Development of recombinant antibody fragments for toxin and microbial contaminant detection and investigations of microcystin and azaspiracid toxicity.

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Supplementary material

In Chapter 4 of the thesis, the anti-MC-LR scFv, 2G1, was modelled using SwissModel and a putative binding pocked was identified using the Computed Atlas of Surface Topography of proteins (CASTp) database. The MC-LR 3D structure was docked into this putative binding pocked using AutoDock Vina. The highest ranked docking pose of the MC-LR molecule docked into the putative 2G1 binding site was visualised using UCFS Chimera 1.12 software.

Supplementary Video 1 presents the 2G1 scFv molecule (represented as a blue ribbon structure) with the MC-LR molecule (represented in gold) docked in the highest ranked docking pose. The 2G1 amino acid (AA) residues highlighted in grey were identified by AutoDock Vina as being in the closest proximity to the MC-LR. Note on nomenclature: the numbering of the AA sequence in this case is different to that of the Kabat numbering system. In this case, numbering begins from the methionine residue. For referencing to the Kabat numbering used in the bulk of the chapter: Pro71 = L-P55; Ser72 = L-S56; Asp73 = L-D57; Leu144 = H-L2; Tyr174 = H-Y32; Glu246 = H-E101; Glu247 = H-E102. Note on colouring; red = oxygen atom; blue = nitrogen atom.

Supplementary Video 2 presents the 2G1 scFv molecule (grey), without the backbone, with the MC-LR molecule (gold) docked in highest ranked docking pose. The framework of the scFv is omitted to improve the clarity of the 8 identified AA residues in close proximity to the MC-LR structure.