

New Pharmacokinetic and Microbiological Prediction Equations to Be Used as Models for the Search of Antibacterial Drugs

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Supplementary Section S1: Internal validation results for each of the selected equations

Table S1. Standard error (SE) and significance (p) of the indices used in the equation RF_{CL}.

Index	SE	p
${}^6\chi_{ch}$	441.367	0.007
$S_{>N-}$	17.6114	0.000
NI_2	278.522	0.000

Table S2. Correlations of the estimates of the regression coefficients of the indices used in the equation RF_{CL}.

Index	${}^6\chi_{ch}$	$S_{>N-}$	NI_2
${}^6\chi_{ch}$	1.000		
$S_{>N-}$	-0.316	1.000	
NI_2	-0.408	0.510	1.000

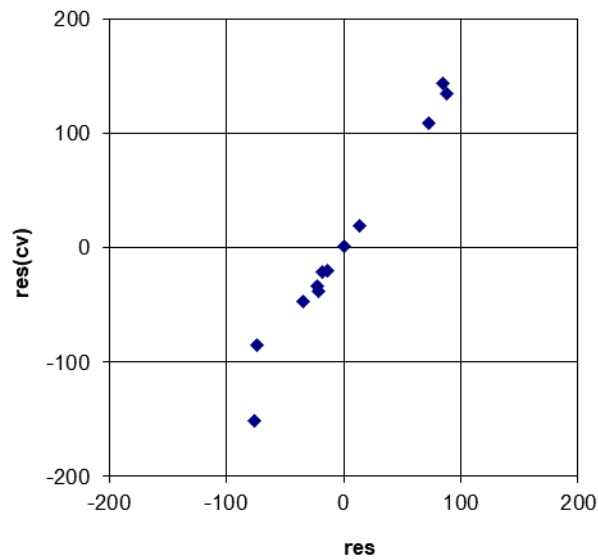
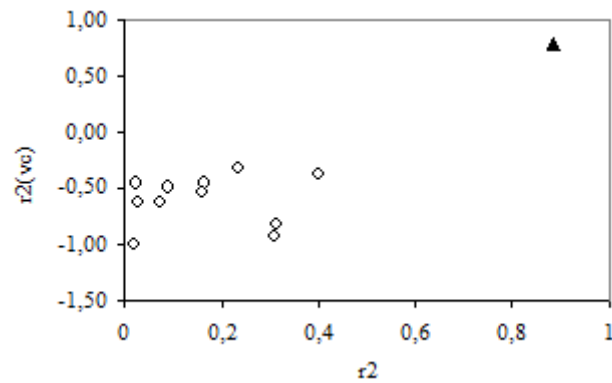
Figure S1. Residual values (res) versus cross-validated residual values (res(cv)) in the equation RF_{CL}.**Figure S2.** Correlation coefficient (r2) versus prediction coefficient (r2(vc)) in the equation RF_{CL}.

Table S3. Standard error (SE) and significance (p) of the indices used in the equation $RF_{MIC50Ea}$.

Index	SE	p
S_{CH2-}	0.0139545	0.000
$S_{>N-}$	0.00827706	0.000
S_{-NH-}	0.00688546	0.000

Table S4. Correlations of the estimates of the regression coefficients of the indices used in the equation $RF_{MIC50Ea}$.

Index	S_{CH2-}	S_{aCa}	S_{-NH-}
S_{CH2-}	1.000		
S_{aCa}	-0.752	1.000	
S_{-NH-}	-0.531	0.355	1.000

Figure S3. Residual values (res) versus cross-validated residual values (res(cv)) in the equation $RF_{MIC50Ea}$.

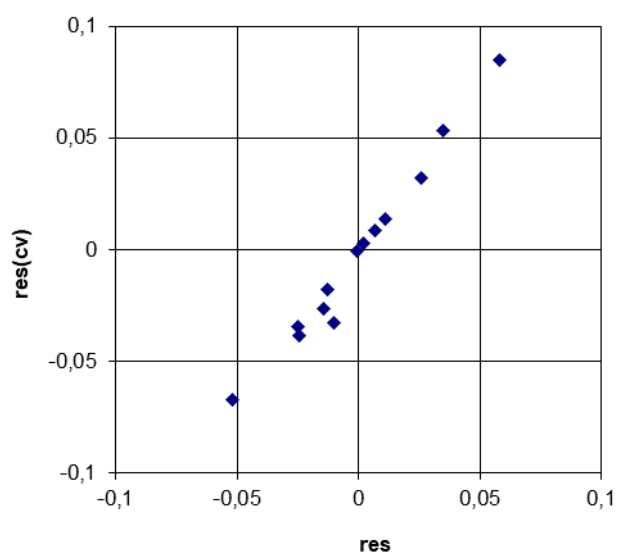


Figure S4. Correlation coefficient (r^2) versus prediction coefficient ($r^2(vc)$) in the equation $RF_{MIC50Ea}$.

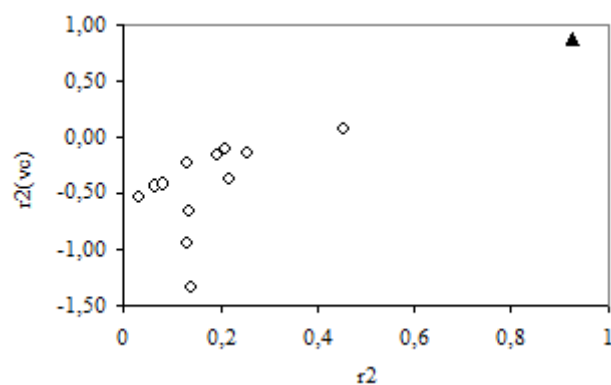


Table S5. Standard error (SE) and significance (p) of the indices used in the equation RF_{MIC50Pm}.

Index.	SE	p
${}^9\chi'_{ch}$	5.78657	0.000
$S_{>N-}$	0.0128396	0.000
S_{-NH-}	0.0181043	0.000

Table S6. Correlations of the estimates of the regression coefficients of the indices used in the equation RF_{MIC50Pm}.

Index.	${}^9\chi'_{ch}$	S_{-CH3}	$S_{>N-}$
${}^9\chi'_{ch}$	1.000		
S_{-CH3}	0.047	1.000	
$S_{>N-}$	0.069	-0.220	1.000

Figure S5. Residual values (res) versus cross-validated residual values (res(cv)) in the equation RF_{MIC50Pm}.

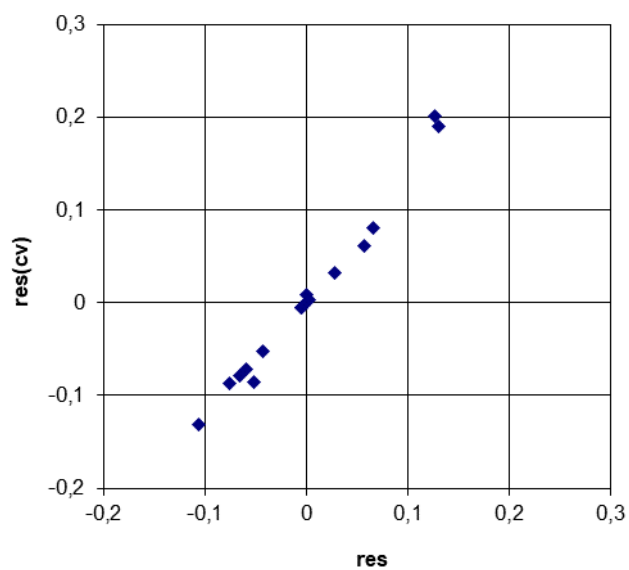


Figure S6. Correlation coefficient (r2) versus prediction coefficient (r2(vc)) in the equation RF_{MIC50Pm}.

