Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

# Distribution study of atorvastatin and its metabolites in rat tissues using combined information from UHPLC/MS and MALDI-Orbitrap-MS imaging

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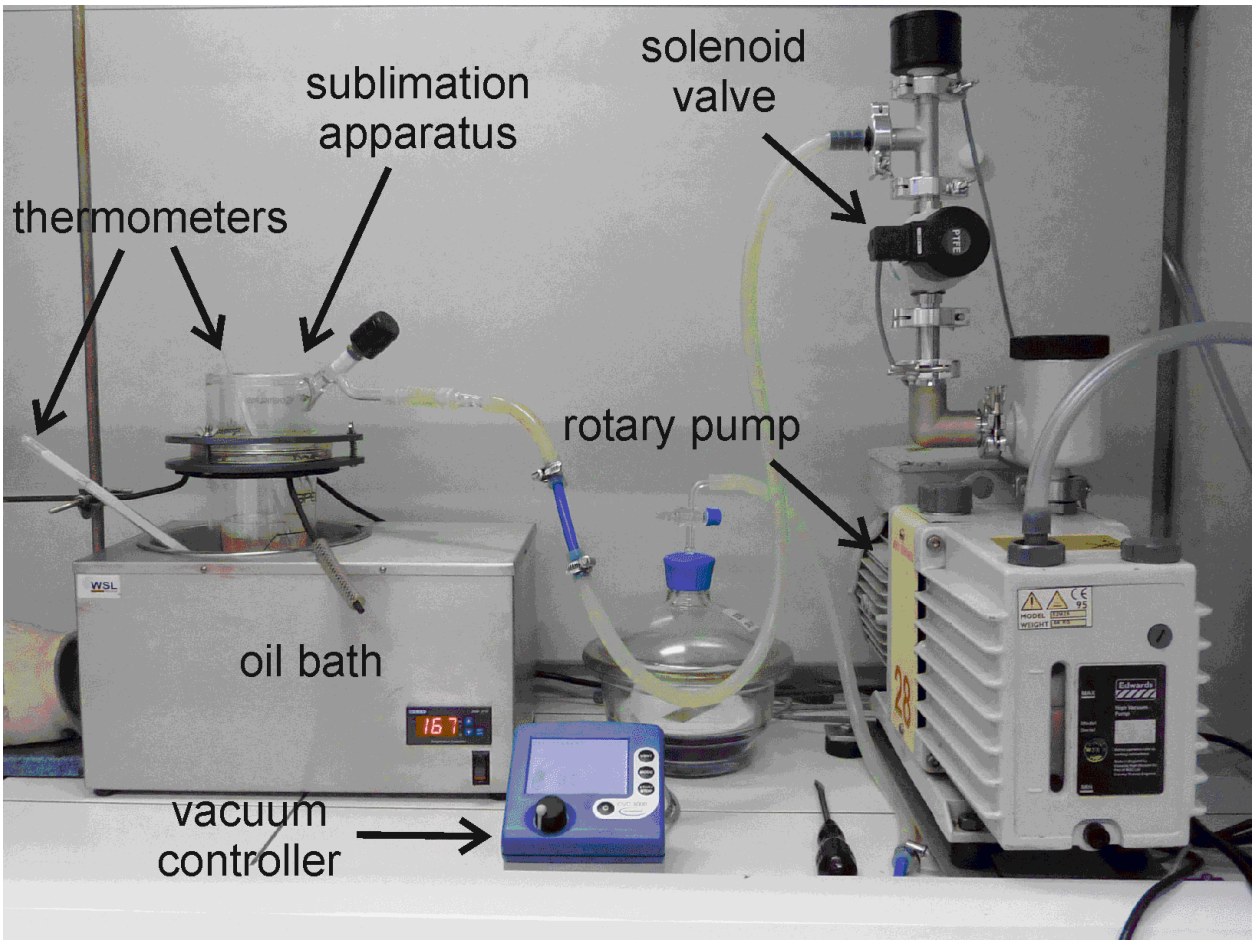


**Fig. S1.** Experimental setup used for the sublimation deposition of matrices

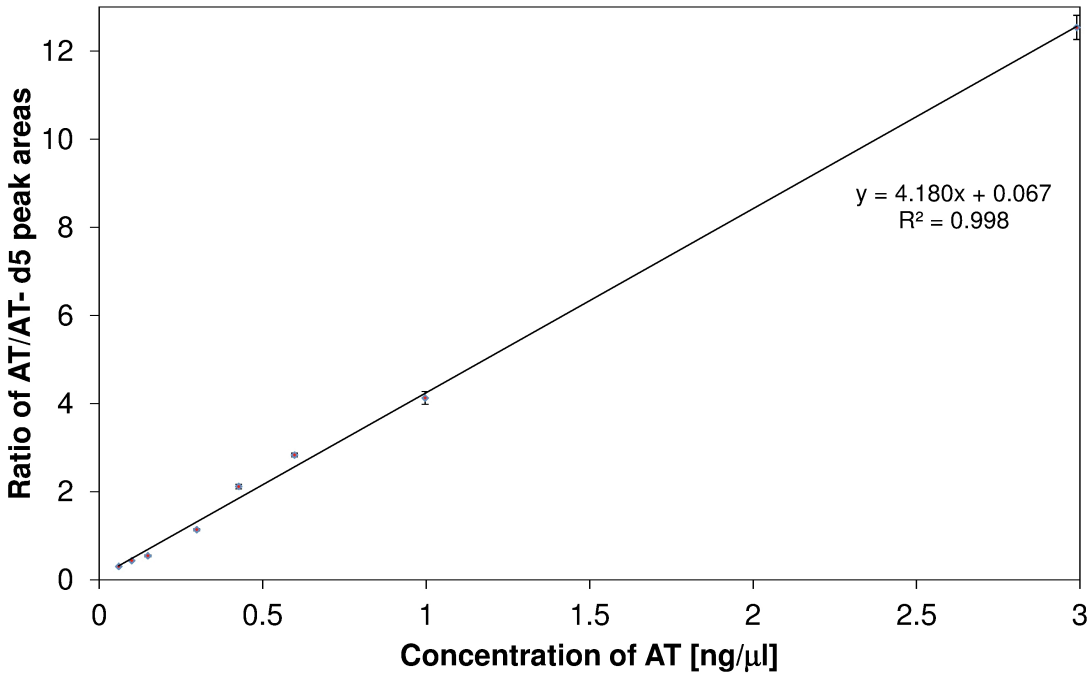


**Fig. S2.** Calibration curve of AT with the normalization to AT-d5. Calibration curve error bars represent the standard deviations of three different measurements (Table S1)

**Table S1.** List of AT standard solutions used for UHPLC/MS quantitation study, their concentrations and experimental values of particular ratios of UHPLC/MS peak areas for AT and its internal standard $EIC_{AT}/EIC_{IS}$

| **Dilution of AT stock solution** | **Concentration [ng/µl]** | **Ratio of UHPLC/MS peak area $EIC_{AT}/EIC_{IS}$** | | | |
|---|---|---|---|---|---|
| | | **analysis 1** | **analysis 2** | **analysis 3** | **average value** |
| 5000x | 0.060 | 0.301 | 0.303 | 0.300 | 0.301 ± 0.001 |
| 3000x | 0.100 | 0.438 | 0.431 | 0.434 | 0.434 ± 0.003 |
| 2000x | 0.149 | 0.533 | 0.571 | 0.524 | 0.543 ± 0.020 |
| 1000x | 0.299 | 1.170 | 1.130 | 1.110 | 1.137 ± 0.025 |
| 700x | 0.427 | 2.070 | 2.190 | 2.090 | 2.117 ± 0.052 |
| 500x | 0.598 | 2.890 | 2.800 | 2.800 | 2.830 ± 0.042 |
| 300x | 0.997 | 4.320 | 4.090 | 3.970 | 4.127 ± 0.145 |
| 100x | 2.990 | 12.290 | 12.920 | 12.400 | 12.537 ± 0.275 |

**Table S2.** Experimental data of UHPLC/MS quantitation study including description of measured rat samples, particular ratios of UHPLC/MS peak areas for AT and its internal standard $EIC_{AT}/EIC_{IS}$ and average of AT concentrations including three sample injections calculated based on the calibration curve

| rat samples | Ratio of UHPLC/MS peak area $EIC_{AT}/EIC_{IS}$ | | | | AT concentration [mg/kg] / [mg/l] |
|---|---|---|---|---|---|
| | analysis 1 | analysis 2 | analysis 3 | average value | |
| liver, slice 1 (7.1 mg) | 1.949 | 1.973 | 2.147 | 2.023 ± 0.088 | 19.78 ± 0.89 |
| liver, slice 2 (9.5 mg) | 2.660 | 2.847 | 2.707 | 2.738 ± 0.080 | 20.17 ± 0.60 |
| liver, slice 3 (9.1 mg) | 2.558 | 2.667 | 2.674 | 2.633± 0.053 | 20.24 ± 0.42 |
| serum | 6.438 | 6.252 | 5.895 | 6.195 ± 0.226 | 0.44 ± 0.02 |
| feces 202 mg (1000x diluted) | 2.602 | 2.502 | 2.684 | 2.596 ± 0.074 | 898 ± 25 |
| urine | < LOD | < LOD | < LOD | - | < LOD |