**Sorption and biodegradation parameters of selected pharmaceuticals in laboratory column experiments**

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**Supplementary details**

**S1 Tandem mass spectrometric determination of pharmaceutics**

**Instrumentation**

Ultrahigh performance liquid chromatography (UHPLC): Agilent 1290 Infinity LC-system consisting of an autosampler 1290 G4226A, a pump 1290 G4220A and a column thermostat 1290 G1316C (Agilent Technologies, Santa Clara, US).

Mass spectrometer (MS): API 4000 QTrap from Sciex (Darmstadt, Germany).

**Chromatographic separation**

Analytical column: Acquity HSS T3, 1,8 µm, 50 x 2,1 mm I.D.

Flow rate: 0.5 ml/min

Temperature: 20°C

Injection volume: 1 µl

Eluents: A: Formic acid/ammoniumformate (10 mmol/l, respectively), B: methanol

Gradient: From 5 % B to 95 % B in 4.5 min; to 100 % B in 0.1 min. At 100 % B for 1.4 min. In 0.1 min to 5 % B again. These conditions are kept constant for 0.9 min (equilibration).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Substance | m/z Q1 | m/z Q3 | DP(V) | CE(V) | CXP(V) | Dwelltime(ms) |
| Caffeine | 195.2 | 110.1 | 72.0 | 33.0 | 9.0 | 50 |
| Caffeine | 195.2 | 179.1 | 75.0 | 36.0 | 9.0 | 50 |
| Antipirine | 189.2 | 104.1 | 75.0 | 34.0 | 6.0 | 50 |
| Antipirine | 189.2 | 161.2 | 74.0 | 25.0 | 9.0 | 50 |
| SMX | 254.1 | 156.2 | 63.0 | 23.0 | 9.0 | 50 |
| Atenolol | 267.2 | 190.2 | 70.0 | 27.0 | 9.0 | 50 |
| Atenolol | 267.2 | 145.0 | 71.0 | 37.0 | 9.0 | 50 |
| Carbamazepine | 237.2 | 194.1 | 70.0 | 28.0 | 9.0 | 50 |
| Carbamazepine | 237.2 | 220.2 | 69.0 | 21.0 | 9.0 | 50 |

DP: Declustering potential
CE: Collision energy
CXP: Cell exit potential

Ion spray voltage was 5500 V, source temperature was 650 °C. Ion source gas 1 and ion source gas 2 were adjusted at 50 psi, collision gas had 11 psi, and curtain gas 20 psi.

**S2 Ion chemistry of the groundwater used in this study: fresh groundwater (Neuherberg) and water at the outlet of G and V columns after one month of equilibration at a constant flow rate of q ≈ 0.5 mL/min (mean and standard deviation from triplet samples).**

|  |  |  |
| --- | --- | --- |
|  |  |  |
|  | Fresh groundwater [mg/L] | G columns[mg/L] | V columns[mg/L] |
| Li+  | 0.00 ± 0.00 | 0.00 ± 0.00 | 0.00 ± 0.00 |
| Na+ | 18.43 ± 0.12 | 18.78 ± 1.25 | 18.19 ± 0.3 |
| NH4+ | 0.00 ± 0.00 | 0.08 ± 0.03 | 0.00 ± 0.00 |
| K+ | 1.01 ± 0.00 | 1.05 ± 0.02 | 1.47 ± 0.39 |
| Mg2+ | 17.10 ± 0.10 | 17.04 ± 0.15 | 15.9 ± 0.88 |
| Ca2+ | 84.63 ± 0.47 | 75.18 ± 3.39 | 76.75 ± 3.58 |
| F- | 0.00 ± 0.00 | 0.00 ± 0.00 | 0.00 ± 0.00 |
| Cl- | 32.57 ± 0.06 | 33.92 ± 2.8 | 32.96 ± 0.47 |
| NO2- | 0.00 ± 0.00 | 0.00 ± 0.00 | 0.00 ± 0.00 |
| Br- | 0.00 ± 0.00 | 0.00 ± 0.00 | 0.00 ± 0.00 |
| NO3- | 6.87 ± 0.06 | 6.57 ± 0.38 | 6.17 ± 0.01 |
| HPO42- | 0.00 ± 0.00 | 0.00 ± 0.00 | 0.00 ± 0.00 |
| SO42- | 7.97 ± 0.06 | 8.30 ± 0.41 | 8.29 ± 0.06 |

**S3 Nitrate and dissolved oxygen (DO) concentrations over time in outflow samples of all six column experiments**