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Supplementary Material

Liquid chromatography-tandem mass spectrometry as a fast and simple method for the determination of several antibiotics in different aqueous matrices

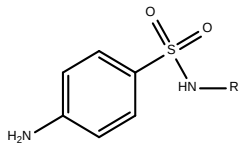
Alexander M. Voigt,[A] Dirk Skutlarek,[A] Christian Timm,[A] Christiane Schreiber,[A] Carsten Felder,[A] Martin Exner[A] and Harald A. Faerber[A,B]

[A]Institute for Hygiene and Public Health, University Hospital Bonn, Medical Faculty, University of Bonn, Building 63, Venusberg-Campus 1, 53127 Bonn, Germany.

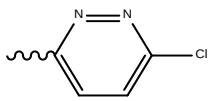
[B]Corresponding author. Email: harald.faerber@ukbonn.de

Sulfonamides

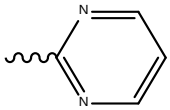
Basic structure



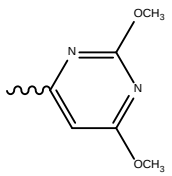
Sulfachloropyridazin (SCP; -/-)



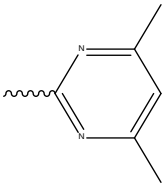
Sulfadiazin (SDZ; H/V)



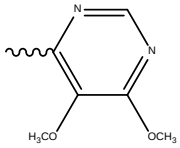
Sulfadimethoxin (SDMX; -/V)



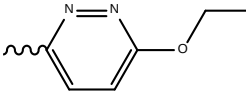
Sulfadimidin (SDMD; -/V)



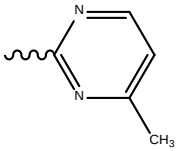
Sulfadoxin (SDX; -/V)



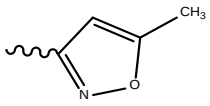
Sulfaethoxypyridazin (SEP; -/-)



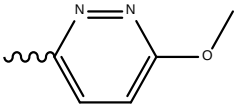
Sulfamerazin (SMZ; -/V)



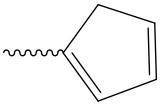
Sulfamethoxazole (SMX; H/V)



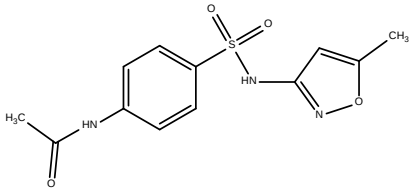
Sulfamethoxypyridazin (SMP; -/V)



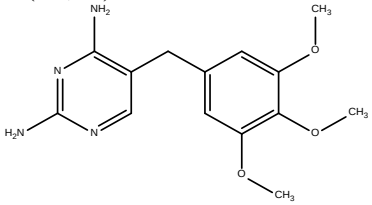
Sulfathiazole (STZ; -/-)



N-Acetyl-Sulfamethoxazole (N4AcSMX; -/-)

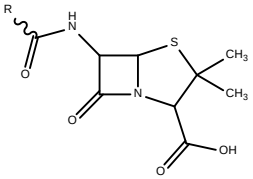


Trimethoprim (TMP; H/V)

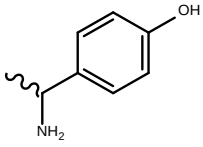


Penicillins and Carbapenems

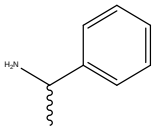
Basic structure



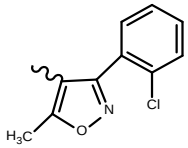
Amoxicillin (AMOX; H/V)



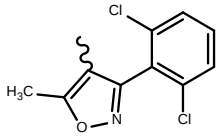
Ampicillin (AMP; H/V)



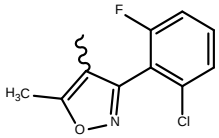
Cloxacillin (CLOX; -/V)



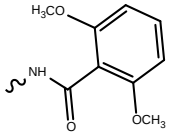
Dicloxacillin (DICLOX; -/-)



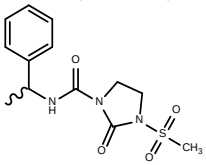
Flucloxacillin (FLU; H/-)



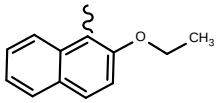
Methicillin (METHI; -/-)



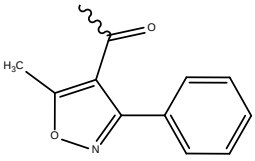
Mezlocillin (MEZLO; H/-)



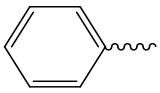
Nafcillin (NAF; -/V)



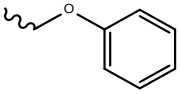
Oxacillin (OXA; -/V)



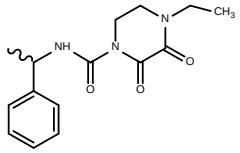
Penicillin G (PEN-G; H/V)



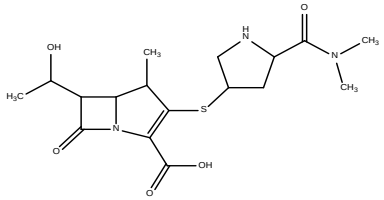
Penicillin V (PEN-V; H/V)



Piperacillin (PIP; H/-)

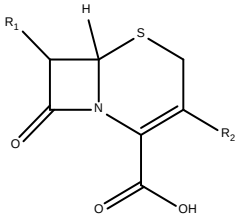


Meropenem (MERO; H/-)

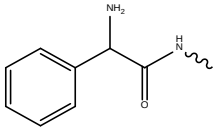


Cephalosporins

Basic structure



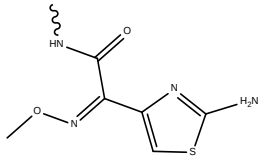
Cefaclor (CEFA; H/-)



R_1:

R_2: Cl

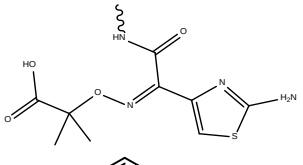
Cefotaxtime (CEFO; H/-)



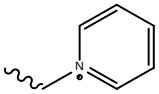
R_1:

R_2:

Ceftazidime (CEFT; H/-)



R_1:

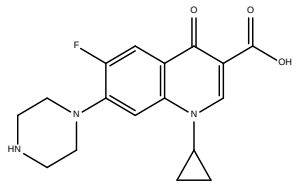


R_2:

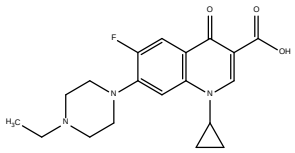
Table S1: Chemical structure (Bryskier, 1999) and the therapeutical field of application, human (H), veterinary medicine (V) and no marketable preparations in Germany (-), based on DIMDI (2018) of the analyzed antibiotics sorted by substance classes.

Fluoroquinolones

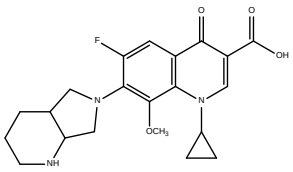
Ciprofloxacin (CIP; H/-)



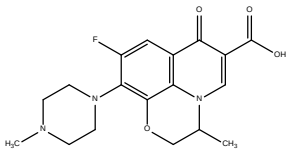
Enrofloxacin (= ENRO; -/V)



Moxifloxacin (MOX; H/-)

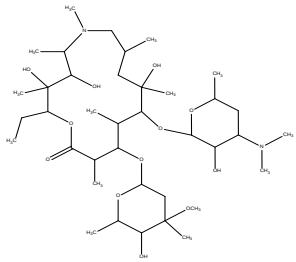


Ofloxacin (OFLOX; H/-)

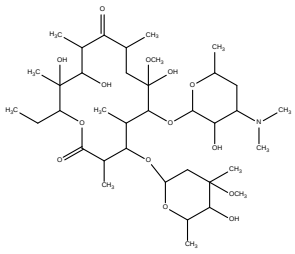


Macrolides

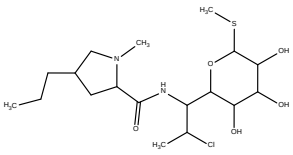
Azithromycin (AZI; H/-)



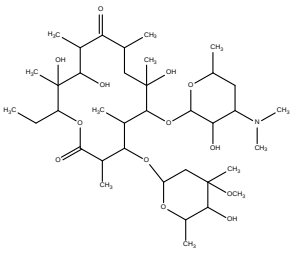
Clarithromycin (CLA; H/-)



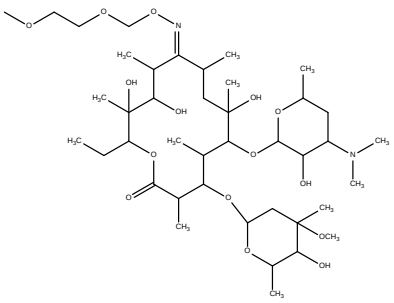
Clindamycin (CLIN; H/V)



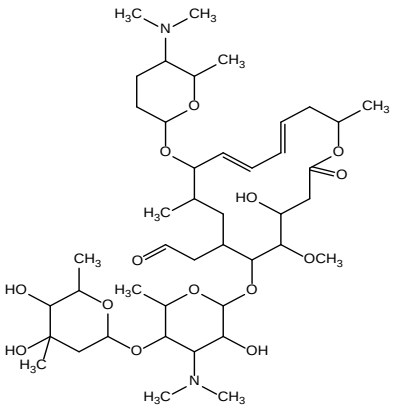
Erythromycin (ERY; H/V)



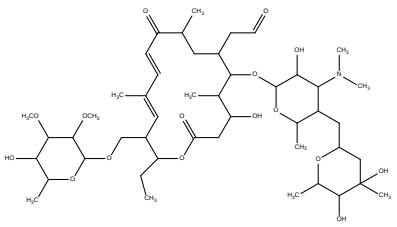
Roxithromycin (ROX; H/-)



Spiramycin (SPIR; H/V)

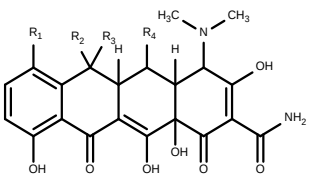


Tylosin (TYL; -/V)



Tetracyclines

Basic structure



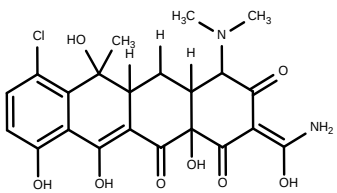
Tetracycline (TC; H/V)	Doxycycline (DOC; H/V)	Oxytetracycline (OTC; H/V)	Chlortetracycline (CTC; H/V)
R_1: H	R_1: H	R_1: H	
R_2: CH_3	R_2: H	R_2: OH	
R_3: OH	R_3: CH_3	R_3: CH_3	
R_4: H	R_4: OH	R_4: OH	

Table S1 (continued): Chemical structure (Bryskier, 1999) and the therapeutical field of application, human (H), veterinary medicine (V) and no marketable preparations in Germany (-), based on DIMDI (2018) of the analyzed antibiotics sorted by their substance classes.

Parameter	DW	SW	GW
pH	8.0 ± 0.1	8.3	6.9
TOC [mg L^{-1}]	0.6 ± 0.2	6.8	0.64
Electric conductivity (25°C , µS cm^{-1})	340 ± 40	579	565
Chlorid [mg L^{-1}]	32 ± 3	61	49
Total amount of phosphate [mg L^{-1}]	< 0.01	< 0.03	0.07
Sulfate [mg L^{-1}]	30 ± 2	64	66
Calcium [mg L^{-1}]	35.7 ± 4.5	59	60
Magnesium [mg L^{-1}]	7.5 ± 0.9	13	14
Turbidity [FNU]	< 0.10	13	0.69

Table S2: Characterization of the blank matrices (DW, SW and GW) by specific water quality parameters

Legend: DW = drinking water; GW = groundwater; SW = surface water; TOC = total organic carbon