Supplementary Materials: Diagnosing microcystin intoxication of canines: Clinicopathological indications, pathological characteristics, and analytical detection in postmortem and antemortem samples

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Table S1. Multiple reaction monitoring (MRM) transitions for targeted analysis of MCs (19 variants), NOD-R and internal standards (*d*7-MC-LR, *d*5-MC-LF) used in LC-MS/MS Analyte.

	Precursor Ion (*m*/*z*)		Fragment Ions (*m*/*z*)	%CE
[DMAdda5]MC-LR	$[M+H]^+$	981.5	539.3, 553.4, 585.4, 599.4, 852.6, 953.6, 963.6	14%
[DMAdda5]MC-LHar	$[M+H]^+$	995.5	375.2, 553.4, 599.4, 866.6, 875.6, 967.6, 977.6	18%
[DAsp3]MC-RR	$[M+2H]^{2+}$	512.9	291.3, 426.3, 445.8, 503.8	28%
MC-RR	$[M+2H]^{2+}$	519.9	298.3, 440.3, 452.8, 455.3, 503.8	20%
NOD-R	$[M+H]^+$	825.5	389.4, 674.5, 691.5, 753.5, 781.5, 808.0	24%
MC-YR	$[M+H]^+$	1045.5	440.3, 599.4, 602.4, 1017.5, 1027.5	20%
MC-HtYR	$[M+H]^+$	1059.5	599.4, 634.4, 1031.6, 1041.6	16%
MC-LR	$[M+H]^+$	995.5	375.2, 553.4, 599.4, 866.6, 875.6, 967.6, 977.6	18%
[DAsp3]MC-LR	$[M+H]^+$	981.5	539.3, 553.4, 585.4, 599.4, 852.6, 953.6, 963.6	14%
[Dha7]MC-LR	$[M+H]^+$	981.5	539.3, 553.4, 585.4, 599.4, 852.6, 953.6, 963.6	14%
[ADMAdda5]MC-LR	$[M+H]^+$	1023.5	553.4, 627.5, 738.8, 963.6, 995.6, 1005.6	25%
MC-HilR	$[M+H]^+$	1009.5	567.4, 599.4	20%
[ADMAdda5]MC-LHar	$[M+H]^+$	1037.6	599.5, 613.4, 641.5, 908.6, 977.6, 1009.5, 1019.6	21%
MC-WR	$[M+H]^+$	1068.6	599.4, 626.3, 939.5, 1040.6	21%
[DLeu1]MC-LR	$[M+H]^+$	1037.6	599.5, 613.4, 641.5, 908.6, 977.6, 1009.5, 1019.6	21%
MC-RY	$[M-H]^-$	1043.5	1001.6, 1025.6	20%
MC-LA	$[M-H]^-$	908.5	780.0, 797.0, 878.0, 891.0	20%
MC-LY	$[M-H]^-$	1000.5	872.0, 889.0, 970.0, 983.0	20%
MC-LW	$[M-H]^-$	1023.6	1005.6	20%
MC-LF	$[M-H]^-$	984.76	966.6	20%
d7-MC-LR	$[M+H]^+$	1002.5	599.54	20%
d5-MC-LF	$[M-H]^-$	984.6	966.6	20%

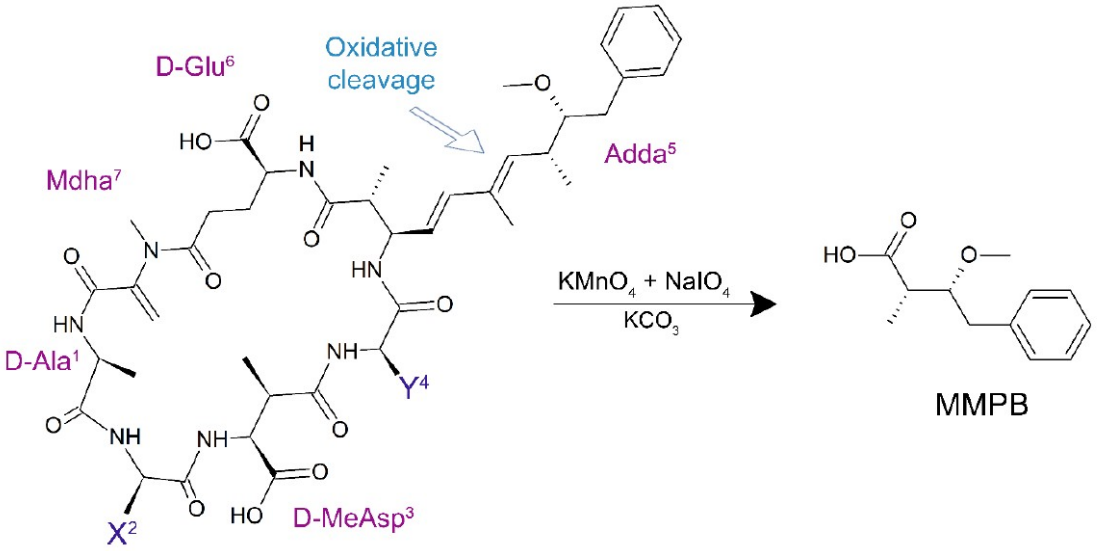

Figure S1. A general representation of the heptapeptide microcystin (left) and the formation of the MMPB molecule following oxidative cleavage of the Adda side chain. The amino acids at X_2 and Y_2 illustrate the sites of amino acid placement responsible for their principal variability and is represented using single letter amino acid code (e.g., L=leucine). Both intact microcystins and MMPB were analyzed in this work.