Supplementary File

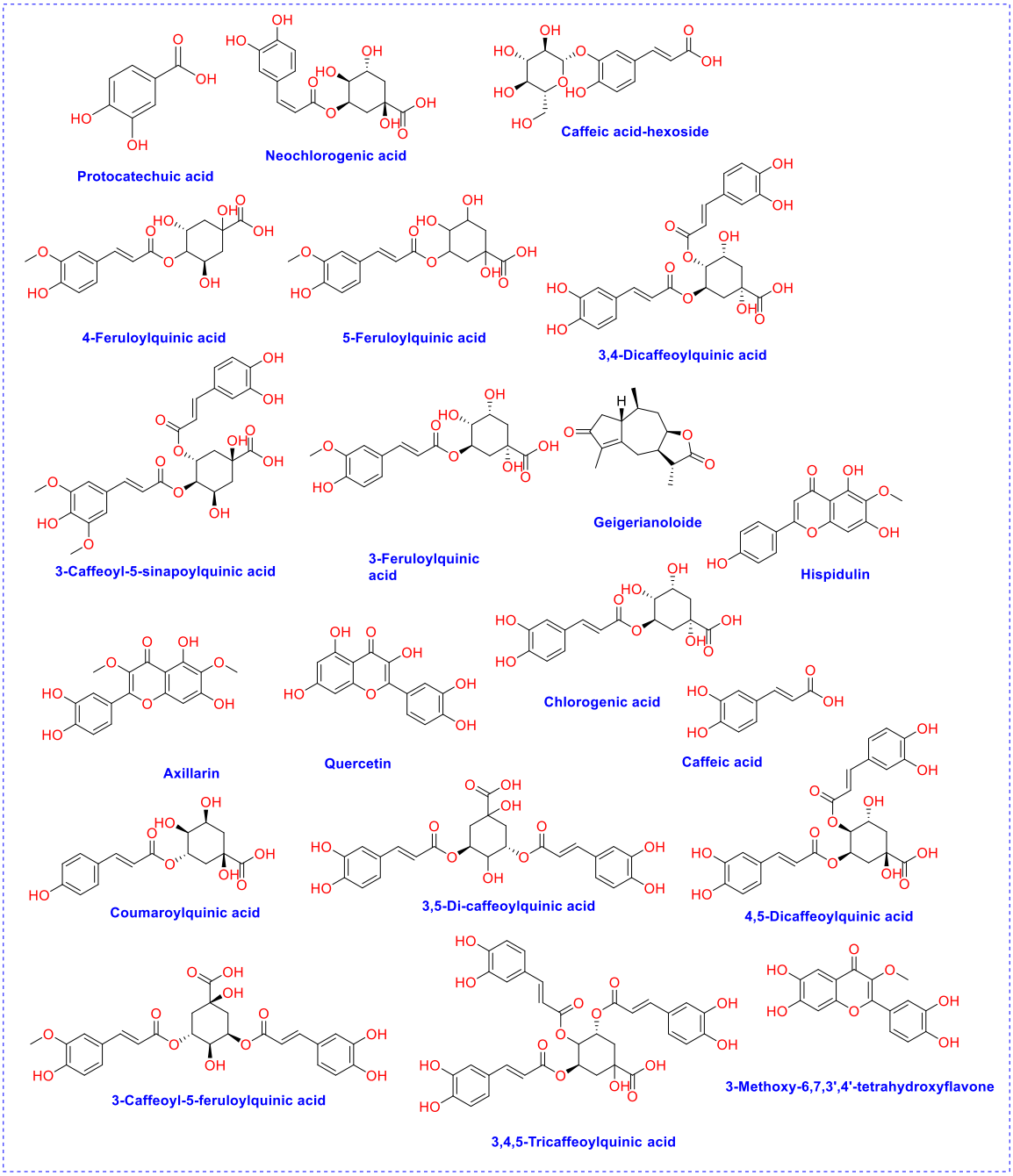

Fig. 1. Chemical structures of the main phytoconstituents of *G. alata.*

Table I The predicted pharmacokinetic properties of *G. alata* reported phytoconstituents.

Phytoconstituent	Intestinal absorption (%)	Vd (L/Kg)	Cl (ml/ min /kg)	CYP-450 enzymes inhibition	BBBP
Protocatechuic acid	71.174	0.05	3.556	No	No
Neochlorogenic	36.377	3.811	2.028	No	No
Caffeic acid-hexoside	50.517	1.384	1.156	No	No
Chlorogenic acid	36.377	3.811	2.028	No	No
Caffeic acid	69.407	0.08	3.221	No	No
Coumaroylquinic acid	43.925	1.008	2.838	No	No
4-Feruloylquinic acid	13.815	0.097	1.12	No	No
5-Feruloylquinic acid	44.764	0.05	2.471	No	No
3,4-Dicaffeoylquinic acid	29.037	42.954	1.102	CYP3A4 substrate	No
3,5-Dicaffeoylquinic acid	44.225	50.119	1.107	CYP3A4 substrate	No
4,5-Dicaffeoylquinic acid	29.037	42.954	0.908	CYP3A4 substrate	No
3-Caffeoyl-5-sinapoylquinic acid	21.891	3.041	1.007	No	No
3-Feruloylquinic acid	44.764	0.05	2.471	No	No
3-Caffeoyl-5-feruloylquinic acid	50.21	0.48	1.161	No	No
3,4,5-Tricaffeoylquinic acid	41.915	33.189	0.627	CYP3A4 substrate	No
Geigerianoloide	99.388	0.193	1.042	No	No
Axillarin	82.651	5.999	2.805	CYP1A2 inhibitor	No
Quercetin	77.207	36.224	2.558	CYP1A2 inhibitor	No
3-Methoxy-5,7,3`,4`-tetrahydroxy-flavone	83.566	0.698	3.954	CYP1A2 inhibitor	No
Hispidulin	84.654	2.344	3.396	CYP3A4 substrate CYP1A2, CYP2C19 & CYP2C9 inhibitor	No

Abbreviations: Vd: Volume of distribution, Cl: Rate of clearance, BBBP: Blood Brain Barrier Penetration

Table II. The predicted drug likeness and toxicity properties of *G. alata* reported phytoconstituents.

Phytoconstituent	**Drug-likeness (Lipinski's rule of five)**	**Major organ toxicity**	**Max. tolerated dose (human) (log mg/kg/day)**	**Oral Rat Acute Toxicity (LD50) (mol/kg)**
Protocatechuic acid	Yes	No	6.486	2.423
Neochlorogenic	1 violation: NH or OH > 5	No	0.735	1.973
Caffeic acid-hexoside	1 violation: NH or OH > 5	AMES toxicity	9.931	1.938
Chlorogenic acid	1 violation: NH or OH > 5	No	0.735	1.973
Caffeic acid	Yes	No	13.964	2.383
Coumaroylquinic acid	Yes	No	0.813	1.737
4-Feruloylquinic acid	Yes	No	18.707	2.115
5-Feruloylquinic acid	Yes	No	19.275	2.025
3,4-Dicaffeoylquinic acid	3 violations: MW > 500, N or O >10, NH or OH>5	No	2.472	2.626
3,5-Dicaffeoylquinic acid	3 violations: MW > 500, N or O>10, NH or OH > 5	No	2.472	2.643
4,5-Dicaffeoylquinic acid	3 violations: MW > 500, N or O >10, NH or OH > 5	No	2.472	2.626
3-Caffeoyl-5-sinapoylquinic acid	3 violations: MW>500, N or O >10, NH or OH > 5	No	2.084	2.604
3-Feruloylquinic acid	Yes	No	19.275	2.025
3-Caffeoyl-5-feruloylquinic acid	3 violations: MW>500, N or O>10, NH or OH > 5	No	2.57	2.534
3,4,5-Tricaffeoylquinic acid	No; 3 violations: MW>500, N or O >10, NH or OH > 5	hERG II inhibitor	2.818	2.511
Geigerianoloide	Yes	No	0.344	1.919
Axillarin	Yes	No	3.206	2.348
Quercetin	Yes	No	3.155	2.471
3-Methoxy-5,7,3`,4`-tetrahydroxy-flavone	Yes	AMES toxicity	9.183	1.836
Hispidulin	Yes	No	1.901	2.402