

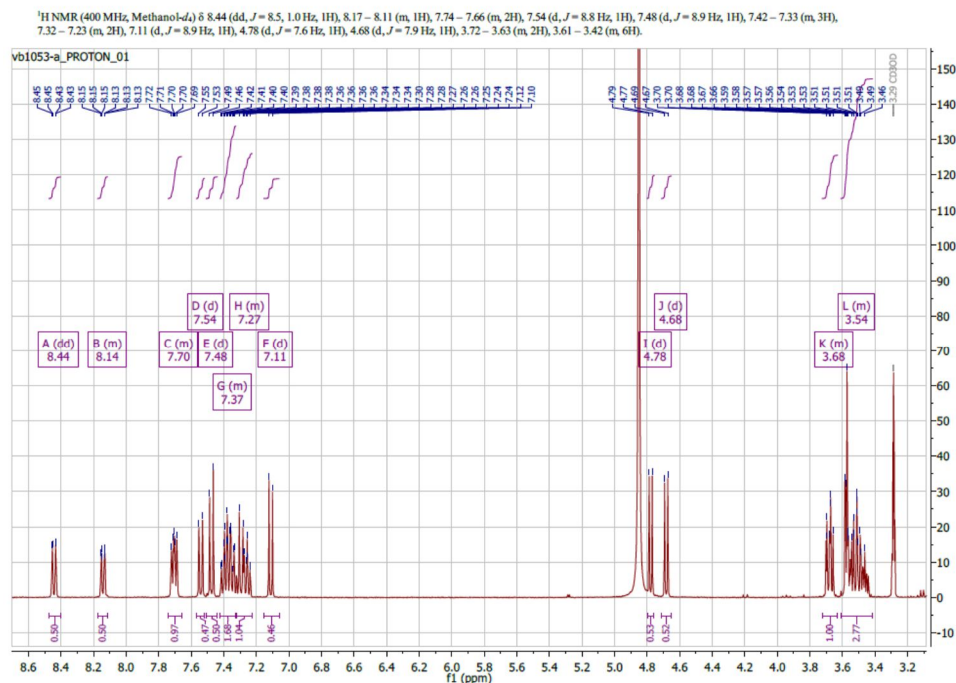
## **Analytical and Bioanalytical Chemistry**

### **Electronic Supplementary Material**

#### **Reliable quantification of 1,2-dihydroxynaphthalene in urine using a conjugated reference compound for calibration**

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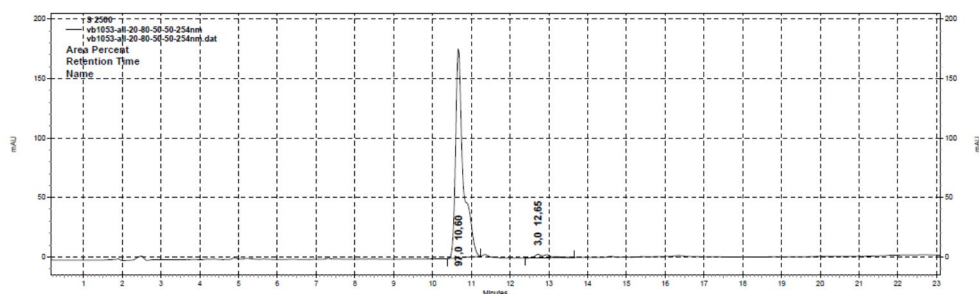
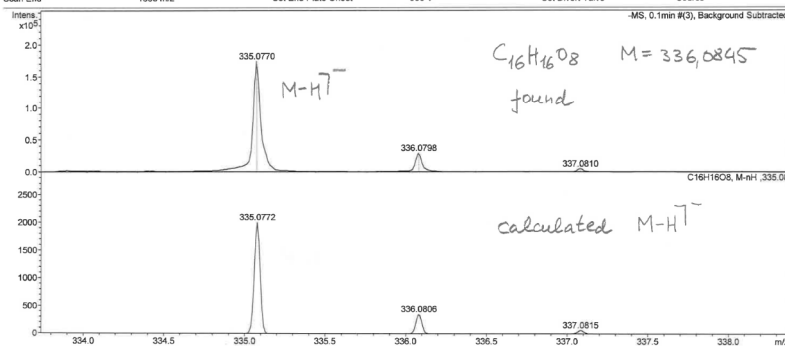
**Fig. S1** <sup>1</sup>H-NMR (in CD<sub>3</sub>OD) and HR-MS spectra (ESI, negative mode) of 1,2-DHN-Glc (vb1053-a) and D<sub>6</sub>-1,2-DHN-Glc (vb1059)



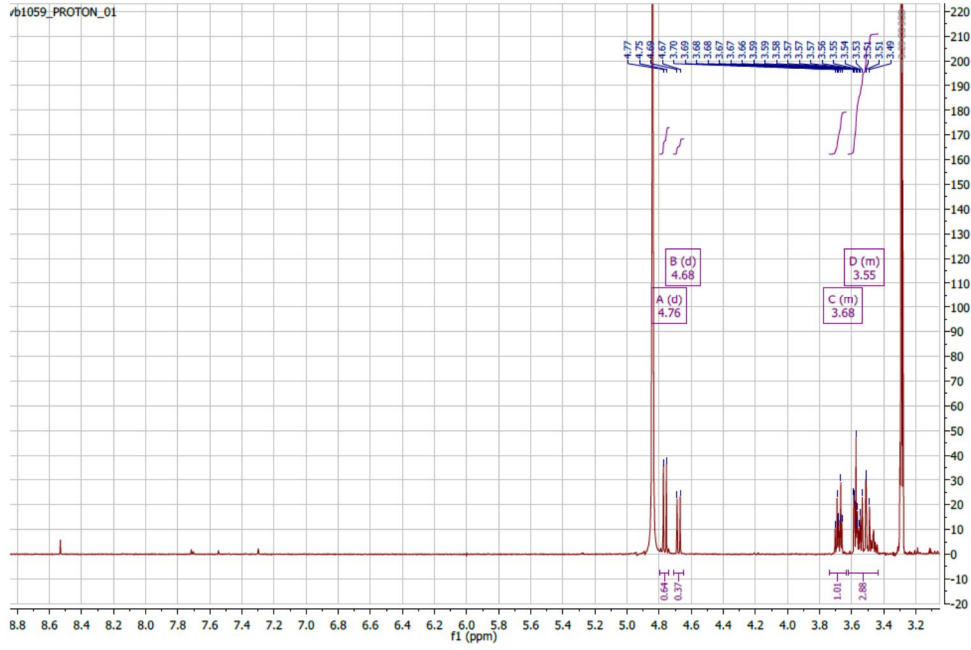
Display Report

<b>Analysis Info</b>	Z:\Data\2017\1704\team270417\neg\VB1053a_low_1_01_96343.d	Acquisition Date	27.04.2017 06:48:42
Analysis Name	hystar_nlm	Operator	BDAL@DE
Method	VB1053a_low	Instrument / Ser#	micrOTOF 10237
Sample Name			
Comment			

<b>Acquisition Parameter</b>	ESI	Ion Polarity	Negative	Set Nebulizer	1.6 Bar
Source Type	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Focus	60 miz	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan Begin	1600 m/z			Set Divert Valve	Source
Scan End					



<sup>1</sup>H NMR (400 MHz, Methanol-d<sub>4</sub>) δ 4.76 (d, J = 7.6 Hz, 1H), 4.68 (d, J = 7.9 Hz, 0H), 3.74 – 3.63 (m, 1H), 3.62 – 3.43 (m, 3H).



### Display Report

<b>Analysis Info</b>	Acquisition Date	27.04.2017 08:53:28
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Method: hystar_ni.m	Instrument / Ser#	micrOTOF 10237
Sample Name: VB1059_low		
Comment:		

<b>Acquisition Parameter</b>	ESI	Ion Polarity	Negative	Set Nebulizer	1.8 Bar
Source Type	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
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Scan End					

