

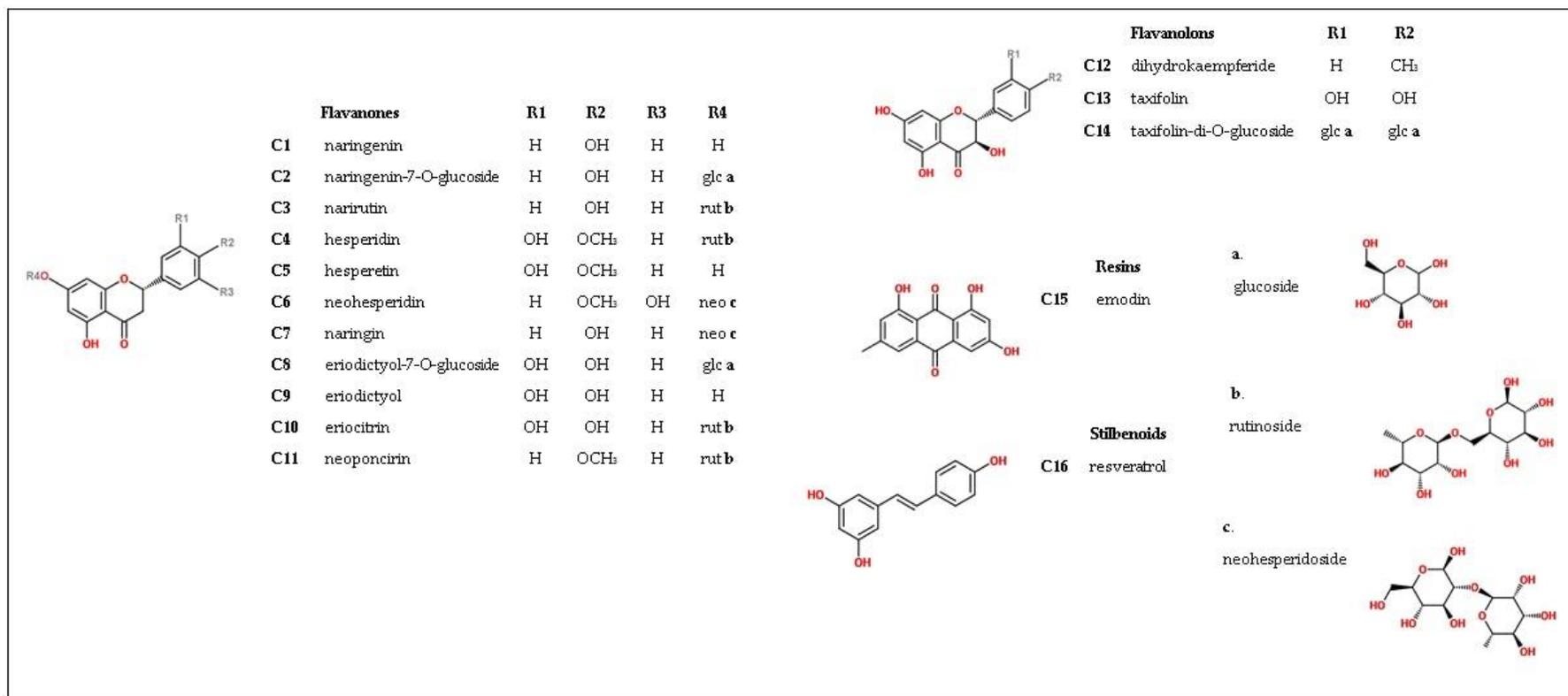
Qualitative and quantitative analysis of polyphenols in *Lamiaceae* herbs – A review

Katerina Tzima^{1,2}, Nigel P. Brunton² and Dilip K. Rai^{1,*}

¹ Department of Food BioSciences, Teagasc Food Research Centre Ashtown, Dublin, D15 KN3K, Ireland

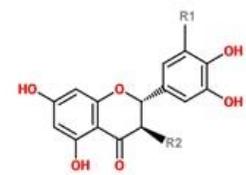
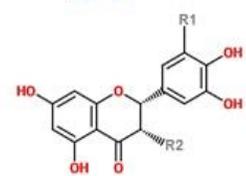
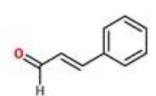
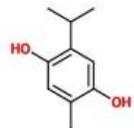
² UCD Institute of Food and Health, University College Dublin, Belfield, Dublin 4, Ireland

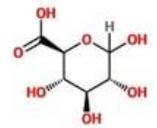
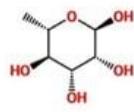
Supplementary Materials



(a)

Figure S1. (a) The chemical structures of the analytical standards or the most abundant polyphenols in the analysed species.

Flavones		R1	R2	R3	R4	R5	R6	R7		Flavan-3-ols		R1	R2	
C17	apigenin	H	OH	H	H	H	H	H		C34	catechin	H	OH	
C18	apigenin-8-C-glucoside	H	OH	H	H	H	H	O-glc a		C35	gallocatechin	OH	OH	
C19	apigenin-7-O-glucoside	H	OH	H	H	H	glc a	H			C36	epicatechin	H	OH
C20	apigenin-7-O-glucuronide	H	OH	H	H	H	gluc d	H			C37	(-)-epigallocatechin	OH	OH
C21	luteolin	OH	OH	H	H	H	H	H				Phenolic aldehydes		
C22	luteolin-7-O-glucoside	OH	OH	H	H	H	glc a	H	C38			cinnamaldehyde		
C23	luteolin-7-O-glucuronide	OH	OH	H	H	H	gluc d	H				Phenolic aldehydes		
C24	chrysoeriol-7-β-O-glucoside	H	OH	OCH ₃	H	H	glc a	H		C39		<i>p</i> -cymene-2,5-diol		
C25	genkwanin	H	OH	H	H	H	CH ₃	H						
C26	homoplantagin	H	OH	H	H	OCH ₃	glc a	H						
C27	nepetin	H	OH	OH	H	OCH ₃	glc a	H						
C28	diosmin	H	OCH ₃	OH	H	H	rha e	H						
C29	diosmetin	OH	OCH ₃	H	H	H	H	H						
C30	3',4',5,7-tetrahydroxy-3-methoxyflavone	H	OH	OH	OCH ₃	H	H	H						
C31	orientin	OH	OH	H	H	H	H	O-glc a						
C32	isorhoifolin	H	OH	H	H	H	rut b	H						
C33	vitexin-2''-O-rhamnoside	H	OH	H	H	H	H	O-rha e						

d.		e.	
glucuronic acid		rhamnose	

(b)

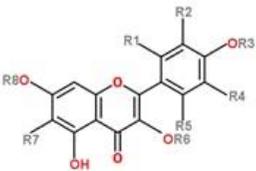
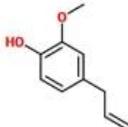
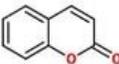
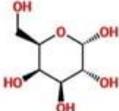
Figure S1. (b) The chemical structures of the analytical standards or the most abundant polyphenols in the analysed species.

Flavonols		R1	R2	R3	R4	R5	R6	R7	R8
C40	quercetin	H	OH	H	H	H	H	H	H
C41	quercetin dihydrate (·2H ₂ O)	H	OH	H	H	H	H	H	H
C42	quercetin-3-O-glucuronide	H	OH	H	H	H	gluc d	H	H
C43	quercetin-3,4'-diglucoside	H	OH	glc a	H	H	glc a	H	H
C44	isoquercitrin	H	OH	H	H	H	glc a	H	H
C45	hyperoside	H	OH	H	H	H	gal f	H	H
C46	rutin	H	H	H	OH	H	rut b	H	H
C47	rutin hydrate (·3H ₂ O)	H	H	H	OH	H	rut b	H	H
C48	kaempferol	H	H	H	H	H	H	H	H
C49	kaempferol-3-O-rutinoside	H	H	H	H	H	rut b	H	H
C50	myricetin	H	OH	H	OH	H	H	H	H
C51	morin	OH	H	H	H	H	H	H	H
C52	fisetin	H	H	H	OH	H	H	H	H
C53	rhamnetin	H	OH	H	H	H	H	H	CH ₃
C54	jaceidin	H	OCH ₃	H	H	H	CH ₃	OCH ₃	H

Hydroxyphenylpropenes	
C55	eugenol

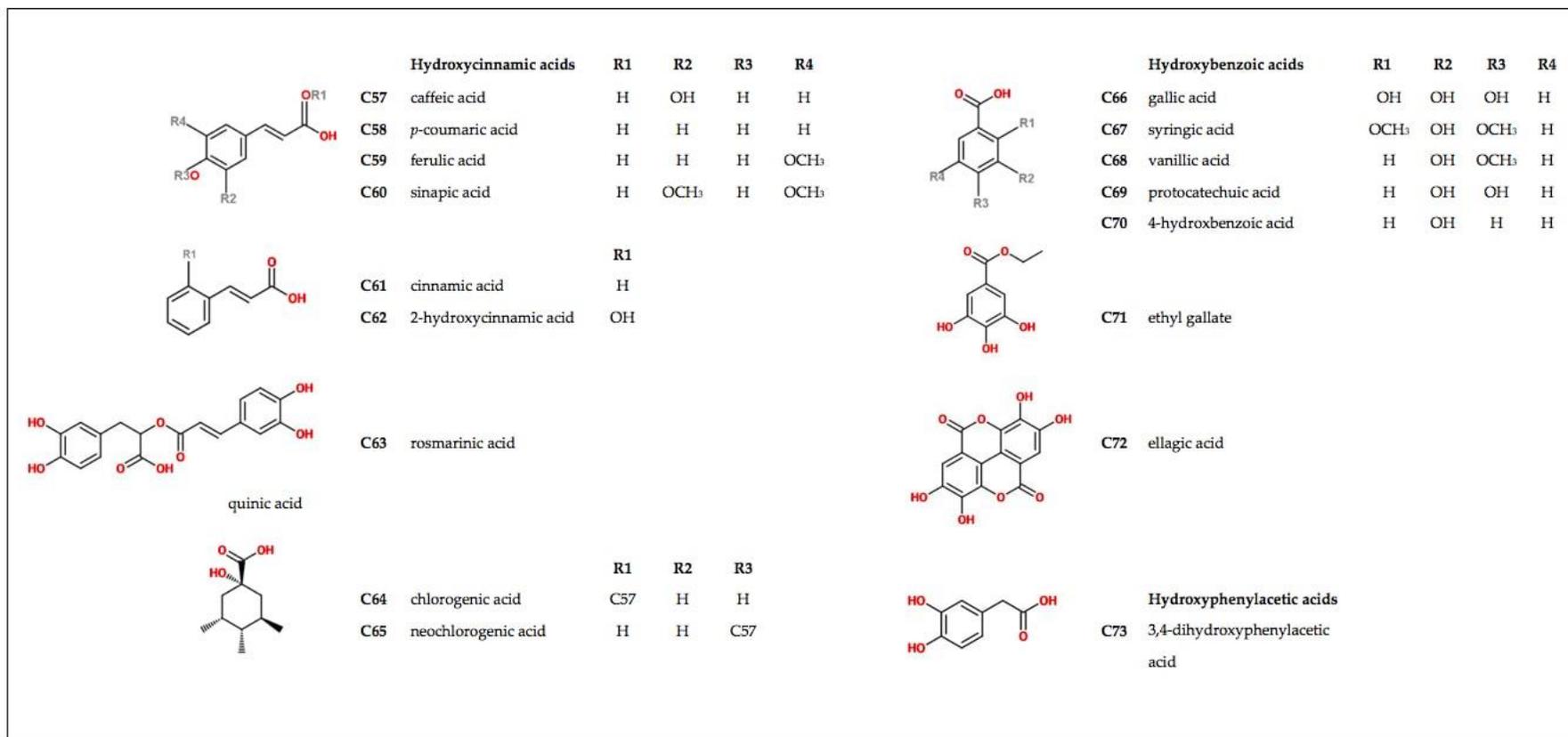
Hydroxycoumarins	
C56	coumarin

f.	galactoside
----	-------------

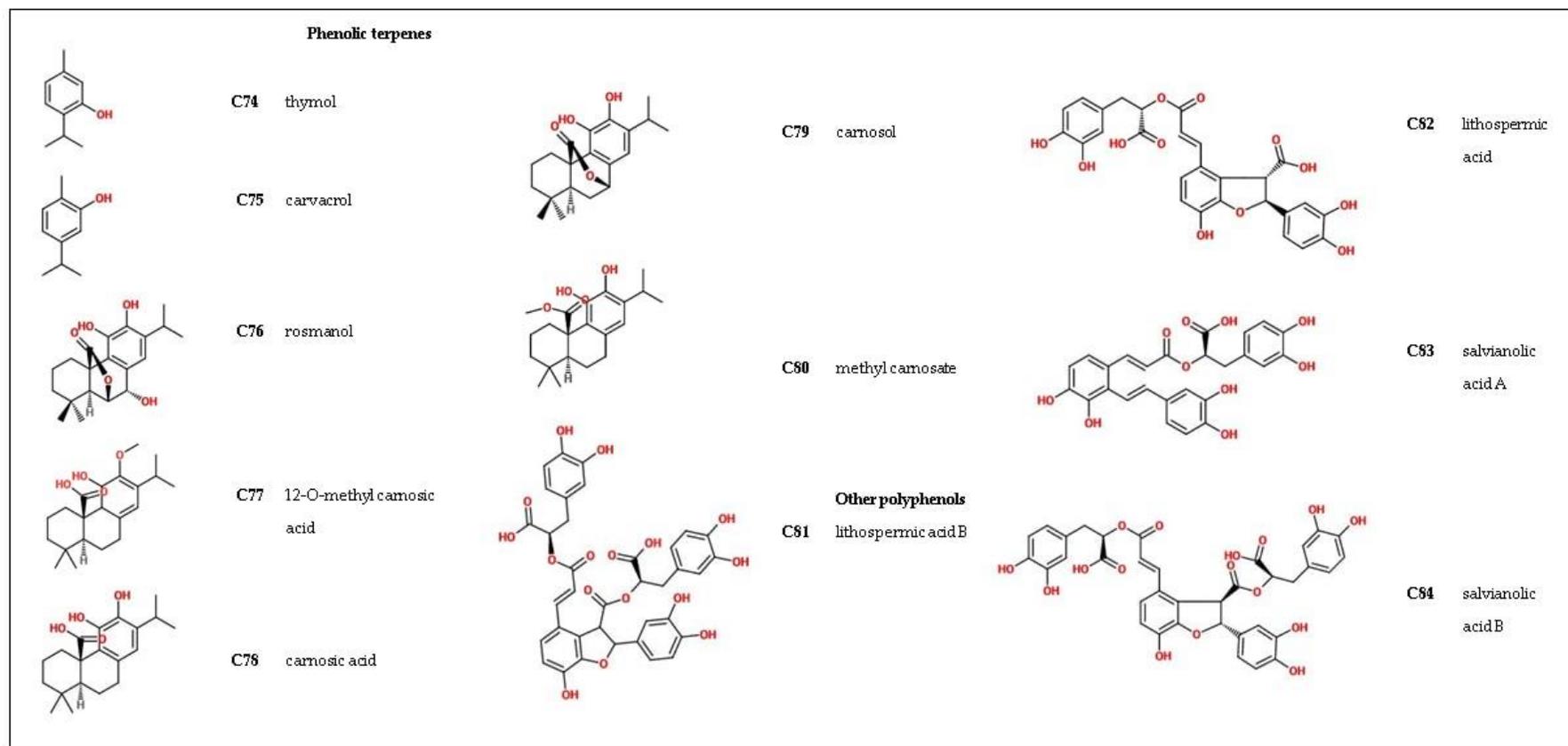
(c)

Figure S1. (c) The chemical structures of the analytical standards or the most abundant polyphenols in the analysed species.



(d)

Figure S1. (d) The chemical structures of the analytical standards or the most abundant polyphenols in the analysed species.



(e)

Figure S1. (e) The chemical structures of the analytical standards or the most abundant polyphenols in the analysed species.

Table S1. (Poly) phenolic compounds identified for the first time in the different researches of Table 2.

<i>Lamiaceae</i> herbs	(Poly) phenolic compounds identified for the first time	Reference
<i>Origanum vulgare</i>	1. apigenin-C-hexoside-C-hexoside	[11]
<i>Mentha australis</i> R. Br <u>Identified for the first time in <i>Mentha</i> genus.</u>	1. neoponcirin 2. biochanin A	[65]
Tunisian <i>Mentha pulegium</i>	1. salvianolic acid B 2. salvianolic acid E 3. isosalvianolic acid B 4. salvialonolic acid I 5. salvianolic acid H 6. lithospermic acid 7. luteolin-6,8-C-dihexose 8. syringetin 9. quercetin, 10. dimethyl ether 11. 2 jaceidin isomers 12. hydroxybenzoic acid hexose isomers 13. dihydroxybenzoic acid hexose 14. vanillic acid hexose 15. syringic acid hexose	[52]
<i>Thymus serpyllum</i>	1. protocatechuic acid 2. protocatechuic acid-hexoside 3. gallic acid 4. rosmarinic acid-glucoside 5. apigenin 6, 8-di-C-glucoside 6. apigenin O-glucuronide 7. luteolin-O-diglucuronide 8. naringin 9. kaempferol O-glucuronide 10. methyl kaempferol O-rutinoside	[64]
<i>Thymus x citriodorus</i>	1. luteolin-7-O-glucuronide (first time in <i>Thymus</i> species) 2. eriodictyol dihexoside with O-glycosidic linkages, (first time in <i>Thymus</i> species) 3. eriodictyol-O-monohexosides (2) (first time in <i>Thymus</i> species) 4. quercetagenin dimethyl ether-O-hexoside (1) (first time in <i>Thymus</i> species) 5. naringenin-O-hexoside (1) (first time in <i>Thymus</i> species) 6. chrysoeriol-7-β-O-glucoside (first time in <i>Thymus</i> species) 7. apigenin-7-β-O-glucuronide (first time in <i>Thymus x citriodorus</i>)	[59]
<i>Thymus vulgaris</i>	1. lithospermic acid B	[2]
<i>Thymus vulgaris</i>	1. sinapic acid-C-hexoside	[11]

<i>Origanum majorana</i>	1. lithospermic acid B	[2]
Tunisian <i>Origanum majorana</i>	1. kaempferol-O-glucuronide 2. sakuranetin 3. salviaonolic acid I 4. luteolin-6,8-C-dihexose (first time in <i>Origanum majorana</i> species) 5. taxifolin (and two isomer derivatives) 6. dihydrokaempferide 7. luteolin-O-glycoside 8. kaempferol-O-sambubioside (not reported in the literature before) 9. luteolin glucoside 10. syringetin 11. quercetin, 12. dimethyl ether 13. 2 jaceidin isomers 14. hydroxybenzoic acid hexose isomers 15. dihydroxybenzoic acid hexose 16. vanillic acid hexose 17. syringic acid hexose	[52]
<i>Satureja hortensis</i>	1. lithospermic acid B	[2]
<i>Rosmarinus officinalis</i>	1. sinapic acid-C-hexoside 2. apigenin-C-hexoside-C-hexoside	[11]
<i>Rosmarinus officinalis</i> <u>Branded extract</u>	1. dihydroxy-dimethoxyflavone derivative 2. dihydroxy-dimethoxyflavone 3. medioresinol derivative 4. dihydroxy-dimethoxyflavone 5. medioresinol-glucuronide 6. isorhamnetin-rutinoside 7. hispidulin-rutinoside 8. 5,6,7,10-tetrahydro-7-hydroxy rosmariquinone derivative 9. isosakuranetin 10. carmosic acid hexoside 11. 5,6,7,10-tetrahydro-7-hydroxyrosmariquinone derivative 12. carmosic acid derivative 13. 40-Methoxytecto-chrysin 14. 5,6,7,10-tetrahydro-7-hydroxy rosmariquinone	[53]
<i>Satureja montana</i> ssp. <i>kitaibelii</i>	1. quinic acid 2. dihydroxybenzoic acid glucoside isomer 1 3. dihydroxybenzoic acid glucoside isomer 2 4. caffeoylquinic acid isomer 1 5. luteolin-7-O-b-glucopyranoside 6. chlorogenic acid 7. caffeoylquinic acid isomer 3 8. caffeoylquinic acid methyl ester 9. dihydroferulic acid 4-O-glucuronide/ 3-methoxy-4,5-dihydroxycinnamic acid glucoside 10. quercetagenin 7-β-D-glucoside 11. quercetin 3-β-D-glucoside 12. acacetin-rutinoside isomer 2 13. apigenin-6,8-di-C-β-D-glucopyranoside/ luteolin-7-O-β-D-rutinoside 14. luteolin-7-β-D-glucuronide	[55]

-
15. kaempferol 3-O-glucoside
 16. patuletin 7-glucoside
 17. dicaffeoylquinic acid isomer 1
 18. dicaffeoylquinic acid isomer 2
 19. dicaffeoylquinic acid isomer 3
 20. apigenin-7-O-β-D-rutinoside
 21. 4-succinyl-3,5-dicaffeoylquinic acid
 22. kaempferol-7-O-rhamnoside
 23. dicaffeoylquinic acid isomer 4
 24. chrysoeriol 7-O-β-D-glucoside
 25. kaempferol 3-O-β-D-glucopyranoside
6''-(3-hydroxy-3-methylglutarate)
 26. acacetin 7-O-rhamnosylgalacturonide
 27. 3,4-dihydroxyphenylacetic acid methyl ester
 28. kaempferol/luteolin
 29. quercetin 3'-methyl ether/6-methoxyluteolin
 30. quercetin 3'-methyl ether/6-methoxyluteolin
 31. tetrahydroxy-dimethoxyflavone
 32. apigenin
 33. luteolin methyl ether isomer 1
 34. luteolin methyl ether isomer 2
 35. 5,6,4'-Trihydroxy-7,3'-dimethoxyflavone/thymusin
 36. 5,6,4'-Trihydroxy-7,3'-dimethoxyflavone/thymusin
 37. trihydroxy-trimethoxyflavone isomer 1
 38. trihydroxy-trimethoxyflavone isomer 2
 39. scutellarein dimethyl ether isomer 1
 40. dihydroxy-trimethoxyflavone
 41. 8-methoxycirsilineol
 42. scutellarein dimethyl ether isomer 2
-

10 *Salvia* ssp.

Identified for the first time in

Salvia spp. (in different species /

with different extraction

solvents).

1. ethyl gallate
2. 3',4',5',7'-tetrahydroxy-3-methoxyflavone
3. hyperoside
4. isorhamnetin-glucoside
5. quercetin 3-glucuronide
6. rhamnetin
7. diosmetin

[3]
