

SUPPLEMENTAL DIGITAL CONTENT (SDC)

Table S1. Compounds used for the final PLS-DA model, along with their chemical formula, spectrometric properties, the standardized coefficients, confidence interval, and associated p-values (Jack-Knifing resampling) for the variable Cr >1.5 mg/dl

Compound	Formula	Properties	Standardized Coefficient	p-value	Confidence Interval
3-Methylindole (Skatole)	C ₉ H ₉ N	m/z: 132,080765 Rt: 3,46 Adduction: [M+H] ⁺	-0.16695299	0.012	-0.29594 to -0.03795
Guaiacol	C ₇ H ₈ O ₂	m/z: 125,059898 Rt: 2,811 Adduction: [M+H] ⁺	-0.15992134	0.040	-0.31206 to -0.00777
Homocarnosine	C ₁₀ H ₁₆ N ₄ O ₃	m/z: 241,129028 Rt: 13,951 Adduction: [M+H] ⁺	0.15774800	0.010	0.03892 to 0.27657
5-Methylcytosine	C ₅ H ₇ N ₃ O	m/z: 126,066383 Rt: 8,141 Adduction: [M+H] ⁺	0.15492272	0.023	0.02254 to 0.28729
Histidine	C ₆ H ₉ N ₃ O ₂	m/z: 156,076614 Rt: 13,985 Adduction: [M+H] ⁺	-0.14781219	0.002	-0.23791 to -0.05770
Xanthosine	C ₁₀ H ₁₂ N ₄ O ₆	m/z: 283,068512 Rt: 8,486 Adduction: [M-H] ⁻	0.14141625	0.029	0.01564 to 0.26718
Choline	C ₅ H ₁₃ NO	m/z: 104,107384 Rt: 15,016 Adduction: [M+H] ⁺	0.13956783	0.028	0.01596 to 0.26317
Glutathione disulfide	C ₂₀ H ₃₂ N ₆ O ₁₂ S ₂	m/z: 613,161499 Rt: 13,655 Adduction: [M+H] ⁺	0.12867136	0.065	-0.00778 to -0.26512
3-Indolepropionic acid	C ₁₁ H ₁₁ NO ₂	m/z: 188,071854 Rt: 2,661 Adduction: [M-H] ⁻	-0.12850942	0.001	-0.19942 to -0.05759
Nicotinate	C ₆ H ₅ NO ₂	m/z: 124,039261 Rt: 8,114 Adduction: [M+H] ⁺	0.12825902	0.074	-0.01247 to 0.26899
α-Lipoic acid	C ₈ H ₁₄ O ₂ S ₂	m/z: 207,051132 Rt: 2,506 Adduction: [M+H] ⁺	-0.12588711	0.047	-0.25017 to -0.00160
Phenylalanine	C ₉ H ₁₁ NO ₂	m/z: 166,086014 Rt: 8,604 Adduction: [M+H] ⁺	0.11587927	0.041	0.00471 to 0.22704
Kynurenic acid	C ₁₀ H ₇ NO ₃	m/z: 188,035202 Rt: 4,198 Adduction: [M-H] ⁻	0.11255399	0.039	0.00591 to 0.21918
L-Kynurenine	C ₁₀ H ₁₂ N ₂ O ₃	m/z: 209,091873 Rt: 8,843 Adduction: [M+H] ⁺	0.11071323	0.020	0.01812 to 0.20330

Urocanic acid	C ₆ H ₆ N ₂ O ₂	m/z: 139,050247 Rt: 7,991 Adduction: [M+H] ⁺	0.10565113	0.233	-0.06970 to 0.28100
N-Butyrylglycine	C ₆ H ₁₁ NO ₃	m/z: 146,081177 Rt: 7,097 Adduction: [M+H] ⁺	0.10469998	0.061	-0.00492 to 0.21432
Indole-3-lactic acid	C ₁₁ H ₁₁ NO ₃	m/z: 204,066437 Rt: 2,615 Adduction: [M-H] ⁻	0.10158428	0.097	-0.01908 to 0.22225
4-Aminohippuric acid	C ₉ H ₁₀ N ₂ O ₃	m/z: 195,076187 Rt: 5,703 Adduction: [M+H] ⁺	0.10137408	0.081	-0.01293 to 0.21568
Indole-3-ethanol	C ₁₀ H ₁₁ NO	m/z: 162,091446 Rt: 2,668 Adduction: [M+H] ⁺	-0.09839586	0.137	-0.22901 to 0.03222
Adenine	C ₅ H ₅ N ₅	m/z: 134,047058 Rt: 7,545 Adduction: [M-H] ⁻	-0.03343797	0.339	-0.10300 to 0.03612
Adenosine	C ₁₀ H ₁₃ N ₅ O ₄	m/z: 268,104065 Rt: 7,39 Adduction: [M+H] ⁺	-0.02616427	0.308	-0.07729 to 0.02496
Deoxyguanosine	C ₁₀ H ₁₃ N ₅ O ₄	m/z: 268,104065 Rt: 7,39 Adduction: [M+H] ⁺	-0.02616427	0.308	-0.07729 to 0.02496