

## Supplementary Information

### Determination of UV-327 and its metabolites in human urine using dispersive liquid-liquid microextraction and gas chromatography-tandem mass spectrometry

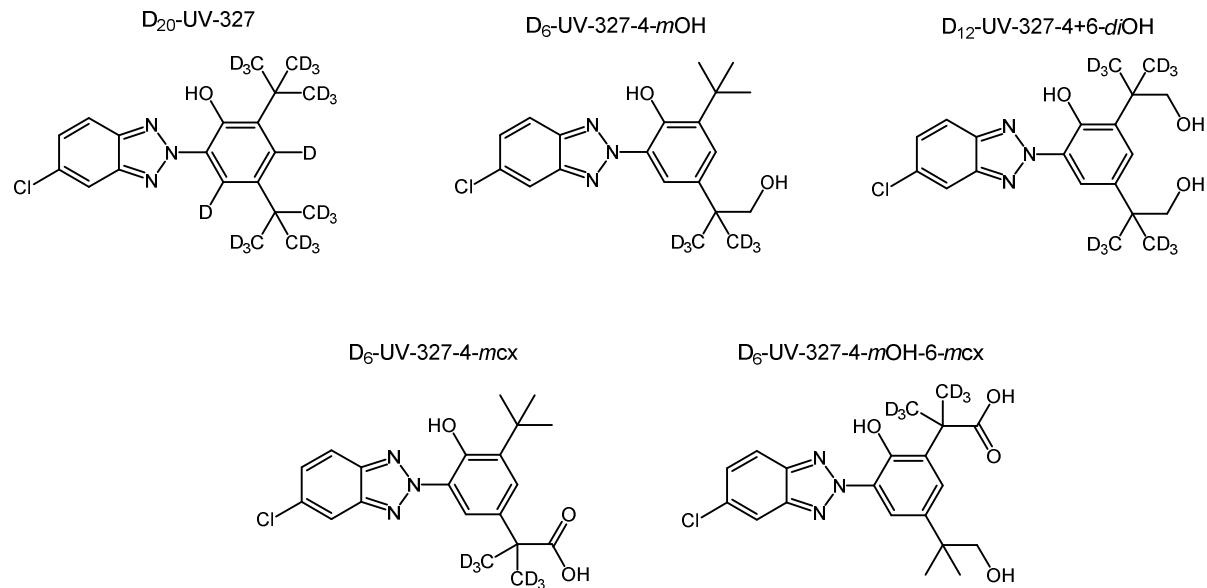
Corinna Fischer, Thomas Göen<sup>\*</sup>

Institute and Outpatient Clinic of Occupational, Social and Environmental Medicine,  
Friedrich-Alexander-Universität Erlangen-Nürnberg, Henkestraße 9–11, 91054 Erlangen, Germany

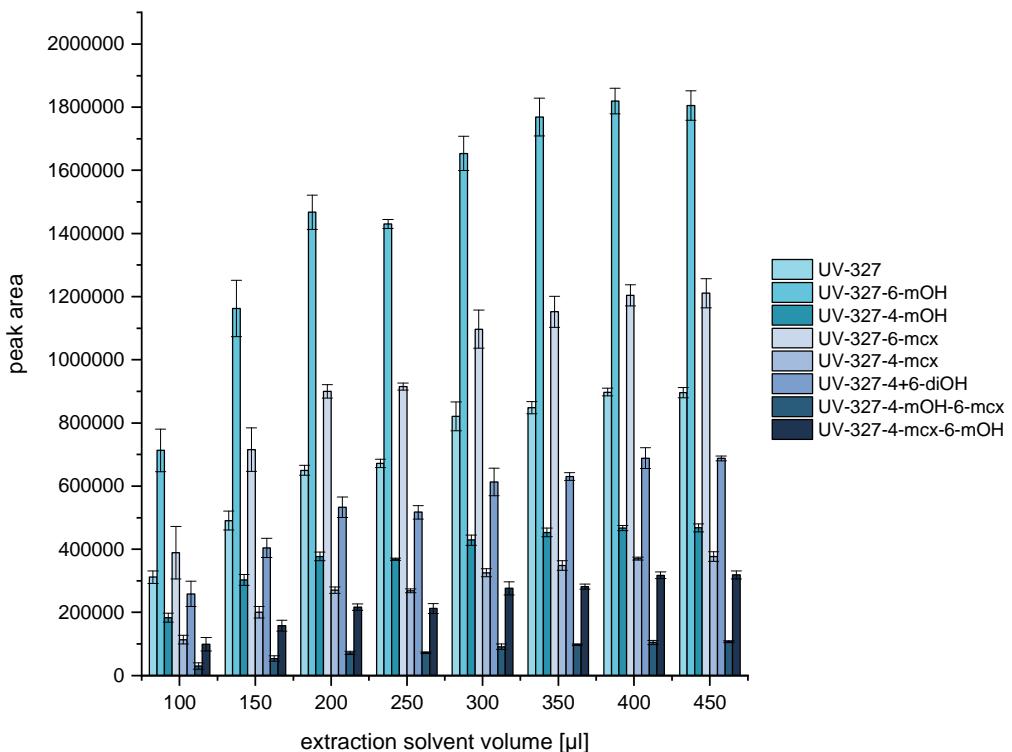
<sup>\*</sup>Corresponding author:

Thomas Göen  
Henkestraße 9–11  
91054 Erlangen  
Tel.: +49 9131 8526121  
[thomas.goeen@fau.de](mailto:thomas.goeen@fau.de)

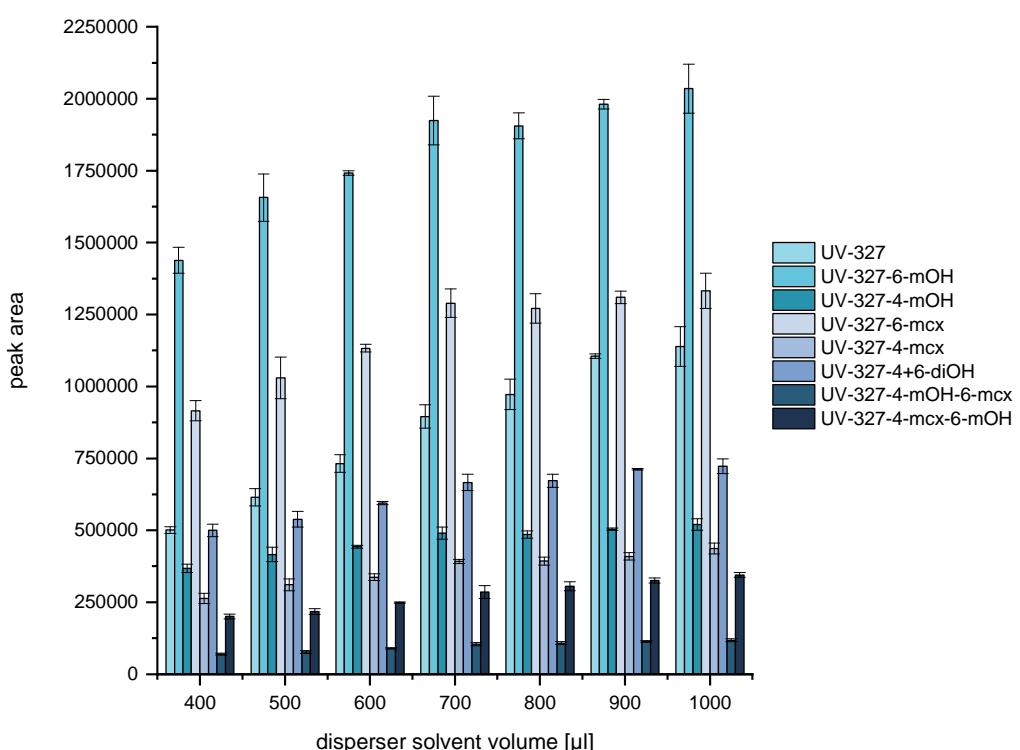
**Fig. SI-1** Chemical structures of the internal standards **D<sub>20</sub>-UV-327** (2-(5-chloro-benzotriazol-2-yl)-4,6-di-(tert-1,1,1-[<sup>2</sup>H<sub>9</sub>]-butyl)- 3,5-(<sup>2</sup>H<sub>1</sub>-2H)-phenol), **D<sub>6</sub>-UV-327-4-mOH** (2-(5-chloro-benzotriazol-2-yl)-4-(1,1-di-(<sup>2</sup>H<sub>3</sub>]-methyl)-2-hydroxyethyl)-6-(*tert*-butyl)phenol), **D<sub>6</sub>-UV-327-4-mcx** (2-(5-chloro-benzotriazol-2-yl)-4-(1,1-di-(<sup>2</sup>H<sub>3</sub>]-methyl)-1-carboxymethyl)-6-(*tert*-butyl)phenol), **D<sub>12</sub>-UV-327-4+6-diOH** (2-(5-chloro-benzotriazol-2-yl)-4,6-di-[1,1-di-(<sup>2</sup>H<sub>3</sub>]-methyl)-2-hydroxyethyl]phenol), and **D<sub>6</sub>-UV-327-4mOH-6-mcx** (2-(5-chloro-benzotriazol-2-yl)-6-(1,1-dimethyl-1-carboxymethyl)-4-(1,1-di-(<sup>2</sup>H<sub>3</sub>]-methyl)-2-hydroxyethyl)phenol)



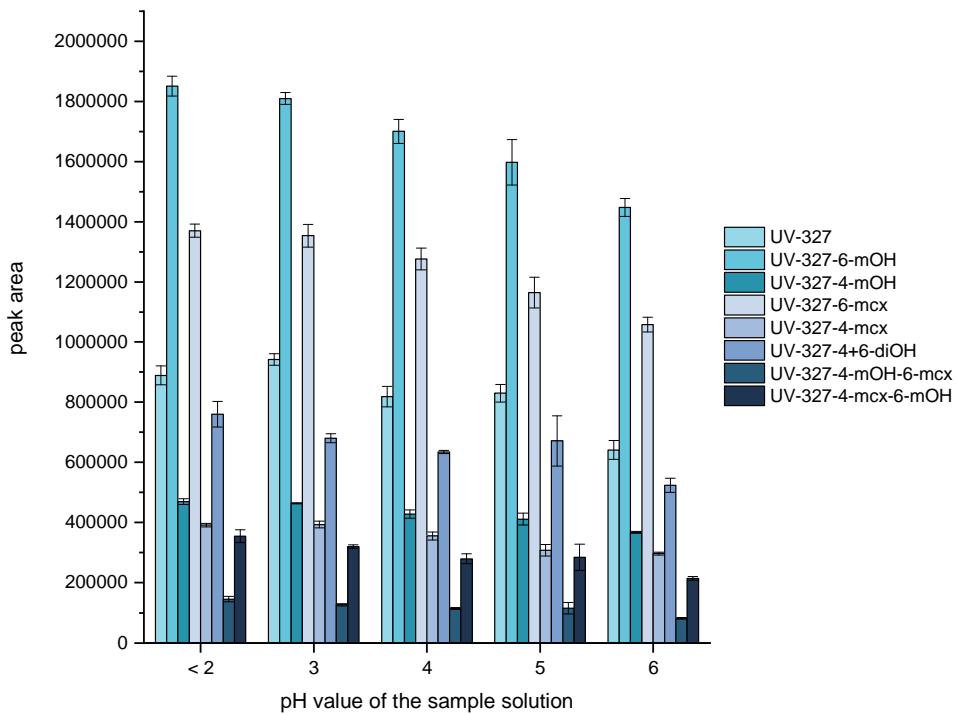
**Fig. SI-2** Effect of the extraction solvent volume ( $n = 3$ ). Extraction solvent (chloroform), 100–450  $\mu$ l; disperser solvent (isopropyl alcohol), 700  $\mu$ l (From left to right: UV-327, UV-327-6-mOH, UV-327-4-mOH, UV-327-6-mcx, UV-327-4-mcx, UV-327-4+6-diOH, UV-327-4-mOH-6-mcx, UV-327-4-mcx-6-mOH)



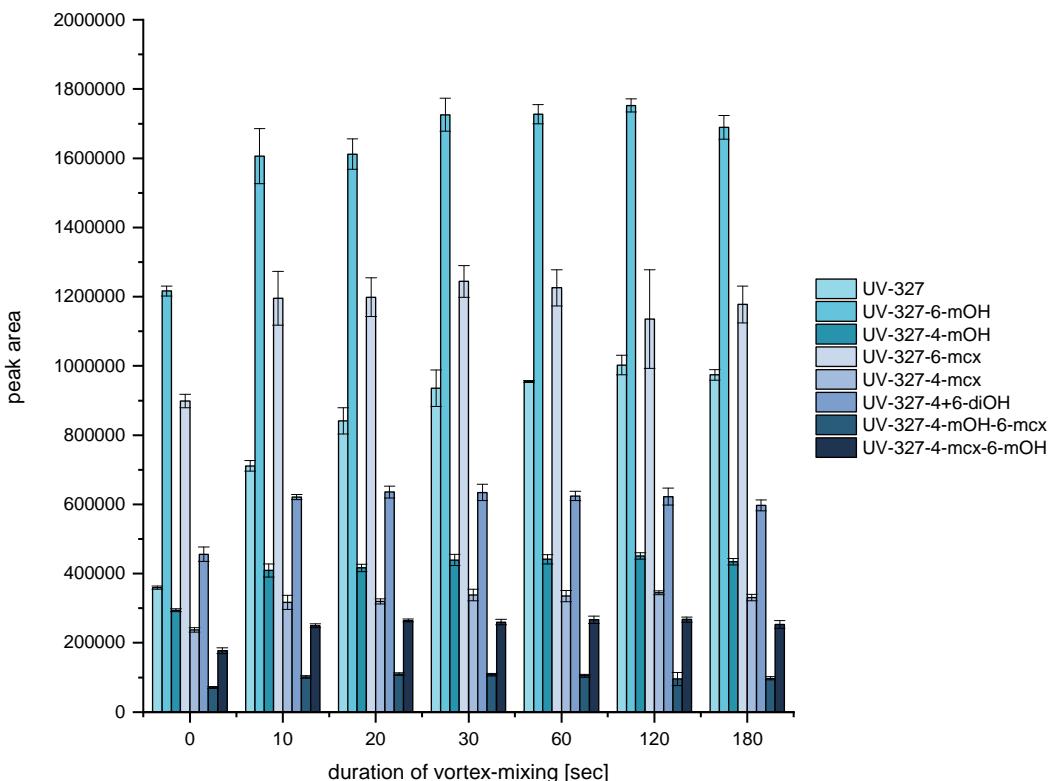
**Fig. SI-3** Effect of the disperser solvent volume ( $n = 3$ ). Extraction solvent (chloroform), 400  $\mu$ l; disperser solvent (isopropyl alcohol), 400–1000  $\mu$ l (From left to right: UV-327, UV-327-6-mOH, UV-327-4-mOH, UV-327-6-mcx, UV-327-4-mcx, UV-327-4+6-diOH, UV-327-4-mOH-6-mcx, UV-327-4-mcx-6-mOH)



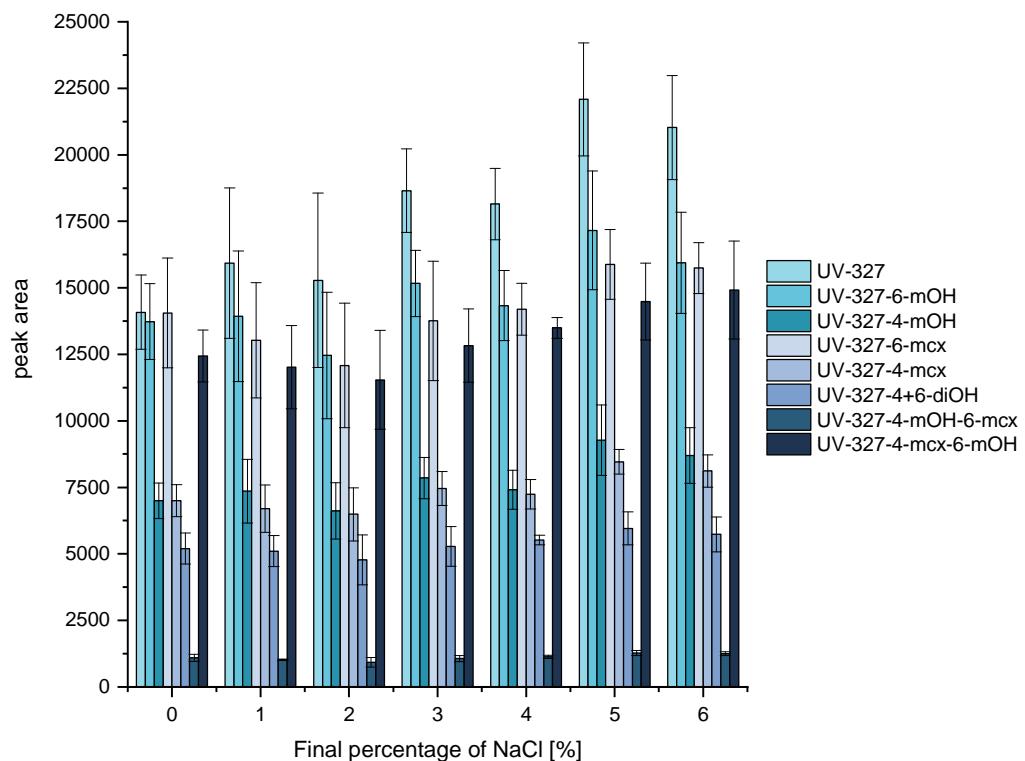
**Fig. SI-4** Effect of the pH value in the range of pH < 2.0 to pH 6.0 (n = 3). Extraction solvent (chloroform), 400 µl; disperser solvent (isopropyl alcohol), 700 µl (From left to right: UV-327, UV-327-6-mOH, UV-327-4-mOH, UV-327-6-mcx, UV-327-4-mcx, UV-327-4+6-diOH, UV-327-4-mOH-6-mcx, UV-327-4-mcx-6-mOH)



**Fig. SI-5** Effect of the duration of vortex-mixing in the range of 0–180 sec (n = 3). Extraction solvent (chloroform), 400 µl; disperser solvent (isopropyl alcohol), 700 µl (From left to right: UV-327, UV-327-6-mOH, UV-327-4-mOH, UV-327-6-mcx, UV-327-4-mcx, UV-327-4+6-diOH, UV-327-4-mOH-6-mcx, UV-327-4-mcx-6-mOH)



**Fig. SI-6** Effect of salt addition in the range of 0–6% NaCl (v/v) ( $n = 3$ ). Extraction solvent (chloroform), 400  $\mu$ l; disperser solvent (isopropyl alcohol), 700  $\mu$ l (From left to right: UV-327, UV-327-6-mOH, UV-327-4-mOH, UV-327-6-mcx, UV-327-4-mcx, UV-327-4+6-diOH, UV-327-4-mOH-6-mcx, UV-327-4-mcx-6-mOH)



**Fig. SI-7** Calibration curves for the determination of UV-327 and its metabolites in urine (ISTD = internal standard)

