

Appendix V - Cited in Chapter 8

Appendix V.I. Compounds present in *Phlomis* spp.

Mass	Compound	Species	References
578.164	Acacetin-7-O- β -glucopyranoside (C27H30O14)	<i>Phlomis aurea</i>	Mohamed et al. (2000)
270.236	Apigenin (C15H10O5)	<i>Phlomis lychnitis</i>	Tomas et al. (1986)
		<i>Phlomis samia</i>	Kyriakopoulou et al. (2001)
432.105	Apigenin-7-glucoside (C21H20O10)	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
		<i>Phlomis floccose</i>	El-Negoumy et al. (1986)
		<i>Phlomis lychnitis</i>	Tomas et al. (1986)
578.163	Apigenin-7-rutinoside (C27H30O14)	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
		<i>Phlomis floccose</i>	El-Negoumy et al. (1986)
?	Apigenin-7-p-coumaroylglucoside	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
		<i>Phlomis floccose</i>	El-Negoumy et al. (1986)
		<i>Phlomis lychnitis</i>	Tomas et al. (1986)
448.100	Astragalinalin (C21H20O11)	<i>Phlomis spinidens</i>	Takeda et al. (2001)
300.063	Chryseriol (C16H12O6)	<i>Phlomis lychnitis</i>	Tomas et al. (1986)
		<i>Phlomis samia</i>	Kyriakopoulou et al. (2001)
		<i>Phlomis fruticosa</i>	Marin et al. (2007)
?	Chryseriol-7-glucuronide	<i>Phlomis fruticosa</i>	Marin et al. (2007)
?	Chrysoeriol-7-glucoside	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
		<i>Phlomis floccosa</i>	El-Negoumy et al. (1986)
		<i>Phlomis lychnitis</i>	Tomas et al. (1986)
		<i>Phlomis fruticosa</i>	Marin et al. (2007)
		<i>Phlomis caucasica</i>	Delazar et al. (2008)
?	Chrysoeriol-7-rutinoside	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
		<i>Phlomis floccosa</i>	El-Negoumy et al. (1986)
		<i>Phlomis caucasica</i>	Delazar et al. (2008)
?	Chryseriol-7-rhamnosylglucoside	<i>Phlomis fruticosa</i>	Marin et al. (2007)
?	Chrysoeriol-7-p-coumaroylglucoside	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
		<i>Phlomis floccosa</i>	El-Negoumy et al. (1986)
		<i>Phlomis lychnitis</i>	Tomas et al. (1986)
		<i>Phlomis purpurea</i>	Tomas-Barberan et al. (1992)
		<i>Phlomis fruticosa</i>	Marin et al. (2007)
		<i>Phlomis fruticosa</i>	Marin et al. (2007)
		<i>Phlomis crinita</i>	Kabouche et al. (2005)
	Chrysoeriol 7-O-(3''-p-coumaroyl)- β -glucoside		
?	Chrysoeriol-7-O(6''- β -d-apiofuranosyl)- β -d-glucopyranoside	<i>Phlomis nisssoli</i>	Bucar et al. (1998)
?	Chrysoeriol-7-O- β -glucopyranoside	<i>Phlomis aurea</i>	Mohamed et al. (2000)
		<i>Phlomis integrifolia</i>	Saracoglu et al. (2003)
		<i>Phlomis lunariifolia</i>	Calis and Kirmizibekmez (2004)
		<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
288.063	Eriodictyol (C15H12O6)	<i>Phlomis fruticosa</i>	Marin et al. (2007)
314.079	Ermanin (C17H14O6)	<i>Phlomis samia</i>	Kyriakopoulou et al. (2001)
302.079	Hesperetin (C16H14O6)	<i>Phlomis fruticosa</i>	Marin et al. (2007)
462.116	Hispidulin-7-glucoside (C22H22O11)	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
464.095	Isoquercitrin (C21H20O12)	<i>Phlomis spinidens</i>	Takeda et al. (2001)
?	Isorhamnetin-3-p-coumaroylglucoside	<i>Phlomis purpurea</i>	Tomas-Barberan et al. (1992)
?	Kaempferol-3-glucosides	<i>Phlomis spectabilis</i>	Kumar et al. (1985)
		<i>Phlomis caucasica</i>	Delazar et al. (2008)
594.137	Kaempferol-3-p-coumaroylglucoside (C30H26O13)	<i>Phlomis purpurea</i>	Tomas-Barberan et al. (1992)
?	Kaempferol-3-(6,8-di-(E)-p-coumaroyl)glucosides	<i>Phlomis spectabilis</i>	Kumar et al. (1985)
?	Kaempferol (7,4-dimethyl ether)-3-glucoside	<i>Phlomis spectabilis</i>	Kumar et al. (1985)

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?	Kaempferol (7,4-dimethyl ether)-3-(6-O-(E)-p-coumaroyl)glucosides	<i>Phlomis spectabilis</i>	Kumar et al. (1985)
?	Kaempferol-3-O- β -d-glucopyranosyl-(1-6)- β -d-glucopyranoside	<i>Phlomis aurea</i>	Aboutabl et al. (2002)
610.153	Lucenin-2 (C27H30O16)	<i>Phlomis aurea</i> <i>Phlomis floccosa</i>	El-Negoumy et al. (1986) El-Negoumy et al. (1986)
286.047	Luteolin (C15H10O6)	<i>Phlomis lychnitis</i> <i>Phlomis crinita</i>	Tomas et al. (1986) Kabouche et al. (2005)
448.100	Luteolin-7-glucoside (C21H20O11)	<i>Phlomis aurea</i> <i>Phlomis floccosa</i> <i>Phlomis lychnitis</i> <i>Phlomis purpurea</i> <i>Phlomis fruticosa</i>	El-Negoumy et al. (1986) El-Negoumy et al. (1986) Tomas et al. (1986) Tomas-Barberan et al. (1992) Marin et al. (2007)
	Luteolin-7-rutinoside		
610.153	Luteolin-7-diglucoside (C27H30O16)	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
594.137	Luteolin-7-p-coumaroylglucoside (C30H26O13)	<i>Phlomis floccosa</i> <i>Phlomis aurea</i> <i>Phlomis floccosa</i> <i>Phlomis lychnitis</i> <i>Phlomis fruticosa</i>	El-Negoumy et al. (1986) El-Negoumy et al. (1986) El-Negoumy et al. (1986) Tomas et al. (1986) Marin et al. (2007)
462.079	Luteolin-7-glucuronide (C21H18O12)	<i>Phlomis fruticosa</i>	Marin et al. (2007)
?	Luteolin-7-rhamnosylglucoside	<i>Phlomis fruticosa</i>	Marin et al. (2007)
?	Luteolin-7-O-[4-O-acetyl- α -rhamnopyranosyl-(1 \rightarrow 2)]- β -glucuronopyranoside	<i>Phlomis lunariifolia</i>	Calis and Kirmizibekmez (2004)
?	Luteolin-7-O- β -glucopyranoside	<i>Phlomis aurea</i> <i>Phlomis lunariifolia</i> <i>Phlomis brunneogaleata</i> <i>Phlomis crinita</i> <i>Phlomis tuberosa</i> <i>Phlomis younghusbandii</i>	Mohamed et al. (2000) Calis and Kirmizibekmez (2004) Kirmizibekmez et al. (2004) Kabouche et al. (2005) Calis et al. (2005) Gao et al. (2007)
580.142	Luteolin-7-O-(6"- β -d-apiofuranosyl)- β -d-glucopyranoside (C26H28O15)	<i>Phlomis nissoli</i>	Bucar et al. (1998)
272.068	Naringenin (C15H12O5)	<i>Phlomis angustissima</i> <i>Phlomis fruticosa</i> <i>Phlomis caucasica</i>	Yalcin et al. (2005) Marin et al. (2007) Delazar et al. (2008)
?	Naringenin-7-glucoside	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
?	Naringenin-7-p-coumaroylglucoside	<i>Phlomis aurea</i>	El-Negoumy et al. (1986)
?	Phlomisflavosides A	<i>Phlomis spinidens</i>	Takeda et al. (2001)
?	Phlomisflavosides B	<i>Phlomis spinidens</i>	Takeda et al. (2001)
462.116	Quercetin-3-O- β -d-glucopyranoside (C22H22O11)	<i>Phlomis aurea</i>	Aboutabl et al. (2002)
610.153	Rutin (C27H30O16)	<i>Phlomis caucasica</i>	Delazar et al. (2008)
492.126	Tricin-7-glucoside (C23H24O12)	<i>Phlomis fruticosa</i>	Marin et al. (2007)
594.158	Vicenin-2 (C27H30O15)	<i>Phlomis aurea</i> <i>Phlomis floccosa</i> <i>Phlomis fruticosa</i>	El-Negoumy et al. (1986) El-Negoumy et al. (1986) Marin et al. (2007)
	Iridoids		
?	8-O-Acetylshanzhiside	<i>Phlomis tuberosa</i>	Ersöz et al. (2001b)
448.158	8-O-Acetylshanzhiside methyl ester (C19H28O12)	<i>Phlomis rigida</i> <i>Phlomis spinidens</i> <i>Phlomis medicinalis</i> <i>Phlomis umbrosa</i> <i>Phlomis younghusbandii</i>	Takeda et al. (2000) Takeda et al. (2001) Yu et al. (2006) Liu et al. (2007) Gao et al. (2007)
?	8-Acetylshanzhigenin methyl ester and 8-acetyl-1-epishanzhigenin methyl ester	<i>Phlomis umbrosa</i>	Guo and Cheng (2001)
?	6-O-Acetyl-shanzhiside methyl ester	<i>Phlomis medicinalis</i>	Yu et al. (2006)
?	Kaempferol (7,4-dimethyl ether)-3-(6-O-(E)-p-coumaroyl)glucosides	<i>Phlomis spectabilis</i>	Kumar et al. (1985)
?	Kaempferol-3-O- β -d-glucopyranosyl-(1-6)- β -d-glucopyranoside	<i>Phlomis aurea</i>	Aboutabl et al. (2002)
		<i>Phlomis angustissima</i>	Yalcin et al. (2005)
?	Barlerin 141	<i>Phlomis rotata</i>	Zhang et al. (1991)
448.158	Barlerin (8-O-acetylshanzhiside methyl ester) (C19H28O12)	<i>Phlomis younghusbandii</i>	Kasai et al. (1994)
566.199	Brunneogaleatoside (C27H34O13)	<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
?	Chlorotuberoside	<i>Phlomis tuberosa</i>	Calis et al. (2005)
?	Dehydropentstemoside	<i>Phlomis rotata</i> <i>Phlomis medicinalis</i>	Zhang et al. (1991) Yu et al. (2006)
?	Deoxypulcheloside I	<i>Phlomis rigida</i>	Takeda et al. (2000)
536.189	5-Deoxypulchelloside I (C26H32O12)	<i>Phlomis longifolia</i> var. <i>longifolia</i> <i>Phlomis lunariifolia</i>	Ersöz et al. (2001a) Calis and Kirmizibekmez (2004)
?	5-Desoxyesamoside	<i>Phlomis tuberosa</i>	Alipieva et al. (2000), Calis et al. (2005)
?	3-Epiphlomurin	<i>Phlomis aurea</i>	Mohamed et al. (2000)
?	8-Epiloganin	<i>Phlomis grandiflora</i> var. <i>grandiflora</i> <i>Phlomis aurea</i>	Takeda et al. (1999) Mohamed et al. (2000), Aboutabl et al. (2002)
?	6- β -hydroxyipolamide	<i>Phlomis rigida</i>	Takeda et al. (2000)

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406.147	Ipolamiide (C17H26O11)	<i>Phlomis linearis</i>	Calis et al. (1991)		
		<i>Phlomis armeniaca</i>	Saracoglu et al. (1995)		
		<i>Phlomis aurea</i>	Mohamed et al. (2000)		
		<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)		
442.142	Lamalbide (C17H26O12)	<i>Phlomis longifolia</i> var. <i>longifolia</i>	Ersöz et al. (2001a)		
		<i>Phlomis tuberosa</i>	Alipieva et al. (2000), Ersöz et al. (2001b), Calis et al. (2005)		
442.142	Lamiide (C17H26O12)	<i>Phlomis linearis</i>	Calis et al. (1991)		
		<i>Phlomis aurea</i>	Mohamed et al. (2000), Aboutabl et al. (2002)		
		<i>Phlomis herba-ventis</i> ssp. <i>pungens</i>	Alipieva et al. (2000)		
		<i>Phlomis pungens</i> var. <i>pungens</i>	Ismailoglu et al. (2002)		
		<i>Phlomis physocalycoside</i>	Ersöz et al. (2003)		
		<i>Phlomis angustissima</i>	Yalcin et al. (2005)		
422.142	Lamiridoside (C17H26O12)	<i>Phlomis rigida</i>	Takeda et al. (2000)		
		<i>Phlomis spinidens</i>	Takeda et al. (2001)		
390.152	Penstemoside (C17H26O10)	<i>Phlomis younghusbandii</i>	Kasai et al. (1994)		
160.999	Phlomiol (C4H4ClN3O2)	<i>Phlomis longifolia</i> var. <i>longifolia</i>	Ersöz et al. (2001a)		
		<i>Phlomis younghusbandii</i>	Gao et al. (2007)		
?	Phlomiside (=gentiobioside)	<i>Phlomis aurea</i>	Aboutabl et al. (2002)		
322.131	Phlomurin (C19H18N2O3)	<i>Phlomis aurea</i>	Mohamed et al. (2000)		
?	Phlorigidoside A (2-O-acetyllamiridoside)	<i>Phlomis rigida</i>	Takeda et al. (2000)		
?	Phlorigidoside B (8-O-acetyl-6- β -hydroxyipolamide)	<i>Phlomis rigida</i>	Takeda et al. (2000)		
?	Phlorigidoside C (5-deoxysesamoside)	<i>Phlomis rigida</i>	Takeda et al. (2000)		
		<i>Phlomis spinidens</i>	Takeda et al. (2001)		
?	Phloyosides I (7-epiplomiol)	<i>Phlomis rotata</i>	Zhang et al. (1991)		
		<i>Phlomis younghusbandii</i>	Kasai et al. (1994)		
		<i>Phlomis mongolica</i>	Li and Zhang (2000)		
		<i>Phlomis tuberosa</i>	Calis et al. (2005)		
		<i>Phlomis medicinalis</i>	Yu et al. (2006)		
		<i>Phlomis umbrosa</i>	Liu et al. (2007)		
?	Phloyosides II	<i>Phlomis younghusbandii</i>	Kasai et al. (1994)		
?	Phloyosides II	<i>Phlomis mongolica</i>	Li and Zhang (2000)		
422.142	Pulchellose-I (C17H26O12)	<i>Phlomis younghusbandii</i>	Gao et al. (2007)		
420.126	Sesamoside (C17H24O12)	<i>Phlomis tuberosa</i>	Alipieva et al. (2000), Calis et al. (2005)		
		<i>Phlomis younghusbandii</i>	Kasai et al. (1994), Gao et al. (2007)		
		<i>Phlomis medicinalis</i>	Yu et al. (2006)		
?	Shanzhigenin methyl ester and 1-epishanzhigenin methyl ester	<i>Phlomis umbrosa</i>	Guo and Cheng (2001)		
406.147	Shanzhiside methyl ester (C17H26O11)	<i>Phlomis rotata</i>	Zhang et al. (1991)		
		<i>Phlomis younghusbandii</i>	Kasai et al. (1994), Gao et al. (2007)		
		<i>Phlomis rigida</i>	Takeda et al. (2000)		
		<i>Phlomis spinidens</i>	Takeda et al. (2001)		
		<i>Phlomis longifolia</i> var. <i>longifolia</i>	Ersöz et al. (2001a)		
		<i>Phlomis tuberosa</i>	Ersöz et al. (2001b), Alipieva et al. (2000), Calis et al. (2005), Calis et al. (2005)		
		<i>Phlomis lunariifolia</i>	Yu et al. (2006)		
		<i>Phlomis medicinalis</i>	Liu et al. (2007)		
		<i>Phlomis umbrosa</i>			
?	6"-Syringyl-sesamoside	<i>Phlomis umbrosa</i>	Liu et al. (2007)		
?	Phenylethylalcohol glycosides				
624.205	Acteoside = verbascoside (C29H36O15)	<i>Phlomis armeniaca</i>	Saracoglu et al. (1995)		
		<i>Phlomis grandiflora</i> var. <i>grandiflora</i>	Takeda et al. (1999)		
		<i>Phlomis aurea</i>	Mohamed et al. (2000)		
		<i>Phlomis longifolia</i> var. <i>longifolia</i>	Ersöz et al. (2001a)		
		<i>Phlomis tuberosa</i>	Ersöz et al. (2001b), Calis et al. (2005)		
		<i>Phlomis samia</i>	Kyriakopoulou et al. (2001)		
		<i>Phlomis physocalys</i>	Ersöz et al. (2003)		
		<i>Phlomis lunariifolia</i>	Calis and Kirmizibekmez (2004)		
		<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)		
		<i>Phlomis crinita</i>	Kabouche et al. (2005)		
		<i>Phlomis umbrosa</i>	Liu et al. (2007)		
		<i>Phlomis caucasica</i>	Delazar et al. (2008)		
		<i>Phlomis lanceolata</i>	Nazemiyeh et al. (2008)		
?	Decaffeoylacteoside	<i>Phlomis tuberosa</i>	Calis et al. (2005)		
		<i>Phlomis umbrosa</i>	Liu et al. (2007)		

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?	Dimethylether myricoside	<i>Phlomis oppositiflora</i>	Calis et al. (2005)
786.258	Echinacoside (C35H46O20)	<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
756.247	Forsythoside B (C34H44O19)	<i>Phlomis armeniaca</i>	Saracoglu et al. (1995)
		<i>Phlomis longifolia</i> var. <i>longifolia</i>	Ersöz et al. (2001a)
		<i>Phlomis tuberosa</i>	Ersöz et al. (2001b), Calis et al. (2005)
		<i>Phlomis spinidens</i>	Takeda et al. (2001)
		<i>Phlomis aurea</i>	Aboutabl et al. (2002)
		<i>Phlomis pungens</i> var. <i>pungens</i>	Ismailoglu et al. (2002)
		<i>Phlomis physocalyx</i>	Ersöz et al. (2003)
		<i>Phlomis lunariifolia</i>	Calis and Kirmizibekmez (2004)
		<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
		<i>Phlomis caucasica</i>	Delazar et al. (2008)
		<i>Phlomis lanceolata</i>	Nazemiyeh et al. (2008)
?	Glucopyranosyl-(1→G (i)-6)-martynoside	<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
?	3-Hydroxy-4-methoxy-β-phenylethoxy-O-[2,3-diacetyl-α-l-rhamnopyranosyl-(1→3)]-4-O-feruloyl-[β-d-apiofuranosyl-(1→6)]-β-d-glucopyranoside(2''',3'''-diacetyl-O-detonyoside D)	<i>Phlomis umbrosa</i>	Liu et al. (2007)
?	3-Hydroxy-4-methoxy-β-phenylethoxy-O-[3,4-diacetyl-α-l-rhamnopyranosyl-(1→3)]-4-O-feruloyl-[β-d-apiofuranosyl-(1→6)]-β-d-glucopyranoside(3''',4'''-diacetyl-O-betonyoside D)	<i>Phlomis umbrosa</i>	Liu et al. (2007)
624.205	Isoverbascoside (C29H36O15)	<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
624.205	Integrifoliosides A (3,4-dihydroxy-β-phenylethoxy-O-β-d-apiofuranosyl-(1→4)-β-l-rhamnopyranosyl-(1→3)-4-O-feruloyl-β-d-glucopyranoside)(C29H36O15)	<i>Phlomis umbrosa</i> <i>Phlomis integrifolia</i>	Liu et al. (2007) Saracoglu et al. (2003)
?	Integrifoliosides B (3-hydroxy-4-methoxy-β-phenylethoxy-O-β-d-apiofuranosyl-(1→4)-α-l-rhamnopyranosyl-(1→3)-4-O-feruloyl-β-d-glucopyranoside)	<i>Phlomis integrifolia</i> <i>Phlomis brunneogaleata</i>	Saracoglu et al. (2003) Kirmizibekmez et al. (2004)
784.278	Leucosceptoside A (C36H48O19)	<i>Phlomis armeniaca</i> <i>Phlomis longifolia</i> var. <i>longifolia</i> <i>Phlomis physocalyx</i> <i>Phlomis tuberosa</i>	Saracoglu et al. (1995) Ersöz et al. (2001a) Ersöz et al. (2003) Calis et al. (2005)
652.236	Martynoside (C31H40O15)	<i>Phlomis physocalyx</i>	Ersöz et al. (2003)
756.248	Myricoside (C34H44O19)	<i>Phlomis oppositiflora</i>	Calis et al. (2005)
?	Myricoside-3''-O-methylether {3,4-dihydroxy-β-phenylethoxy-O-β-d-apiofuranosyl-(1→3)-α-l-rhamnopyranosyl-(1→3)-4-O-feruloyl-β-d-glucopyranoside}	<i>Phlomis oppositiflora</i>	Calis et al. (2005)
?	2-Phenylethyl-O-β-Xylopyranosyl-(1→2)-β-glucopyranoside	<i>Phlomis aurea</i>	Mohamed et al. (2000)
?	Phlomisethanoside	<i>Phlomis grandiflora</i> var. <i>grandiflora</i>	Takeda et al. (1999)
?	Physocalycoside (3-hydroxy-4-methoxy-β-phenylethoxy-O-[α-l-rhamnopyranosyl-(1→2)-α-l-rhamnopyranosyl-(1→3)]-4-O-feruloyl-[β-d-glucopyranosyl-(1→6)]-β-d-glucopyranoside)	<i>Phlomis physocalycoside</i>	Ersöz et al. (2003)
756.248	Samioside (C34H44O19)	<i>Phlomis angustissima</i>	Yalcin et al. (2005)
?	Samioside (1-O-3,4-(dihydroxyphenyl)ethyl β-d-apiofuranosyl-(1→4)-α-l-rhamnopyranosyl-(1→3)-4-O-caffeoyl-β-d-glucopyranoside)	<i>Phlomis samia</i> <i>Phlomis umbrosa</i>	Kyriakopoulou et al. (2001) Liu et al. (2007)
?	Serratumoside A {3-hydroxy,4-methoxy-β-phenylethoxy-O-β-d-apiofuranosyl-(1→3)-β-l-rhamnopyranosyl-(1→3)-4-O-feruloyl-β-d-glucopyranoside}	<i>Phlomis oppositiflora</i>	Calis et al. (2005)
?	Wiedemannioside C	<i>Phlomis physocalyx</i>	Ersöz et al. (2003)
770.263	Alyssonoside (C35H46O19)	<i>Phlomis pungens</i> var. <i>pungens</i> <i>Phlomis integrifolia</i> <i>Phlomis angustissima</i> <i>Phlomis umbrosa</i>	Ismailoglu et al. (2002) Saracoglu et al. (2003) Yalcin et al. (2005) Liu et al. (2007)
?	Cistanoside B	<i>Phlomis mongolica</i>	Li and Zhang (2000)
786.258	Phlinoside A (3,4-dihydroxy-β-phenylethoxy-O-β-d-glucopyranosyl-(1→2)-α-l-rhamnopyranosyl-(1→3)-4-O-caffeoyl-β-d-glucopyranoside) (C35H46O20)	<i>Phlomis linearis</i>	Calis et al. (1990)
756.247	Phlinoside B (3,4-dihydroxy-β-phenylethoxy-O-β-d-xylopyranosyl-(1→2)-α-l-rhamnopyranosyl-(1→3)-4-O-caffeoyl-β-d-glucopyranoside) (C34H44O19)	<i>Phlomis linearis</i> <i>Phlomis armeniaca</i>	Calis et al. (1990) Saracoglu et al. (1995)

Cont. Appendix V.I.

770.263	Phlinoside C (3,4-dihydroxy- β -phenylethoxy-O- α -l-rhamnopyranosyl-(1 \rightarrow 2)- α -l-rhamnopyranosyl-(1 \rightarrow 3)-4-O-caffeoyl- β -d-glucopyranoside) (C35H46O)	<i>Phlomis linearis</i> <i>Phlomis armeniaca</i> <i>Phlomis lanceolata</i>	Calis et al. (1990) Saracoglu et al. (1995) Nazemiyeh et al. (2008)
770.263	Phlinoside D (3,4-dihydroxy- β -phenylethoxy-O- β -d-xylopyranosyl-(1 \rightarrow 2)- α 1 \rightarrow 3)-4-O-feruloyl- β -d-glucopyranoside) (C35H46O19)	<i>Phlomis linearis</i>	Calis et al. (1991)
784.278	Phlinoside E (3,4-dihydroxy- β -phenylethoxy-O- α -l-rhamnopyranosyl (1 \rightarrow 2)- α -l-rhamnopyranosyl-(1 \rightarrow 3)-4-O-feruloyl- β -d-glucopyranoside) (C36H48O19)	<i>Phlomis linearis</i>	Calis et al. (1991)
?	Phlinoside F (β -[3-hydroxy,4-methoxyphenyl]ethyl-O- $[\beta$ -xylopyranosyl(1 \rightarrow 2)- α -rhamnopyranosyl-(1 \rightarrow 3)]-O-4-O-feruloyl- β -glucopyranoside	<i>Phlomis angustissima</i>	Yalcin et al. (2005)
?	Teucroside	<i>Phlomis armeniaca</i>	Saracoglu et al. (1995)
	Acetophenone glycosides		
	4-Hydroxyacetophenone 4-O-(6'-O- β -d-apiofuranosyl)- β -d-glucopyranoside		
	Acridone alkaloid		
576.438	Daucosterol (C35H60O6)	<i>Phlomis younghusbandii</i>	Gao et al. (2007)
	Aliphatic alcohol glycoside		
?	Lunarioside-1-octen-3-yl-O- β -apiofuranosyl-(1 \rightarrow 6)-O- $[\beta$ -glucopyranosyl-(1 \rightarrow 2)]- β -glucopyranoside	<i>Phlomis lunariifolia</i>	Calis and Kirmizibekmez (2004)
	Benzyl alcohol glycosides		
?	Benzyl alcohol-O- β -xylopyranosyl-(1 \rightarrow 2)- β -glucopyranoside	<i>Phlomis aurea</i>	Mohamed et al. (2000)
	Caffeic acid esters		
354.095	Chlorogenic acid (C16H18O9)	<i>Phlomis brunneogaleata</i> <i>Phlomis longifolia</i> var. <i>Longifolia</i>	Kirmizibekmez et al. (2004) Ersöz et al. (2001a)
?	3-O-Caffeoylquinic acid methyl ester	<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
336.084	5-O-Caffeoylshikimic acid (C16H16O8)	<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
	Diterpenoid glycosyl esters		
?	Baiyunoside	<i>Phlomis medicinulis</i>	Katagari et al. (1991)
436.136	Phlomisoside I (Phlorhizin C21H24O10)?	<i>Phlomis younghusbandii</i>	Katagari et al. (1991), Kasai et al. -1994
436.136	Phlomisoside II (Phlorhizin C21H24O10)?	<i>Phlomis medicinulis</i>	Katagari et al. (1991)
?	Phlomisoside III (β -d-xylopyranosyl(1 \rightarrow 2)- β -d-glucopyranosyl ester-15,16-epoxy-8,13 (16),14-labdatrien-19-oic acid)	<i>Phlomis younghusbandii</i>	Katagari et al. (1991), Kasai et al. -1994
?	Phlomisoside IV (α -l-rhamnopyranosyl (1 \rightarrow 2)- β -d-glucopyranosyl ester-15,16-epoxy-8,13 (16),14-labdatrien-19-oic acid)	<i>Phlomis younghusbandii</i>	Katagari et al. (1991), Kasai et al. -1994
	Lignans		
?	Lariciresinol-4'-O- β -d-glucoside	<i>Phlomis spinidens</i>	Takeda et al. (2001)
742.268	Liriodendrin (C34H46O18)	<i>Phlomis aurea</i> <i>Phlomis brunneogaleata</i>	Mohamed et al. (2000) Kirmizibekmez et al. (2004)
	Megastigmane glucosides		
1.429.669	Citroside (C70H92ClN17O14)	<i>Phlomis grandiflora</i> var. <i>grandiflora</i> <i>Phlomis spinidens</i>	Takeda et al. (1999) Takeda et al (2001)
388.209	Phlomuroside (C19H32O8)	<i>Phlomis aurea</i> <i>Phlomis lunariifolia</i>	Mohamed et al. (2000) Calis and Kirmizibekmez (2004)
	Monoterpen glycosides		
?	Betulalbuside A	<i>Phlomis armeniaca</i> <i>Phlomis lunariifolia</i>	Saracoglu et al. (1995) Calis and Kirmizibekmez (2004)
?	8-Hydroxylinaloyl 3-O- β -d-glucopyranoside	<i>Phlomis armeniaca</i>	Saracoglu et al. (1995)
	Neolignan glucosides		
?	Dehydrodiconiferylalcohol 9'-O- β -d-glucopyranoside	<i>Phlomis lunariifolia</i> <i>Phlomis tuberosa</i>	Calis and Kirmizibekmez (2004) Calis et al. (2005)
?	(7S, 8R)-Dehydroconiferyl alcohol-8-5'-dehydroconiferyl aldehyde 4-O- β -d-glucopyranoside	<i>Phlomis oppositiflora</i>	Calis et al. (2005)
?	Dihydrodehydrodiconiferyl alcohol-9-O- β -d-glucopyranoside	<i>Phlomis chimerae</i> <i>Phlomis lunariifolia</i> <i>Phlomis tuberosa</i>	Ersöz et al. (2002) Calis and Kirmizibekmez (2004) Calis et al. (2005)
?	Dihydrodehydrodiconiferyl alcohol 9'-O- β -d-glucopyranoside	<i>Phlomis lunariifolia</i> <i>Phlomis tuberosa</i>	Calis and Kirmizibekmez (2004) Calis et al. (2005)
534.114	Longifloroside A ((-)-4-O-methyldehydrodiconiferyl alcohol-9'-O- β -d-glucopyranoside) (C22H27ClO13)	<i>Phlomis chimerae</i>	Ersöz et al. (2002)

Cont. Appendix V.I.

	(-)-4-O-Methylidihydrodehydrodiconiferyl alcohol-9'-O-β-d-glucopyranoside	<i>Phlomis chimerae</i>	Ersöz et al. (2002)
	Nortriterpens		
?	28-Noroleana-16,21-diene-3α,19α,23,29-tetrol	<i>Phlomis spectabilis</i>	Kumar et al. (1992)
?	28-Noroleana-16,21-diene-3α,19α,29-triol-23-al.	<i>Phlomis spectabilis</i>	Kumar et al. (1992)
?	(17S)-2α,18',23-Trihydroxy-3,19-dioxo-19(18→17)-abeo-28-norolean-12-en-25-oi acid β-d-glucopyranosyl ester	<i>Phlomis viscosa</i> C, alis et al. (2004)	
	Oleanane-type triterpen glycosides		
?	29-(β-d-glucopyranosyloxy)-2α,3β,23-trihydroxyolean-12-en-28-oic acid	<i>Phlomis viscosa</i>	C, alis et al. (2004)
?	30-(β-d-glucopyranosyloxy)-2α,3β,23-trihydroxyolean-12-en-28-oic acid	<i>Phlomis viscosa</i>	C, alis et al. (2004)
	Phenolic glycosides		
372.142	Syringin (C17H24O9)	<i>Phlomis aurea</i> <i>Phlomis lunariifolia</i>	Mohamed et al. (2000) Calis and Kirmizibekmez (2004)
	Pyrrolidinium derivatives		
?	(2S,4R)-2-Carboxy-4-(E)-p-coumaroyloxy-1,1-dimethylpyrrolidinium inner salt	<i>Phlomis brunneogaleata</i>	Kirmizibekmez et al. (2004)
?	[(2S,4R)-1,1-dimethyl-4-(E)-p-coumaroyloxyproline inner salt		
?	β-Sitosterol 3-O-β-d-glucopyranoside and 1-methyl-O-β-d-glucopyranoside	<i>Phlomis tuberosa</i>	Calis et al. (2005)
?	Syringaresinol-4-O-β-d-Glucopyranoside	<i>Phlomis angustissima</i>	Yalcin et al. (2005)

Appendix V.II. Metabolites present in all samples after 6h.

	R5I_6h	R5C_6h	R4I_6h	R4C_6h	R3I_6h	R3C_6h	R2I_6h	R2C_6h	R1I_6h	R1C_6h	6h
73,01407	755	11	1613	870	538	70	1199	329	118	124	10
101,9366	4075	5423	5011	8218	6619	11678	1455	352	225	300	10
133,0134	95	648	5390	1391	2532	3429	1224	8953	18	161	10
142,0205	300	4639	165820	4774	109736	41199	9444	11463	382	467	10
170,1396	1180	655	226	288	535	63	1089	105	57	105	10
209,0235	1172	330	1061	980	2173	598	401	2475	337	96	10
298,3365	8	272	218	1120	283	173	450	1243	280	264	10
314,3132	205	813	73	4	641	54	205	1598	347	139	10
325,0818	94	26	1640	44	905	857	571	1165	193	239	10
372,1577	87	682	2028	498	1418	3334	1591	8237	397	442	10
379,3486	307	503	347	275	317	47	1658	1731	171	10	10
403,9081	238	589	75	306	1243	2364	778	6711	942	644	10
413,3724	2510	1133	4120	1030	9343	13107	4368	23383	4108	400	10
441,4033	5575	6442	6141	1440	11979	16476	10338	22172	9829	658	10
447,3585	13652	1729	35611	311	39026	48496	55167	31887	11235	1686	10
464,3724	3517	8974	35643	2908	100063	135677	105032	53694	30394	453	10
467,8014	412	208	518	180	31	1369	8468	8649	636	509	10
469,4374	11793	3447	5832	4683	11773	10024	21523	5430	4890	79	10
506,4438	6236	1516	18033	10130	15727	19870	18481	2634	4893	1298	10
518,4688	537	156	2118	652	1282	3230	2926	3849	596	90	10
554,5379	5183	2149	12578	1933	13905	23366	19035	15654	3467	568	10
558,478	11285	2455	14175	216	25741	28156	23098	7845	1973	91	10
560,4932	8816	2188	24748	13059	30828	36926	27219	6417	2680	255	10
561,5245	2321	65	1941	1207	617	5384	3297	5560	3155	162	10
565,536	28993	10550	24469	2665	33415	51602	65426	17504	5296	556	10
580,5597	6219	848	8426	1443	1364	6963	11839	6181	2347	150	10
581,4761	10083	3354	6379	776	11077	14549	19920	4126	77	819	10
584,5722	2856	2879	2299	964	6976	9684	8534	12371	4713	293	10
587,5449	40	171	210	794	4818	5222	6700	10205	5117	566	10
591,5529	27778	5460	24138	3227	30458	57464	85298	9042	2048	95	10
592,5547	10924	6214	21752	1664	25292	37044	35778	15299	8612	75	10
594,576	6252	3941	21271	1382	33235	51309	39659	54948	31430	269	10
597,5079	18324	443	27909	3504	35416	54805	49244	9275	5516	525	10
597,5723	4518	347	3737	1632	12822	19642	15602	19410	3098	151	10
598,511	11070	5679	17815	3101	18839	24815	14978	11164	5001	47	10
599,5234	24133	1051	25181	2871	53796	74175	68997	4587	222	148	10
602,5391	20319	14215	29320	6391	40003	54480	42875	11931	3077	201	10
606,5712	12097	6204	22741	3515	31857	40733	40682	8758	6016	538	10
607,4942	4001	1155	3425	625	7837	8996	9248	10123	556	103	10

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608,5012	2543	1259	3444	426	4011	4970	3051	6660	66	191	10
608,5838	8054	3150	17977	988	24589	34179	33677	14863	8582	890	10
609,5089	8687	2694	7295	161	13928	13148	11821	5859	269	1200	10
609,5994	13959	747	15960	1870	15789	27407	36609	8346	4051	24	10
612,4753	509	218	135	185	643	425	246	4209	275	446	10
614,5718	61	3480	2545	853	13636	16635	19482	36833	39382	78	10
619,5888	25704	7330	11042	1430	21243	49806	72217	20206	12987	56	10
621,6006	13433	2545	8130	2645	7196	25577	51774	8960	5194	291	10
623,6137	9986	329	4526	751	3068	14118	32316	9920	3446	155	10
624,5285	10953	3995	7531	117	8621	15120	15421	13841	2216	817	10
637,6287	2406	2585	6566	2450	12213	21097	18952	6770	2178	292	10
638,6284	1187	2838	14178	378	15753	26601	15390	20742	4776	1045	10
640,5591	2798	3353	7808	317	14931	20175	7478	15221	2738	122	10
645,6025	12103	2001	13274	677	25822	47477	35726	5188	1498	209	10
648,6732	449	582	767	1594	579	2050	923	5018	4732	86	10
652,6483	2123	1921	8694	4556	10961	16754	16578	8774	2698	964	10
653,6404	1227	39	4429	2706	6772	9913	4372	5436	1639	227	10
654,576	3172	436	5521	1020	14245	15834	6300	43904	22667	1068	10
654,6544	726	1388	2590	1855	5805	9215	6119	5225	3409	54	10
664,647	2900	6735	7737	4917	7444	16440	25637	10394	3675	287	10
665,657	4828	3320	2274	2060	2582	10194	22366	2104	4773	352	10
677,6623	6607	3505	4257	948	9506	28037	23322	7977	2767	508	10
679,6764	3673	2243	1669	1260	7149	16146	14506	3855	2551	704	10
681,6059	4331	351	4443	4240	10064	15013	1543	2043	3009	110	10
684,6219	4365	2877	11742	4098	19445	26733	7615	141366	111068	535	10
696,6278	1074	1577	1994	2431	11556	12597	6565	15070	10303	65	10
696,7012	236	384	1925	1794	3924	7424	1231	4426	3568	183	10
705,6912	4511	1853	2805	119	6887	12496	17281	1573	53	1332	10
709,6372	3644	584	1125	741	5939	6136	5365	3287	2836	333	10
721,6381	2030	2483	1297	723	4282	4155	674	1597	565	618	10
776,2387	686	317	45	24	215	363	593	1512	406	272	10
792,5775	933	723	6669	8027	5624	515	2868	2230	472	339	10
848,7888	1310	1759	13480	3085	19801	22198	24853	57772	66312	2053	10
874,8069	9770	7934	13346	6136	31499	43360	13456	20480	37277	56	10
901,8267	11635	4347	12857	7215	29963	39929	26543	20125	27812	632	10
934,8115	165	195	473	660	2157	465	15756	8950	1436	173	10
1260,776	457	69	87	198	182	319	293	77	1522	1210	10
1633,585	491	1364	2350	361	5635	534	895	2018	180	408	10
1817,887	171	215	222	190	284	513	182	862	1438	5658	10
1991,276	227	62	178	150	420	235	164	263	2018	369	10

Appendix V.III. Metabolites present in all samples after 12h.

	R5I_12h	R5C_12h	R4I_12h	R4C_12h	R3I_12h	R3C_12h	R2I_12h	R2C_12h	R1I_12h	R1C_12h	12h	6h
119,9501	505	704	171	115	264	154	300	83	51	231	10	10
126,0397	92	44	10	6	144	45	273	992	52	90	10	10
140,537	72	63	901	3	18	168	571	216	113	65	10	10
141,8989	3283	4120	942	1067	9377	7427	70	302	107	331	10	10
240,061	122	427	1305	424	253	229	212	657	211	265	10	10
245,0319	966	1786	3046	790	1280	1815	3596	6300	910	1934	10	10
248,8829	238	784	965	5	942	927	389	449	405	252	10	10
278,845	449	70	1123	37	121	131	1072	1052	1872	497	10	10
296,0756	474	483	679	497	203	111	108	542	100	328	10	10
350,2954	867	1350	269	528	1919	1415	212	452	2008	231	10	10
351,291	412	1121	83	523	543	264	672	1155	219	318	10	10
353,8267	325	1222	235	158	2096	2195	1549	1043	347	356	10	10
391,3836	695	82	14	116	124	61	998	1034	38	65	10	10
396,3294	12629	341	1003	948	1288	2926	2919	148	1252	3071	10	10
411,3578	82849	3573	12489	137	17179	30065	9426	2518	6180	6778	10	10
416,3669	29864	1114	2283	3101	27484	35190	5827	3401	594	397	10	10
423,3583	114362	7561	15290	539	26764	42345	25079	14085	5918	6370	10	10
429,1134	1441	560	4177	2192	3054	2126	16596	25306	183	4096	10	10
429,3664	16718	7349	2253	17089	3801	5309	1584	6142	8202	7580	10	10

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431,3275	52433	3353	16139	3768	13560	23566	18179	1290	199	47	10
436,3616	35412	2392	2963	1023	8830	14236	5038	2123	1195	217	10
440,3924	29780	456	839	636	3408	9122	4526	1686	196	280	10
446,3971	5313	588	2241	705	700	1197	33	2760	887	1112	10
447,3585	151016	2365	26105	2016	45768	78602	29178	16475	14453	3928	10
449,3353	1378	14542	1771	26915	3141	1695	16379	1833	4629	2957	10
452,2908	579	156	1405	341	533	593	63	146693	444	931	10
457,3949	19763	1270	413	926	1889	5589	2689	4117	816	479	10
459,3916	27483	344	4028	83	5109	9070	951	13377	2860	2990	10
468,4266	37637	43	975	781	1812	5523	6728	916	236	115	10
469,4374	105505	8037	1180	3512	18005	32752	12599	3040	7895	1448	10
473,377	137793	5246	29987	754	32967	54049	36798	1435	2779	2434	10
480,4551	5621	449	259	583	672	894	446	1564	144	158	10
485,2867	1006	1013	7907	172	432	997	430	8474	2	1833	10
488,4004	59149	5052	5453	20725	17972	30015	9140	7489	3322	7482	10
489,4088	226200	8033	20852	1569	65508	99139	69621	2409	321	952	10
490,4124	87916	3188	8267	716	26849	38804	18659	10063	368	1772	10
496,4831	17518	761	471	439	1229	7224	2095	6117	535	98	10
497,3772	42258	2508	6047	1738	8195	17743	2977	2421	4158	2110	10
499,3938	94932	2758	7099	906	20968	35712	23575	2718	837	1076	10
504,4286	106931	4733	9092	629	24063	38488	19751	4012	1913	878	10
508,4842	13216	460	653	568	1515	6090	2277	1582	866	311	10
509,4903	3358	120	672	499	2319	7690	1031	12303	1271	37	10
514,4142	46298	862	1046	745	9846	18231	4449	2912	132	1044	10
515,4258	198305	8299	15033	2943	53427	95281	57081	3380	54	337	10
517,4416	302845	12729	25042	1148	71849	118225	77531	2366	586	145	10
518,4451	121997	3917	9398	251	31693	54536	23231	5891	1943	743	10
525,5023	164598	9178	10148	872	39628	60124	35743	4217	980	334	10
536,4914	154842	6701	15572	7423	37381	56461	32223	4252	2695	713	10
554,4935	15681	391	574	682	2455	4388	965	1894	21	504	10
555,4592	136381	3125	13847	76	34336	57204	33173	4537	1089	902	10
558,478	106437	4810	7596	42	28051	46661	16154	6121	1157	122	10
560,4932	133610	8342	17462	1572	38308	63871	24345	1630	1184	399	10
561,5051	277549	6814	23855	1713	69268	120125	71945	3857	2550	84	10
564,5227	160007	6800	17813	7359	51791	72249	29936	9209	1568	30	10
566,5371	140189	5614	17529	3647	42996	64214	26011	26656	3910	22	10
567,5506	136661	7029	7728	549	27694	51239	29322	7910	2011	300	10
569,7798	933	1398	845	391	3658	2491	9063	6729	1965	1012	10
577,7888	2339	2494	1232	262	1564	1925	11764	13914	2374	457	10
580,5597	30146	4104	6511	1325	8053	12854	9643	6597	1683	151	10
583,4917	141450	9630	12332	723	27866	54928	36957	2104	1088	662	10
588,5258	151147	5341	17820	5887	27970	55546	33278	2564	1467	470	10
597,5079	179479	5608	16336	1129	43835	76769	35261	4652	7950	1815	10
598,511	95439	7098	11311	3932	24625	44412	6988	9343	4441	256	10
603,553	269031	20753	22130	3071	57450	122333	70327	8016	6504	1069	10
606,5712	152729	7817	14947	166	45038	73503	34093	4621	4094	877	10
608,5838	135906	4079	14430	1208	39171	64986	27565	11474	5231	629	10
612,5273	66331	6126	6695	282	20342	31638	9711	12126	1661	593	10
613,5428	176301	11415	15967	591	44395	83482	40499	11313	3969	413	10
616,5626	148494	11103	10903	1191	36003	71586	28257	17434	4877	24	10
634,6038	144927	738	12207	1028	43139	86744	14527	17272	10211	2166	10
635,6182	135924	7617	2689	1452	20865	66958	24586	12213	10151	792	10
637,5418	58223	1191	4880	437	11523	28756	9211	2086	1457	926	10
639,5573	90248	7672	7721	2902	16972	47062	19753	7373	572	349	10
643,5882	140913	9234	8353	1491	30922	78846	33968	8226	2704	75	10
644,5897	101511	5132	12760	4228	38134	70172	17842	9351	2040	357	10
667,6691	19449	430	511	733	135	6301	2738	406	183	480	10
668,5929	41934	2521	963	1280	9505	21689	1164	12730	3440	239	10
669,605	81102	7121	4304	962	6585	32798	21516	4461	1871	381	10
680,6803	47879	1986	1652	1237	12311	30767	4162	3997	460	131	10
691,6776	43754	581	1466	1649	14665	36950	8590	985	1108	78	10
730,6998	28971	2397	2765	1080	14519	32328	6579	3324	661	569	10

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744,7119	16866	958	1948	647	11862	20139	3677	834	2194	1301	10
745,7241	11890	2746	804	183	6713	16712	4570	2565	1228	275	10
756,7165	14771	2502	1742	115	4162	12989	1251	9502	4122	387	10
773,758	4184	1357	658	94	4106	9630	1780	4467	466	80	10
886,7221	1385	6945	18053	69239	268	239	160822	504	554	799	10
909,7058	390	4534	516	5882	971	1832	3437	729	3534	5323	10
922,6934	667	524	2033	233	345	1514	75	2451	240	737	10
934,8115	522	618	746	4451	571	1119	33670	4680	1297	424	10
937,5039	170	855	213	232	120	50	61	843	24	282	10
940,7336	1786	988	7138	19392	628	154	21446	113	464	430	10
1094,664	1166	855	9015	2964	569	612	9646	112	479	297	10
1441,209	248	54	63	153	124	357	11384	362	7	307	10
1501,556	505	203	5520	265	791	661	762	340	55	785	10
1578,618	474	438	655	41	259	168	541	387	72	133	10
1644,699	128	147	753	279	116	242	370	567	51	115	10
1736,269	2540	3082	46486	1918	86	260	9902	50	277	176	10
1800,524	14	341	311	237	68	257	31	37	69	10	10

Appendix V.IV. Metabolites present in all samples after 24h.

	R5I_24h	R5C_24h	R4I_24h	R4C_24h	R3I_24h	R3C_24h	R2I_24h	R2C_24h	R1I_24h	R1C_24h	24h
54,97244	1322	478	2262	657	3050	3139	271	2497	6	64	10
100,9477	145	93	162	196	280	277	251	7599	44	2797	10
164,0928	4147	167	5453	1972	271	3865	3101	3085	48	352	10
216,1091	201	850	309	355	1485	2229	2217	1742	150	257	10
241,9492	534	387	1558	787	2167	926	73	649	48	89	10
276,642	3401	2494	2230	613	36	1092	942	1200	908	579	10
288,1919	260	409	2255	549	414	1483	4996	958	802	859	10
295,1215	130069	498612	1388218	802008	183838	303952	102210	104592	36278	28920	10
296,1251	20939	91188	259614	157059	38916	58748	11991	11756	10219	11314	10
299,1872	6139	3870	17384	2905	6957	7160	6687	12616	9990	6654	10
301,2772	332	178	1575	207	777	1867	28	6106	181	423	10
311,1172	253619	198148	363858	315867	88797	110566	13302	85415	17831	11027	10
312,1201	49828	41220	73482	63978	14401	22234	2800	15415	5466	2135	10
332,1468	533	3475	11506	363	184	340	711	525	336	554	10
333,0999	8984	10312	12802	20010	1702	6851	1276	3832	1225	714	10
351,291	306	14	2551	425	84	173	209	361	95	432	10
357,27	630	106	107	317	358	951	3994	3319	242	730	10
365,1274	30471	20476	16573	16648	1514	2810	73	1213	1129	3651	10
373,2988	2242	107	331	787	872	170	2519	1483	739	32	10
388,2471	159	1	1031	651	259	1227	1701	956	234	204	10
392,0807	7091	4676	12827	16829	845	5756	191	2773	1463	450	10
396,3294	14607	483	7892	50	1961	2009	4693	4003	793	1909	10
403,2942	33580	822	34677	22236	11799	9059	11356	10225	3897	2257	10
404,2976	6732	713	5781	4135	1226	1136	1168	4438	859	147	10
409,2722	907	760	8008	1368	826	695	6196	2894	88	604	10
411,3578	110894	100	30793	6643	12389	13230	1413	36357	9317	8209	10
423,3583	152878	2745	44563	15682	15936	23005	12887	68636	8412	6766	10
427,2971	10170	76	3988	1020	2410	1807	7051	11948	228	1039	10
436,3616	49292	1402	5536	3849	3536	8355	10415	24081	2074	1980	10
437,3742	201119	4347	25041	11281	10376	24445	36702	114277	853	1237	10
440,3924	42950	203	1510	1120	2714	3196	8125	11643	627	529	10
444,3351	11468	4234	6306	4319	6276	4207	1561	2549	3301	5893	10
450,3784	79270	674	9525	5084	7953	13168	19694	34510	884	1219	10
453,4058	198805	3920	17634	7070	15415	27893	26831	92059	899	1690	10
455,4191	117939	1899	6929	5081	8821	12956	8084	60964	1976	2358	10
457,3949	32152	352	2973	1016	584	2376	197	6541	318	1034	10
459,2758	251	46	1084	507	263	1979	6183	3170	214	283	10
459,882	1518	284	308	156	2101	1829	6001	4087	3337	3094	10
461,376	240203	3962	138014	12164	26822	32427	10800	123557	19942	35231	10

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463,3912	294972	12369	36456	15983	17114	36475	54497	163988	317	3208	10
464,3982	106924	1800	11364	5327	8807	14315	22598	58436	2993	2576	10
465,4066	302198	6204	22201	9122	18100	39250	49201	150574	847	1940	10
467,422	257789	2356	13445	6270	7756	20378	41779	121268	2292	1981	10
470,4659	12339	58	260	64	114	1336	664	3607	247	472	10
471,3612	96931	1534	10661	8860	2241	11463	11373	42573	1886	3350	10
473,377	194236	6424	37494	16528	14337	30086	33446	98550	5546	4452	10
476,3035	624	771	2438	1536	1595	4377	6626	4268	337	298	10
477,4076	331398	8498	35202	19238	22070	49308	56552	164322	614	1128	10
479,4233	337580	6667	29918	22077	31790	58303	59626	162607	1153	3430	10
481,4385	266530	6285	13845	11899	26616	47481	38309	126705	1378	4315	10
483,4532	146817	1609	8137	4582	13816	23655	13523	63000	1684	1726	10
487,3932	190799	8647	27046	13223	27882	39494	35409	107088	343	3010	10
489,4283	7977	754	194	1316	1501	2456	1679	6902	450	629	10
491,424	331298	14752	26201	16016	33017	53110	56888	162554	916	1957	10
491,4454	7856	363	438	987	1093	3433	985	5708	407	761	10
493,4395	348955	5109	24080	15026	33021	52027	61233	176682	1658	3588	10
495,4548	278872	3302	14888	10847	23627	34270	42709	136727	1275	4042	10
496,4582	132486	3453	6225	2969	12070	15063	16698	49934	1316	2329	10
496,4831	19748	111	907	994	1467	3765	2019	9809	365	977	10
499,3938	135751	1133	15958	5581	7312	16130	19609	67222	1162	2554	10
499,4764	22334	871	62	765	1113	2206	2356	6757	335	716	10
500,3967	46129	906	2081	984	2448	4563	6798	21374	669	1755	10
501,411	242676	6744	22091	13146	13465	38871	49557	149432	709	2161	10
503,4249	347133	7579	29893	20538	22614	52400	71999	183145	265	1308	10
505,4402	400658	9700	32199	8863	25278	51686	78388	205116	496	1863	10
507,4558	416430	14558	28539	14789	26337	55833	64451	199673	9420	5471	10
509,4705	334003	7118	19417	12445	21387	44229	55097	171072	2977	7102	10
511,4856	197245	2203	11245	3535	9605	25547	23387	83036	943	2242	10
512,4883	93104	632	1813	4793	5286	12109	9272	36373	1054	1824	10
513,4109	147750	4786	16515	13705	16853	37164	19610	76321	2161	195	10
515,4258	248024	7472	23000	18970	24275	53263	54259	141590	57	1273	10
517,4416	361690	10712	42706	28944	44033	75135	71711	187335	963	2741	10
518,4451	138400	1884	16307	14742	19192	27918	21643	72418	1021	2599	10
518,4688	10625	163	837	700	1003	2349	1179	5628	28	78	10
519,4571	401246	15307	37634	22185	51787	87279	73651	208441	1916	5027	10
523,396	39445	119	10095	717	5041	7235	1654	11602	1692	1554	10
523,4865	336077	9087	21559	14407	40487	68396	47785	175136	5045	7545	10
525,4113	75669	2455	8446	4504	9309	17085	8314	37582	660	425	10
525,5023	206568	4924	13569	9657	23207	37579	26661	90275	1418	1975	10
531,4585	392433	6776	48113	29899	40702	75706	55639	217624	5971	2220	10
532,4608	151678	757	16756	9962	14729	24901	23782	72324	1696	165	10
533,4725	401051	9647	32836	19949	36774	64777	73315	207551	2673	3204	10
535,4878	435362	15893	30877	25896	25560	62279	43826	188430	34401	4637	10
537,413	45237	2251	20647	8127	2597	3976	3600	17445	689	1142	10
537,5032	354038	10908	14969	9570	14397	46384	57292	187247	3386	5838	10
538,5065	200304	537	11846	12607	12596	29769	36461	112758	3806	12466	10
539,4274	85493	1688	6018	2685	5078	11847	12495	43092	4003	120	10
539,5179	225479	7010	10405	9928	6077	23281	32546	104822	1520	5054	10
541,4429	171409	6990	14039	9194	10013	20748	21451	82996	353	3657	10
544,4643	139312	2081	14328	9835	8296	23830	17505	94238	5151	9046	10
545,4739	384225	15472	31742	16951	27604	61851	77078	209006	1425	10888	10
547,4887	405490	14941	22164	16433	19351	58637	71478	208794	2985	12528	10
549,5036	423059	14924	33010	16693	27325	68228	33912	197474	6269	19670	10
550,5051	219485	5403	17094	19640	19474	44356	42778	110195	5700	10955	10
551,5187	300148	8466	13241	12233	18200	45942	42902	147697	2383	4684	10
552,522	133102	247	12283	8374	15535	25445	22810	65180	2296	6124	10
553,5367	216666	6458	13756	12773	15103	36791	28591	110658	5560	7633	10
555,4592	166387	2923	23611	12565	17447	35820	23537	85069	2614	1575	10
556,4626	71754	467	8461	5835	6772	15648	16901	44239	457	1387	10

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556,5779	4857	55	440	687	1637	3114	463	2543	262	569	10
557,4748	264749	12361	19820	16159	28684	55414	53318	144919	634	2040	10
557,5278	43748	640	333	225	2422	7234	2988	17209	4250	5213	10
558,478	125434	3749	11828	7849	16173	29600	15715	59291	718	2784	10
561,5051	343640	5260	25991	22494	36870	75079	63358	184283	5008	7668	10
561,5245	10946	966	879	1975	1711	5319	2415	13648	1898	5720	10
563,5202	348833	14577	32366	29966	35060	78367	58703	176720	13817	1899	10
564,5227	192937	1333	23468	19357	28230	43792	38762	101577	4035	9319	10
565,4453	50241	1930	77	55	7426	11550	4501	20174	989	1163	10
565,536	273393	12963	13163	18333	23350	49134	50416	146495	3420	6512	10
566,5371	166233	252	13902	18893	21537	34194	38138	90022	4294	13267	10
567,4604	97051	2413	6821	2394	10887	16478	7882	43317	919	2067	10
567,5506	165357	4973	10575	8030	14465	29088	26941	85745	1636	5151	10
569,4756	164066	8826	15988	8056	20449	34630	23948	91490	1157	3295	10
571,4907	258049	12622	16463	14256	23430	52003	50716	146736	176	3950	10
573,5079	359169	5952	29192	24867	27492	71129	53568	225415	10936	22442	10
574,5092	180773	5374	21907	17334	16686	35177	24848	86685	1445	3988	10
575,5231	360020	7232	23437	13970	19352	67694	56319	217792	14143	35330	10
577,4473	28197	640	2200	515	2177	6348	2233	21674	518	2047	10
577,5365	372955	6846	16914	14537	5260	43934	14936	107473	3693	9528	10
577,7888	1408	1539	544	673	2190	4075	2360	11381	19	1186	10
579,4614	69169	2655	5203	2724	2217	6603	9704	30952	5	706	10
579,5506	254557	6846	16685	9996	374	27608	41205	124439	969	2652	10
580,5597	37484	452	667	4881	949	8216	11380	29125	1622	5132	10
581,4761	102666	2152	8137	4945	6297	14833	12138	52987	549	2528	10
581,5434	5940	1534	1047	1080	976	1948	4247	6941	421	1588	10
583,4917	178382	4036	16135	11989	12951	28247	26888	93656	1107	2577	10
584,4907	102130	646	6454	5698	10567	18592	16071	65600	1144	3007	10
586,5107	137491	751	11299	11946	12690	26582	22261	78372	998	7577	10
587,5231	339278	8719	19534	17228	19450	61543	66890	185330	365	13119	10
588,5258	179127	7098	15903	22011	9592	32219	38365	91461	1037	4666	10
589,5392	363496	11724	20635	16488	19658	66652	59665	202376	11948	16662	10
591,5529	353721	7648	19962	23352	14885	61008	66663	183258	2707	7940	10
593,5684	287326	3301	16945	15592	12759	49710	51811	148912	4015	6967	10
595,5825	179011	3293	9753	9930	10733	34924	30672	93999	2469	6062	10
596,4971	73840	2296	8853	5692	5582	18694	658	38295	147	2030	10
596,5399	43059	1623	1068	1436	3940	8570	3935	20398	1033	1960	10
597,5079	212312	4428	27435	19449	24993	52334	19284	111850	4116	2784	10
597,5723	100570	464	4990	4965	7630	22182	13080	42941	1699	5081	10
598,511	113286	7183	11364	10201	14002	28732	6677	55505	3308	4722	10
601,5385	353127	4575	32455	28659	40209	95990	60671	279003	12879	22341	10
602,5391	193025	7325	25480	26148	32123	52447	40387	124761	1514	10418	10
603,5382	28522	391	1762	3076	9051	15406	599	42110	2660	6033	10
603,553	311713	6807	30632	23893	26372	69880	60498	187166	4911	12422	10
605,5693	310916	7847	18591	28130	31711	63522	63323	183247	2367	8758	10
607,4942	49860	1776	4818	985	5038	9845	5985	25494	469	1223	10
607,5707	33229	5395	4168	4750	9750	13002	14607	29169	328	1522	10
609,4553	2004	196	686	624	1240	2414	828	3241	107	1063	10
609,5089	89067	1161	5459	4482	8438	19224	8546	42530	313	2999	10
611,5244	137859	4019	10729	12757	11950	22443	20162	74020	543	3258	10
612,5273	82478	559	5608	6722	9138	19765	11822	47492	2531	6671	10
613,5428	217699	3307	17259	14591	21363	45788	42896	142199	5421	11197	10
613,5927	36457	286	1307	1274	1232	3902	1652	19916	2481	5709	10
615,5558	242445	8675	13045	9793	16504	36965	50289	153874	1624	13057	10
616,5626	183694	5155	9212	12709	15059	39250	43356	126131	4552	16502	10
617,57	236936	4322	4527	7799	4698	36860	51798	143091	581	4341	10
619,4984	40160	1047	2350	1138	2004	5209	1826	17323	885	2855	10
619,5888	271760	5707	10368	15408	4741	44216	54692	178071	7689	17466	10
621,5103	53372	580	2493	1675	1489	6990	2745	26787	1237	2182	10
621,6006	193989	70	8992	8775	632	20288	37478	113656	3500	8141	10

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623,5274	90222	4042	5973	2794	2876	18140	13516	75057	1416	7343	10
624,5285	75441	4210	7540	4905	4790	15820	10550	53523	2814	6289	10
625,5411	140779	4468	10838	6882	6781	21771	24111	75761	4398	9934	10
626,5442	78736	3283	3903	4973	5385	15901	8337	57443	6388	13735	10
629,5714	213100	4636	13893	16833	6870	32961	29030	140608	7215	16031	10
633,6015	187942	3584	9470	9286	6182	37434	37071	117575	690	7782	10
635,6182	155546	984	4702	5628	10766	35033	19149	103160	9956	14576	10
637,5418	71200	482	7462	4018	8171	18480	7921	34769	732	3762	10
638,5453	41086	566	1870	3987	5909	12001	3237	17400	575	3368	10
639,5573	111626	3688	11234	10308	11989	27565	16143	57743	893	3236	10
639,6158	67218	406	9979	4104	8822	19886	2013	46000	7678	8004	10
641,5726	143673	1412	13011	16235	16837	37468	25545	83646	1720	5645	10
642,5756	103743	191	9219	11926	19826	38608	8768	81644	10693	23638	10
643,5882	154101	2773	14386	12666	17794	43847	28529	97632	1680	8464	10
645,6025	147770	1830	11207	9122	15580	39948	29155	98309	718	4764	10
647,5315	19475	306	884	85	2456	4426	634	10815	1295	3851	10
647,6174	152500	5063	4687	5631	13488	42803	31609	96922	427	8669	10
649,6314	125685	719	7479	7520	8332	29099	21787	83716	3732	7996	10
653,5734	93374	811	6185	3055	10978	24300	22951	61053	2392	4865	10
655,5883	113354	738	6893	6963	7825	24707	14638	80833	3886	10511	10
659,6186	129791	1756	4820	6424	10665	25070	23689	81880	499	3483	10
661,6348	121713	738	5158	6096	2606	25433	27867	87004	2380	5109	10
662,4848	1775	142	265	451	428	604	2962	4260	294	6531	10
663,6465	121710	747	3596	454	2321	19845	26566	78072	2684	4386	10
664,647	102431	793	5744	11575	3139	18920	37488	83601	4154	6225	10
666,5912	18962	2156	3443	2578	3340	5548	3624	16449	1916	9850	10
667,6691	20558	768	325	1190	81	3084	4725	12355	599	278	10
668,5929	56507	1602	2095	1850	4846	12208	6886	32477	3526	7805	10
669,605	94632	980	4199	5098	213	14716	13097	61929	983	4732	10
671,6176	121248	3734	4996	6469	6007	27636	17150	91965	7059	11345	10
673,6335	105259	2698	5326	5355	2719	21624	14125	64949	140	2052	10
677,6623	93694	2218	4025	5749	4818	21273	17967	64943	4364	3455	10
678,6662	80172	507	5295	7599	6071	23090	28821	60916	4015	5264	10
687,6491	68619	1915	5112	5055	8690	27535	11586	40863	1575	3870	10
689,6638	68155	479	5663	5976	8019	25496	12130	39975	1133	8401	10
693,6885	43080	2753	2350	4408	5595	13582	1950	26536	2867	3002	10
695,6222	39792	921	3960	2264	5080	12735	318	23072	1437	2041	10
695,6957	13068	397	589	308	2304	5342	49	8959	1175	796	10
697,6376	47708	645	526	1699	6291	15113	2885	33905	5798	5036	10
699,649	60235	267	4514	1891	6686	21155	1843	51226	7188	8117	10
707,6227	22965	380	2240	644	434	5299	158	13225	802	1008	10
715,6805	40663	693	1636	3097	1997	13905	5544	26169	1274	3370	10
717,6907	42052	1662	2303	1031	3956	12879	8377	25978	186	2634	10
729,6949	26970	1592	2804	3098	7230	15437	859	14198	3877	7425	10
736,7476	10405	144	576	593	1883	5558	2452	14600	226	3640	10
742,6995	19632	616	3816	5211	5384	8168	4548	21204	3420	3344	10
791,7104	3052	763	1692	829	2597	4127	17	13832	2266	2284	10
811,4923	7470	8696	89490	26842	500	922	1002	3418	466	411	10
826,7938	1808	6369	16224	12144	24398	46323	16587	120064	12826	8346	10
827,7971	1447	737	3530	1330	4169	8003	2924	17999	1360	230	10
839,4892	20431	27599	31806	14319	1142	7082	50	1103	475	345	10
874,8069	9220	4414	12692	15928	21987	37375	1656	169278	21854	40153	10
900,8231	7511	4686	7659	18441	29591	54329	17996	240877	25632	30248	10
945,6721	27829	21411	51767	12023	7778	7982	9018	19710	1362	628	10
947,6793	6219	3334	11821	2643	1902	2166	2289	2615	896	1313	10
952,7136	4107	6624	1622	17	2073	1268	1333	3735	406	2637	10
965,691	23709	20902	50469	13346	5426	6674	11139	9659	2172	709	10
966,6939	7744	5867	13423	2807	1618	1370	676	1426	247	815	10
982,6991	155312	123437	298416	70726	32510	39339	70069	104072	276	1198	10
983,702	52411	42154	100438	23278	11443	14444	20792	34534	1489	2750	10

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984,7052	14569	11131	23133	7055	3065	3604	2701	835	56	2917	10
991,7132	29741	24827	74128	15922	4443	4778	9210	15668	447	2199	10
992,2151	11375	10673	26346	4758	1251	2434	3442	4496	1299	396	10
992,6873	47054	38351	16744	640	13419	14930	16661	22349	2110	63	10
1000,729	25875	20864	27788	6303	6112	4268	2472	18489	2943	667	10
1254,838	12232	9894	192077	2853	387	174	5271	12732	139	81	10
1257,35	7563	5497	3551	469	1531	2641	659	262	179	431	10
1323,282	16695	7534	6176	2145	785	916	2813	6281	362	39	10
1348,945	7381	5203	645	69	348	513	306	2608	349	298	10
1353,283	5051	3472	2437	1204	154	519	667	1400	662	172	10
1633,585	472	2146	4021	1639	1629	2436	2250	7265	50	72	10
1657,509	8008	3568	1009	1306	161	78	1167	3489	257	122	10
1725,75	1054	832	7653	2218	96	177	35	1325	195	233	10
1728,732	2794	1781	2246	1464	332	38	617	756	214	358	10
1734,263	5469	3874	42051	9588	223	354	3014	6701	196	611	10
1735,268	14457	11165	102263	21775	295	162	9125	17119	236	62	10
1818,638	7756	6671	16526	3495	263	83	4424	5937	311	243	10
1980,941	67903	49696	849056	192436	158	696	42386	114989	389	146	10
1983,417	60375	39031	163549	68459	236	427	34800	68890	421	206	10
1986,396	17977	11754	4076	5532	139	157	3520	15203	127	66	10
1986,896	8219	5562	3772	2414	18	196	3529	6312	150	162	10

Appendix V.V. Metabolites present in all samples after 48h.

	R5I_48h	R5C_48h	R4I_48h	R4C_48h	R3I_48h	R3C_48h	R2I_48h	R2C_48h	R1I_48h	R1C_48h	48h
54,97244	1857	832	1730	2583	3866	5400	42	1256	439	61	10
60,97302	4458	779	4664	2470	4643	4245	622	1540	483	104	10
120,9932	107088	2815	91498	84100	129664	123458	24847	45046	22171	52	10
123,029	6554	6783	2261	8922	14311	4793	7143	8646	9025	1890	10
128,0053	1033	92	486	9879	7905	5753	209	1648	591	107	10
129,9934	30089	101	29680	28077	43043	35351	14001	18705	9847	103	10
130,0709	65	806	106	517	572	377	555	312	648	73	10
137,968	325	37	1248	1096	1098	2021	90	748	284	449	10
139,9527	538	452	599	566	1000	1063	217	322	121	164	10
143,9815	8752	2513	5719	49465	36047	27086	2037	5050	2682	2605	10
144,009	53326	721	35931	57508	76711	73489	11770	19198	9375	4458	10
163,9544	914	302	3980	1573	3118	3804	806	7697	1022	55	10
164,0928	4547	5338	2008	6797	7021	5270	1255	664	1718	234	10
165,9538	936	115	2970	929	5495	4019	360	5001	1324	22	10
169,0722	2926	158	23010	387	9118	10172	29703	21670	32135	798	10
171,9801	907	209	1497	222	1800	1713	193	217	325	277	10
202,0794	2327	891	7853	30941	18325	8826	693	1135	628	214	10
223,9662	432	135	260	499	444	66	204	111	18	87	10
257,0869	15808	2952	24603	10058	12008	7717	2933	6642	2951	92	10
325,2409	477	3851	62972	436	6755	5971	2180	4719	1344	5053	10
343,2887	6306	2740	23170	966	410	1465	219	4717	865	3505	10
344,2163	2345	1663	53085	305	17362	20001	4451	21454	6905	562	10
368,2984	6305	402	23784	170	712	1476	559	2669	954	1484	10
374,3692	1435	133	556	123	195	1168	1125	1233	368	27	10
375,2623	6396	135	82884	878	6961	6872	2505	5623	3445	296	10
379,3486	5994	370	2753	339	629	651	1208	434	528	176	10
400,356	9238	668	13599	592	1352	1543	443	1946	420	76	10
422,3479	41280	856	25270	1680	8218	7517	588	7541	1840	1072	10
431,3275	85782	170	45583	12774	9043	13674	19206	34847	17740	340	10

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433,3427	165210	184	30059	13811	12813	29712	34931	77462	36122	1922	10
434,2566	758	916	303	37	1631	1149	181	1935	525	117	10
436,3616	52224	2711	23117	5090	4265	9155	5241	16240	6761	1266	10
437,3742	222995	8248	16524	13932	16590	31117	44215	90373	39680	1895	10
439,3899	182336	2879	5141	7229	12252	27060	24938	55145	25065	950	10
440,3924	43486	1672	8603	1021	2469	4692	3900	9791	5246	813	10
447,3585	226673	3909	51260	20788	37255	49397	25334	95954	44154	12901	10
449,375	253043	1261	13529	19468	32994	51136	44553	100417	52279	3867	10
450,3784	92200	1588	36622	4530	10296	15890	11409	25855	10655	79	10
453,4058	213512	6652	6669	15114	18923	34560	26420	68621	29908	682	10
455,4191	137761	4306	9101	5181	10870	17359	10482	38288	15523	2008	10
462,3798	93751	8848	23874	1929	4603	9674	2705	20760	14052	14788	10
463,3912	330702	16519	23099	26613	21056	42230	64157	132053	67231	2840	10
465,4066	340578	9063	8265	22395	21628	47231	59550	118630	63100	1914	10
466,4344	12282	572	566	267	792	1306	650	1912	2053	676	10
467,422	280619	13327	5922	10123	10210	27530	40479	94951	44095	1651	10
469,4374	160185	3636	105177	4398	10062	10008	10397	40692	18211	4098	10
470,4396	66897	198	23636	2156	2593	3426	3450	9695	6218	3239	10
471,3612	111299	4742	14060	6073	5324	15278	11544	28536	16739	3044	10
471,4086	49889	1409	5365	698	399	4450	2836	11336	3523	1598	10
473,377	203584	12923	19231	11166	14381	35983	28323	75245	41373	8516	10
474,3807	67598	3758	13953	1118	2737	9501	4375	17736	8609	4002	10
475,3931	372645	7354	17204	27793	30445	60547	48106	125863	60421	5256	10
476,3967	127051	4445	23716	3697	10639	20111	5134	29607	12924	2205	10
477,4076	363183	12049	4591	25378	27491	59494	64216	130041	66738	1614	10
477,4306	3873	256	599	131	420	1332	1470	239	931	598	10
479,4233	386722	13653	3411	27150	34595	64985	67933	122925	67986	2000	10
480,4551	8604	577	391	891	244	612	89	1668	682	117	10
485,3767	110135	290	7705	5783	11664	19684	15353	31252	17095	5209	10
485,4215	58230	1214	2589	669	3341	6736	1201	5596	4335	1272	10
486,4986	4624	384	366	259	520	594	36	72	109	99	10
487,3932	223393	13612	15245	19135	26656	50582	43913	81307	44039	2087	10
489,4088	319923	17565	3816	15082	32499	63014	61514	118585	65782	7165	10
489,4283	7266	2119	1164	1149	2202	2535	3222	4150	2333	144	10
490,4124	130933	4406	12978	8304	17307	25440	18382	35773	18449	4813	10
491,424	375647	18478	85	16050	30815	59312	64403	134030	63992	1945	10
492,4273	166736	2588	14123	8058	13465	25952	21019	47221	20458	864	10
493,4395	402263	16290	12046	21083	27063	60114	64997	136207	66972	2683	10
494,4426	155648	3089	18300	7278	11263	22049	22806	48402	24231	734	10
495,4548	311494	9030	6060	9000	19360	42909	46035	100797	44853	1675	10
496,4582	146239	6692	13190	5813	9030	15768	16926	37107	18183	2804	10
496,4831	27328	902	1190	1257	57	3830	2421	5089	1798	1441	10
497,3772	67932	165	8324	3137	5097	9086	2824	16538	8185	6715	10
497,4696	168590	4247	1489	4672	8646	21458	18784	56686	19278	878	10
498,4278	50897	23	3424	814	146	3027	2317	6220	3126	422	10
498,4713	92869	943	9898	2976	648	7475	9657	21514	9416	915	10
499,3938	146007	4859	11840	8976	7581	22770	24189	51191	25470	2139	10
499,4764	24397	118	1338	801	2012	3499	1307	2490	1474	602	10
500,3967	53202	1502	11434	943	3607	6845	4327	11248	7200	1745	10
501,411	275651	12220	13150	20533	13962	43567	55267	117018	60792	3013	10
502,4131	103424	347	11596	5276	2008	12356	14387	31117	14326	1977	10
503,4249	387903	19299	21635	34233	27602	54066	76391	155733	81738	1133	10
504,4286	158199	6848	23076	10811	12382	24004	26085	52951	28186	5202	10
505,4402	452496	14400	14408	29277	19794	55451	87811	170896	83897	2866	10
507,4558	476492	21687	7882	25062	19525	60195	59056	158127	78676	15479	10
508,4591	198281	5462	25874	11183	10465	27306	29403	64686	35494	3750	10
508,4842	21351	559	274	1543	929	3039	3061	3130	3078	880	10
509,4705	383405	12550	11260	21418	17030	46245	58957	117887	62774	3071	10
510,4771	183240	327	21510	7835	6822	24385	26365	45099	26908	3615	10
511,3946	84438	1693	6893	4707	6397	15276	7934	25022	12567	789	10

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511,4856	229213	7112	2545	8784	7718	27061	29138	65403	25199	1500	10
512,4883	105919	3058	12651	4025	6170	11824	11141	20820	11652	969	10
513,4109	167864	9279	4554	13470	20782	35555	16619	61740	23378	170	10
513,4555	75745	619	621	3618	3631	7829	4065	6821	4210	223	10
513,4954	46153	1294	1744	157	1935	5776	2705	3901	2863	1397	10
514,4142	67414	3421	6556	4805	8081	14740	5674	14853	5265	940	10
515,4258	288573	10269	1886	20117	23933	58241	54043	117791	54694	479	10
516,4291	118737	456	5276	6237	10949	21698	16444	36083	17770	818	10
517,4416	422702	19333	5280	29583	38089	79611	73204	148354	74717	1445	10
518,4451	175816	4334	12384	14258	16338	29925	24473	50039	25862	2089	10
518,4688	9164	1504	894	1603	1569	3548	1592	4605	1535	453	10
519,4571	460659	20420	2788	29552	48084	94848	79718	167060	80790	2954	10
521,4721	487918	19728	623	29045	42577	80398	72544	148121	67259	3498	10
522,475	215042	2009	21687	10052	22360	46192	32335	63799	31191	1274	10
523,396	50929	3605	5684	1565	3728	9036	959	9359	5465	3251	10
524,4891	222149	1139	21110	10202	23846	43506	30323	58902	34642	6034	10
525,4113	86406	4478	6026	4918	9600	14840	7701	23561	11223	1721	10
525,5023	241814	16764	1357	8957	19155	37598	28051	71785	28885	2310	10
528,4346	95048	19	9963	4008	10602	17113	7228	23185	9238	1567	10
528,5115	29119	68	3502	2202	1898	5616	2032	1893	2333	1162	10
529,4443	330693	17123	9631	19512	28517	66516	53193	121866	54198	731	10
530,4502	162102	416	10791	6523	13337	29956	18804	44946	18205	1801	10
531,4585	446927	32468	47916	21827	49262	82698	53147	171701	78182	5576	10
531,482	12389	1168	952	1442	1873	4159	700	1618	1509	886	10
532,4608	174984	7456	30169	10436	19069	28140	18316	58097	25514	1660	10
533,4725	460927	23271	18846	27050	32884	66845	76668	172757	78890	4229	10
535,4717	2834	3008	1638	1313	1265	1631	4873	5919	9200	980	10
536,4914	226164	4191	48794	18365	15351	32243	30590	68273	40699	7697	10
537,413	53236	15191	2359	559	1762	5129	3538	12025	5464	1723	10
537,5032	402468	22093	18116	19439	22154	43569	56957	132287	63404	4608	10
538,5065	233262	1896	44017	11382	14054	32785	42383	61281	45100	7846	10
539,4274	100924	5245	8204	5892	3486	12891	3367	30956	14581	1393	10
539,5179	253548	10846	15235	14095	7329	21980	34161	71211	32841	2782	10
540,5184	140820	604	24608	4745	6079	14122	19431	32259	20865	2902	10
541,4429	186326	8897	15498	13557	7545	26676	24297	61879	27289	1742	10
542,4462	84590	1077	16507	4245	3508	11597	10162	21569	9594	718	10
543,4584	320824	22293	11725	23954	9446	44665	58457	123157	55813	863	10
543,4958	69854	2383	1235	1688	3751	11919	7852	13196	9381	2272	10
544,4643	158023	5695	23593	13961	7422	27373	23596	45719	29798	4063	10
545,4739	458443	27822	16575	25822	26457	63493	81814	151808	79394	5090	10
546,4823	246766	847	35944	15640	16410	40664	46612	71450	39320	5118	10
547,4887	474024	24442	12114	31833	20157	56166	77737	149823	75956	8704	10
549,5036	510865	16867	22714	32609	26037	69509	36453	95632	42839	11074	10
550,5051	253650	524	45816	20773	18595	45446	37705	62198	42142	7817	10
551,4291	60031	3496	4426	1664	3769	13568	5359	13450	5217	380	10
551,5055	55454	1836	7439	5651	10154	19403	18516	29578	21834	3772	10
551,5187	348622	13158	2145	16162	18648	48771	42089	104027	45172	2870	10
552,522	160570	2057	20482	9152	15518	28065	27135	34671	25636	3211	10
553,4434	106258	2450	3170	3823	8122	21281	10000	26036	9558	35	10
553,5121	11291	560	880	2185	2811	4420	2923	6417	4192	1017	10
553,5367	259525	7106	10135	11670	18154	37416	30008	69698	31379	4896	10
555,4592	192456	8452	1676	13575	18829	37722	21773	63614	25255	791	10
555,5223	127947	574	18669	3293	10637	18224	3942	3788	8927	4817	10
556,4626	86444	2119	8515	3394	8102	16267	14232	31037	15602	485	10
556,5246	99866	443	12869	2508	8501	18254	10795	13154	14279	5280	10
556,5779	6421	72	487	367	1171	3060	1128	2621	1703	523	10
557,4748	315214	14783	1594	17979	31405	55914	53673	111842	48747	962	10
558,478	143477	5999	14555	9585	14454	28743	17359	39746	20824	971	10
559,4904	409149	23939	11486	25997	43818	81481	64022	130703	62710	3053	10
560,4932	185357	4362	24079	14237	23743	42225	29531	56956	28940	1426	10

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561,5051	404065	7667	8523	23094	36907	76090	60373	135239	64685	6695	10
561,5245	11434	1687	1263	288	2876	5135	2590	1760	5643	3743	10
563,5038	14384	1237	5849	3456	1026	6514	2202	2928	5933	2957	10
563,5202	420601	34384	13810	17736	47852	80553	26774	139776	61924	6489	10
564,5227	219616	2301	43854	16267	32058	50050	37229	55734	41037	7245	10
565,536	325976	18190	2773	15601	31637	48275	44203	103776	50187	4326	10
566,5371	185883	2500	42494	16096	25087	34225	36655	45895	37745	9785	10
567,4604	107205	4198	2648	6648	7099	18017	9342	28441	12543	618	10
567,5506	195789	6295	8090	6981	16216	27156	23081	55410	27441	3592	10
568,5551	135976	949	33086	10173	16133	27186	21890	33141	22691	5796	10
569,4756	188069	11368	14982	10318	17995	36843	24147	61902	27078	3566	10
571,4907	298903	18724	13835	16672	25365	52346	51466	118445	49562	2479	10
572,4939	139016	2258	21317	9893	13365	23711	21466	34118	22876	6264	10
573,5079	413415	21990	20465	24276	38209	67963	62218	137672	73855	9737	10
574,5092	194513	8658	32913	19393	25104	32883	26231	55074	30840	2489	10
575,5231	425647	19138	11543	23895	25956	63800	53575	102561	74819	28502	10
578,536	254980	1776	67768	17258	19346	36907	32655	56838	43980	15513	10
579,4614	78757	4202	8150	4145	175	9189	9879	25846	9443	578	10
579,5506	300980	13878	8174	17633	12617	20939	43099	90269	41587	1961	10
580,5597	57710	1772	8162	5475	6418	9733	11940	18138	10283	2493	10
581,4761	124061	7610	9551	8098	6298	18051	11389	38212	13972	1461	10
581,5655	228477	9711	10585	7327	8768	20492	32186	60901	34175	3225	10
582,4788	57538	748	21436	881	2343	4446	789	12310	3538	1182	10
582,5709	154905	2647	42169	9266	9465	22112	32844	46566	30419	5045	10
583,4917	199846	9410	15573	18612	10769	30514	27080	70132	28822	1602	10
583,5563	136196	4341	17077	2831	4853	17061	9781	22295	15034	4015	10
584,4907	111111	1405	28710	7707	9766	21362	14076	40014	17739	857	10
584,5722	71691	1530	21334	4379	2886	8855	8088	11146	10803	3331	10
585,5074	313636	15696	7047	16665	10183	42465	52812	110255	53541	2569	10
586,5107	156081	2612	20800	8601	9306	25493	24918	39391	24456	643	10
587,5231	408021	20652	12318	23958	21600	56772	71899	128679	70076	2339	10
587,5449	2339	687	390	1135	2298	3418	3039	6030	3647	2433	10
588,5258	207963	4960	40058	22262	15261	32749	40448	60018	37629	2003	10
589,5392	416925	23023	8263	20374	25458	65961	59208	130042	74938	12108	10
590,5426	246052	3300	47627	19780	26862	52611	40194	48001	42098	7853	10
591,5529	409670	19433	5894	19210	20687	55868	70560	136205	68349	5017	10
592,5547	233971	772	55267	16168	24309	37347	39781	48869	51106	11790	10
593,5684	336763	11108	3643	14100	20391	46350	50223	108452	52192	5096	10
595,5825	209432	8721	9562	5683	18303	32076	30340	60115	31012	5263	10
596,5399	48116	289	6186	2096	5566	11183	2314	7260	2956	2059	10
597,5079	248632	10191	13724	16694	28716	54115	31353	86988	31245	727	10
597,5723	125470	735	8947	3606	9206	20567	11042	18229	11097	2184	10
598,511	125321	2552	15674	14085	17797	33918	10053	28009	14721	2092	10
599,5234	343094	10668	3875	15983	39695	69209	49748	116266	51814	2451	10
601,5385	422091	15465	14428	27935	48876	90788	69172	187035	81095	11942	10
602,5391	224219	9293	44648	20526	34929	56826	40189	74211	44692	5240	10
603,5382	30252	1902	22013	498	7973	17937	3423	13883	9288	4340	10
604,5554	255111	5305	58180	17336	46382	71571	35789	24514	50310	27038	10
605,4789	31362	387	16173	782	4929	7974	2136	4901	1970	1402	10
605,5693	374246	24309	8536	19270	39233	61929	65402	136696	65318	6124	10
606,5712	216384	6009	52086	11595	30580	47206	42115	67569	49510	11156	10
607,4942	58189	1545	20746	3695	4590	10293	5595	17575	5353	1329	10
607,5707	39878	2070	8800	6526	7837	10395	11828	17639	10675	1885	10
607,585	256156	14152	3116	6613	22386	41318	40124	101935	45118	5282	10
608,5012	29259	745	11900	2581	3083	4947	1788	2195	2080	1394	10
608,5838	191157	749	47223	10119	24874	33363	41855	50655	50055	11488	10
609,5089	103872	5413	7186	4376	8367	16414	10367	28459	10104	1886	10
609,5994	187803	9752	10665	9860	11864	26424	33346	71659	31667	4095	10
610,5142	54843	250	9402	1695	5469	9828	2978	10524	5603	1732	10
611,5244	157044	5097	8857	11005	12884	26227	21125	52469	21626	2339	10

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611,5886	107712	1197	34810	4781	13907	17096	9417	12432	13460	6114	10
612,5273	97278	906	17814	7947	8040	19820	10632	26314	13582	2384	10
612,6066	55148	1695	29685	3501	5547	7831	7819	11386	9223	3896	10
613,5428	249230	6955	21644	15394	20595	48011	37101	97207	45488	7449	10
614,5439	137335	5365	23164	10448	12934	29883	18505	27061	23000	6989	10
615,5558	280569	19655	10403	9331	19966	41631	46576	99074	51707	5007	10
616,5626	208689	9598	43603	12178	17031	43575	41686	62676	46632	7558	10
617,57	280495	18751	7037	7419	9814	35321	53090	114996	49782	3467	10
619,4984	50126	627	7227	2199	1038	6122	1646	5738	2804	2136	10
619,5888	302970	14713	9222	12156	9362	44600	52932	113371	57458	10677	10
620,5925	205537	1212	57572	9888	19559	39841	22376	41561	50724	28790	10
621,5103	64880	2268	11236	1664	3040	8135	817	14240	5172	2648	10
621,6006	222601	10220	16516	7112	7657	25687	38872	83187	40563	6135	10
622,6023	163184	2162	50902	14263	6751	20218	43474	46382	46068	13871	10
623,5274	105678	5383	21993	5444	2191	18295	12892	56895	16198	3310	10
623,6137	144696	5530	13688	3283	986	13280	25185	53699	24029	3645	10
624,5285	90584	4899	27887	7413	4891	17403	6846	26470	11267	3737	10
625,5411	167444	9237	30033	9642	7073	24045	20060	47379	20120	5389	10
626,5442	90602	5327	27681	8105	6206	17967	8261	8446	10160	9040	10
627,5563	202582	6793	11208	10014	12066	29649	32084	70410	32726	3814	10
629,5714	240330	13206	8172	14771	8571	41122	34117	70601	41602	5970	10
630,5738	158954	6825	39275	13601	10222	32652	31876	28390	31388	4349	10
631,5898	256736	11807	5643	7688	16749	47606	35257	87668	43065	10385	10
633,6015	226355	9023	3851	5933	16051	39054	39647	76565	34024	4721	10
635,5257	52460	608	7852	2150	5764	11309	3684	8669	4083	694	10
635,6182	180493	8692	4265	1410	12970	35142	24176	60130	30824	11143	10
637,5418	85502	621	3424	3130	5835	16623	6937	17565	7818	2096	10
637,6287	108945	2910	13515	7333	7920	23022	18591	37703	16264	2651	10
639,5573	124203	6345	5893	10029	14011	30224	12045	36064	13898	4139	10
640,5591	78587	1198	11026	2114	11544	23449	5388	17190	11630	6143	10
640,6393	43509	272	27446	2593	9528	13968	6608	8415	6389	2528	10
641,5726	165580	10511	3204	10065	23726	37763	22707	55004	23790	4480	10
642,5756	115817	1895	20655	3464	19204	38169	10476	9739	19349	12923	10
643,5882	181022	10890	1996	9878	24402	42049	28544	64408	31208	3070	10
645,6025	171706	11425	4111	5262	21137	38138	27349	67117	26404	2631	10
648,6248	173884	1985	42942	5750	32233	56816	22723	32607	40274	30035	10
649,6314	144163	4044	9475	3605	15598	28360	23006	58391	24336	5720	10
651,557	54129	1012	3457	1348	5749	10211	6634	9967	5013	568	10
651,6446	101193	5229	13973	1395	10967	16549	18804	42785	16278	3269	10
652,6483	85742	1329	48395	4740	13039	17839	17345	31833	21028	3254	10
653,5734	104999	4326	32587	3268	14531	25856	10239	33824	13736	3676	10
653,6404	59875	964	18952	3933	8907	12550	5150	14883	6773	2212	10
654,6544	48585	875	26028	2012	9523	12195	5338	12141	7999	2648	10
655,5883	133504	11253	15340	7763	13453	23249	17792	42940	22058	5472	10
657,6038	144358	6038	11688	2333	8371	28495	16156	45967	24672	8892	10
658,6057	114154	649	39534	5281	13905	30585	20974	20478	24942	7950	10
659,6186	143224	6985	12490	3004	11604	26985	24232	65656	25754	1854	10
661,6348	136865	6714	11086	3634	11399	23746	19004	61690	19949	1358	10
663,6465	136813	8710	13218	1754	7289	16890	25298	63331	23817	2772	10
664,647	120371	3353	67497	3541	6471	16032	31385	48081	29841	4410	10
666,6596	82403	3887	185546	1354	28882	24707	188	33508	18709	5878	10
667,5856	108374	6324	62238	1806	9517	29881	1034	27817	16080	13084	10
668,5929	57162	2108	17890	2076	5499	12396	6000	6678	8947	4765	10
669,605	115189	8329	5845	6059	5538	15370	14732	42463	15813	2074	10
671,6176	139751	7603	13724	3952	12477	27202	13272	43943	21810	4774	10
672,619	105321	1991	49060	6669	18276	27735	15085	4555	15942	12181	10
673,6335	121335	5797	14309	4428	6093	22444	18730	43469	19423	2981	10
675,6484	119770	3823	10036	1537	9497	24650	24103	47825	18826	2324	10
676,6511	95005	4742	34495	5355	15294	31151	23179	30710	26623	7067	10
677,6623	106751	2219	10493	1245	7986	21676	14598	46493	17629	3781	10

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678,6662	90255	1300	37111	3727	12804	23409	19992	32347	22557	5464	10
679,6764	72835	3549	7749	1124	7119	15227	10925	28126	11936	2447	10
680,6803	60683	1663	44938	1411	11733	17099	13027	18685	13867	3725	10
687,6491	80338	7434	9025	2302	14221	25273	7121	27291	8632	3237	10
689,6638	75069	2397	8577	2063	11391	25037	9087	19138	9445	3811	10
691,6776	61386	1852	6673	1030	11428	19123	9681	30962	8336	2886	10
692,6798	60881	2480	28250	125	14636	23891	13819	24106	11365	1412	10
693,6074	28916	572	9317	679	5492	6808	4061	6884	1359	274	10
700,6523	48917	2245	27843	365	10571	17627	3178	2106	5188	3968	10
705,6912	52646	1938	7649	47	4046	12346	7451	27669	7899	912	10
706,6972	47046	1126	22698	2895	4402	9621	10576	25802	9918	1136	10
714,6683	48117	1169	16220	1870	6505	8720	7029	3419	9042	5357	10
717,6907	46723	1590	6773	134	5366	12446	6541	15024	5197	1437	10
718,6995	43700	1475	14069	2609	7787	14843	5832	14436	6782	1089	10
720,7123	35103	1288	14517	2075	6032	9888	9932	17592	4319	715	10
732,7172	30404	1612	7203	2278	10628	15119	6501	12573	2863	675	10
743,7102	20806	1306	4299	352	5860	9807	1544	14377	84	574	10
826,7938	6	3534	28579	6542	26356	51670	8953	67233	20799	6073	10
900,8231	2244	8627	52603	820	64728	59776	7720	66016	35581	25636	10
1633,585	142	1457	2118	1171	2841	3349	1863	3967	794	590	10

Appendix V.VI. Metabolites present in all samples after 72h.

	R5I_72h	R5C_72h	R4I_72h	R4C_72h	R3I_72h	R3C_72h	R2I_72h	R2C_72h	R1I_72h	R1C_72h	72h
72,06723	3222	1186	272	386	2007	1820	76	737	197	124	10
117,9862	2182	2239	3608	2696	4661	6667	530	79	153	113	10
123,029	1251	7	9931	14607	9324	7686	5698	7028	474	3211	10
141,8989	3922	6689	9950	8568	1573	10418	186	205	51	14	10
147,0293	11	8617	20618	23812	7143	1569	5753	18666	236	335	10
216,1091	243	65	2341	319	3331	1999	646	633	188	210	10
240,0792	766	3584	3765	8338	16940	20404	2095	5684	780	1209	10
241,9492	812	430	329	6212	1594	1361	97	431	132	127	10
245,9107	8125	10672	12528	9000	17665	18151	1214	999	665	148	10
362,2884	35	733	1525	1677	394	1149	808	2065	287	332	10
369,8364	872	1042	554	203	1445	1436	460	463	280	294	10
469,4374	167714	4150	12342	17911	6682	30367	4131	24775	536	2443	10
471,4086	56791	353	764	49	926	4534	183	2653	590	472	10
526,5311	17600	885	1517	182	1721	4706	61	2991	232	125	10
563,5202	435510	29788	33332	26774	47052	80504	2273	82711	1248	5846	10
568,5848	8940	732	541	557	914	3798	446	2149	1061	272	10
601,5216	6513	943	2476	819	2034	3903	97	1481	90	379	10
603,5382	25815	455	11108	1453	9004	17049	903	5787	1142	3264	10
633,6015	236477	3337	18405	7362	9758	33775	1800	54898	1007	743	10
666,6596	83809	3508	46334	1952	34213	17363	2075	5631	1558	1216	10
677,6623	115807	3474	13384	2181	5382	23704	788	25372	3004	2227	10
696,7012	15686	505	10166	473	6663	6568	2613	235	955	1739	10
709,6372	42834	4867	5939	2462	3091	9484	4489	1674	1475	205	10
790,704	2615	2486	3073	838	5572	3225	995	4836	3168	1629	10
889,6674	10	353	1454	93	1585	133	496	20	1195	1293	10
932,6565	439	1430	1768	3636	747	150	423	77	606	276	10

Appendix V.VII. The five metabolites present constitutively in the roots in nine out of ten time-points.

	R5I_72h	R5I_48h	R5I_24h	R5I_12h	R5I_6h	R5C_72h	R5C_48h	R5C_24h	R5C_12h	R5C_6h
558,478	149887	143477	125434	106437	11285	4054	5999	3749	4810	2455
580,5597	70247	57710	37484	30146	6219	0	1772	452	4104	848
597,5079	250578	248632	212312	179479	18324	9431	10191	4428	5608	443
598,511	131783	125321	113286	95439	11070	5665	2552	7183	7098	5679
677,6623	115807	106751	93694	81165	6607	3474	2219	2218	3666	3505

R4I_72h	R4I_48h	R4I_24h	R4I_12h	R4I_6h	R4C_72h	R4C_48h	R4C_24h	R4C_12h	R4C_6h
15301	14555	11828	7596	14175	7091	9585	7849	42	216
10935	8162	667	6511	8426	4595	5475	4881	1325	1443
12720	13724	27435	16336	27909	19617	16694	19449	1129	3504
16406	15674	11364	11311	17815	10003	14085	10201	3932	3101
13384	10493	4025	3619	4257	2181	1245	5749	0	948

R3I_72h	R3I_48h	R3I_24h	R3I_12h	R3I_6h	R3C_72h	R3C_48h	R3C_24h	R3C_12h	R3C_6h
15689	14454	16173	28051	25741	35090	28743	29600	46661	28156
2886	6418	949	8053	1364	4935	9733	8216	12854	6963
24775	28716	24993	43835	35416	53331	54115	52334	76769	54805
15793	17797	14002	24625	18839	32110	33918	28732	44412	24815
5382	7986	4818	11284	9506	23704	21676	21273	42128	28037

R2I_72h	R2I_48h	R2I_24h	R2I_12h	R2I_6h	R2C_72h	R2C_48h	R2C_24h	R2C_12h	R2C_6h
0	17359	15715	16154	23098	21929	39746	59291	6121	7845
382	11940	11380	9643	11839	12429	18138	29125	6597	6181
0	31353	19284	35261	49244	60337	86988	111850	4652	9275
0	10053	6677	6988	14978	17918	28009	55505	9343	11164
788	14598	17967	18529	23322	25372	46493	64943	3709	7977

R1I_72h	R1I_48h	R1I_24h	R1I_12h	R1I_6h	R1C_72h	R1C_48h	R1C_24h	R1C_12h	R1C_6h		ALL
679	20824	718	1157	1973	350	971	2784	122	91		49
1571	10283	1622	1683	2347	1119	2493	5132	151	150		49
4080	31245	4116	7950	5516	338	727	2784	1815	525		49
2017	14721	3308	4441	5001	648	2092	4722	256	47		49
3004	17629	4364	3294	2767	2227	3781	3455	401	508		49

Appendix V.VIII. Search at Pubchem compound for metabolite:

➤ **m/z=558.478 - H= 557.4700 (557.469 and 557.471)**

1. AC1MT3TE; 4-oxo-N-[4-(2,3,4,5,6-pentafluorophenoxy)phenyl]-2,6-diphenyl-1,4

MW: 557.470858 g/mol MF: C28H17F5NO2PS

IUPAC name: 4-oxo-N-[4-(2,3,4,5,6-pentafluorophenoxy)phenyl]-2,6-diphenyl...

CID: 3544509 (unlikely)

2. Phosphorimidic acid, (diphenoxyphosphinyl)-, triphenyl ester; AGN-PC-00KY1M; CTK0E8201 ...

MW: 557.470124 g/mol MF: C30H25NO6P2

IUPAC name: diphenoxyphosphorylimino(triphenoxy)- S^{I} -phosphane

CID: 13111765

3. AGN-PC-042QS4; N,N-bis(diphenoxyphosphoryl)aniline

MW: 557.470124 g/mol MF: C30H25NO6P2

IUPAC name: N,N-bis(diphenoxyphosphoryl)aniline

CID: 23412864

4. SureCN4245900

MW: 557.469876 g/mol MF: C24H24F5N5O5

IUPAC name: 2,6-difluoro-N-[4-[5-(3-morpholin-4-ylpropylamino)-1,3,4-oxa...

CID: 68973144

➤ **m/z=580.5597 (578.9920=578.9910 to 578.9930)**

1. Octadecanoic acid, 2-methyl-, anhydride; 91357-09-4; ACMC-20luas ...

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: 2-methyloctadecanoyl 2-methyloctadecanoate

CID: 71328160

2. SureCN987670

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: 4-methyl-2-(4-methyl-2-pentadecyloxetan-2-yl)oxy-2-pentadecy...

CID: 66868327

3. octadecanoyl icosanoate; AGN-PC-0DBGN8

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: octadecanoyl icosanoate

CID: 60209074

4. hexadecanoyl docosanoate; AGN-PC-0DBDVQ

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: hexadecanoyl docosanoate

CID: 60205038

5.

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: [(7R)-18-methylnonadecan-7-yl] (Z,12R)-12-hydroxyoctadec-9-e...

CID: 57489994

6. AGN-PC-01XRNC; 9-Octadecenoic acid, 12-hydroxy-, 2-octyldodecyl ester

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: 2-octyldodecyl 12-hydroxyoctadec-9-enoate

CID: 73450280

7. ACMC-20mrcl; 9-Octadecenoic acid, 12-hydroxy-, 2-octyldodecyl ester, (Z)- (9CI); 125093-27-8

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: icosan-9-yl 12-hydroxyoctadec-9-enoate

CID: 71340306

8.

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: 2-[1-[1-(oxiran-2-yl)heptadecoxy]heptadecyl]oxirane

CID: 56611579

9.

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: 2-octyldodecyl (12R)-12-hydroxyoctadec-9-enoate

CID: 54450109

10.

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: nonadecanoyl nonadecanoate

CID: 54406478

11.

MW: 578.992360 g/mol MF: C38H74O3

IUPAC name: (12R)-12-hydroxy-2-(2-octyldodecyl)octadec-9-enoic acid
CID: 54139886

12. OCTYLDODECYL RICINOLEATE; 9-Octadecenoic acid,12-hydroxy-, 2-octyldodecyl ester, (Z)- (9CI); CTK4B4220 ...
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: icosan-9-yl (12R)-12-hydroxyoctadec-9-enoate
CID: 53891347

13.
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: (2R)-3-[(3S,11S)-3,11-dimethyltetradecoxy]-2-[(3R)-3-methyl-...
CID: 42627332

14.
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: icosan-9-yl (Z)-12-hydroxyoctadec-9-enoate
CID: 25125276

15. AGN-PC-03ZTGC; 3-oxoicosan-2-yl octadecanoate
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 3-oxoicosan-2-yl octadecanoate
CID: 23149578

16. AGN-PC-02Q46C; 1-oxohexadecan-3-yl docosanoate
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 1-oxohexadecan-3-yl docosanoate
CID: 19980185

17. AGN-PC-02Q469; 1-oxotetradecan-3-yl tetracosanoate
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 1-oxotetradecan-3-yl tetracosanoate
CID: 19980182

18.
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-octyldodecyl (E)-12-hydroxyoctadec-9-enoate
CID: 18548272

19.
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: (4S)-4-(dotriacont-31-enoxymethyl)-2,2-dimethyl-1,3-dioxolan...
CID: 10817039

20. AC1NTDJ7; Stearic acid, 2-(1-octadecenyloxy)ethyl ester, (E)-; 2-[(1E)-1-Octadecenyloxy]ethyl stearate ...
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-[(E)-octadec-1-enoxy]ethyl octadecanoate
CID: 5378765

21. AC1NTDJ4; 2-[(1Z)-1-Octadecenyloxy]ethyl stearate; 2-[(Z)-octadec-1-enoxy]ethyl octadecanoate ...
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-[(Z)-octadec-1-enoxy]ethyl octadecanoate
CID: 5378764

22. 2-[(9Z)-9-Octadecenyloxy]ethyl stearate; AC1NTDI4; 2-[(Z)-octadec-9-enoxy]ethyl octadecanoate ...
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-[(Z)-octadec-9-enoxy]ethyl octadecanoate
CID: 5378750

23. AC1NSL54; 2-octadecoxyethyl (Z)-octadec-9-enoate; 2-(Octadecyloxy)ethyl (9Z)-9-octadecenoate ...

MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-octadecoxyethyl (Z)-octadec-9-enoate
CID: 5365193

24. AC1NSKSN; 9-Octadecenoic acid, 2-(octadecyloxy)ethyl ester; 2-octadecoxyethyl (E)-octadec-9-enoate ...
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-octadecoxyethyl (E)-octadec-9-enoate
CID: 5365023

25. CTK8I1216
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-octadec-1-enoxyethyl octadecanoate
CID: 628379

26. CTK8J3535; 9-Octadecenoic acid 2-(octadecyloxy)ethyl ester; 56599-42-9
MW: 578.992360 g/mol MF: C38H74O3
IUPAC name: 2-octadecoxyethyl octadec-9-enoate
CID: 545689

m/z:677.6623 (676.6544: 676.6534 to 676.6574) Selection from Bioactive compounds

1. AGN-PC-03X4GP; methyl 2-[4-[(4E,6Z)-4,6-bis[4-(1-methoxy-1-oxopropan-2-yl)oxy-6-oxocyclohexa-2,4-dien-1-ylidene]-1,3,5-triazinan-2-ylidene]-3-oxocyclohexa-1,5-dien-1-yl]oxybutanoate
MW: 677.654600 g/mol MF: C34H35N3O12
IUPAC name: methyl 2-[4-[4,6-bis[4-(1-methoxy-1-oxopropan-2-yl)oxy-6-oxo...
CID: 74012123

2. SureCN10943916
MW: 677.654600 g/mol MF: C34H35N3O12
IUPAC name: [(4S)-4-[(2R,4S,5R,6R)-4-amino-5-methoxy-6-methyloxan-2-yl]o...
CID: 70477817

3. SureCN10943905
MW: 677.654600 g/mol MF: C34H35N3O12
IUPAC name: [(2S,4S)-4-[(2R,4S,5S,6S)-4-amino-5-methoxy-6-methyloxan-2-y...
CID: 70477813

4. SureCN4312728
MW: 677.654600 g/mol MF: C34H35N3O12
IUPAC name: 2-[4-[(2S)-2-amino-3-[4-(3-hydroxy-2-methoxycarbonylphenoxy)...
CID: 68998664

5. SureCN9176973
MW: 677.654600 g/mol MF: C34H35N3O12
IUPAC name: N'-amino-N-[3-hydroxy-2-methyl-6-[[[(1S,3S)-3,5,12-trihydroxy...
CID: 67788816

6.
MW: 677.654600 g/mol MF: C34H35N3O12
IUPAC name: methyl 2-[4-[(4Z,6Z)-4,6-bis[4-(1-methoxy-1-oxopropan-2-yl)o...
CID: 59873926

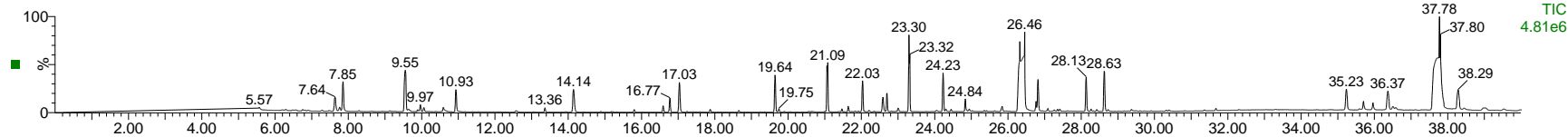
7. SureCN10821895
MW: 677.654600 g/mol MF: C34H35N3O12
IUPAC name: 2-[2-[2-[2-[bis(carboxymethyl)amino]-5-(6-ethoxycarbonyl-1H-...
CID: 53869228

Appendix V.X. Exudate samples at 72 h analysed by GC-MS after derivatization. Ref=reference; E_Chal=challenged; E_Ctrl=control; E_Z=zoospores; E_MSS=Mineral Salt Solution.

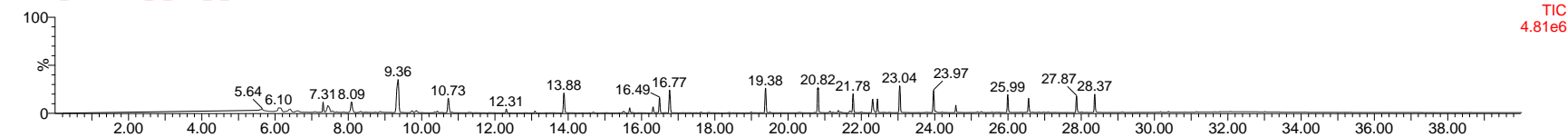
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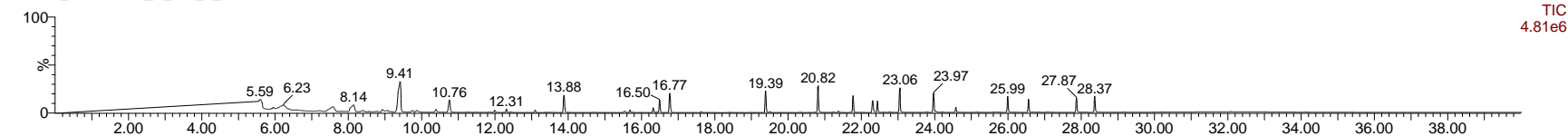
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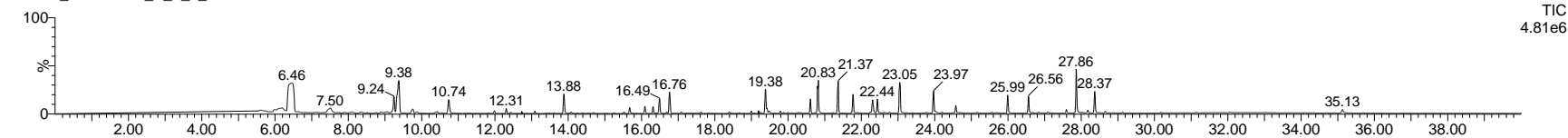
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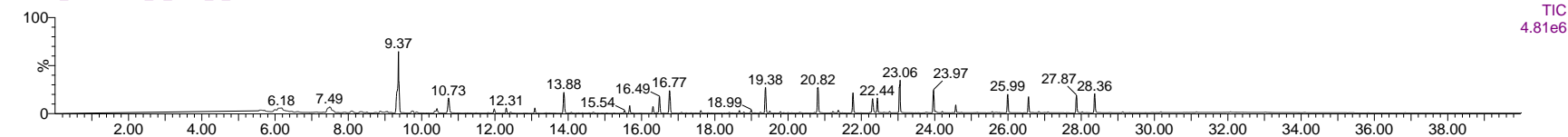
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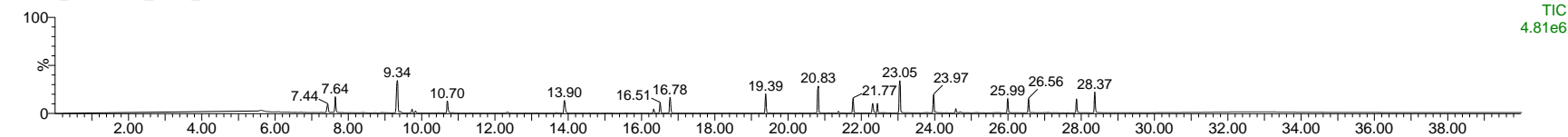
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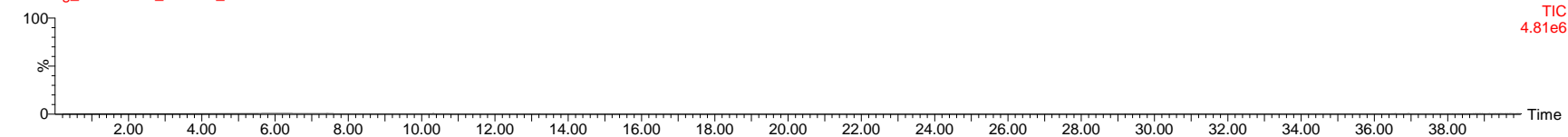
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dneves_201311106_Blank_04



Tshering_201311105_Hexane_03



Time

Appendix V.XI. Comparison of means and T-test for metabolite m/z 355.0929, m/z 355.1442 and m/z 355.2116.

Estatísticas de grupo					
	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz355.0929	Control	20	914,10	2031,567	454,272
	Challenged	20	429,85	565,662	126,486

Teste de amostras independentes										
	Teste de Levene para igualdade de variâncias		teste-t para Igualdade de Médias							
	Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença		
								Inferior	Superior	
Peak_intensity_mz355.0929	Variancias iguais assumidas	4,732	,036	1,027	38	,311	484,250	471,553	-470,350	1438,059
	Variancias iguais não assumidas			1,027	21,928	,316	484,250	471,553	-493,876	1462,376

Estatísticas de grupo					
	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz355.1442	Control	20	1289,80	2546,299	569,370
	Challenged	20	1177,05	2150,786	480,930

Teste de amostras independentes										
	Teste de Levene para igualdade de variâncias		teste-t para Igualdade de Médias							
	Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença		
								Inferior	Superior	
Peak_intensity_mz355.1442	Variancias iguais assumidas	,011	,915	,151	38	,881	112,750	745,303	-1386,036	1621,536
	Variancias iguais não assumidas			,151	36,966	,881	112,750	745,303	-1387,423	1622,923

Estatísticas de grupo					
	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz355.2116	Control	20	4225,50	5812,322	1299,675
	Challenged	20	5230,30	10681,364	2388,426

Teste de amostras independentes										
	Teste de Levene para igualdade de variâncias		teste-t para Igualdade de Médias							
	Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença		
								Inferior	Superior	
Peak_intensity_mz355.2116	Variancias iguais assumidas	1,270	,267	-,370	38	,714	-1804,800	2719,142	-6509,414	4498,814
	Variancias iguais não assumidas			-,370	29,345	,714	-1804,800	2719,142	-6593,231	4553,631

Appendix V.XII. Comparison of means and T-test for metabolite m/z 181.0354 and m/z 181.0713.

Estatísticas de grupo					
	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz181.0354	Control	20	18983,30	21569,856	4823,166
	Challenged	20	938,85	1395,511	312,046

Teste de amostras independentes										
	Teste de Levene para igualdade de variâncias		teste-t para Igualdade de Médias							
	Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença		
								Inferior	Superior	
Peak_intensity_mz181.0354	Variancias iguais assumidas	20,146	,000	3,733	38	,001	18044,450	4833,250	6290,047	27829,853
	Variancias iguais não assumidas			3,733	18,159	,001	18044,450	4833,250	7934,022	28154,878

Estatísticas de grupo					
	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz181.0713	Control	20	7994,10	10660,294	2383,714
	Challenged	20	2459,25	2764,201	618,094

Teste de amostras independentes										
	Teste de Levene para igualdade de variâncias		teste-t para Igualdade de Médias							
	Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença		
								Inferior	Superior	
Peak_intensity_mz181.0713	Variancias iguais assumidas	12,891	,001	2,248	38	,030	5534,850	2462,546	549,686	10520,014
	Variancias iguais não assumidas			2,248	21,543	,035	5534,850	2462,546	421,560	10648,148

Appendix V.XIII. Comparison of means and T-test for metabolite m/z 169.0722, m/z 169.0342 and m/z 169.0859.

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz169.0722	Control	20	3587,75	5575,274	1246,669
	Challenged	20	14114,60	17351,628	3879,942

Teste de amostras independentes										
		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Peak_intensity_mz169.0722	Variâncias iguais assumidas	34,422	,000	-2,583	38	,014	-10526,850	4075,308	-18776,879	-2276,621
	Variâncias iguais não assumidas			-2,583	22,882	,017	-10526,850	4075,308	-18959,677	-2094,023

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz169.0342	Control	20	2717,75	2086,447	466,544
	Challenged	20	512,40	944,736	211,249

Teste de amostras independentes										
		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Peak_intensity_mz169.0342	Variâncias iguais assumidas	7,172	,011	4,306	38	,000	2285,350	512,142	1168,673	3242,127
	Variâncias iguais não assumidas			4,306	26,477	,000	2285,350	512,142	1153,549	3257,151

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz169.0859	Control	20	165,85	216,255	48,356
	Challenged	20	5208,90	9886,571	2210,704

Teste de amostras independentes										
		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Peak_intensity_mz169.0859	Variâncias iguais assumidas	22,345	,000	-2,281	38	,028	-5043,050	2211,233	-9519,458	-566,642
	Variâncias iguais não assumidas			-2,281	19,018	,034	-5043,050	2211,233	-9670,915	-415,185

Appendix V.XIV. Comparison of means and T-test for metabolite m/z 139.1062 and m/z 139.0242

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz139.1062	Control	20	34059,95	26833,170	6000,079
	Challenged	20	37703,10	50465,787	11284,493

Teste de amostras independentes										
		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Peak_intensity_mz139.1062	Variâncias iguais assumidas	18,938	,002	-.285	38	,777	-3643,150	12780,482	-29515,884	22229,584
	Variâncias iguais não assumidas			-.285	28,948	,778	-3643,150	12780,482	-29784,209	22497,909

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz139.0242	Control	20	38987,95	66780,553	14932,586
	Challenged	20	2929,65	5035,897	1126,061

Teste de amostras independentes										
		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Peak_intensity_mz139.0242	Variâncias iguais assumidas	9,187	,004	2,408	38	,021	36058,300	14974,983	5743,031	66373,569
	Variâncias iguais não assumidas			2,408	19,216	,026	36058,300	14974,983	4738,137	67377,463

Appendix V.XV. Comparison of means and T-test for metabolite m/z 211.1925 and m/z

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz211.1925	Control	20	555,35	1169,107	261,420
	Challenged	20	1095,40	1232,689	275,638

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias					95% Intervalo de Confiança da Diferença	
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	Inferior	Superior
Peak_intensity_mz211.1925	Variancias iguais assumidas	2,327	,135	-1,422	38	,163	-540,050	379,890	-1309,098	228,998
	Variancias iguais não assumidas			-1,422	37,894	,163	-540,050	379,890	-1309,169	229,069

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz211.201	Control	20	1750,95	1371,616	306,703
	Challenged	20	1465,85	3434,756	768,035

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias					95% Intervalo de Confiança da Diferença	
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	Inferior	Superior
Peak_intensity_mz211.201	Variancias iguais assumidas	2,336	,135	,345	38	,732	285,100	827,009	-1389,092	1959,292
	Variancias iguais não assumidas			,345	24,910	,733	285,100	827,009	-1418,471	1989,671

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz211.0463	Control	20	40403,50	36862,136	8242,624
	Challenged	20	1066,05	2286,413	511,258

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias					95% Intervalo de Confiança da Diferença	
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	Inferior	Superior
Peak_intensity_mz211.0463	Variancias iguais assumidas	24,054	,000	4,763	38	,000	39337,450	8258,465	22619,062	56955,838
	Variancias iguais não assumidas			4,763	19,146	,000	39337,450	8258,465	22961,213	56813,687

Estatísticas de grupo

	Condition	N	Média	Desvio Padrão	Erro padrão da média
Peak_intensity_mz211.1553	Control	20	3156,70	6716,607	1501,879
	Challenged	20	6499,80	7345,923	1642,598

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias					95% Intervalo de Confiança da Diferença	
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	Inferior	Superior
Peak_intensity_mz211.1553	Variancias iguais assumidas	1,925	,173	-1,592	38	,141	-3343,100	2225,707	-7848,907	1162,607
	Variancias iguais não assumidas			-1,592	37,699	,141	-3343,100	2225,707	-7849,968	1163,788

Appendix V.XV. Search for m/z 149.01 and m/z 198.04 <http://www.massbank.eu/MassBank/jsp/Result.jsp>

MassBank | Database | Quick Search | [Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID:


Quick Search Results

[mass calculator](#) [user manual](#)

Search Parameters :
 Exact Mass of Compound: 149.01 (Tolerance: 0.11)
 Instrument Type: CE-ESI-TOF, HPLC-ESI-TOF, LC-ESI-ITTOF, LC-ESI-QIT, LC-ESI-TOF, ESI-FTICR, LC-ESI-IT, LC-ESI-Q, LC-ESI-QQ, UPLC-ESI-QTOF, ESI-ITFT, LC-ESI-ITFT, LC-ESI-QFT, LC-ESI-QTOF
 MS Type: MS
 Ion Mode: Positive [Edit / Resubmit Query](#)

Results : 3 Hit. (1 - 3 Displayed)

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Name	Formula / Structure	ExactMass	ID
L-Methionine 3 spectra	C5H11NO2S 	149.05105	

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
Quick Search Results

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Search Parameters :
 Exact Mass of Compound: 198.04 (Tolerance: 0.11)
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 MS Type: MS
 Ion Mode: Positive [Edit / Resubmit Query](#)

Results : 4 Hit. (1 - 4 Displayed)

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Name	Formula / Structure	ExactMass	ID
Guafenesin 4 spectra	C10H14O4 	198.08921	

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