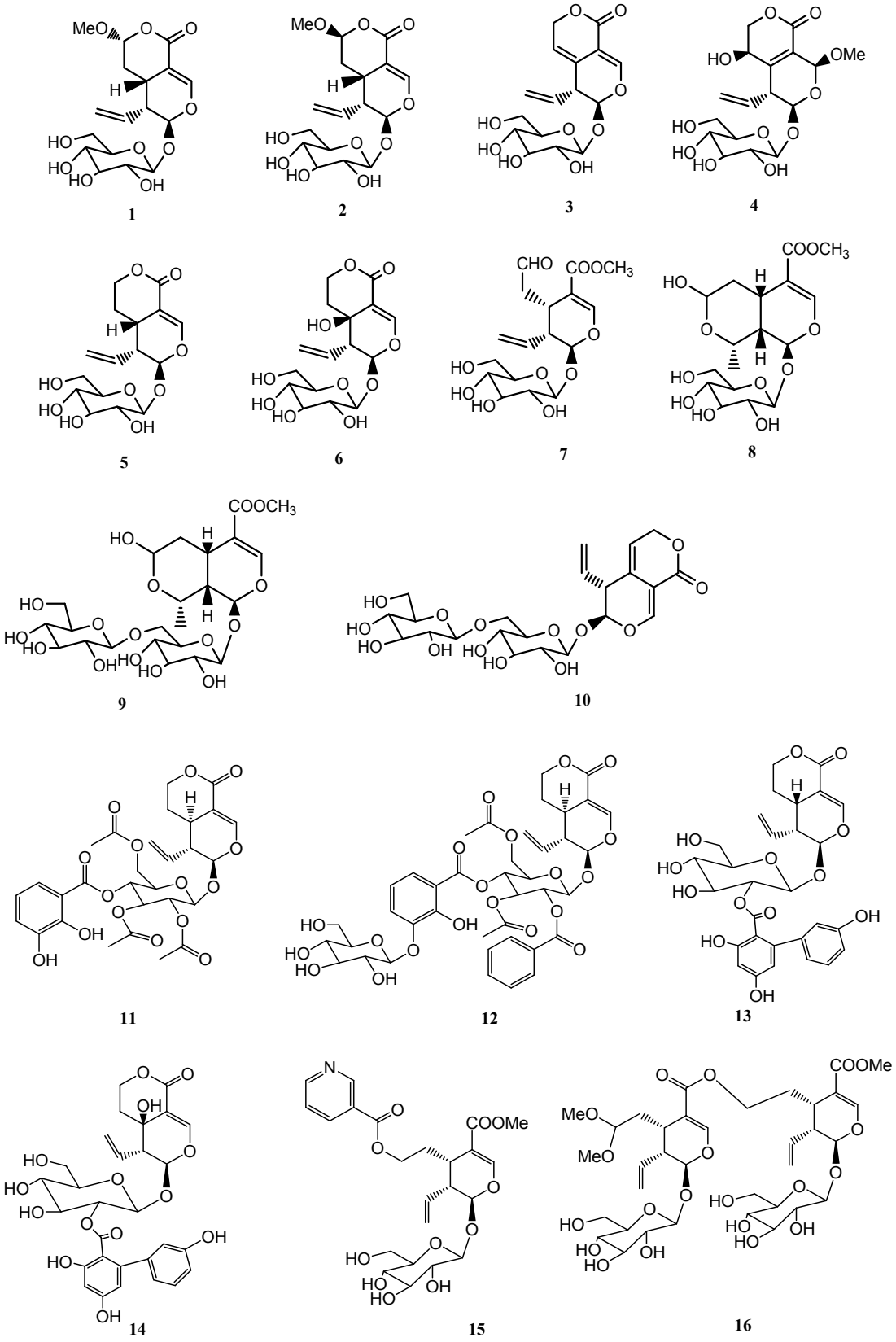
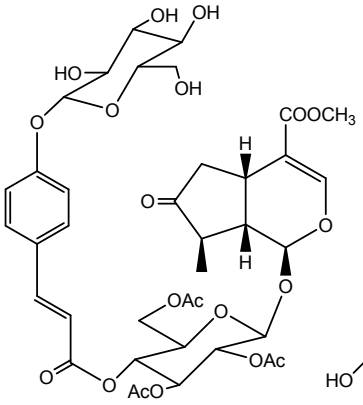
Supplementary Fig. 1 all the structures of the studied compounds 29 iridoids, seco-iridoids and analogss for CYP3A4 and CYP2D6.





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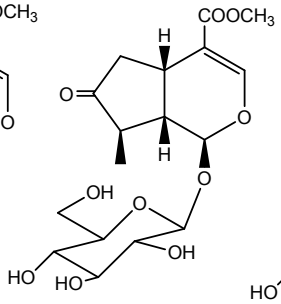

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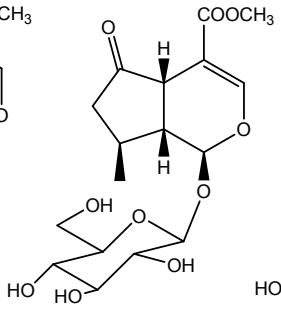

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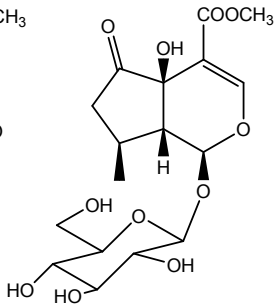

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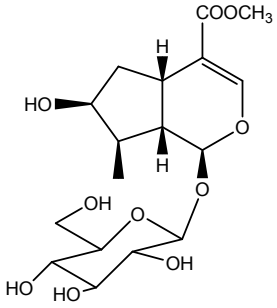

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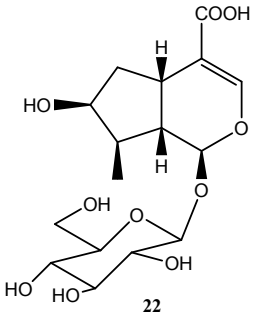

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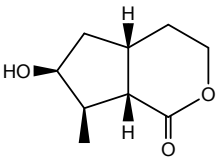

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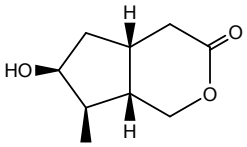

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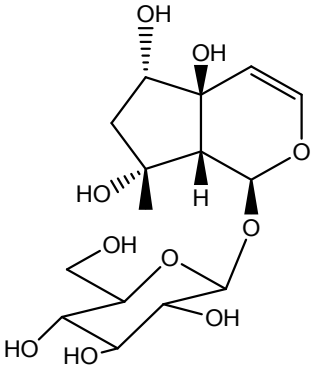

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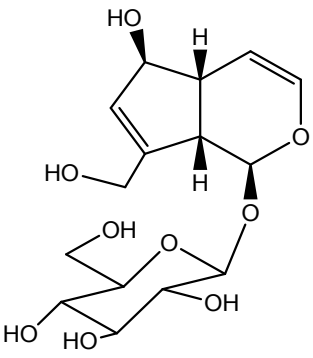

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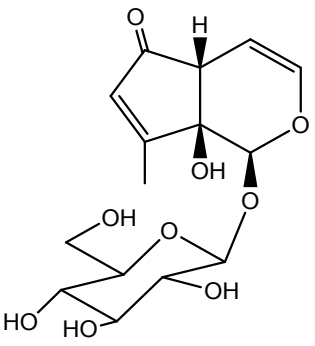

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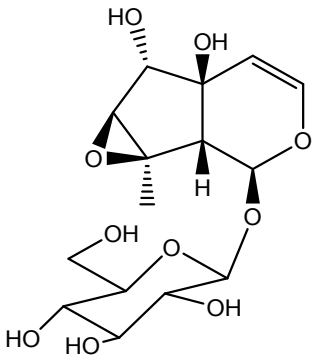

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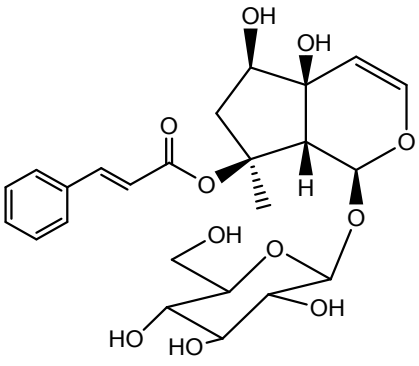

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Supplementary Table 1

Name	Formula	docking score	
		iridoids,seco-iridoids	analogs glycoside
(1S, 5R, 9R)- deglucosyltrifloroside	$C_{29}H_{32}O_{15}$	10.7289	
(1S,5R,9R)-scabraside	$C_{40}H_{44}O_{20}$	9.2446	9.5001
2',3',6'-tri-*O*-acetyl-4′-O-*trans*-*p*-(0-β-D –glucopyranosyl)coumaroyl-7-ketologanin	$C_{38}H_{46}O_{20}$	11.4408	10.568
6′-O-β-D-glucopyanosylmorroniside	$C_{23}H_{36}O_{16}$	8.4985	6.5528
6-epiharpagide	$C_{16}H_{24}O_{11}$	8.8441	4.6417
6'-*O*-β-*D*-Glucosylgentiopicroside	$C_{22}H_{30}O_{14}$	8.1932	4.6684
7-ketologanin	$C_{17}H_{24}O_{10}$	7.886	4.0923
7-α-methoxysweroside	$C_{17}H_{24}O_9$	6.4357	4.706
7β-[(E)-4'-*O*-(β-*D*-glucopyranosyl) caffeoyloxy]-sweroside	$C_{25}H_{28}O_{13}$	8.0927	6.6074
7-β-methoxysweroside	$C_{17}H_{24}O_9$	6.6872	6.0397
Aucubin	$C_{15}H_{22}O_9$	8.9447	4.9157
Boonein	$C_{10}H_{16}O_2$	3.0591	
Cornin	$C_{17}H_{24}O_{10}$	8.058	6.5485
Epi-vogeloside	$C_{17}H_{24}O_{10}$	8.8783	5.261
Gentiopicroside	$C_{16}H_{20}O_9$	8.1959	3.3757
Harpagoside	$C_{24}H_{30}O_{10}$	7.2965	6.0545
Hastatoside	$C_{17}H_{24}O_{11}$	8.5396	7.8332
Isoboonein	$C_{10}H_{16}O_2$	3.9274	
Loganic acid	$C_{16}H_{24}O_{10}$	6.9448	4.2461
Loganin	$C_{17}H_{26}O_{10}$	7.6903	4.2461
Morroniside	$C_{17}H_{26}O_{11}$	7.6797	6.5528
Procumbide	$C_{15}H_{22}O_{10}$	6.7485	4.2994

Qinjiaoside	$C_{17}H_{24}O_{11}$	6.1195	5.0323
Secologanoside	$C_{17}H_{24}O_{10}$	7.3734	6.7208
Sweroside	$C_{16}H_{22}O_{9}$	6.6642	5.1294
Swertiamarin	$C_{16}H_{22}O_{10}$	6.5268	4.8952
Teuhircoside	$C_{16}H_{22}O_{8}$	7.1964	4.2369
Tripterospermumcin A	$C_{23}H_{29}NO_{11}$	9.7259	8.7587
Tripterospermumcin B	$C_{35}H_{52}O_{20}$	8.2867	8.8845
Vogeloside	$C_{17}H_{24}O_{10}$	6.9525	6.2281
Amarogentin	$C_{29}H_{30}O_{13}$	8.6151	
Amaroswerin	$C_{29}H_{30}O_{14}$	9.7123	