

Table S2 Phytochemical compounds determined within Ferulinae members in Iran (with chemical formula) inferred from Table S1.

Compound name	Type	Formula
Flavouring Agent		
(Aromatic compound)		
1,15-hexadecadinene		C ₁₆ H ₃₀
10-epi- γ-eudesmol		C ₁₅ H ₂₆ O
2-methyloctane	Alkanes	CH ₃ (CH ₂) ₅ CH(CH ₃) ₂
cauferoside		C ₃₀ H ₄₀ O ₁₀
citronellyl acetate		C ₁₂ H ₂₂ O ₂
exo-fenchyl acetate		C ₁₂ H ₂₀ O ₂
Farnesiferol A		C ₂₄ H ₃₀ O ₄
ferolin		C ₂₂ H ₃₀ O ₄
feropodin		C ₁₅ H ₂₀ O ₂
Ferulin		C ₁₅ H ₁₆ O ₃
ferutin		C ₂₀ H ₂₆ O ₅
geranyl propionate		C ₁₃ H ₂₂ O ₂
isobornyl acetate		C ₁₂ H ₂₀ O ₂
naphthalene	benzenoid polycyclic aromatic hydrocarbon	C ₁₀ H ₈
nonanal		C ₉ H ₁₈ O
nonane	linear alkane	C ₉ H ₂₀
norinone	bicyclic ketone	C ₉ H ₁₄ O
α-D- xylofuranoside,		C ₈ H ₁₆ O ₅
methyl 2,5-di-O-methyl-		
α-terpinyl n-pentanoate		C ₁₅ H ₂₆ O ₂
α- Terpinyl pentanoate		
Coumarins		
conferol acetate		C ₂₆ H ₃₂ O ₅
Conferone		C ₂₄ H ₂₈ O ₄
cumarin		C ₉ H ₆ O ₂
farnesiferone A		
Iso-pimpinellin	dimethylpsoralen	C ₁₃ H ₁₀ O ₅
Osthol		C ₁₅ H ₁₆ O ₃
Disulfide		
(E)-1-propenyl sec-butyl disulfide		C ₇ H ₁₄ S ₂
(E)-sec-Butyl propenyl disulfide		
(Z)-sec-Butyl propenyl disulfide		C ₇ H ₁₄ S ₂
1-methylpropyl-(1E)-disulfide		C ₇ H ₁₄ S ₂
(=(E)-sec-Butyl propenyl disulfide)		
1-methylpropyl-(1Z)-disulfide		C ₇ H ₁₄ S ₂
disulphane		F ₂ S ₂
methylpropyl (1Z)-disulfide		C ₇ H ₁₄ S ₂
Hexadecanoic acid	fatty acid	C ₁₆ H ₃₂ O ₂
geranyl isovalerate	fatty alcohol esters	C ₁₅ H ₂₆ O ₂
Tetradecanal	fatty aldehyde	C ₁₄ H ₂₈ O
hexadecanal	fatty aldehyde	C ₁₆ H ₃₂ O
Flavanoide		
astragalin	flavanoide	C ₂₁ H ₂₀ O ₁₁
cirsiliol	dimethoxyflavone	C ₁₇ H ₁₄ O ₇
eupatorin	trimethoxyflavone	C ₁₈ H ₁₆ O ₇
luteolin	flavone	C ₁₅ H ₁₀ O ₆
nepetin	O-methylated flavone	C ₁₆ H ₁₂ O ₇
quercetin	flavonoid	C ₁₅ H ₁₀ O ₇
rutin	bioflavonoid	C ₂₇ H ₃₀ O ₁₆
salvigenin	flavonoid	C ₁₈ H ₁₆ O ₆
scoparone	flavonoid	C ₁₁ H ₁₀ O ₄
Furocoumarin		
badrakemin		C ₂₆ H ₃₂ O ₆
badrakemin acetate		C ₂₆ H ₃₂ O ₅
badrakemone		C ₂₄ H ₂₈ O ₄
opoferzin	guaianolide	C ₂₀ H ₂₂ O ₅
caffein acid	hydroxycinnamic acid	C ₉ H ₈ O ₄
p-coumaric acid	hydroxyl phenyl group	C ₉ H ₈ O ₃

Monoterpenes

(E)- β- ocimene	C ₁₀ H ₁₆
(Z)- β- ocimene	C ₁₀ H ₁₆
allo-ocimene	C ₁₀ H ₁₆
auraptene	monoterpene coumarin ether
bornyl acetate	monoterpene ester
Camphene	monoterpene bicyclic
Carvone	
cis- β-ocimene	C ₁₀ H ₁₆
citronellol	monoterpoid acyclic
Endo fenchyl acetate	monoterpoids bicyclic
Eucalyptol	
Geranyl acetate	
iso-sylvestrene	
limonene	monoterpene cyclic
Linalool	terpene alcohol
myrcene	
β-myrcene	C ₁₀ H ₁₆
myrtenol	monoterpoids bicyclic
p-cymen-9-ol	C ₁₀ H ₁₆ O
p-cymene	C ₁₀ H ₁₄
pinocarveol	alkylbenzene
sabinene	C ₁₀ H ₁₆ O
sabinene	C ₁₀ H ₁₆
terpinene	
α-Terpinene	C ₁₀ H ₁₆
β-Terpinene	
γ-Terpinene	
δ-terpinene	
terpinolene	
thymol methyl ether	C ₁₀ H ₁₆
trans-isolimonene	C ₁₁ H ₁₆ O
trans-pinocarveol	C ₁₀ H ₁₆
trans-sabinol	monoterpoids bicyclic
trans-verbenol	monoterpene bicyclic
α- phellandrene	monoterpene alcohols bicyclic
α-fenchene	monoterpene cyclic
α-terpineol	monoterpene alcohol
α-terpinyl acetate	C ₁₂ H ₂₀ O ₂
α-thujene	C ₁₀ H ₁₆
β-myrcene	C ₁₀ H ₁₆
β-ocimene	C ₁₀ H ₁₆
β-phellandrene	monoterpene cyclic
β-pinene	C ₁₀ H ₁₆
α-pinene	C ₁₀ H ₁₆
γ-terpinene	
δ- 3-carene	C ₁₀ H ₁₆
δ-3-Carene	C ₁₀ H ₁₆

β-dihydroagrofuran

β-amyrin

Phenolic compounds

caffeic acid

carvacrol

chlorogenic acid

Elemicine

Farnesiferol B

ferulic acid

gallic acid

Myristicin

p-coumaric acid

phenolic glycoside

thymol

α-asarone

ferutinin

Strols

daucosterol

naphthoquinone**pentacyclic triterpenol**

C₃₀H₅₀O

polyphenol

monoterpoid phenol

polyphenol

phenylpropene

terpene lactones

polyphenol

ellagitannins (Phenolic acid)

phenylpropene

polyphenol

phenolic glycoside

monoterpoid phenol

phenylpropanoid

phytoestrogen

C₁₀H₁₄O

C₁₂H₁₆O₃

C₂₂H₃₀O₄

C₁₀H₁₄O

C₁₂H₁₆O₃

C₂₂H₃₀O₄

C₃₅H₆₀O₆

phytosterol glycosides	Phytosterol glycosides	
β -sitosterol	phytosterols	$C_{29}H_{50}O$
Stigmasterol	unsaturated phytosterol	$C_{29}H_{48}O$
Sesquiterpenes		
(E)- caryophyllene	sesquiterpene bicyclic	$C_{15}H_{24}$
(E)- nerolidol	sesquiterpene alcohol	$C_{15}H_{26}O$
7-epi- γ -eudesmol	sesquiterpenoid carbocyclic	$C_{15}H_{26}O$
aristolone		$C_{15}H_{22}O$
bicyclogermacrene	sesquiterpenoids isolepidozane	$C_{15}H_{24}$
bornyl angelate		$C_{15}H_{24}O_2$
Bulnesol	sesquiterpenoid guaiane	$C_{15}H_{26}O$
Carotol	sesquiterpene alcohol	$C_{15}H_{26}O$
caryophillene oxide		$C_{15}H_{24}O$
chimganidin		$C_{23}H_{32}O_5$
dehydro-sesquicineole	sesquiterpenes	$C_{15}H_{24}O$
epi- α -cadinol	sesquiterpenoid alcohol	$C_{15}H_{26}O$
epi- α -muurolol	sesquiterpenoid	$C_{15}H_{26}O$
Epi- γ -eudesmol	eudesmane sesquiterpenoid	$C_{15}H_{26}O$
Eremophilene		$C_{15}H_{24}$
germacrene D		$C_{15}H_{24}$
germacrene D-4-ol	sesquiterpenoid	$C_{15}H_{26}O$
Germacrene B	sesquiterpenoid	$C_{15}H_{24}$
glubolol	sesquiterpenoid	$C_{15}H_{26}O$
Guaiol	sesquiterpenoid alcohol	$C_{15}H_{26}O$
guaioyl acetate	sesquiterpenoid	$C_{17}H_{28}O_2$
Hinesol	sesquiterpenoid	$C_{15}H_{26}O$
humulane esters	Sesquiterpenoids	
isolongifolene	sesquiterpenoid	
karaferin	Sesquiterpene alcohols, guaiane esters	
karaferinin	Sesquiterpene alcohols, guaiane esters	
longiborneol		
spathulenol	sesquiterpenoid tricyclic	$C_{15}H_{26}O$
Valerianol	sesquiterpenoid	$C_{15}H_{24}O$
α -bisabolol	sesquiterpene alcohol monocyclic	$C_{15}H_{26}O$
α -cadinol	sesquiterpenoid alcohol	$C_{15}H_{26}O$
α -eudesmol	sesquiterpenoid	$C_{15}H_{26}O$
α -gurjunene		$C_{15}H_{24}$
α -muurolol	sesquiterpenoid alcohol	$C_{15}H_{26}O$
α -ylangene	sesquiterpenoid	$C_{15}H_{24}$
β -bisabolene		$C_{15}H_{24}$
β -caryophyllene	sesquiterpene bicyclic	$C_{15}H_{24}$
β -chamigrene		$C_{15}H_{24}$
β -elemene		$C_{15}H_{24}$
β -eudesmol	sesquiterpenoid carbocyclic	$C_{15}H_{26}O$
β -himachalene	sesquiterpenoid lippifoliane	$C_{15}H_{24}$
γ -elemene		$C_{15}H_{24}$
δ -cadinene	sesquiterpene bicyclic	$C_{15}H_{24}$
Sesquiterpene coumarins		
Asacoumarin A		$C_{24}H_{30}O_5$
Asacoumarin B		$C_{24}H_{30}O_5$
assafoetidin		$C_{24}H_{30}O_4$
Assafoetidinol A		
Assafoetidinol B		
conferol		$C_{24}H_{30}O_4$
Epi-conferdione		$C_{24}H_{26}O_5$
epi-samarcandin		$C_{24}H_{32}O_5$
epi-samarcandin acetate		
ethyl galbanate		$C_{11}H_{18}O_3$
farnesiferol C		
farnesiferone B		
fekrynl acetate		$C_{26}H_{34}O_5$
ferilin		$C_{24}H_{30}O_4$
Feselol		$C_{24}H_{30}O_4$
flabellilobin A		
flabellilobin B		
franesiferol A		$C_{24}H_{30}O_4$
franesiferol B		$C_{24}H_{30}O_4$

franesiferol C		C ₂₄ H ₃₀ O ₄
galbanic acid		C ₂₄ H ₃₀ O ₅
gummosin		
gumoside A		C ₃₅ H ₄₈ O ₁₄
gumoside B		C ₃₀ H ₄₀ O ₁₀
isosamarcandin		C ₂₉ H ₃₈ O ₆
kamolonol		C ₂₄ H ₃₀ O ₅
kamolonol acetate		
Karatavincinol A		C ₂₄ H ₃₂ O ₅
Lehmferin		C ₂₄ H ₃₀ O ₄
ligupersin A		C ₂₄ H ₂₈ O ₅
methyl galbanate		C ₂₅ H ₃₂ O ₅
microlobin		C ₂₆ H ₃₂ O ₆
persicaosides A		
persicaosides A-D		
szowitsiacoumarin A		
szowitsiacoumarin B		
tadshiferin		
umbelliferone		
Umbelliprenin		C ₂₄ H ₃₀ O ₃
Sesquiterpene lactones		
Copaene	sesquiterpenes tricyclic	C ₁₅ H ₂₄
Diversolides A-G		
feruhodin B		
feruhodin A		
ferulidin		C ₁₅ H ₁₈ O ₄
guaianolide		
isobadkhsin		
oopodin		C ₂₀ H ₂₆ O ₄
opoferdin		
semopodin		
Cardenolide	steroid	C ₂₃ H ₃₄ O ₂
Sulfur containing compounds		
2-ethylthiopyridine	monosulfide	C ₇ H ₉ NS
Foetithiophene A	monosulfide	C ₈ H ₁₀ O ₂ S
Foetithiophene B	monosulfide	C ₈ H ₁₀ O ₂ S
2,3,4-trimethylthiophene =	monosulfide	C ₇ H ₁₀ S
Thiophene, 2,3,4-trimethyl		
2,3,4,5-tetramethylthiophene		
2,5-diethylthiophene =	monosulfide	C ₈ H ₁₂ S
Thiophene, 2,5-diethyl		
foetisulfide D	Tetrasulfide	C ₈ H ₁₄ S ₄
foetisulfide A		
foetisulfide B		
foetisulfide C		
foetithiophene A		
foetithiophene B		
dimethyl trisulphide	trisulfide	C ₂ H ₆ S ₃
foetisulfide C	trisulfide	C ₈ H ₁₆ O ₂ S ₃
foetisulfide A	trisulfide	C ₈ H ₁₆ OS ₃
Terpenoid coumarins		
ferocaulicin		C ₂₆ H ₃₀ O ₆
microlobidene		C ₂₄ H ₃₀ O ₄