

Supplemental table S2: Atorvastatin metabolite concentrations in the time-series experiment on primary human hepatocytes of Individual 2

	AS	ASL	ASpOH	ASoOH	ASLpOH	ASLoOH
time [min]	Extracellular Concentrations [pmol ml ⁻¹]					
0	8803.3 ±785.4	56.1 ±5.1	n.d.	n.d.	n.d.	n.d.
30	6709.7 ±536.9	20.0 ±2.8	2.1 ±0.4	10.5 ±1.8	n.d.	n.d.
60	6416.5 ±297.9	26.2 ±1.5	10.0 ±0.9	47.7 ±1.5	1.3 ±0.4	n.d.
120	6571.1 ±133.0	30.7 ±2.2	77.7 ±8.9	272.5 ±10.8	3.4 ±0.7	4.8 ±0.2
240	5284.9 ±288.6	40.4 ±3.2	341.9 ±29.8	875.2 ±23.6	6.4 ±1.0	9.4 ±0.4
360	4676.7 ±175.7	35.8 ±2.0	561.9 ±25.0	1348.3 ±94.3	6.6 ±1.0	9.7 ±0.4
480	4271.2 ±968.2	34.1 ±1.9	754.1 ±36.0	1666.4 ±75.0	7.6 ±1.1	10.4 ±0.3
720	2626.6 ±65.5	29.9 ±2.1	1131.7 ±82.2	2082.3 ±93.1	10.2 ±0.9	19.2 ±0.9
time [min]	Intracellular Concentrations [pmol ml ⁻¹]					
30	31162.9 ±2469.3	350.3 ±29.7	837.1 ±19.4	592.4 ±13.0	79.7 ±4.8	n.d.
60	29251.8 ±2815.3	398.6 ±29.8	1350.6 ±16.6	857.0 ±80.2	86.0 ±2.8	n.d.
120	30829.5 ±98.1	459.0 ±39.0	2634.3 ±72.7	1784.9 ±190.6	135.7 ±5.1	32.4 ±8.8
240	27117.8 ±1142.2	518.2 ±28.4	3165.4 ±282.0	2077.5 ±272.3	157.1 ±10.0	51.5 ±6.4
360	22432.9 ±2525.3	422.5 ±68.6	4342.4 ±599.7	2489.7 ±142.0	164.7 ±21.8	63.8 ±21.8
480	19098.5 ±1589.6	359.7 ±40.6	4045.3 ±522.4	2704.5 ±210.9	133.1 ±9.8	45.8 ±16.7
720	13392.5 ±347.0	313.1 ±22.5	5554.6 ±463.9	3716.2 ±459.9	148.1 ±14.6	74.5 ±12.2

Extracellular concentrations (upper part) and intracellular concentrations (lower part) of Atorvastatin metabolites, Atorvastatin acid and lactone (AS and ASL) and corresponding para- and ortho-hydroxy-metabolites (acids: ASpOH and ASoOH; lactones: ASLpOH and ASLoOH) at the defined time-points with mean and standard deviation (n=3) from measurements per LC-MS/MS (n.d.: not determinable; n.o.: not observed).