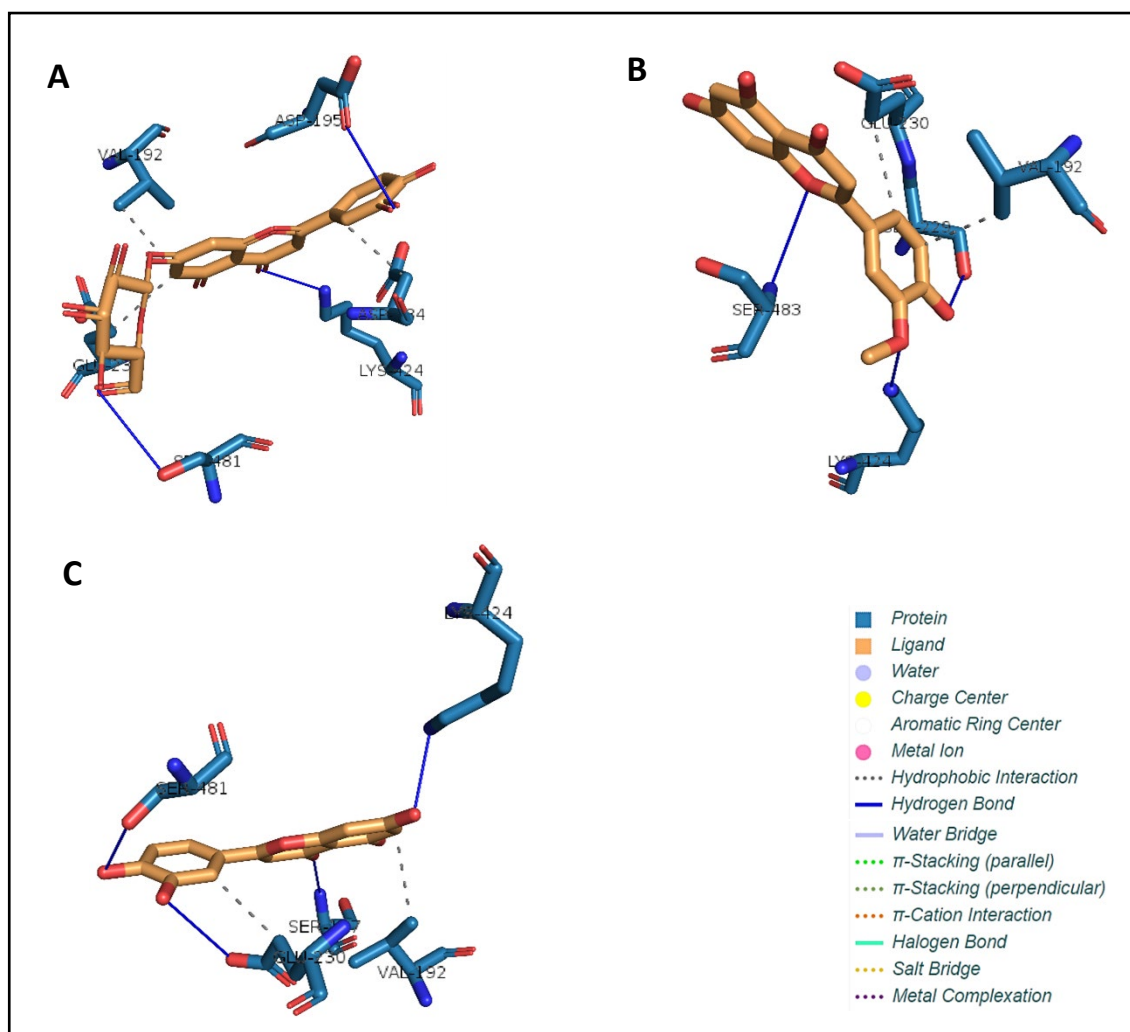


Figure 1. Interactions between the ligands and the amino acid residues of the active site: **A.** Luteolin 7-O- β -D-glucopyranoside ($C_{21}H_{20}O_{11}$), **B.** Chrysoeriol ($C_{16}H_{12}O_6$) and **C.** Luteolin ($C_{15}H_{10}O_6$) in complexes with target nsp4 (QHD43415_4).

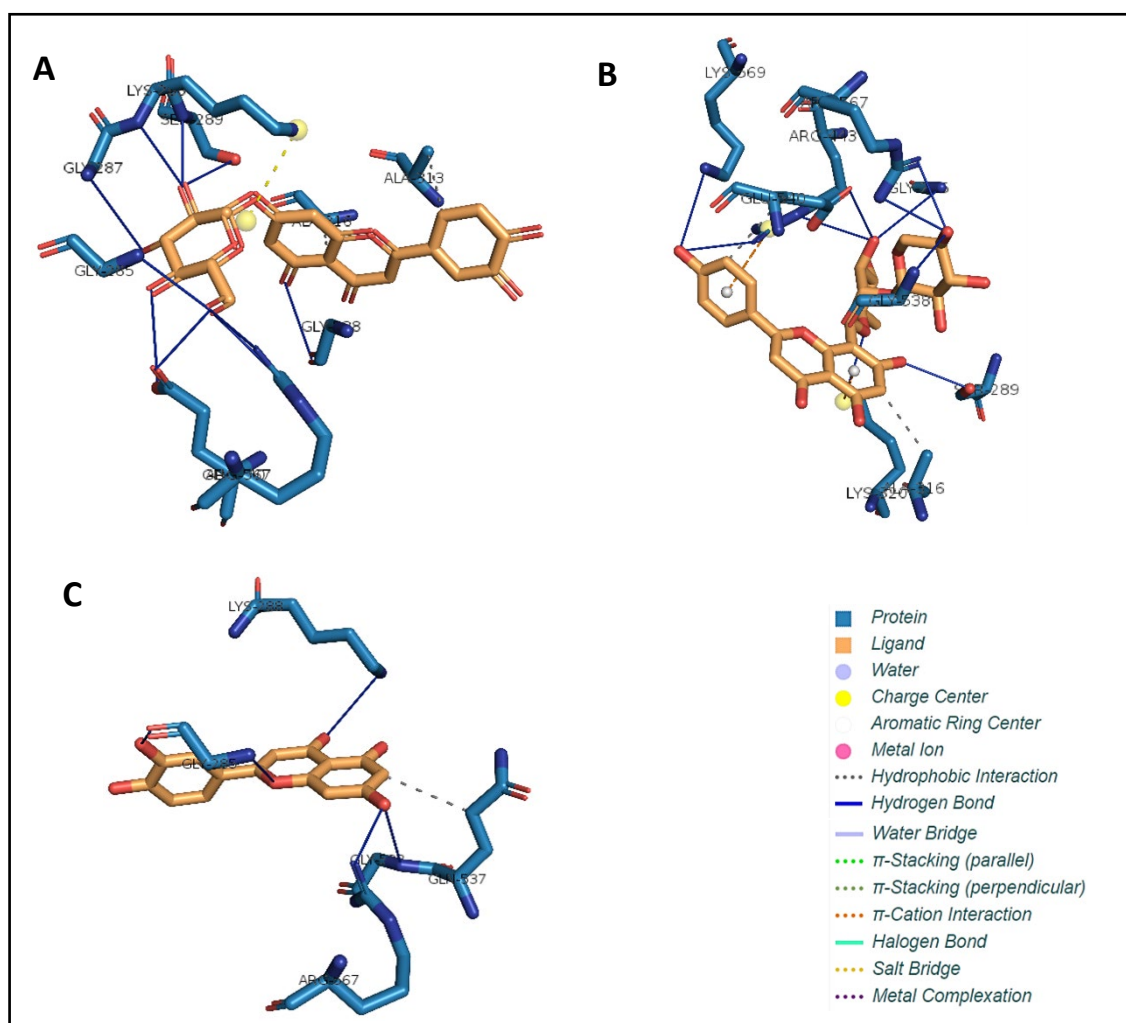


Figure 2. Interactions between ligands and amino acid residues at the active site: **A.** Luteolin-7-O-β-D-glucopyranoside ($C_{21}H_{20}O_{11}$), **B.** Vitexin-2''-O-xyloside ($C_{26}H_{28}O_{14}$) and **C.** Luteolin ($C_{15}H_{10}O_6$) in complexes with the Helicase target (QHD43415_12).

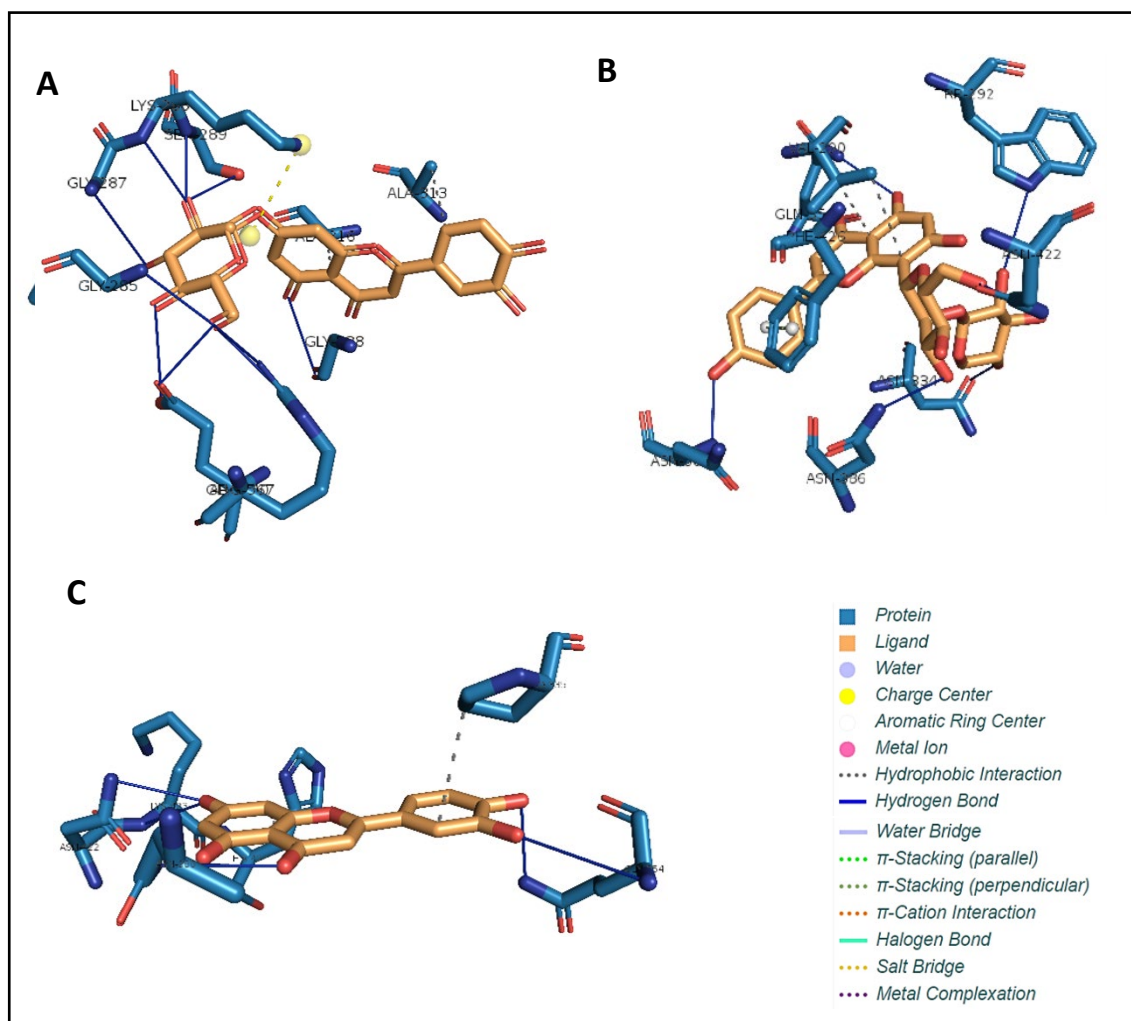


Figure 3. Interactions between ligands and amino acid residues at the active site: **A** Luteolin-7-O- β -D-glucopyranoside ($C_{21}H_{20}O_{11}$), **B** Vitexin-2''-O-xyloside ($C_{26}H_{28}O_{14}$) and **C** Luteolin ($C_{15}H_{10}O_6$) in complexes with the ExoN target (QHD43415_13).

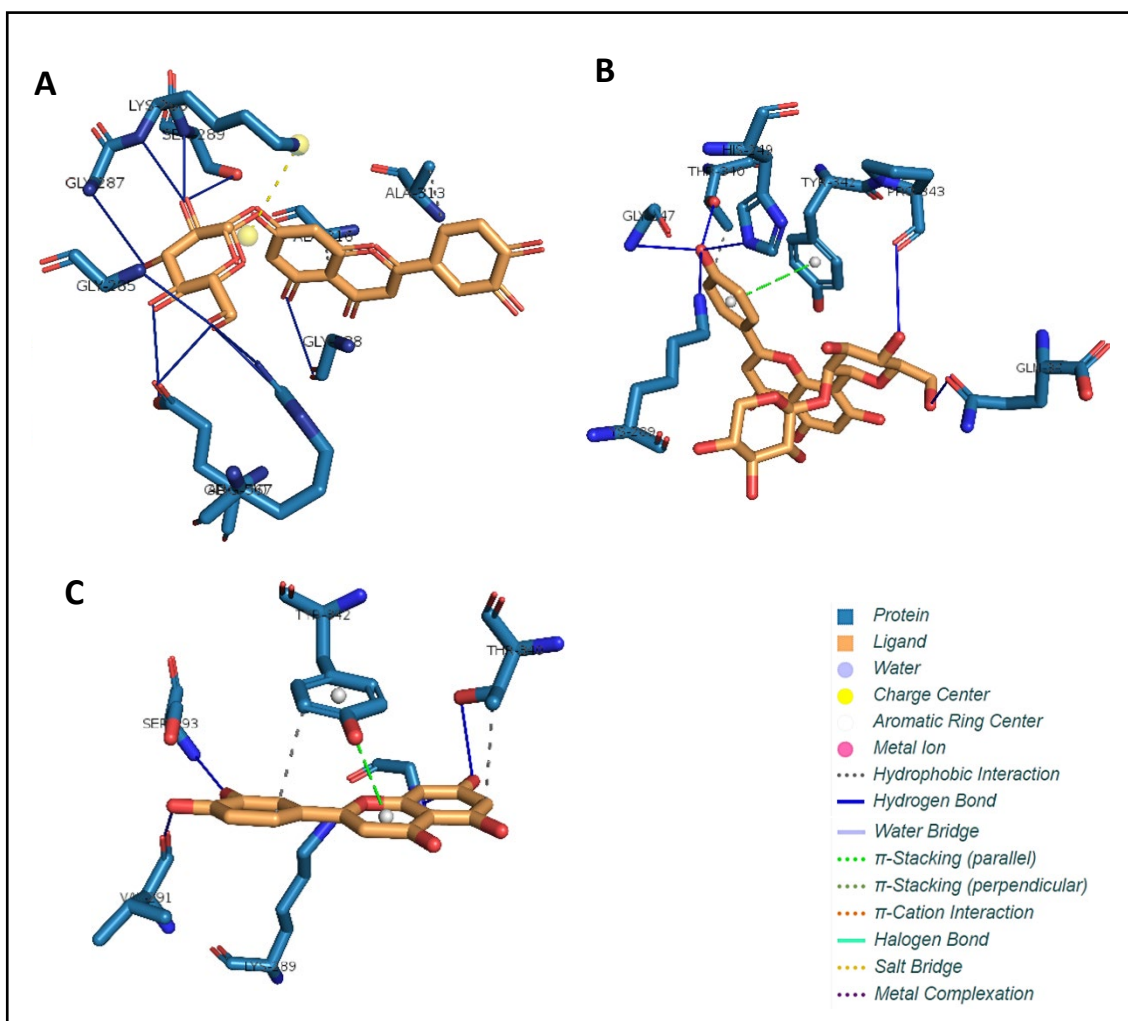
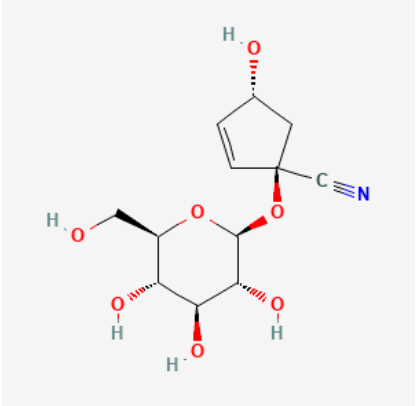
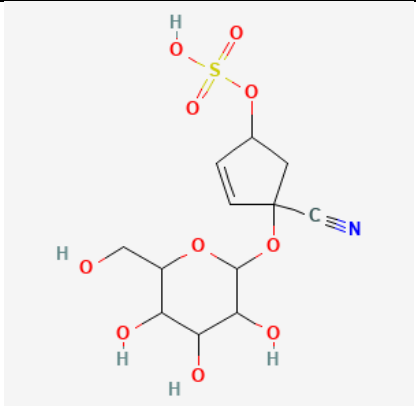
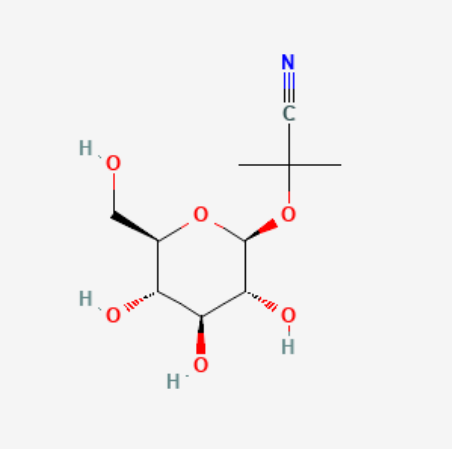
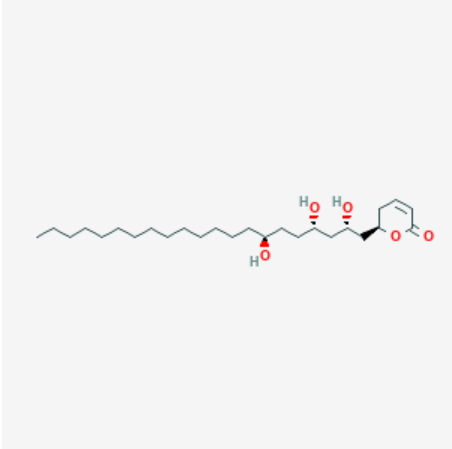


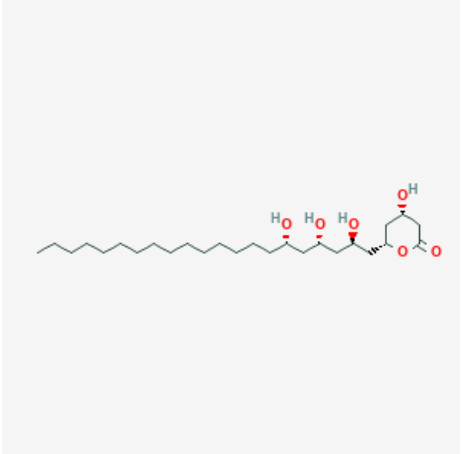
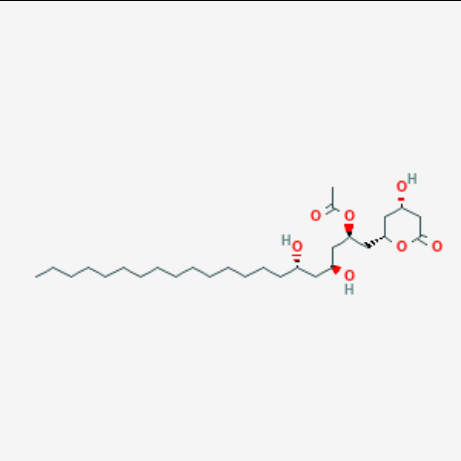
Figure 4. Interactions between the ligands and the amino acid residues of the active site: **A.** Luteolin-7-O-β-D-glucopyranoside ($C_{21}H_{20}O_{11}$), **B.** Vitexin-2''-O-xyloside ($C_{26}H_{28}O_{14}$) and **C.** Luteolin ($C_{15}H_{10}O_6$) in complexes with the target QHD43415_14 (Uridylate-specific endoribonuclease –NendoU).

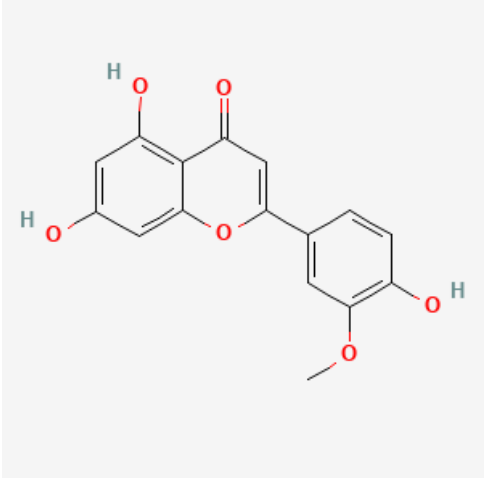
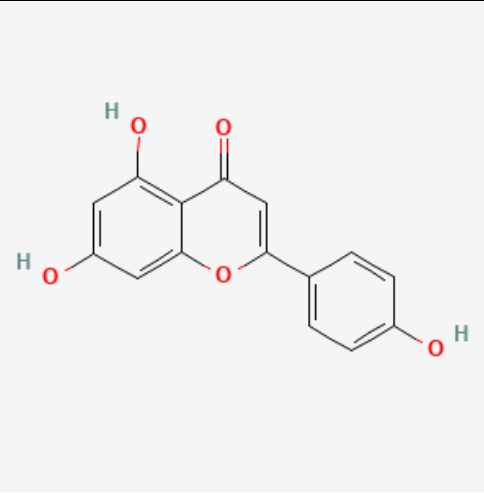
TABLE

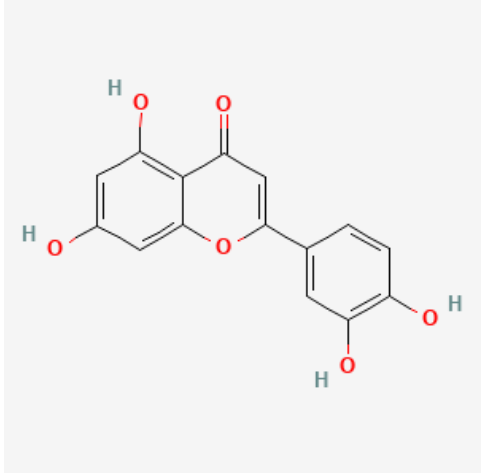
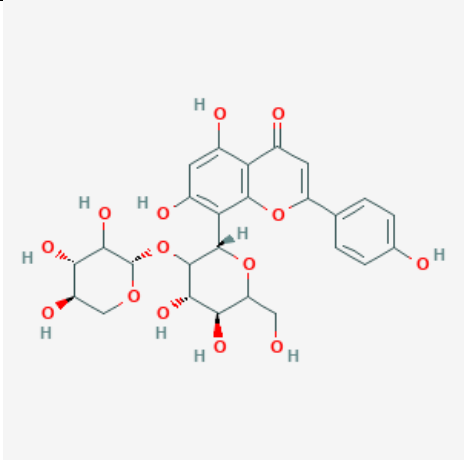
Table 1. Relationship between chemical groups, compounds and where they are found in *Passiflora foetida* with their possible biological effects.

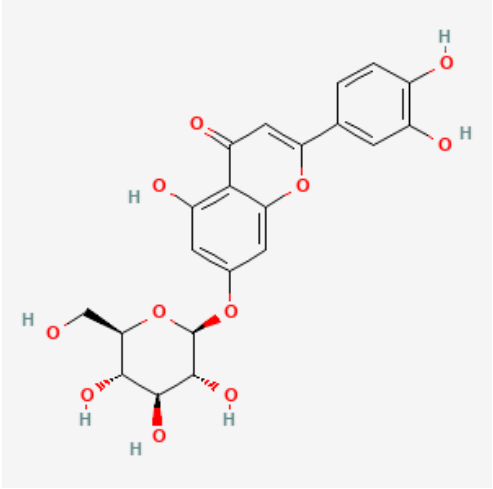
CHEMICAL GROUP	STRUCTURE	NAME ¹	PART OF THE PLANT WHERE IT WAS OBTAINED
Cyanogenic glycoside	 Volkenin	(1 <i>R</i> ,4 <i>R</i>)-4-hydroxy-1-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxycyclopent-2-ene-1-carbonitrile	Aerial parts (as mixed parts) ²
	 Tetraphyllin B Sulfate	[4-cyano-4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxycyclopent-2-en-1-yl] hydrogen sulfate	Aerial parts (as mixed parts) ²

CHEMICAL GROUP	STRUCTURE	NAME ¹	PART OF THE PLANT WHERE IT WAS OBTAINED
Cyanogenic glycoside	 Linamarin	2-methyl-2-[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropanenitrile	Aerial parts (as mixed parts) ²
α-Pyrone polyketides	 Passifloricin A	(2 <i>R</i>)-2-[(2 <i>S</i> ,4 <i>S</i> ,7 <i>S</i>)-2,4,7-trihydroxyhenicosyl]-2,3-dihydropyran-6-one	Leaf resin ³

CHEMICAL GROUP	STRUCTURE	NAME ¹	PART OF THE PLANT WHERE IT WAS OBTAINED
α-Pyrone polyketides	 Passifloricin B	(4 <i>S</i> ,6 <i>R</i>)-4-hydroxy-6-[(2 <i>R</i> ,4 <i>S</i> ,6 <i>S</i>)-2,4,6-trihydroxyhenicosyl]oxan-2-one	Leaf resin ³
	 Passifloricin C	[(2 <i>R</i> ,4 <i>S</i> ,6 <i>S</i>)-4,6-dihydroxy-1-[(2 <i>S</i> ,4 <i>S</i>)-4-hydroxy-6-oxooxan-2-yl]henicosan-2-yl] acetate	Leaf resin ³

CHEMICAL GROUP	STRUCTURE	NAME ¹	PART OF THE PLANT WHERE IT WAS OBTAINED
Flavonoids	 Chrysoeriol	5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)chromen-4-one	Stem bark ⁴
	 Apigenin	5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one	Stem bark ⁴

CHEMICAL GROUP	STRUCTURE	NAME ¹	PART OF THE PLANT WHERE IT WAS OBTAINED
Flavonoids	 Luteolin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxychromen-4-one	Stem bark ⁴
	 Vitexin-2''-O-xyloside	8-[(2 <i>S</i> ,4 <i>S</i> ,5 <i>S</i>)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2 <i>S</i> ,4 <i>S</i> ,5 <i>R</i>)-3,4,5-trihydroxyoxan-2-yl]oxyoxan-2-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one	Stem bark ⁴

CHEMICAL GROUP	STRUCTURE	NAME ¹	PART OF THE PLANT WHERE IT WAS OBTAINED
Flavonoids	 Luteolin 7-O-β-D-glucopyranoside	2-(3,4-dihydroxyphenyl)-5-hydroxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	Stem bark ⁴

¹ Chemical name obtained according to IUPAC (International Union of Pure and Applied Chemistry), computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14).

² According to Andersen, L.; Andersen, A.; Jaroszewski, J.W. Cyanogenesis of *Passiflora foetida*. Phytochemistry, 47(6), 1049-1050, 1998.

³ According to Echeverri, F.; et al.. Passifloricins, polyketides α-pirones from *Passiflora foetida* resin. Phytochemistry, 56(8), 881-885, 2001.

⁴ According to Nguyen, T.Y. et al.. Anti-inflammatory flavonoids isolated from *Passiflora foetida*. Natural Product Communications, 10(6), 929-931, 2015.