Supporting Information for

Identification of novel urolithin metabolites in human feces and urine after the intake of a pomegranate extract

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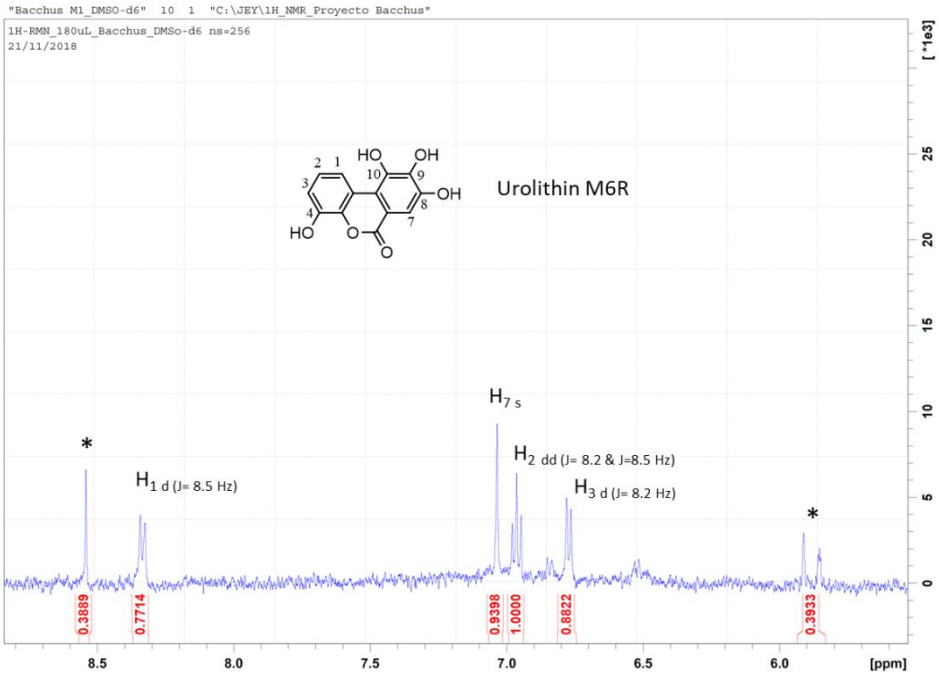
Supplementary Table 1. UPLC-QTOF-MS/MS fragments of the main urolithins at collision energy 30V. In bold, the most intense fragments. In red the fragments with the highest intensity.

	Exact mass	MS/MS fragments	Molecular formula	Mass loss
Urolithin D	259.0248	**242.0226**	-	-17
		213.0199	$C_{12}H_5O_4$	-46
Urolithin M6	259.0248	242.0220	-	-18
		231.0309	$C_{12}H_7O_5$	-28
		213.0101	$C_{12}H_5O_4$	-46
		203.0357	$C_{11}H_7O_4$	-56
		187.0400	$C_{11}H_7O_3$	-72
		175.0420	$C_{10}H_7O_3$	-84
		159.0454	$C_{10}H_7O_2$	-100
Urolithin M6R	259.0248	241.0148	$C_{13}H_5O_5$	-18
		231.0303	$C_{12}H_7O_5$	-28
		213.0201	$C_{12}H_5O_4$	-46
		203.0358	$C_{11}H_7O_4$	-56
		185.0243	$C_{11}H_5O_3$	-74
		159.0455	$C_{10}H_7O_2$	-100
		129.0343	C_9H_5O	-130
Urolithin C	243.0299	226.0275	-	-17
		215.0355	$C_{12}H_7O_4$	-28
		199.0399	$C_{12}H_7O_3$	-44
		187.0398	$C_{11}H_7O_3$	-56
		171.0438	$C_{11}H_7O_2$	-72
		143.0495	$C_{10}H_7O$	-100
Urolithin CR	243.0299	**226.0276**	-	-17
		215.0353	$C_{12}H_7O_4$	-28
		197.0251	$C_{12}H_5O_3$	-46
		187.0402	$C_{11}H_7O_3$	-56
		171.0438	$C_{11}H_7O_2$	-72
Urolithin M7	243.0299	**198.0332**	-	-45
		187.0400	$C_{11}H_7O_3$	-56
		173.0239	$C_{10}H_5O_3$	-70
		147.0452	$C_9H_7O_2$	-96
Urolithin M7R	243.0299	226.0278	-	-17
		215.0336	$C_{12}H_7O_4$	-28
		199.0359	$C_{12}H_7O_3$	-44
		187.0401	$C_{11}H_7O_3$	-56
		171.0454	$C_{11}H_7O_2$	-72
		143.052	$C_{10}H_7O$	-100
Isourolithin A	227.0350	198.0325	-	-29
		183.0456	$C_{12}H_7O_2$	-44
		171.0458	$C_{11}H_7O_2$	-56
		159.0453	-	-68
Urolithin A	227.0350	210.0319	-	-17
		198.0335	-	-29
		182.0371	-	-45
		171.0444	$C_{11}H_7O_2$	-56

		154.0426	-	-73
Urolithin AR	227.0350	**210.0324** 198.0333 182.0378 171.0455 154.0429	- - - $C_{11}H_7O_2$ -	-17 -29 -45 -56 -73
Urolithin B	211.0401	**167.0504** 155.0495 **139.0548**	$C_{12}H_7O$ - $C_{11}H_7$	-44 -56 -72
Urolithin BR	211.0401	**183.0452** 167.0557 **155.0500**	$C_{12}H_7O_2$ $C_{12}H_7O$ $C_{11}H_7O$	-28 -44 -56

Supplementary Figure 1



Supplementary Figure 1. ^{1}H NMR spectrum of urolithin M6R (4,8,9,10-tetrahydroxy urolithin). (*) Contaminants.