

Supplemental table S3: Atorvastatin metabolite concentrations in the time-series experiment on primary human hepatocytes of Individual 3

	AS		ASL		ASpOH		ASoOH		ASLpOH		ASLoOH	
time [min]	Extracellular Concentrations [pmol ml ⁻¹]											
0	9041.0	±195.5	27.8	±2.0	n.d.		n.d.		n.d.		n.d.	
30	8344.6	±2257.8	27.0	±3.4	n.d.		n.d.		n.d.		n.d.	
60	8580.2	±1810.9	32.1	±6.7	10.8	±0.2	28.7	±0.9	n.d.		n.d.	
120	7439.3	±1331.9	51.6	±16.0	36.9	±2.9	90.4	±13.3	5.2	±0.1	6.0	±0.3
240	7035.6	±949.8	46.3	±12.7	224.7	±18.2	475.3	±33.9	7.0	±0.2	7.6	±0.6
480	4884.2	±652.5	60.6	±1.2	780.7	±26.4	1412.3	±25.4	10.1	±0.3	10.3	±0.8
720	4301.0	±153.6	38.7	±5.0	1087.5	±63.0	1747.6	±40.2	11.0	±1.3	12.1	±0.8
960	2530.3	±153.2	31.4	±10.2	1485.6	±69.7	2179.2	±76.0	14.5	±2.9	16.5	±3.9
1200	1968.0	±262.9	23.8	±2.7	1815.7	±46.9	2344.2	±87.5	18.5	±0.7	20.9	±0.9
time [min]	Intracellular Concentrations [pmol ml ⁻¹]											
30	29613.3	±1767.5	389.8	±5.6	663.0	±19.3	433.5	±70.6	203.3	±3.0	n.d.	
60	38633.4	±5714.4	437.2	±55.1	3316.3	±536.8	1492.3	±169.8	222.6	±6.7	n.d.	
120	33630.5	±7944.7	483.7	±97.1	5683.9	±1294.6	2227.9	±640.3	243.9	±24.8	65.9	±20.5
240	31980.2	±1907.7	611.9	±58.6	7413.0	±462.1	2935.0	±462.1	297.5	±11.4	119.9	±50.9
480	27551.1	±3830.0	562.1	±101.0	10260.4	±2006.2	3724.9	±630.7	318.7	±34.5	147.2	±7.0
720	17601.2	±591.4	393.0	±57.1	8615.2	±590.5	2797.6	±576.7	275.4	±23.5	112.1	±48.1
960	13855.9	±1555.3	311.3	±17.0	12896.4	±875.7	3946.7	±466.6	323.5	±12.3	130.9	±67.3
1200	9622.1	±403.5	280.9	±23.4	15129.2	±1102.4	3628.3	±166.4	359.8	±23.6	152.8	±30.8

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).