

## Supplementary Material

**Table S1.** Hydrolysis constant values of Mn<sup>2+</sup> at different temperatures and ionic strengths in NaCl.

Species	logβ <sup>a)</sup>			
	<i>t</i> = 15°C		<i>t</i> = 25°C	<i>t</i> = 37°C
	<i>I</i> = 0.15 <sup>b)</sup>	<i>I</i> = 0.15 <sup>b)</sup>	<i>I</i> = 0.48 <sup>b)</sup>	<i>I</i> = 0.96 <sup>b)</sup>
MOH <sup>+</sup>	-10.6(1)	-10.46	-10.70	-10.95
M <sub>2</sub> (OH) <sub>3</sub> <sup>+</sup>	-26.35(2)	-24.47	-24.69	-24.92
Ref.	c)	d)	d)	d)

<sup>a)</sup> Refer to the reaction: pM<sup>2+</sup> + qH<sub>2</sub>O = M<sub>p</sub>(OH)<sub>q</sub><sup>(2p-q)</sup> + qH<sup>+b)</sup> in mol L<sup>-1</sup>; <sup>c)</sup> unpublished data, this work; <sup>d)</sup> literature data.

**Table S2.** Protonation constant values of *Amp* and *Amox* at different temperatures and ionic strengths in NaCl.

t/°C	L	Species <sup>a)</sup>	logβ <sup>H</sup>			Ref.
			I = 0.15 <sup>b)</sup>	I = 0.5 <sup>b)</sup>	I = 1 <sup>b)</sup>	
15	<i>Amp</i>	LH	7.317			c)
15		LH <sub>2</sub>	9.899			
25		LH	7.051	7.095	7.244	
25		LH <sub>2</sub>	9.638	9.660	9.805	
37		LH	6.757			
37		LH <sub>2</sub>	9.351			
15	<i>Amox</i>	LH	9.706			c)
15		LH <sub>2</sub>	17.287			
15		LH <sub>3</sub>	19.783			
25		LH	9.565	9.482	9.533	
25		LH <sub>2</sub>	16.865	16.807	16.972	
25		LH <sub>3</sub>	19.427	19.404	19.615	
37		LH	9.400			
37		LH <sub>2</sub>	16.395			
37		LH <sub>3</sub>	19.049			

<sup>a)</sup> Refer to the reaction L + rH = LH<sub>r</sub>, charges omitted for simplicity; <sup>b)</sup> in mol L<sup>-1</sup>; <sup>c)</sup> F. Crea, D. Cucinotta, C. De Stefano, D. Milea, S. Sammartano, G. Vianelli Modelling solubility, acid-base properties and activity coefficients of 3 amoxicillin, ampicillin and (+)6-aminopenicillanic acid, in NaCl(aq) at different ionic strengths and temperatures Eur. J. Pharm. Sci. 47 (2012) 661-677.

**Table S3.** Recalculated formation constant values for Mn<sup>2+</sup>-*Amp* and Mn<sup>2+</sup>-*Amox* species at different ionic strengths and temperatures.

L	Species	logβ <sup>a)</sup>			
		<i>t</i> = 15°C		<i>t</i> = 25°C	<i>t</i> = 37°C
		<i>I</i> = 0.15 <sup>b)</sup>	<i>I</i> = 0.15 <sup>b)</sup>	<i>I</i> = 0.48 <sup>b)</sup>	<i>I</i> = 0.96 <sup>b)</sup>
<i>Amp</i>	MnLH	9.58(12) <sup>c)</sup>	9.52(14) <sup>c)</sup>	9.16(9) <sup>c)</sup>	8.73(13) <sup>c)</sup>
	MnL	2.32(3)	2.23(9)	2.14(6)	2.18(9)
<i>Amox</i>	MnLH <sub>2</sub>	19.88(2)	19.63(5)	19.68(4)	20.11(4)
	MnLH	12.43(5)	12.70(6)	12.59(6)	12.56(9)
<sup>a)</sup> Refer to the reaction M+ L + rH = MLH <sub>r</sub> , charges omitted for simplicity; <sup>b)</sup> in mol L <sup>-1</sup> ; <sup>c)</sup> ≥95% of confidence interval.					