

Supplementary Materials: Cylindrospermopsin- and Deoxycylindrospermopsin-Producing *Raphidiopsis raciborskii* and Microcystin-Producing *Microcystis* spp. in Meiktila Lake, Myanmar

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Table S1. Identities of microcystins detected by LC-HRMS/MS analysis in *M. aeruginosa* strains AB2017/14 and /15, their retention times (t_R), concentrations, elemental compositions, observed m/z values in positive and negative ionisation modes, whether they matched retention times in reference samples and whether characteristic microcystin product ions were observed. All compounds are microcystins, the confidence in the identity of the congener varies depending on the availability of standards for retention time reference and on the information obtained from the LC-HRMS analysis and chemical reactivity.^a

| Concentration | | | | | | | | | | Accurate mass | | | | | | | | | | | |
|---------------|--------------------------------|--------------|--------------------------------|--------------------|-----------|-------|--------------------|-------|---|---------------|----------|------------|------------|------------|------------|-----|-------|-----|-----|---------|--|
| AB2017/14 | | | | | AB2017/15 | | | | | Positive | | | | | Negative | | | | | MC Frag | |
| Compound name | Confidence | | <i>t</i> _R (min) | μg g ⁻¹ | % | | μg g ⁻¹ | % | Neutral formula | RDBE | <i>z</i> | <i>m/z</i> | Δ (ppm) | <i>m/z</i> | Δ (ppm) | Ref | Thiol | Pos | Neg | | |
| 1 | [D-Asp ³]MC-RR | Confirmed | Known | 4.18 | 2.4 | 0.21 | 1002.4 | 7.21 | C ₄₈ H ₇₃ N ₁₃ O ₁₂ | 19 | 2 | 512.7825 | 0.3 | 1022.5443 | 1.4 | A | Yes | Yes | Yes | | |
| 2 | [Dha ⁷]MC-RR | Probable | Known | 4.53 | 0.1 | 0.01 | 31.8 | 0.23 | C ₄₈ H ₇₃ N ₁₃ O ₁₂ | 19 | 2 | 512.7819 | −0.9 | 1022.5454 | 2.5 | B | Yes | Yes | No | | |
| 3 | MC-RR | Confirmed | Known | 4.55 | 19.4 | 1.74 | 1458.0 | 10.49 | C ₄₉ H ₇₅ N ₁₃ O ₁₂ | 19 | 2 | 519.7903 | 0.3 | 1036.5597 | −0.2 | A | Yes | Yes | Yes | | |
| 4 | [D-Asp ³]MC-ER | Probable | Known | 6.14 | ND | - | 119.6 | 0.86 | C ₄₇ H ₆₈ N ₁₀ O ₁₄ | 19 | 1 | 997.5016 | 2.7 | 995.4858 | 1.4 | C | Yes | Yes | Yes | | |
| 5 | MC-LR-Cys ^b | Probable | Known | 6.16 | 0.1 | 0.01 | ND | - | C ₅₂ H ₈₁ N ₁₁ O ₁₄ S | 18 | 2 | 558.7908 | −1.3 | 1114.5657 | 4.0 | | No | Yes | Yes | | |
| 6 | MC-(H2)YR | Probable | Known | 6.18 | 32.4 | 2.90 | ND | - | C ₅₂ H ₇₄ N ₁₀ O ₁₃ | 21 | 1 | 1047.5516 | 0.6 | 1045.5378 | 1.3 | | Yes | Yes | Yes | | |
| 7 | [D-Asp ³]MC-(H2)YR | Probable | New | 6.20 | 32.9 | 2.95 | ND | - | C ₅₁ H ₇₂ N ₁₀ O ₁₃ | 21 | 1 | 1033.5370 | 1.6 | 1031.5224 | 1.6 | | Yes | Yes | Yes | | |
| 8 | [D-Asp ³]MC-(H4)YR | Probable | Known | 6.27 | 0.6 | 0.05 | 148.1 | 1.07 | C ₅₁ H ₇₄ N ₁₀ O ₁₃ | 20 | 1 | 1035.5525 | 1.5 | 1033.5381 | 1.6 | B | Yes | Yes | Yes | | |
| 9 | MC-ER | Probable | New | 6.55 | 0.6 | 0.05 | 37.8 | 0.27 | C ₄₈ H ₇₀ N ₁₀ O ₁₄ | 19 | 1 | 1011.5158 | 1.2 | 1009.5015 | 1.5 | | Yes | Yes | Yes | | |
| 10 | [D-Asp ³]MC-YR | Probable | Known | 6.59 | ND | - | 144.1 | 1.04 | C ₅₁ H ₇₀ N ₁₀ O ₁₃ | 22 | 1 | 1031.5204 | 0.7 | 1029.5072 | −1.2 | | Yes | Yes | No | | |
| 11 | MC-(H4)YR | Probable | Known | 6.64 | 6.4 | 0.57 | 310.8 | 2.24 | C ₅₂ H ₇₆ N ₁₀ O ₁₃ | 20 | 1 | 1049.5683 | 1.6 | 1047.5540 | 1.9 | B | Yes | Yes | Yes | | |
| 12 | [Mser ⁷]MC-LR | Probable | Known | 6.80 | 0.4 | 0.04 | 13.3 | 0.10 | C ₄₉ H ₇₆ N ₁₀ O ₁₃ | 17 | 1 | 1013.5668 | 0.2 | 1011.5530 | 0.9 | B | No | Yes | No | | |
| 13 | [D-Asp ³]MC-LR | Confirmed | Known | 6.89 | 40.8 | 3.65 | 1870.3 | 13.45 | C ₄₈ H ₇₂ N ₁₀ O ₁₂ | 18 | 1 | 981.5416 | 1.2 | 979.5273 | 1.5 | A | Yes | Yes | Yes | | |
| 14 | MC-YR | Confirmed | Known | 6.99 | 9.1 | 0.81 | 317.4 | 2.28 | C ₅₂ H ₇₂ N ₁₀ O ₁₃ | 22 | 1 | 1045.5369 | 1.5 | 1043.5224 | 2.6 | A | Yes | Yes | Yes | | |
| 15 | MC-MR ^{b,c} | Probable | Known | 6.99 | 3.6 | 0.32 | ND | - | C ₄₈ H ₇₂ N ₁₀ O ₁₂ S | 18 | 1 | 1013.5135 | 1.0 | 1011.4999 | 1.9 | | Yes | Yes | Yes | | |
| 16 | MC-Y(OMe)R | Probable | Known | 7.07 | 7.2 | 0.64 | ND | - | C ₅₃ H ₇₄ N ₁₀ O ₁₄ | 22 | 1 | 1075.5475 | 1.5 | 1073.5329 | 1.5 | B | Yes | Yes | Yes | | |
| 17 | MC-LR | Confirmed | Known | 7.12 | 183.0 | 16.38 | 3332.5 | 23.97 | C ₄₉ H ₇₄ N ₁₀ O ₁₂ | 18 | 1 | 995.5568 | 0.7 | 993.5435 | 2.0 | A | Yes | Yes | Yes | | |
| 18 | [Dha ⁷]MC-LR | Confirmed | Known | 7.13 | 0.8 | 0.07 | 37.4 | 0.27 | C ₄₈ H ₇₂ N ₁₀ O ₁₂ | 18 | 1 | 981.5410 | 0.6 | 979.5289 | 3.1 | A | Yes | No | No | | |
| 19 | Unidentified MC | Unidentified | New | 7.15 | 59.0 | 5.28 | ND | - | C ₅₄ H ₇₁ N ₁₁ O ₁₃ | 25 | 1 | 1082.5322 | 1.5 | 1080.5170 | 0.9 | | Yes | Yes | Yes | | |
| 20 | MC-KynR | Probable | Known | 7.35 | 4.5 | 0.40 | ND | - | C ₅₃ H ₇₃ N ₁₁ O ₁₃ | 23 | 1 | 1072.5478 | 1.5 | 1070.5332 | 1.4 | B | Yes | No | Yes | | |
| 21 | MC-HiIR | Confirmed | Known | 7.38 | 41.8 | 3.74 | 17.9 | 0.13 | C ₅₀ H ₇₆ N ₁₀ O ₁₂ | 18 | 1 | 1009.5726 | 0.9 | 1007.5582 | 1.0 | A | Yes | Yes | Yes | | |
| 22 | Unidentified | Unidentified | New | 7.38 | 59.6 | 5.34 | ND | - | C ₅₄ H ₇₁ N ₁₁ O ₁₃ | 25 | 1 | 1082.5321 | 1.4 | 1080.5169 | 0.8 | | Yes | Yes | Yes | | |
| 23 | MC-OiaR | Tentative | Known | 7.40 | 102.4 | 9.17 | ND | - | C ₅₄ H ₇₃ N ₁₁ O ₁₃ | 24 | 1 | 1084.5460 | −0.2 | 1082.5311 | −0.5 | | Yes | Yes | Yes | | |
| 24 | [D-Asp ³]MC-RE | Probable | New | 7.43 | ND | - | 110.1 | 0.79 | C ₄₇ H ₆₈ N ₁₀ O ₁₄ | 19 | 1 | 997.5004 | 1.5 | 995.4857 | 1.3 | | Yes | Yes | Yes | | |
| 25 | MC-FR | Confirmed | Known | 7.48 | 255.2 | 22.85 | ND | - | C ₅₂ H ₇₂ N ₁₀ O ₁₂ | 22 | 1 | 1029.5408 | 0.4 | 1027.5269 | 1.1 | A | Yes | Yes | Yes | | |

| | | | | | | | | | | | | | | | | | | | |
|--------|----------------------------|--------------|-------|-------|------|-------|--------|-------|---|----|---|-----------|------|-----------|------|---|-----|-----|-----|
| 26 | MC-WR | Confirmed | Known | 7.64 | 0.7 | 0.06 | ND | - | C ₅₄ H ₇₃ N ₁₁ O ₁₂ | 24 | 1 | 1068.5517 | 0.3 | 1066.5380 | 1.2 | A | Yes | Yes | Yes |
| 27 | MC-RE | Probable | New | 7.79 | 3.8 | 0.34 | 1281.0 | 9.21 | C ₄₈ H ₇₀ N ₁₀ O ₁₄ | 19 | 1 | 1011.5161 | 0.4 | 1009.5015 | 1.4 | | Yes | Yes | Yes |
| 28 | MC-RA | Probable | Known | 8.24 | 13 | 1.16 | ND | - | C ₄₆ H ₆₈ N ₁₀ O ₁₂ | 18 | 1 | 953.5100 | 1.0 | 951.4955 | 1.0 | D | Yes | Yes | Yes |
| 29 | MC-Rabu | Probable | Known | 8.83 | 7.1 | 0.64 | ND | - | C ₄₇ H ₇₀ N ₁₀ O ₁₂ | 18 | 1 | 967.5255 | 0.8 | 965.5116 | 1.5 | D | Yes | Yes | Yes |
| 30 | MC-(H2)YG | Probable | New | 9.06 | 5.4 | 0.48 | ND | - | C ₄₈ H ₆₅ N ₇ O ₁₃ | 20 | 1 | 948.4720 | 0.7 | 946.4577 | 1.0 | | Yes | Yes | Yes |
| 31 | MC-RM ^b | Probable | New | 9.23 | 0.2 | 0.02 | ND | - | C ₄₈ H ₇₂ N ₁₀ O ₁₂ S | 18 | 1 | 1013.5095 | -3.0 | 1011.4966 | -1.3 | | Yes | Yes | No |
| 32 | MC-(H2)YA | Probable | New | 9.34 | 10.1 | 0.90 | ND | - | C ₄₉ H ₆₇ N ₇ O ₁₃ | 20 | 1 | 962.4880 | 1.1 | 960.4738 | 1.4 | | Yes | Yes | Yes |
| 33 | Unidentified MC | Unidentified | New | 9.50 | 12 | 1.07 | ND | - | C ₅₀ H ₆₆ N ₈ O ₁₁ | 22 | 1 | 955.4929 | 0.5 | 953.4783 | 0.5 | | Yes | Yes | Yes |
| 34 | Unidentified MC | Unidentified | New | 9.78 | 2.3 | 0.21 | ND | - | C ₅₁ H ₆₈ N ₈ O ₁₁ | 22 | 1 | 969.5089 | 0.9 | 967.4942 | 0.7 | | Yes | Yes | Yes |
| 35 | Unidentified MC | Unidentified | New | 9.96 | 3.7 | 0.33 | ND | - | C ₅₁ H ₆₇ N ₇ O ₁₃ | 22 | 1 | 986.4877 | 0.7 | 984.4735 | 1.1 | | Yes | Yes | No |
| 36 | [D-Asp ³]MC-EE | Probable | Known | 11.43 | ND | - | 403.3 | 2.90 | C ₄₆ H ₆₃ N ₇ O ₁₆ | 19 | 1 | 970.4421 | 1.8 | 968.4272 | 1.4 | C | Yes | Yes | Yes |
| 37 | MC-EE | Probable | New | 12.58 | 0.9 | 0.08 | 1533.5 | 11.03 | C ₄₇ H ₆₅ N ₇ O ₁₆ | 19 | 1 | 984.4578 | 1.8 | 982.4432 | 1.7 | | Yes | Yes | Yes |
| 38 | [D-Asp ³]MC-LE | Probable | New | 12.82 | 1.2 | 0.11 | 358.8 | 2.58 | C ₄₇ H ₆₇ N ₇ O ₁₄ | 18 | 1 | 954.4832 | 1.4 | 952.4690 | 1.8 | | Yes | Yes | Yes |
| 39 | [D-Asp ³]MC-LA | Probable | Known | 13.32 | 6.5 | 0.58 | ND | - | C ₄₃ H ₆₅ N ₇ O ₁₂ | 17 | 1 | 896.4770 | 0.7 | 894.4631 | 1.4 | | Yes | Yes | Yes |
| 40 | MC-LE | Probable | New | 13.69 | 12.9 | 1.15 | 1376.1 | 9.90 | C ₄₈ H ₆₉ N ₇ O ₁₄ | 18 | 1 | 968.4982 | 0.7 | 966.4849 | 2.0 | | Yes | Yes | Yes |
| 41 | MC-LA | Confirmed | Known | 14.87 | 44.8 | 4.01 | ND | - | C ₄₆ H ₆₇ N ₇ O ₁₂ | 17 | 1 | 910.4920 | -0.1 | 908.4788 | 1.4 | A | Yes | Yes | Yes |
| 42 | MC-HilA | Probable | New | 15.29 | 5.9 | 0.53 | ND | - | C ₄₇ H ₆₉ N ₇ O ₁₂ | 17 | 1 | 924.5076 | -0.1 | 922.4942 | 1.1 | | Yes | Yes | Yes |
| 43 | MC-WA | Probable | Known | 15.88 | 4.4 | 0.39 | ND | - | C ₅₁ H ₆₆ N ₈ O ₁₂ | 23 | 1 | 983.4874 | 0.1 | 981.4737 | 1.0 | | Yes | Yes | Yes |
| 44 | MC-FA | Probable | Known | 15.95 | 42.3 | 3.79 | ND | - | C ₄₉ H ₆₅ N ₇ O ₁₂ | 21 | 1 | 944.4767 | 0.4 | 942.4629 | 1.1 | | Yes | Yes | Yes |
| 45 | MC-LAbu | Probable | Known | 16.09 | 16.6 | 1.49 | ND | - | C ₄₇ H ₆₉ N ₇ O ₁₂ | 17 | 1 | 924.5078 | -1.1 | 922.4943 | 1.2 | D | Yes | Yes | Yes |
| 46 | MC-HilAbu | Probable | New | 16.55 | 2.2 | 0.20 | ND | - | C ₄₈ H ₇₁ N ₇ O ₁₂ | 17 | 1 | 938.5233 | 0.0 | 936.5110 | 2.3 | | Yes | Yes | Yes |
| 47 | MC-WAbu | Probable | Known | 17.20 | 13.4 | 1.20 | ND | - | C ₅₂ H ₆₈ N ₈ O ₁₂ | 23 | 1 | 997.5030 | 0.0 | 995.4898 | 1.4 | | Yes | Yes | Yes |
| 48 | MC-FAbu | Probable | Known | 17.39 | 26.4 | 2.36 | ND | - | C ₅₀ H ₆₇ N ₇ O ₁₂ | 21 | 1 | 958.4921 | 0.0 | 956.4784 | 0.9 | | Yes | Yes | Yes |
| 49 | MC-LV | Probable | Known | 17.62 | 3.6 | 0.32 | ND | - | C ₄₈ H ₇₁ N ₇ O ₁₂ | 17 | 1 | 938.5228 | -0.6 | 936.5106 | 1.9 | | Yes | Yes | Yes |
| 50 | MC-LL | Probable | Known | 17.93 | 3.9 | 0.35 | ND | - | C ₄₉ H ₇₃ N ₇ O ₁₂ | 17 | 1 | 952.5388 | -0.2 | 950.5254 | 1.0 | D | Yes | Yes | Yes |
| 51 | MC-FV | Probable | New | 18.40 | 0.7 | 0.06 | ND | - | C ₅₁ H ₆₉ N ₇ O ₁₂ | 21 | 1 | 972.5072 | -0.5 | 970.4944 | 1.3 | | Yes | Yes | No |
| 52 | iso-MC-LL | Tentative | New | 18.49 | 1.2 | 0.11 | ND | - | C ₄₉ H ₇₃ N ₇ O ₁₂ | 17 | 1 | 952.5388 | -0.2 | 950.5262 | 1.8 | | Yes | Yes | Yes |
| 53 | MC-WV | Probable | New | 18.54 | 2.9 | 0.26 | ND | - | C ₅₃ H ₇₀ N ₈ O ₁₂ | 23 | 1 | 1011.5166 | -1.9 | 1009.5041 | 0.0 | | Yes | Yes | Yes |
| 54 | MC-WL | Probable | Known | 18.74 | 2.8 | 0.25 | ND | - | C ₅₄ H ₇₂ N ₈ O ₁₂ | 23 | 1 | 1025.5337 | -0.6 | 1023.5210 | 1.3 | | Yes | Yes | Yes |
| 55 | iso-MC-FV | Tentative | New | 18.79 | 2.1 | 0.19 | ND | - | C ₅₁ H ₆₉ N ₇ O ₁₂ | 21 | 1 | 972.5073 | -0.5 | 970.4942 | 1.1 | | Yes | Yes | Yes |
| 56 | iso-MC-WL | Tentative | New | 19.16 | 1.3 | 0.12 | ND | - | C ₅₄ H ₇₂ N ₈ O ₁₂ | 23 | 1 | 1025.5344 | 0.2 | 1023.5216 | 1.9 | | Yes | Yes | Yes |
| Total: | | | | 1117 | | 100.0 | 13904 | 100.0 | | | | | | | | | | | |

^a Concentration expressed per weight of biomass and as a percentage of total microcystins detected in each culture; Proposed elemental composition and calculated number of rings plus double-bond equivalents (RDBE); Accurate mass measured by LC-HRMS, with observed mass errors and charge z in positive mode (all negative ions were singly-charged); Ref, reference; A, standard, or minor analogue in a standard; B, samples from Yilmaz et al.¹; C, *Planktothrix prolificus* from Mallia et al.²; D, Bloom samples from L. Victoria³; Thiol, reacted with mercaptoethanol indicating presence of Mdha⁷ or Dha⁷ (Miles et al.⁴); MC Frags, characteristic microcystin fragments (Figure 2) observed in either positive or negative ionization modes; ^b Reacted with Oxone/DMSO, confirming the presence of an oxidisable sulfide moiety.⁵; ^c A good quality confirmatory MS/MS spectrum of the Oxone/DMSO oxidation product, MC-M(O)R, was obtained showing the characteristic product ions for this compound.⁵

References:

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