

Supplementary Material (ESI) for Molecular BioSystems
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ID	Annotation	Mode	m/z	² RelArea ± SD (×1000)			DL/HC		DL/DLS	
				Plasma			Ratio	³ p-value	Ratio	³ p-value
				HC	DL	DLS				
<i>Fatty acid</i>										
AN_231	FA(12:1)	A	197.16	0.8 ± 0.3	0.7 ± 0.2	0.8 ± 0.1	0.9	0.73	0.9	0.59
AN_232	FA(12:0)	A	199.17	1.4 ± 0.4	2.4 ± 0.2	1.3 ± 0.4	1.8	0.02	1.9	0.013
AN_233	FA(13:0)	A	213.19	N.D.	0.4 ± 0.2	0.3	N.A.	N.A.	1.2	N.A.
AN_234	FA(14:3)	A	221.16	3.1 ± 0.8	4.5 ± 1.1	3.3 ± 0.4	1.5	0.15	1.3	0.20
AN_235	FA(14:2)	A	223.17	0.9 ± 0.1	1.0 ± 0.3	1.0 ± 0.4	1.1	0.55	1.0	0.97
AN_236	FA(14:1)	A	225.19	0.7 ± 0.1	1.2 ± 0.6	0.8 ± 0.2	1.8	0.28	1.5	0.39
AN_237	FA(14:1)	A	225.19	0.7 ± 0.3	3.2 ± 1.1	1.4 ± 0.6	4.4	0.05	2.3	0.08
AN_238	FA(14:0)/Myristic acid	A	227.20	21.9 ± 7.0	44.0 ± 7.8	23.3 ± 3.8	2.0	0.02	1.9	0.03
AN_239	FA(15:1)	A	239.20	1.6 ± 1.9	2.8 ± 0.7	1.1 ± 0.2	1.8	0.38	2.6	0.03
AN_240	FA(15:1)	A	239.20	2.8 ± 0.6	6.7 ± 0.8	3.4 ± 1.0	2.4	3.2E-03	2.0	0.011
AN_241	FA(15:0)/Pentadecanoic acid	A	241.22	6.7 ± 0.4	10.0 ± 1.1	7.4 ± 0.9	1.5	0.02	1.4	0.04
AN_242	3-Hydroxytetradecanoic acid	A	243.20	0.4 ± 0.2	0.9 ± 0.2	0.6 ± 0.1	2.3	0.10	1.6	0.13
AN_243	FA(16:3)	A	249.19	0.5 ± 0.1	1.4 ± 0.2	0.7 ± 0.2	3.0	8.2E-03	2.0	0.02
AN_244	FA(16:2)	A	251.20	2.1 ± 0.4	5.1 ± 0.3	3.4 ± 1.0	2.5	1.1E-03	1.5	0.09
AN_245	FA(16:1)	A	253.22	79.5 ± 25.4	266.2 ± 68.3	129.7 ± 45.2	3.3	0.03	2.1	0.05
AN_246	FA(16:0)	A	255.23	794.5 ± 56.0	1295.7 ± 140.2	962.2 ± 215.2	1.6	0.015	1.3	0.10
AN_247	FA(17:3)	A	263.20	N.D.	0.9 ± 0.1	0.5 ± 0.2	N.A.	N.A.	1.7	0.25
AN_248	FA(17:2)	A	265.22	0.9 ± 0.2	2.8 ± 0.4	1.5 ± 0.6	3.0	3.8E-03	2.0	0.04
AN_249	FA(17:1)	A	267.23	17.6 ± 5.4	34.2 ± 4.5	20.8 ± 7.2	1.9	0.02	1.6	0.06
AN_250	FA(17:0)	A	269.25	37.6 ± 1.4	57.3 ± 4.0	46.8 ± 6.4	1.5	8.2E-03	1.2	0.09
AN_251	FA(18:4)	A	275.20	0.6 ± 0.1	1.8 ± 0.1	0.9 ± 0.3	3.1	3.5E-04	2.0	0.03
AN_252	FA(18:3)	A	277.22	300.0 ± 77.6	800.4 ± 82.0	401.9 ± 156.9	2.7	1.6E-03	2.0	0.03
AN_253	FA(18:2)	A	279.23	1547.4 ± 217.6	2977.0 ± 181.8	2024.4 ± 546.8	1.9	1.1E-03	1.5	0.08
AN_254	FA(18:1)/Oleic acid	A	281.25	1399.2 ± 285.3	2545.1 ± 367.2	1778.6 ± 507.4	1.8	0.015	1.4	0.11
AN_255	FA(18:0)/Stearic acid	A	283.27	481.6 ± 81.2	710.9 ± 85.6	566.6 ± 114.1	1.5	0.03	1.3	0.16
AN_256	Methyl palmitic acid	C	288.29	5.0 ± 0.9	6.2 ± 1.8	6.0 ± 1.8	1.3	0.36	1.0	0.89
AN_257	FA(19:2)	A	293.25	0.7 ± 0.2	1.4 ± 0.1	0.9 ± 0.1	2.0	0.02	1.7	0.007
AN_258	FA(19:1)	A	295.27	10.6 ± 2.0	16.3 ± 2.6	11.7 ± 1.9	1.5	0.04	1.4	0.07
AN_259	FA(19:0)	A	297.28	3.8 ± 0.6	6.6 ± 0.9	4.7 ± 0.7	1.8	0.014	1.4	0.05
AN_260	FA(20:5)	A	301.22	2.9 ± 0.7	6.7 ± 0.8	4.0 ± 0.9	2.3	3.2E-03	1.7	0.02
AN_261	FA(20:4)/Arachidonic acid	A	303.23	43.7 ± 6.7	87.3 ± 5.0	59.4 ± 14.2	2.0	1.2E-03	1.5	0.06
AN_262	FA(20:3)	A	305.25	1.8 ± 0.3	4.1 ± 0.3	3.0 ± 0.8	2.3	5.3E-04	1.4	0.12
AN_263	FA(20:3)	A	305.25	8.0 ± 1.8	16.4 ± 1.3	10.7 ± 2.1	2.0	3.9E-03	1.5	0.02
AN_264	FA(20:2)	A	307.27	13.4 ± 2.5	24.6 ± 2.7	16.3 ± 1.9	1.8	6.5E-03	1.5	0.02
AN_265	FA(20:1)	A	309.28	13.5 ± 1.4	23.9 ± 1.5	18.4 ± 3.6	1.8	8.4E-04	1.3	0.11
AN_266	FA(20:0)	A	311.30	2.7 ± 0.4	6.4 ± 1.1	4.4 ± 1.1	2.3	0.02	1.5	0.09
AN_267	FA(21:0)	A	325.31	0.3	0.9 ± 0.2	0.6 ± 0.1	3.4	N.A.	1.5	0.08
AN_268	FA(22:5)	A	329.25	13.5 ± 2.2	26.7 ± 2.9	21.7 ± 2.4	2.0	4.1E-03	1.2	0.09
AN_269	FA(22:4)	A	331.27	8.7 ± 2.0	16.1 ± 1.2	12.5 ± 1.8	1.8	9.6E-03	1.3	0.05
AN_270	FA(22:3)	A	333.28	0.6	1.1 ± 0.2	1.1 ± 0.2	1.8	N.A.	1.1	0.64
AN_271	FA(22:2)	A	335.30	0.5 ± 0.0	1.1 ± 0.2	0.9 ± 0.3	2.3	0.014	1.2	0.38
AN_272	FA(22:1)/Erucic acid	A	337.31	1.4 ± 0.4	3.0 ± 0.6	2.1 ± 0.6	2.2	0.02	1.4	0.12
AN_273	FA(22:0)	A	339.33	1.1 ± 0.1	8.8 ± 1.4	5.2 ± 1.6	7.9	9.9E-03	1.7	0.04
AN_274	Ethyl arachidonic acid	C	350.31	15.8 ± 3.0	22.7 ± 1.2	21.3 ± 4.7	1.4	0.04	1.1	0.66
AN_275	FA(23:0)	A	353.34	0.7 ± 0.1	1.4 ± 0.5	1.0 ± 0.3	1.9	0.13	1.5	0.26
AN_276	FA(24:5)	A	357.28	0.5 ± 0.2	1.1 ± 0.1	0.9	2.2	0.07	1.2	N.A.
AN_277	FA(24:4)	A	359.30	0.4 ± 0.0	0.7 ± 0.1	0.5 ± 0.1	1.8	0.02	1.4	0.03
AN_278	FA(24:2)	A	363.33	0.5 ± 0.0	1.5 ± 0.1	1.3 ± 0.2	2.8	3.2E-03	1.2	0.14
AN_279	FA(24:1)	A	365.34	2.5 ± 0.3	7.9 ± 3.1	6.8 ± 2.5	3.2	0.09	1.2	0.67
AN_280	FA(24:0)/n-Tetracosanoic acid	A	367.36	1.7 ± 0.4	3.7 ± 0.9	2.0 ± 0.5	2.1	0.04	1.9	0.06
AN_281	FA(25:3)	A	375.33	0.6 ± 0.3	7.1 ± 2.5	2.2 ± 0.6	12.0	0.04	3.3	0.07
AN_282	FA(25:0)	A	381.38	0.5 ± 0.1	0.9 ± 0.2	0.4 ± 0.0	1.6	0.08	2.3	0.05
AN_283	FA(26:2)	A	391.36	0.2	2.5 ± 0.5	1.2 ± 0.1	10.5	N.A.	2.1	0.05
AN_284	FA(26:0)	A	395.39	0.5 ± 0.1	0.9 ± 0.2	0.4 ± 0.1	1.8	0.07	2.1	N.A.
<i>Acyl-carnitine</i>										
AN_285	AC(13:1)	C	356.28	1.0 ± 0.3	N.D.	1.0 ± 0.4	N.A.	N.A.	N.A.	N.A.
AN_286	AC(14:3)	C	366.26	0.7 ± 0.1	N.D.	0.8 ± 0.3	N.A.	N.A.	N.A.	N.A.
AN_287	AC(14:2)	C	368.28	2.4 ± 0.6	N.D.	3.9 ± 0.6	N.A.	N.A.	N.A.	N.A.
AN_288	AC(14:1)	C	370.29	5.8 ± 0.8	N.D.	9.0 ± 1.8	N.A.	N.A.	N.A.	N.A.
AN_289	AC(14:0)	C	372.31	5.9 ± 1.2	3.4 ± 2.6	10.3 ± 6.9	0.6	0.24	0.3	0.22
AN_290	AC(15:0)	C	386.33	1.8 ± 0.6	1.6 ± 0.6	2.5 ± 1.0	0.9	0.68	0.6	0.26
AN_291	AC(16:2)	C	396.31	3.5 ± 0.8	0.4	6.0 ± 1.1	0.10	N.A.	0.06	N.A.
AN_292	AC(16:1)	C	398.33	9.5 ± 0.2	4.5 ± 2.5	13.3 ± 9.2	0.5	0.07	0.3	0.23
AN_293	AC(16:0)	C	400.34	44.6 ± 11.0	71.9 ± 28.4	124.8 ± 36.2	1.6	0.23	0.6	0.12
AN_294	AC(17:1)	C	412.33	1.8 ± 0.3	0.6 ± 0.2	1.8 ± 0.5	0.3	7.0E-03	0.3	0.05
AN_295	AC(17:0)	C	414.36	3.3 ± 0.8	6.2 ± 1.9	10.0 ± 1.7	1.9	0.10	0.6	0.06
AN_296	AC(18:2)	C	424.34	57.9 ± 12.0	25.2 ± 11.7	69.3 ± 43.4	0.4	0.03	0.4	0.22
AN_297	AC(18:1)	C	426.36	54.4 ± 6.2	64.3 ± 37.4	122.1 ± 55.7	1.2	0.69	0.5	0.22
AN_298	AC(18:0)	C	428.37	26.8 ± 7.7	78.3 ± 36.9	134.2 ± 19.4	2.9	0.13	0.6	0.10
AN_299	AC(20:1)	C	454.39	1.9 ± 0.3	4.7 ± 1.8	6.1 ± 1.2	2.4	0.11	0.8	0.33
AN_300	AC(20:0)	C	456.40	1.2 ± 0.0	4.9 ± 1.1	5.2 ± 0.3	4.1	0.03	0.9	0.69
AN_301	AC(21:0)	C	470.42	0.3	1.0 ± 0.2	1.0 ± 0.0	3.7	N.A.	1.1	0.46

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AN_302	AC(22:0)	C	484.43	1.1 ± 0.2	3.0 ± 0.5	2.7 ± 0.5	2.6	*	0.011	1.1	0.57
AN_303	AC(23:0)	C	498.45	0.9 ± 0.1	2.0 ± 0.6	1.6 ± 0.4	2.3		0.08	1.2	0.41
<i>Bile acids</i>											
AN_304	Cholesterol	C	369.36	557.9 ± 62.5	5560.9 ± 1592.4	4010.0 ± 2470.8	10.0	*	0.03	1.4	0.42
AN_305	Lithocholic acid	A	375.29	6.0 ± 3.7	3.9 ± 0.5	1.7 ± 0.4	0.6		0.39	2.3	* 3.7E-03
AN_306	Ursodeoxycholic acid	A	391.29	111.3 ± 51.7	32.2 ± 8.0	32.2 ± 8.3	0.3	*	9.7E-04	1.0	0.99
AN_307	Chenodeoxycholic acid	A	391.29	379.5 ± 257.1	116.2 ± 41.9	50.5 ± 10.9	0.3		0.13	2.3	0.10
AN_308	Cholic acid	A	407.28	5.6 ± 2.1	2.4 ± 0.5	1.8 ± 0.6	0.4	*	0.012	1.3	0.27
AN_309	Glycolithocholic acid	A	432.32	3.0 ± 1.4	2.8 ± 2.3	1.3 ± 0.4	0.9		0.27	2.1	* 0.02
AN_310	Glycochenodeoxycholic acid	A	448.31	17.4 ± 11.9	12.3 ± 9.5	4.3 ± 2.0	0.7		0.55	2.8	0.28
AN_311	Glycodeoxycholic acid	A	448.31	3.0 ± 1.4	2.8 ± 2.3	1.3 ± 0.4	0.9		0.88	2.1	0.39
AN_312	Glycocholic acid	A	464.30	2.2 ± 0.6	1.9 ± 0.4	1.3 ± 0.3	0.8		0.57	1.4	0.16
AN_313	Taurochenodeoxycholic acid	A	498.30	0.9 ± 0.3	0.8 ± 0.2	0.3 ± 0.1	0.8		0.39	2.5	0.06
AN_314	Taurocholic acid	A	514.29	1.9 ± 0.6	1.6 ± 0.4	0.8	0.8		0.33	2.0	N.A.
<i>Steroids</i>											
AN_315	Androsterone	C	308.26	1.6 ± 0.4	1.8 ± 0.2	1.4 ± 0.4	1.1		0.60	1.3	0.19
AN_316	Cortisolone	C	347.22	6.1 ± 5.1	18.0 ± 4.1	17.2 ± 12.0	3.0	*	0.04	1.0	0.92
AN_317	18-Hydroxycorticosterone	C	363.22	1.1 ± 0.1	1.4 ± 0.3	0.5 ± 0.0	1.3		0.41	2.6	0.17
AN_318	Campesterol	C	383.37	24.6 ± 1.5	143.5 ± 49.9	91.5 ± 72.3	5.8		0.05	1.6	0.37
AN_319	4-Cholestan-3-one	C	385.35	1.3	39.8 ± 7.4	23.9 ± 8.5	30.4		N.A.	1.7	0.07
AN_320	5 α -Cholestan-3-one	C	387.37	4.3 ± 0.6	49.3 ± 15.9	31.1 ± 18.3	11.5	*	0.04	1.6	0.27
AN_321	Dihydrotachysterol	C	399.36	N.D.	16.0 ± 4.0	15.1 ± 9.5			N.A.	1.1	0.88
AN_322	Hecogenin	C	431.32	3.6 ± 0.4	6.1 ± 1.0	4.4 ± 0.3	1.7	*	0.03	1.4	0.08
AN_323	α -Tocopherol	C	431.39	95.0 ± 23.2	1212.4 ± 80.5	1232.3 ± 125.1	12.8	*	8.3E-04	1.0	0.83
AN_324	α -Tocopherol acetate	C	490.42	0.9 ± 0.0	4.5 ± 1.3	2.5 ± 0.5	5.0	*	0.04	1.8	0.11
<i>Flavonoids</i>											
AN_325	Isoliquiritigenin	A	255.07	0.4 ± 0.2	0.6 ± 0.2	0.4 ± 0.1	1.3		0.50	1.3	0.45
AN_326	Naringenin	A	271.06	0.8 ± 0.2	0.9 ± 0.2	N.D.	1.1		0.69	N.A.	N.A.
AN_327	6-Hydroxyapigenin	A	285.04	4.4 ± 0.8	4.3 ± 0.6	3.1 ± 1.0	1.0		0.91	1.4	0.17
AN_328	Kaempferol	C	287.05	0.8 ± 0.1	0.7 ± 0.3	1.5 ± 0.5	1.0		0.25	0.5	0.13
AN_329	Phyllodulcin	C	287.09	1.4 ± 1.3	0.8 ± 0.2	1.0 ± 0.6	0.6		0.52	0.8	0.70
AN_330	Quercetin	A	301.04	1.0 ± 0.3	1.2 ± 0.2	0.6 ± 0.1	1.1		0.40	1.8	* 0.05
<i>Others</i>											
AN_331	Retinol	C	287.23	21.5 ± 3.3	17.3 ± 1.1	20.2 ± 2.6	0.8		0.15	0.9	0.19
AN_332	Ricinoleic acid	A	297.24	6.5 ± 5.0	16.2 ± 0.6	9.1 ± 1.9	2.5	*	1.7E-04	1.8	* 0.015
AN_333	Sphingosine	C	300.29	6.4 ± 0.3	4.4 ± 0.5	2.6 ± 0.6	0.7	*	9.6E-03	1.7	* 0.02
AN_334	Mandelonitrile	C	134.06	5.7 ± 3.1	3.8 ± 0.5	3.1 ± 0.1	0.7		0.41	1.2	0.15
AN_335	Simvastatin	C	419.28	N.D.	N.D.	30.3 ± 6.0	N.A.		N.A.	N.A.	N.A.

¹ Peaks were detected in LC-TOF MS measurement for cation mode (C) or anion mode (A).

² Raw area values of each sample were normalized (see *Experimental Procedures*), and standard deviations (SDs) were calculated ($n = 3$).

³ p -value (Student's t test)

⁴ Detected only from one time in each group.

* $p < 0.05$

DL: untreated Watanabe heritable hyperlipidemic rabbits; DLS: simvastatin-treated Watanabe heritable hyperlipidemic rabbits; HC: Japanese white healthy control rabbits

N.D.: Not Detected, N.A.: Not Available