Supplementary Information

Diversity, Bioactivity Profiling and Untargeted Metabolomics of the Cultivable Gut Microbiota of Ciona intestinalis

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Figure S1. Venn diagram of exclusive and shared peaks of three *Streptomyces* sp. extracts (CHG40-GYM, CHG48-GYM, CHG64-GYM) and one *N. prasina* extract (CKG58-GYM).
Figure S2. Putatively identified compounds detected in crude extracts of microorganisms associated with the gut of C. intestinalis. Chemical structures are labelled with their respective peak number (see Tables S5-S10).
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Figure S3. FBMN of *Streptomyces* sp. extract CHG48-GYM. The width of edges represents the cosine similarity between two nodes. See Table S5 for putatively annotated compounds.
Figure S4. FBMN of *Micromonospora* sp. extract CKG20-GYM. The width of edges represents the cosine similarity between two nodes. The FBMN was generated with edges having cosine score above 0.8. See Table S6 for putatively annotated compounds.
Figure S5. FBMN of *Bacillus* sp. extract CKG24-GYM. The width of edges represents the cosine similarity between two nodes. See Table S7 for putatively annotated compounds.
Figure S6. FBMN of *Trichoderma* sp. extracts CHG34-CAG and CHG34-PDA. The width of edges represents the cosine similarity between two nodes. Nodes are color-coded by the respective extracts: light green: CHG34-CAG, dark green: CHG34-PDA. ISF: abundant in source fragments of detected metabolites. See Table S8 for putatively annotated compounds.
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Figure S9. Experimental (black) and library (green) MS/MS spectra of bonactin (14), putatively identified in *Streptomyces* sp. extract CHG48-GYM. The spectral match was generated by the online platform GNPS [1].

Figure S10. Experimental (black) and library (green) MS/MS spectra of homononactyl homononactate (18), putatively identified in *Streptomyces* sp. extract CHG48-GYM. The spectral match was generated by the online platform GNPS [1].
Figure S11. Annotated MS/MS spectra of putatively novel lipopeptides detected in *Trichoderma* sp. extracts CHG34-CAG and CHG34-PDA. The putative amino acid sequences were predicted based on the experimentally determined MS/MS fragmentation pattern of m/z 770.5386 [M+H]+ (103; top) and m/z 754.5423 [M+H]+ (105; bottom; here shown for extract CHG34-PDA). Ala: alanine, Gly: glycine, Leu/Ile: (iso)leucine, Leuol/Ileol: (iso)leucinol, Oc: octanoyl, Ser: serine, Val: valine.
Figure S12. Comparative metabolome analyses of Penicillium sp. extracts CKG23-CAG and CKG23-PDA. (a) Venn diagram of shared and exclusive peaks detected in extract CKG23-CAG (light purple) and CKG23-PDA (dark purple). (b) Zearalenone cluster produced by Penicillium sp. isolate CKG23 (see Figure S8 for full FBMN). The width of edges represents the cosine similarity between two nodes. (c) Putatively annotated metabolites of the zearalenone cluster are displayed with their \textit{m/z} values and observed adducts. Compound numbers are in accordance with Table S10.
Table S1. Taxonomic classification of microbial strains isolated from the gut of *C. intestinalis* sampled in Helgoland and Kiel Fjord. Strain codes are based on the respective sampling location and sampled tissue (CHG = *C. intestinalis* from Helgoland, gut; CKG = *C. intestinalis* from Kiel Fjord, gut). The three closest related strains are given according to the BLAST search [2]. RG = risk group (according to TRBA 460 and TRBA 466). Acc. no.: Accession number.

| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|----------|----------|---------------------------------|---------------------------------|----------------------------------------|-----|
| CHG1        | MB               | MW065489 | 16S      | Uncultured *Vibrio* sp.         | MG554543.1                      | *Vibrio* sp. (Vibrionales)             | 1   |
|             |                  |          |          | Uncultured *Vibrio* sp.         | MG554505.1                      |                                        |     |
|             |                  |          |          | *Vibrio owensii*                | CP025797.1                      |                                        |     |
| CHG2        | MB               | MW065490 | 16S      | *Ruegeria* sp.                  | KY363633.1                      | *Ruegeria atlantica* (Rhodobacterales) | 1   |
|             |                  |          |          | *Ruegeria* sp.                  | KX833139.1                      |                                        |     |
|             |                  |          |          | *Ruegeria atlantica*            | JN128252.1                      |                                        |     |
| CHG3        | MB               | MW065491 | 16S      | Bacterium b1cb16                | EF207071.1                      | *Shewanella* sp. (Alteromonadales)     | 1   |
|             |                  |          |          | *Shewanella piezotolerans*      | MF975607.1                      |                                        |     |
|             |                  |          |          |                                  | CP000472.1                      |                                        |     |
| CHG4        | MB               | MW065492 | 16S      | *Citrobacter amalonaticus*       | MG238567.1                      | *Citrobacter* sp. (Enterobacterales)  | 2   |
|             |                  |          |          | *Citrobacter farmeri*           | CP022695.1                      |                                        |     |
|             |                  |          |          | *Citrobacter* sp.               | LT556085.1                      |                                        |     |
| CHG5        | MB               | MW065493 | 16S      | *Shewanella woodyi*             | NR_114412.1                     | *Shewanella woodyi* (Alteromonadales)  | 1   |
|             |                  |          |          | *Shewanella woodyi*             | NR_074846.1                     |                                        |     |
|             |                  |          |          | *Shewanella woodyi*             | CP000961.1                      |                                        |     |
| CHG6        | TSB              | MW065494 | 16S      | *Shewanella schlegeliana*       | MG388302.1                      | *Shewanella* sp. (Alteromonadales)     | 1   |
|             |                  |          |          | *Shewanella sairae*             | AB274769.1                      |                                        |     |
|             |                  |          |          | *Shewanella schlegeliana*       | AB274767.1                      |                                        |     |
| CHG7        | TSB              | MW065495 | 16S      | *Shewanella putrefaciens*       | MG976650.1                      | *Shewanella* sp. (Alteromonadales)     | 2   |
|             |                  |          |          | *Shewanella hafniensis*         | MF612155.1                      |                                        |     |
|             |                  |          |          | *Shewanella xiamenensis*        | MF033476.1                      |                                        |     |
| CHG8        | TSB              | MW065496 | 16S      | *Shewanella* sp.                | KJ748462.1                      | *Shewanella* sp. (Alteromonadales)     | 2   |
|             |                  |          |          | *Shewanella* sp.                | KJ748460.1                      |                                        |     |
|             |                  |          |          | *Shewanella algae*              | KX218308.1                      |                                        |     |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|----------|----------|--------------------------------|---------------------------------|---------------------------------------|-----|
| CHG9        | TSB              | MW065497 | 16S      | *Escherichia coli*             | CP025753.1                      | *Escherichia coli* (Enterobacterales)  | 2   |
|             |                  |          |          | *Escherichia coli*             | CP025747.1                      |                                       |     |
|             |                  |          |          | *Escherichia coli*             | CP025739.1                      |                                       |     |
| CHG10       | CMN              | MW065498 | 16S      | *Vibrio alginolyticus*         | KY229785.1                      | *Vibrio sp.* (Vibrionales)            | 2   |
|             |                  |          |          | *Vibrio alginolyticus*         | JN188414.1                      |                                       |     |
|             |                  |          |          | *Vibrio alginolyticus*         | KY684259.1                      |                                       |     |
| CHG11       | CMN              | MW065499 | 16S      | *Ruegeria sp.*                 | KY363633.1                      | *Ruegeria atlantica* (Rhodobacterales) | 1   |
|             |                  |          |          | *Ruegeria sp.*                 | KX833139.1                      |                                       |     |
|             |                  |          |          | *Ruegeria atlantica*           | HQ908680.1                      |                                       |     |
| CHG12       | CMN              | MW065500 | 16S      | Uncultured bacterium clone     | KX078089.1                      | *Shewanella sp.* (Alteromonadales)    | 1   |
|             |                  |          |          | SanDiego.a2585                 | KF799676.1                      |                                       |     |
|             |                  |          |          | Uncultured bacterium clone     | KF799675.1                      |                                       |     |
|             |                  |          |          | SanDiego.a2547                 |                                  |                                       |     |
| CHG16       | WSP              | MW065501 | 16S      | *Vibrio sp.*                   | MK533523.1                      | *Vibrio sp.* (Vibrionales)            | 1   |
|             |                  |          |          | *Vibrio sp.*                   | MK533517.1                      |                                       |     |
|             |                  |          |          | *Vibrio owensii*               | CP033138.1                      |                                       |     |
| CHG19       | WSP              | MW064137 | ITS      | Fungal sp. isolate whc1        | MH465392.1                      | *Arthrinium sp.* (Xylariales)         | 1   |
|             |                  |          |          | *Arthrinium arundinis*         | KX778674.1                      |                                       |     |
|             |                  |          |          | *Arthrinium sacchari*          | KX778672.1                      |                                       |     |
| CHG20       | WSP              | MW065502 | 16S      | *Citrobacter freundii*         | CP027849.1                      | *Citrobacter freundii* (Enterobacterales) | 2   |
|             |                  |          |          | *Citrobacter freundii complex* | CP026231.1                      |                                       |     |
|             |                  |          |          | *Citrobacter freundii*         | CP011657.1                      |                                       |     |
| CHG21       | WSP              | MW065503 | 16S      | *Citrobacter braakii*          | MH368419.1                      | *Citrobacter braakii* (Enterobacterales) | 2   |
|             |                  |          |          | *Citrobacter sp.*              | MH368123.1                      |                                       |     |
|             |                  |          |          | *Citrobacter braakii*          | CP022049.2                      |                                       |     |
| CHG22       | WSP              | MW064138 | ITS      | Uncultured *Penicillium clone* | KT581734.1                      | *Penicillium hoeksii* (Eurotiales)    | 1   |
|             |                  |          |          | WPW-OTU-32                     | NR_137913.1                     |                                       |     |
|             |                  |          |          | *Penicillium hoeksii*          | KX305048.1                      |                                       |     |
|             |                  |          |          | *Penicillium hoeksii*          |                                  |                                       |     |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|---------|----------|-------------------------------|-------------------------------|---------------------------------------|-----|
| CHG24       | WSP              | MW064139| ITS      | Aspergillus niger Fungal sp. SNB-LAPI-7-61 Aspergillus niger | MG647867.1 KU977335.1 MH050790.1 | Aspergillus sp. (Eurotales) | 2   |
| CHG25       | WSP              | MW064140| ITS      | Penicillium expansum Penicillium sp. Penicillium ulaiense | MF303721.1 KP403971.1 LN871568.1 | Penicillium sp. (Eurotales) | 1   |
| CHG26       | WSP              | MW064141| ITS      | Uncultured Galactomyces clone P71B Geotrichum candidum Geotrichum candidum | MG193553.1 MH680587.1 MF782775.1 | Galactomyces candidum (Saccharomycetales) | 1   |
| CHG28       | WSP              | MW064142| ITS      | Trichoderma harzianum Trichoderma sp. Trichoderma harzianum | MF871539.1 MH285106.1 KY750434.1 | Trichoderma sp. (Hypocreales) | 1   |
| CHG29       | PDA              | MW064143| ITS      | Uncultured Didymella clone 191_K9ov Stagonosporopsis cucurbitacearum | KF525844.1 KY430454.1 KU168143.1 | Phoma sp. (Pleosporales) | 1   |
| CHG32       | TSB              | MW065504| 16S      | Vibrio ruminonis Vibrio sp. Vibrio owensii | AP018685.1 MG262453.1 MH368433.1 | Vibrio sp. (Vibrionales) | 1   |
| CHG34       | WSP              | MW064144| ITS      | Trichoderma sp. Trichoderma harzianum Trichoderma harzianum | MF871539.1 KY750434.1 | Trichoderma sp. (Hypocreales) | 1   |
| CHG35       | PDA              | MW064145| ITS      | Penicillium sp. Penicillium antarcticum Penicillium atrovenetum | KY401117.1 KP016829.1 KF679753.1 | Penicillium sp. (Eurotales) | 1   |
| CHG38       | WSP              | MW064146| ITS      | Fusarium graminearum Fusarium graminearum Fusarium graminearum | MK079896.1 MK079895.1 MK079894.1 | Fusarium sp. (Hypocreales) | 1   |
| CHG39       | WSP              | MW065505| 16S      | Bacillus subtilis Bacillus subtilis Bacillus velezensis | MG977677.1 MG976620.1 MG970354.1 | Bacillus sp. (Bacillales) | 1   |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|----------|----------|--------------------------------|---------------------------------|----------------------------------------|-----|
| CHG40       | TSB              | MW065506 | 16S      | Streptomyces sp.               | KY613504.1                      | Streptomyces sp. (Streptomycetales) | 1   |
|             |                  |          |          | Streptomyces parvus            | KY213676.1                      |                                        |     |
|             |                  |          |          | Streptomyces lavendulae        | KY213666.1                      |                                        |     |
| CHG41       | TSB              | MW065507 | 16S      | Bacillus licheniformis         | KY886241.1                      | Bacillus licheniformis (Bacillales)  | 1   |
|             |                  |          |          | Uncultured bacterium clone OTU3| KP975259.1                      |                                        |     |
|             |                  |          |          | Streptomyces sp.               | KC522129.1                      |                                        |     |
| CHG42       | TSB              | MW065508 | 16S      | Shewanella algae               | NR_114236.1                     | Shewanella sp. (Alteromonadales)      | 2   |
|             |                  |          |          | Shewanella alga                | NR_117771.1                     |                                        |     |
|             |                  |          |          | Shewanella halodatis           | NR_117770.1                     |                                        |     |
| CHG43       | MB               | MW065509 | 16S      | Vibrio splendidus              | MH010050.1                      | Vibrio sp. (Vibrionales)              | 2   |
|             |                  |          |          | Vibrio sp.                     | MG788349.1                      |                                        |     |
|             |                  |          |          | Vibrio anguillarum             | CP023433.1                      |                                        |     |
| CHG44       | MB               | MW064147 | ITS      | Aspergillus oryzae             | MH625703.1                      | Aspergillus sp. (Eurotiales)          | 2   |
|             |                  |          |          | Aspergillus oryzae             | MH578599.1                      |                                        |     |
|             |                  |          |          | Aspergillus flavus              |                                 |                                        |     |
| CHG47       | WSP              | MW064148 | ITS      | Arthrinium sp.                 | MH059547.1                      | Arthrinium sp. (Xylariales)           | 1   |
|             |                  |          |          | Arthrinium sp.                 | MH059539.1                      |                                        |     |
|             |                  |          |          | Arthrinium arundinis           | MK256947.1                      |                                        |     |
| CHG48       | WSP              | MW065510 | 16S      | Streptomyces sp.               | MG637270.1                      | Streptomyces sp. (Streptomycetales)  | 1   |
|             |                  |          |          | Streptomyces pratensis         | MG637268.1                      |                                        |     |
|             |                  |          |          | Streptomyces pratensis         | MK484235.1                      |                                        |     |
| CHG49       | PDA              | MW064175 | 18S      | Uncultured fungus clone nco40d10c1| KC670836.1                      | Pleosporaceae (Pleosporales)          | 1   |
|             |                  |          |          | Uncultured fungus clone nco40a09c1| KC670799.1                      |                                        |     |
|             |                  |          |          | Pyrenophora tritici-repentis    | U42486.1                        |                                        |     |
| CHG52       | WSP              | MW064149 | ITS      | Penicillium cosmopolitanum     | MH864385.1                      | Penicillium sp. (Eurotiales)          | 1   |
|             |                  |          |          | Penicillium cosmopolitanum     | MH864384.1                      |                                        |     |
|             |                  |          |          | Penicillium cosmopolitanum     | MH864377.1                      |                                        |     |
| CHG53       | PDA              | MW064150 | ITS      | Trichoderma sp.                | MH794211.1                      | Trichoderma sp. (Hypocreales)         | 1   |
|             |                  |          |          | Trichoderma sp.                | MH284929.1                      |                                        |     |
|             |                  |          |          | Trichoderma koningii           | KX343123.1                      |                                        |     |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|---------|----------|---------------------------------|---------------------------------|----------------------------------------|-----|
| CHG56      | TSB              | MW064151 | ITS      | Aspergillus nidulans            | MG459155.1, MH041155.1, MG991576.1 | Aspergillus sp. (Eurotiales)          | 1   |
| CHG59      | PDA              | MW064152 | ITS      | Tamaricola sp.                  | MG977427.1, MG977425.1, KU714703.1 | Tamaricola sp. (Pleosporales)         | 1   |
| CHG60      | TSB              | MW064153 | ITS      | Peroneutypa sp.                 | MF359647.1, EU436688.1, JQ922161.1 | Peroneutypa sp. (Xylariales)          | 1   |
| CHG61      | TSB              | MW065511 | 16S      | Uncultured bacterium clone      | FN434816.1, MG554532.1, CP022468.1 | Vibrio sp. (Vibrionales)             | 2   |
| CHG64      | TSB              | MW065512 | 16S      | Streptomyces microflavus        | MG855947.1, MH251131.1, MH250821.1 | Streptomyces sp. (Streptomycetales)   | 1   |
| CKG1       | MB               | MW065513 | 16S      | Pseudomonas sp.                 | KX621130.1, KJ814609.1, DQ005209.1 | Pseudomonas sp. (Pseudomonadales)     | 1   |
| CKG2       | MB               | MW065514 | 16S      | Rhodococcus sp.                 | MG515722.1, LN867321.1, NR_145614.1 | Rhodococcus sp. (Corynebacteriales)   | 2   |
| CKG3       | MB               | MW065515 | 16S      | Shewanella sp.                  | FR821223.1, FR744880.1, KX271676.1 | Shewanella sp. (Alteromonadales)      | 1   |
| CKG4       | MB               | MW065516 | 16S      | Vibrio sp.                     | MG788349.1, CP023433.1, CP023293.1 | Vibrio sp. (Vibrionales)             | 2   |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|---------|----------|---------------------------------|---------------------------------|----------------------------------------|-----|
| CKG5        | MB               | MW065517| 16S      | Nocardiopsis alba                | MH843138.1                      | Nocardiopsis sp. (Streptosporangiales) | 1   |
|             |                  |         |          |                                 | MH843137.1                      |                                        |     |
|             |                  |         |          |                                 | MH843136.1                      |                                        |     |
| CKG6        | MB               | MW065518| 16S      | Shewanella aestuarii             | KX271676.1                      | Shewanella aestuarii (Alteromonadales) | 1   |
|             |                  |         |          |                                 | KX271675.1                      |                                        |     |
|             |                  |         |          |                                 | KX271674.1                      |                                        |     |
| CKG7        | MB               | MW065519| 16S      | Vibrio owensii                   | LC369696.1                      | Vibrio sp. (Vibrionales)               | 1   |
|             |                  |         |          |                                 | MG896198.1                      |                                        |     |
|             |                  |         |          |                                 | MG896189.1                      |                                        |     |
| CKG8        | MB               | MW065520| 16S      | Vibrio sp.                       | MG788349.1                      | Vibrio sp. (Vibrionales)               | 2   |
|             |                  |         |          |                                 | CP023433.1                      |                                        |     |
|             |                  |         |          |                                 | CP023293.1                      |                                        |     |
| CKG9        | CMN              | MW065521| 16S      | Vibrio sp.                       | MG788349.1                      | Vibrio sp. (Vibrionales)               | 2   |
|             |                  |         |          |                                 | CP023433.1                      |                                        |     |
|             |                  |         |          |                                 | CP023293.1                      |                                        |     |
| CKG10       | CMN              | MW065522| 16S      | Uncultured Vibrio sp. clone HH101354 | MG554532.1                      | Vibrio sp. (Vibrionales)               | 2   |
|             |                  |         |          |                                 | MG554529.1                      |                                        |     |
|             |                  |         |          |                                 | CP022446.1                      |                                        |     |
| CKG11       | CMN              | MW065523| 16S      | Shewanella aestuarii             | KX271676.1                      | Shewanella aestuarii (Alteromonadales) | 1   |
|             |                  |         |          |                                 | KX271675.1                      |                                        |     |
|             |                  |         |          |                                 | KX271674.1                      |                                        |     |
| CKG12       | TSB              | MW065524| 16S      | Vibrio owensii                   | MG896198.1                      | Vibrio sp. (Vibrionales)               | 1   |
|             |                  |         |          |                                 | CP026321.1                      |                                        |     |
|             |                  |         |          |                                 | KY655411.1                      |                                        |     |
| CKG13       | TSB              | MW065525| 16S      | Uncultured marine bacterium isolate | KJ814609.1                      | Pseudomonas sp. (Pseudomonadales)      | 1   |
|             |                  |         |          | TGGGE gel band 22TGGGE1          | JQ012964.1                      |                                        |     |
|             |                  |         |          | Pseudomonas sp.                  | MG687270.1                      |                                        |     |
| CKG14       | TSB              | MW065526| 16S      | Shewanella sp.                   | FR821223.1                      | Shewanella sp. (Alteromonadales)       | 1   |
|             |                  |         |          |                                 | FR744880.1                      |                                        |     |
|             |                  |         |          |                                 | KX271676.1                      |                                        |     |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|---------|----------|--------------------------------|---------------------------------|----------------------------------------|-----|
| CKG15       | TSB              | MW065527| 16S      | Shewanella sp.                 | MF045123.1                      | Shewanella (Alteromonadales)             | 1   |
| CKG16       | TSB              | MW064154| ITS      | Eutypa lata                    | MF359647.1                      | Eutypa lata (Xylariales)                | 1   |
| CKG19       | TSB              | MW065528| 16S      | Bacillus pumilus               | CP027034.1                      | Bacillus sp. (Bacillales)              | 2   |
| CKG20       | TSB              | MW065529| 16S      | Micromonospora sp.             | EU437811.1                      | Micromonospora sp. (Micromonosporales) | 1   |
| CKG21       | CMN              | MW065530| 16S      | Bacillus hwajinpoensis         | MG651497.1                      | Bacillus hwajinpoensis (Bacillales)     | 1   |
| CKG22       | PDA              | MW064155| ITS      | Penicillium antarcticum        | MH828228.1                      | Penicillium sp. (Eurotiales)            | 1   |
| CKG23       | WSP              | MW064156| ITS      | Penicillium antarcticum        | MH828228.1                      | Penicillium sp. (Eurotiales)            | 1   |
| CKG24       | WSP              | MW065531| 16S      | Bacillus subtilis              | KC428745.1                      | Bacillus sp. (Bacillales)              | 1   |
| CKG25       | WSP              | MW064157| ITS      | Geotrichum candidum            | KF713521.1                      | Galactomyces candidum (Saccharomycetales) | 1   |
| CKG27       | WSP              | MW065532| 16S      | Bacillus muralis               | MF506797.1                      | Bacillus sp. (Bacillales)              | 2   |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|-----------------|---------|----------|---------------------------------|---------------------------------|----------------------------------------|----|
| CKG29       | WSP             | MW065533 | 16S      | *Bacillus amyloliquefaciens*    | MG136848.1                   | *Bacillus* (Bacillales)               | 1  |
|             |                 |         |          | *Bacillus amyloliquefaciens*    | MG136846.1                   |                                        |    |
|             |                 |         |          | *Bacillus subtilis*             | MG977677.1                   |                                        |    |
| CKG30       | WSP             | MW065534 | 16S      | *Bacillus pumilus*              | CP027034.1                   | *Bacillus* (Bacillales)               | 2  |
|             |                 |         |          | *Bacillus pumilus*              | KY623354.1                   |                                        |    |
|             |                 |         |          | *Bacillus zhongzhouensis*       | MG937731.1                   |                                        |    |
| CKG31       | PDA             | MW065535 | 16S      | *Vibrio* sp.                    | LC416561.1                   | *Shewanella kairetica* (Alteromonadales) | 1  |
|             |                 |         |          | *Shewanella* sp.                | MH333258.1                   | *Shewanella kairetica* (Alteromonadales) |    |
|             |                 |         |          |                                  | KX078089.1                   |                                        |    |
| CKG32       | WSP             | MW064158 | ITS      | *Fusarium graminearum*          | MF800908.1                   | *Fusarium* (Hypocreales)              | 1  |
|             |                 |         |          | *Fusarium graminearum*          | KY466827.1                   | *Fusarium* (Hypocreales)              |    |
|             |                 |         |          | *Fusarium graminearum*          | KY466825.1                   |                                        |    |
| CKG33       | WSP             | MW064159 | ITS      | *Mucor hiemalis*                | HQ845045.1                   | *Mucor hiemalis* (Mucorales)          | 1  |
|             |                 |         |          | *Mucor hiemalis*                | HM037964.1                   | *Mucor hiemalis* (Mucorales)          |    |
|             |                 |         |          | *Mucor hiemalis*                | HM037963.1                   |                                        |    |
| CKG36       | TSB             | MW065536 | 16S      | *Bacillus sp.*                  | CP020437.2                   | *Bacillus* (Bacillales)               | 2  |
|             |                 |         |          | *Bacillus cereus*               | MG977683.1                   | *Bacillus* (Bacillales)               |    |
|             |                 |         |          | *Bacillus cereus*               | MG966498.1                   |                                        |    |
| CKG37       | CMN             | MW064160 | ITS      | *Sarocladium strictum*          | MH880255.1                   | *Sarocladium strictum* (Hypocreales)  | 1  |
|             |                 |         |          | *Sarocladium strictum*          | LC314675.1                   | *Sarocladium strictum* (Hypocreales)  |    |
|             |                 |         |          | *Sarocladium strictum*          | MF663649.1                   |                                        |    |
| CKG38       | CMB             | MW065537 | 16S      | *Pseudomonas sp.*               | KT710819.1                   | *Pseudomonas anguilliseptica* (Pseudomonadales) | 1  |
|             |                 |         |          | *Pseudomonas sp.*               | KT710818.1                   | *Pseudomonas anguilliseptica* (Pseudomonadales) |    |
|             |                 |         |          | *Pseudomonas sp.*               | JX177684.1                   |                                        |    |
| CKG39       | TSB             | MW065538 | 16S      | *Bacillus licheniformis*        | MG980062.1                   | *Bacillus* (Bacillales)               | 1  |
|             |                 |         |          | *Bacillus licheniformis*        | MG280960.1                   | *Bacillus* (Bacillales)               |    |
|             |                 |         |          | *Bacillus licheniformis*        | MG189544.1                   |                                        |    |
| CKG40       | WSP             | MW065539 | 16S      | Uncultured *Klebsiella* sp. clone JXS1-28 | JN873189.1             | *Klebsiella* (Enterobacterales)      | 2  |
|             |                 |         |          | *Klebsiella* sp.                | KM873628.1                   | *Klebsiella* (Enterobacterales)      |    |
|             |                 |         |          | *Raoultella ornithinolytica*    | CP010557.1                   |                                        |    |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|----------|----------|-------------------------------|---------------------------------|----------------------------------------|----|
| CKG42       | WSP              | MW064161 | ITS      | *Elaphocordyceps* sp.         | KC237381.1                      | *Elaphocordyceps* sp. (Hypocreales)    | 1  |
|             |                  |          |          |                               | KC237380.1                      |                                        |    |
|             |                  |          |          |                               | KX034386.1                      |                                        |    |
| CKG43       | WSP              | MW065540 | 16S      | *Bacillus subtilis*           | MG928427.1                      | *Bacillus* sp. (Bacillales)            | 1  |
|             |                  |          |          | *Bacillus siamensis*          | KY962351.1                      |                                        |    |
|             |                  |          |          |                               | KY962340.1                      |                                        |    |
| CKG44       | WSP              | MW064162 | ITS      | Uncultured *Neonectria coccinea* AEW3_110 | KJ022022.1                      | *Neonectria coccinea* (Hypocreales)    | 1  |
|             |                  |          |          |                               | KF823598.1                      |                                        |    |
|             |                  |          |          |                               | KC660506.1                      |                                        |    |
| CKG45       | WSP              | MW064163 | ITS      | *Purpureocillium lilacinum*   | KY007618.1                      | *Purpureocillium lilacinum* (Hypocreales) | 2  |
|             |                  |          |          |                               | MH865347.1                      |                                        |    |
|             |                  |          |          |                               | MH865301.1                      |                                        |    |
| CKG46       | TSB              | MW065541 | 16S      | *Nocardiopsis* sp.            | MK045298.1                      | *Nocardiopsis prasina* (Streptosporangiales) | 1  |
|             |                  |          |          | *Nocardiopsis prasina*        | MF594115.1                      |                                        |    |
|             |                  |          |          |                               | MF170851.1                      |                                        |    |
| CKG47       | CMN              | MW065542 | 16S      | *Vibrio* sp.                  | MG788349.1                      | *Vibrio* sp. (Vibrionales)             | 2  |
|             |                  |          |          | *Vibrio anguillarum*          | CP023433.1                      |                                        |    |
|             |                  |          |          |                               | CP023293.1                      |                                        |    |
| CKG49       | WSP              | MW064164 | ITS      | *Mucor circinelloides*        | MH911362.1                      | *Mucor circinelloides* (Mucorales)     | 1  |
|             |                  |          |          |                               | KC329629.1                      |                                        |    |
|             |                  |          |          |                               | JX241658.1                      |                                        |    |
| CKG50       | CMN              | MW065543 | 16S      | *Sporosarcina* sp.            | KX108967.1                      | *Sporosarcina* sp. (Bacillales)        | 1  |
|             |                  |          |          | *Sporosarcina* sp.            | KT368976.1                      |                                        |    |
|             |                  |          |          |                               | KF800793.1                      |                                        |    |
| CKG51       | CMN              | MW064165 | ITS      | *Penicillium polonicum*       | KY978579.1                      | *Penicillium* sp. (Eurotiales)         | 1  |
|             |                  |          |          |                               | KY993979.1                      |                                        |    |
|             |                  |          |          |                               | KY092668.1                      |                                        |    |
| CKG52       | CMN              | MW065544 | 16S      | *Vibrio* sp.                  | MG788349.1                      | *Vibrio* sp. (Vibrionales)             | 2  |
|             |                  |          |          | *Vibrio anguillarum*          | CP023433.1                      |                                        |    |
|             |                  |          |          |                               | CP023293.1                      |                                        |    |
| Strain code | Isolation medium | Acc. no. | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|----------|----------|---------------------------------|----------------------------------|----------------------------------------|----|
| CKG53       | CMN               | MW065545 | 16S      | *Streptomyces* sp.              | MK134635.1                       | *Streptomyces* sp. (Streptomycetales) | 2  |
| CKG54       | CMB               | MW064176 | 18S      | *Cordyceps farinosa* Fungal sp. J271 Isaria farinosa | MH857775.1 KC242713.1 KC242708.1 | *Cordyceps farinosa* (Hypocreales) | 1  |
| CKG55       | MB                | MW065546 | 16S      | *Nocardiopsis alba* Nocardiopsis alba Nocardiopsis alba | MH333283.1 MF321814.1 MF321809.1 | *Nocardiopsis alba* (Streptosporangiales) | 1  |
| CKG57       | CMB               | MW064166 | ITS      | *Aaosphaeria arxii* Arthopyrenia sp. Massarina igniaria | MH861193.1 KU747910.1 KR534712.1 | *Arthopyrenia* sp. (Pleosporales) | 1  |
| CKG58       | CMB               | MW065547 | 16S      | *Nocardiopsis* sp.              | MK045298.1 MF594115.1 MF170851.1 | *Nocardiopsis* prasina (Streptosporangiales) | 1  |
| CKG60       | MB                | MW065548 | 16S      | *Enterobacter* sp.              | MF429589.1 MH392488.1 MG75538.1 | *Citrobacter* sp. (Enterobacterales) | 2  |
| CKG62       | PDA               | MW064167 | ITS      | *Trichoderma* sp. *Trichoderma* hirae *Trichoderma* harzianum | MK290992.1 MK288146.1 MK209008.1 | *Trichoderma* sp. (Hypocreales) | 1  |
| CKG63       | WSP               | MW064168 | ITS      | *Penicillium* psychrosexualis *Penicillium* psychrosexualis *Penicillium* psychrosexualis | MH864839.1 MH864838.1 MH864787.1 | *Penicillium* sp. (Eurotiales) | 1  |
| CKG64       | CMB               | MW064169 | ITS      | *Penicillium* polonicum *Penicillium* polonicum *Penicillium* polonicum | MK271277.1 MK267441.1 MK07720.1 | *Penicillium* sp. (Eurotiales) | 1  |
| CKG66       | CMB               | MW064170 | ITS      | Uncultured fungus clone ZB042802405(86) Fungal sp. strain PS14 *Acrostalagmus* luteolbus | MF962944.1 MH456880.1 KT824244.1 | *Acrostalagmus* luteolbus (Hypocreales) | 1  |
| Strain code | Isolation medium | Acc. no.  | Amplicon | Closest related species (BLAST) | Acc. no. closest related species | Lowest taxonomic classification (order) | RG |
|-------------|------------------|-----------|----------|---------------------------------|----------------------------------|-----------------------------------------|----|
| CKG67_I     | CMB              | MW064171  | ITS      | Purpureocillium lilacinum       | LC413751.1                      | Purpureocillium lilacinum (Hypocreales) | 2  |
|             |                  |           |          | Purpureocillium lilacinum       | MF996819.1                      |                                         |    |
|             |                  |           |          | Purpureocillium lilacinum       | KF706346.1                      |                                         |    |
| CKG67_II    | WSP              | MW065549  | 16S      | Nocardiosis alba                | MH333283.1                      | Nocardiosis alba (Streptosporangiales) | 1  |
|             |                  |           |          | Nocardiosis alba                | MH071379.1                      |                                         |    |
|             |                  |           |          | Nocardiosis alba                | MF321814.1                      |                                         |    |
| CKG68       | WSP              | MW064172  | ITS      | Purpureocillium lilacinum       | MH865347.1                      | Purpureocillium lilacinum (Hypocreales) | 2  |
|             |                  |           |          | Purpureocillium lilacinum       | MH865301.1                      |                                         |    |
|             |                  |           |          | Purpureocillium lilacinum       | MH865154.1                      |                                         |    |
| CKG70       | TSB              | MW064173  | ITS      | Plectosphaerella cucumerina     | MH791266.1                      | Plectosphaerella cucumerina (Glomerellales) | 1  |
|             |                  |           |          | Fungal sp. strain S255T         | KU839553.1                      |                                         |    |
|             |                  |           |          | Fungal sp. strain S255S         | KU839552.1                      |                                         |    |
| CKG71       | TSB              | MW064174  | ITS      | Sarocladium strictum           | KY465763.1                      | Sarocladium strictum (Hypocreales)       | 1  |
|             |                  |           |          | Fungal sp. strain S254T         | KU839539.1                      |                                         |    |
|             |                  |           |          | Fungal sp. strain S254S         | KU839538.1                      |                                         |    |
Table S2. Antimicrobial and anticancer activities (% inhibition at a test concentration of 100 µg/mL) of microbial crude extracts. Inhibition values are given as average values of the two biological and two technical replicates. Some bacterial isolates were only cultivated on MB medium, since they did not grow on GYM medium. Extracts selected by the bioactivity selection criterion (see Section 2.3.) are highlighted in blue. MRSA: Methicillin-resistant *Staphylococcus aureus*, Efm: *Enterococcus faecium*, Ab: *Acinetobacter baumannii*, Ec: *Escherichia coli*, Kp: *Klebsiella pneumoniae*, Psa: *Pseudomonas aeruginosa*, Ca: *Candida albicans*, Cn: *Cryptococcus neoformans*, A375: Malignant melanoma, A549: Lung carcinoma, HCT116: Colon cancer, MB231: Breast cancer; “-”: Inhibition ≤20%; in bold: Inhibition values ≥80%; AC: extract was selected based on high anticancer activity (inhibition ≥80%); AM: extract was selected based on high antimicrobial activity (inhibition ≥80%).

| Strain | Identification       | Medium | MRSA | Efm | Ab | Ec | Kp | Psa | Ca | Cn | A375 | A549 | HCT116 | MB231 | Selected? |
|--------|----------------------|--------|------|-----|----|----|----|-----|----|----|------|------|--------|-------|-----------|
| CHG2   | *Ruegeria atlantica* | MB     | 73   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -      | -     | 36        |
| CHG3   | *Shewanella sp.*    | MB     | 92   | 52  | -  | -  | -  | -   | -  | -  | -    | -    | -      | -     |           |
| CHG5   | *Shewanella woodyi* | MB     | 95   | 78  | -  | -  | -  | -   | -  | -  | -    | -    | -      | -     |           |
| CHG6   | *Shewanella sp.*    | GYM    | 100  | 92  | -  | -  | -  | -   | -  | -  | -    | -    | -      | -     |           |
| CHG12  | *Shewanella sp.*    | MB     | 88   | 100 | -  | -  | -  | -   | -  | -  | -    | -    | -      | -     | 26        |
| CHG16  | *Vibrio sp.*        | MB     | 98   | 100 | -  | -  | -  | -   | -  | -  | -    | -    | -      | -     |           |
| CHG19  | *Arthrinium sp.*    | CAG    | -    | -   | -  | -  | -  | 65  | -  | 71 | 78   | 75   | 78     |       |           |
|        |                      | PDA    | -    | -   | -  | -  | -  | 26  | -  | 53 | 25   | 44   |        |       |           |
| CHG22  | *Penicillium hoeksi*| CAG    | 85   | -   | -  | -  | -  | -   | -  | 25 | 31   | 25   | 29     |       |           |
|        |                      | PDA    | 84   | -   | -  | -  | -  | -   | -  | 63 | 48   | 59   | 48     |       |           |
| CHG25  | *Penicillium sp.*   | CAG    | 99   | 100 | 98 | 100| 100| 100 | -  | 98 | 93   | 98   | 92     | Yes (AC)|           |
|        |                      | PDA    | 98   | 84  | 97 | 100| 100| 100 | 99 | 99 | 98   | 99   | 95     | Yes (AC)|           |
| CHG26  | *Galactomyces candidum* | CAG   | 96   | 33  | -  | -  | -  | -   | -  | -  | -    | -    | -      |       |           |
|        |                      | PDA    | 54   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -      |       |           |
| CHG29  | *Phoma sp.*         | CAG    | -    | -   | -  | -  | -  | -   | -  | -  | -    | -    | -      |       |           |
|        |                      | PDA    | -    | -   | -  | -  | -  | -   | -  | -  | -    | -    | -      |       |           |
| CHG32  | *Vibrio sp.*        | MB     | 79   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -      |       |           |
| CHG34  | *Trichoderma sp.*   | CAG    | 41   | -   | -  | -  | -  | 24  | -  | 97 | 96   | 95   | 93     | Yes (AC)|           |
|        |                      | PDA    | 94   | 100 | -  | -  | -  | 100 | 92 | 98 | 99   | 99   | 98     | Yes (AC & AM)|       |
| CHG35  | *Penicillium sp.*   | CAG    | 100  | 100 | 99 | 99 | 100| 84  | -  | 21 | 72   | 93   | 95     | 64    | Yes (AC)  |
| Strain   | Identification       | Medium | MRSA | Efm | Ab | Ec | Kp | PsA | Ca | Cn | A375 | A549 | HCT116 | MB231 | Selected?   |
|----------|----------------------|--------|------|-----|----|----|----|-----|----|----|------|------|---------|-------|-------------|
| CHG38    | Fusarium sp.         | PDA    | 98   | 74  | 98 | 98 | 100| 77  | -  | -  | 89   | 98   | 98      | 72    | Yes (AC)    |
|          |                      | CAG    | 100  | 100 | -  | -  | -  | 92  | 96 | 98 | 65   | 93   | 40      |       |             |
| CHG39    | Bacillus sp.         | GYM    | 97   | 100 | -  | -  | -  | -   | -  | -  | 69   | 73   | 48      | 69    |             |
|          |                      | MB     | 96   | 94  | -  | -  | -  | -   | -  | -  | 30   | 29   | -       | 31    |             |
| CHG40    | Streptomyces sp.     | GYM    | 100  | 100 | -  | -  | -  | 61  | 37 | 98 | 99   | 98   | 99      |       | Yes (AC)    |
|          |                      | MB     | 100  | 87  | -  | -  | -  | -   | -  | -  | 51   | 51   | 55      | 61    |             |
| CHG41    | Bacillus licheniformis | GYM   | 69   | -   | -  | -  | -  | -   | -  | -  | 62   | 33   | 38      | 51    |             |
|          |                      | MB     | 66   | -   | -  | -  | -  | -   | -  | -  | 25   | 33   | -       | 33    |             |
| CHG48    | Streptomyces sp.     | GYM    | 100  | 100 | -  | -  | -  | 100 | 97 | 98 | 92   | 88   | 93      |       | Yes (AC & AM)|
|          |                      | MB     | 100  | 100 | -  | -  | -  | 72  | 71 | 69 | 71   | 74   |         |       |             |
| CHG49    | Pleosporaceae        | CAG    | 99   | 84  | 97 | 100| 100| 100 | 38 | 53 | 99   | 95   | 98      | 94    | Yes (AC)    |
|          |                      | PDA    | 98   | 68  | 98 | 100| 100| 82  | 28 | -  | 97   | 97   | 98      | 53    |             |
| CHG52    | Penicillium sp.      | CAG    | 92   | 88  | -  | -  | -  | 30  | -  | -  | 30   | 33   | -       |       |             |
|          |                      | PDA    | 95   | 96  | -  | -  | -  | -   | -  | -  | 72   | 71   | 69      | 71    |             |
| CHG53    | Trichoderma sp.      | CAG    | -    | -   | -  | -  | -  | -   | -  | -  | 20   | -    | -       |       |             |
|          |                      | PDA    | -    | -   | -  | -  | -  | -   | -  | -  | -    | -    | -       |       |             |
| CHG56    | Aspergillus sp.      | CAG    | 67   | -   | -  | -  | -  | -   | 22 | 26 | 34   | 34   | 46      |       |             |
|          |                      | PDA    | 70   | -   | -  | -  | -  | -   | 30 | 37 | 34   | 34   | 59      |       |             |
| CHG59    | Tamariccola sp.      | CAG    | 92   | -   | 36 | -   | -  | -   | -  | -  | -    | -    | -       |       |             |
|          |                      | PDA    | 91   | -   | 37 | -   | -  | -   | -  | -  | -    | -    | -       |       |             |
| CHG60    | Peroneutypa sp.      | CAG    | 35   | -   | 33 | -   | -  | -   | -  | -  | 47   | 35   | 46      |       |             |
|          |                      | PDA    | 32   | -   | -  | -  | -  | -   | 33 | 36 | 25   | -    | -       |       |             |
| CHG64    | Streptomyces sp.     | GYM    | 100  | 97  | -  | -  | -  | 99  | 98 | 99 | 98   | 98   | 98      |       | Yes (AC)    |
|          |                      | MB     | 100  | 98  | -  | -  | -  | 58  | 23 | 50 |      |      |         |       |             |
| CKG5     | Nocardiopsis sp.     | GYM    | -    | 46  | -  | -  | -  | -   | -  | -  | 29   | -    | 48      | -     |             |
| CKG6     | Shewanelia aestuarii | MB     | 100  | 94  | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     |             |
| Strain  | Identification          | Medium | MRSA | Efm | Ab | Ec | Kp | Psa | Ca | Cn | A375 | A549 | HCT116 | MB231 | Selected? |
|---------|-------------------------|--------|------|-----|----|----|----|-----|----|----|------|------|---------|-------|-----------|
| CKG7    | Vibrio sp.              | MB     | 34   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     | -         |
| CKG12   | Vibrio sp.              | MB     | 100  | 74  | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     | -         |
| CKG13   | Pseudomonas sp.         | MB     | 35   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     | -         |
| CKG15   | Shewanella colwelliana  | MB     | 100  | 100 | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     | -         |
| CKG16   | Eutypa lata             | CAG    | 46   | -   | 31 | -  | -  | -   | -  | 26 | 34   | 33   | -       | -     | Yes (AC)  |
|         |                         | PDA    | -    | -   | 29 | -  | -  | -   | -  | 33 | 26   | 32   | -       | -     |           |
| CKG20   | Micromonospora sp.      | GYM    | 100  | 100 | -  | -  | -  | -   | 98 | 100| 99   | 100  | -       | -     | Yes (AC)  |
|         |                         | MB     | 53   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     |           |
| CKG21   | Bacillus hwajinpoensis  | GYM    | 65   | -   | -  | -  | -  | -   | -  | -  | 20   | -    | -       | -     |           |
|         |                         | MB     | 100  | 100 | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     |           |
| CKG23   | Penicillium sp.         | CAG    | 100  | 98  | 100| 100| 100| 89  | -  | -  | 97   | 98   | 98      | 97    | Yes (AC)  |
|         |                         | PDA    | 100  | 100| 98  | 100| 100| 75  | -  | 41 | 95   | 98   | 77      | 92    | Yes (AC)  |
| CKG24   | Bacillus sp.            | GYM    | 100  | 100 | -  | -  | -  | -   | 94 | 72 | 98   | 63   | 34      | -     | Yes (AC & AM) |
|         |                         | MB     | 100  | 100 | -  | -  | -  | -   | -  | 51 | 54   | 43   | 59      |       |           |
| CKG25   | Galactomyces candidum   | CAG    | 100  | 100| 100| 100| 100| 85  | -  | -  | 96   | 99   | 92      | 82    | Yes (AC)  |
|         |                         | PDA    | 99   | 99  | 100| 100| 100| 93  | -  | -  | 98   | 99   | 99      | 93    | Yes (AC)  |
| CKG31   | Shewanella kaireticia   | GYM    | 100  | 100| 34 | -  | -  | -   | -  | -  | 27   | 26   | 25      |       |           |
|         |                         | MB     | 100  | 100| 34 | -  | -  | -   | -  | -  | 20   | -    | -       | -     |           |
| CKG32   | Fusarium sp.            | CAG    | 100  | 100| -  | -  | -  | -   | 89 | 40 | 61   | 20   | 29      | -     | Yes (AM)  |
|         |                         | PDA    | 99   | 86  | -  | -  | -  | 60  | -  | 21 | -    | -    | -       | -     |           |
| CKG33   | Mucor hiemalis          | CAG    | 62   | -   | -  | -  | -  | -   | -  | -  | 27   | 27   | 48      |       |           |
|         |                         | PDA    | 77   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     |           |
| CKG37   | Sarocladium strictum    | CAG    | 100  | 94  | -  | 38 | -  | -   | -  | -  | -    | -    | -       | -     |           |
|         |                         | PDA    | 95   | 47  | -  | 41 | -  | -   | -  | 78 | 48   | 58   | 56      |       |           |
| CKG38   | Pseudomonas anguilliseptica | GYM   | 100  | 100| -  | -  | -  | -   | 85 | 49 | 68   | 24   | 91      | 88    | Yes (AC & AM) |
|         |                         | MB     | 100  | 97  | -  | -  | -  | -   | 80 | 73 | -    | -    | -       | -     | Yes (AM)  |
| CKG39   | Bacillus sp.            | GYM    | -    | -   | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     |           |
|         |                         | MB     | 37   | -   | -  | -  | -  | -   | -  | -  | -    | -    | -       | -     |           |
| Strain   | Identification                  | Medium | MRSA | Efm | Ab  | Ec  | Kp  | Psa | Ca  | Cn  | A375 | A549 | HCT116 | MB231 | Selected?   |
|----------|---------------------------------|--------|------|-----|-----|-----|-----|-----|-----|-----|------|------|--------|-------|-------------|
| CKG42    | *Elaphocordyces* sp.            | CAG    | 76   | -   | -   | -   | -   | -   | 37  | -   | -    | -    | -      | -     |             |
|          |                                 | PDA    | 82   | 66  | -   | -   | -   | 35  | 38  | 26  | -    | -    | -      | -     |             |
| CKG43    | *Bacillus* sp.                  | GYM    | 92   | 100 | -   | -   | -   | -   | 38  | -   | 24   | -    | -      | -     |             |
|          |                                 | MB     | 94   | 100 | -   | -   | -   | -   | 26  | -   | -    | -    | -      | -     |             |
| CKG44    | *Neonectria coccinea*           | CAG    | 54   | -   | -   | -   | -   | -   | 24  | -   | -    | -    | 28     | -     |             |
|          |                                 | PDA    | -    | -   | -   | -   | -   | -   | -   | -   | -    | -    | -      | -     |             |
| CKG49    | *Mucor circinelloides*          | CAG    | 89   | 98  | -   | -   | -   | -   | 21  | 35  | 44   | 22   | -      | -     |             |
|          |                                 | PDA    | 100  | 100 | -   | -   | -   | -   | 66  | 37  | 79   | 43   | -      | -     |             |
| CKG50    | *Sporosarcina* sp.              | GYM    | 100  | 96  | -   | -   | -   | -   | -   | -   | -    | -    | -      | -     |             |
|          |                                 | MB     | 100  | 98  | -   | -   | -   | -   | -   | -   | -    | -    | 20     | -     |             |
| CKG54    | *Cordyceps farinosa*            | CAG    | 98   | 95  | -   | -   | -   | -   | 56  | -   | 30   | -    | -      | -     |             |
|          |                                 | PDA    | 99   | 97  | -   | -   | -   | -   | 52  | 24  | 42   | -    | -      | -     |             |
| CKG57    | *Arthopyrenia* sp.              | CAG    | 66   | -   | -   | -   | -   | -   | -   | -   | -    | -    | -      | -     |             |
|          |                                 | PDA    | 52   | -   | -   | -   | -   | -   | -   | -   | -    | -    | -      | -     |             |
| CKG58    | *Nocardiosis prasina*           | GYM    | 81   | 98  | -   | -   | -   | -   | 81  | 54  | 99   | 99   | 99     | 98    | Yes (AC & AM) |
|          |                                 | MB     | 100  | 99  | -   | -   | -   | -   | 31  | 26  | -    | 38   | -      | 61    |             |
| CKG62    | *Trichoderma* sp.               | CAG    | 30   | -   | -   | -   | -   | -   | 88  | -   | 28   | -    | -      | -     |             |
|          |                                 | PDA    | 70   | 100 | -   | 31  | -   | -   | 93  | 74  | 98   | 98   | 99     | 98    | Yes (AC & AM) |
| CKG63    | *Penicillium* sp.               | CAG    | 96   | 25  | 26  | -   | -   | 21  | 36  | -   | 45   | 50   | 30     | 64    |             |
|          |                                 | PDA    | 76   | 22  | 84  | 71  | 82  | 59  | -   | 51  | 80   | 49   | 77     | -     | Yes (AC)   |
| CKG64    | *Penicillium* sp.               | CAG    | -    | -   | -   | -   | -   | 37  | -   | -   | 21   | -    | 37     | -     |             |
|          |                                 | PDA    | 70   | -   | -   | -   | -   | -   | -   | -   | 34   | 30   | 45     | -     |             |
| CKG66    | *Acrostalagmus luteolalus*      | CAG    | 100  | 100 | 86  | 28  | -   | 22  | -   | -   | 87   | 89   | 83     | 89    | Yes (AC)   |
|          |                                 | PDA    | 87   | 51  | -   | -   | -   | -   | -   | -   | 25   | 70   | -      | -     |             |
| CKG70    | *Plectosphaerella* cucumerina   | CAG    | 56   | -   | -   | -   | -   | -   | -   | -   | -    | -    | -      | -     |             |
|          |                                 | PDA    | 69   | -   | -   | -   | -   | -   | -   | -   | -    | -    | -      | -     |             |
Table S3. Statistical comparison of chemically distinct bacterial crude extracts. ANOSIM was based on Euclidean distance. Group 1 included the following extracts: *Pseudomonas anguilliseptica* extracts CKG38-GYM and CKG38-MB and *Streptomyces* sp. extracts CHG40-GYM and CHG64-GYM.

| Comparison                                      | R value | p value |
|------------------------------------------------|---------|---------|
| All                                            | 1       | 0.0001  |
| Group 1 x Group 2 (CHG48-GYM, CKG58-GYM)       | 1       | 0.0022  |
| Group 1 x Group 3 (CKG20-GYM)                   | 1       | 0.0229  |
| Group 1 x Group 4 (CKG24-GYM)                   | 1       | 0.0232  |

Table S4. Statistical comparison of chemically distinct fungal crude extracts. ANOSIM was based on Euclidean distance. Group 1 included the following extracts: *Acrostalagmus luteoalbus* extract CKG66-CAG, *Galactomyces candidum* extracts CKG25-CAG and CKG25-PDA, *Penicillium* sp. extracts CHG25-CAG, CHG25-PDA, CHG35-CAG, CHG35-PDA, CKG23-CAG and CKG63-PDA and *Pleosporaceae* extracts CHG49-CAG and CHG49-PDA.

| Comparison                                      | R value | p value |
|------------------------------------------------|---------|---------|
| All                                            | 0.8363  | 0.0001  |
| Group 1 x Group 2 (CHG34-CAG, CHG34-PDA, CKG62-PDA) | 0.9369  | 0.0001  |
| Group 1 x Group 3 (CHG38-CAG, CHG38-PDA, CKG32-CAG) | 0.6822  | 0.0001  |
| Group 1 x Group 4 (CKG23-PDA)                   | 0.9996  | 0.0055  |
Table S5. Putatively identified compounds produced by *Streptomyces* sp. extract CHG48-GYM. Putative annotations were based on the accurate mass, the predicted putative molecular formulae (MF), the retention time (Rt), the fragmentation pattern and the biological origin. *MF with best ppm error displayed; IC: Identification confidence level [3]; Nf: No fragmentation detected or below noise threshold (5e3); Ref = reference(s).

| No. | m/z value | Adduct | Rt (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Ref |
|-----|-----------|--------|----------|-----|-------------|------------------------|----|------------------------|----------------|-----------------|-----|
| 1   | 225.1104  | [M+H]+ | 3.07     | 1.8 | C₉H₁₀N₂O₄   | 181.1201, 164.1114, 141.9593, 97.9700 | 4  | n.a.                  |                |                 |     |
| 2   | 208.0976  | [M+H]+ | 3.1      | 1   | C₈H₁₀N₂O₃   | 190.0865, 166.0866, 164.1073, 146.0968, 135.0804, 131.0732, 122.0962, 118.0657 | 3  | Streptazolin          | Oxazolidone alkaloid | *Streptomyces viridochromogenes* [4] |     |
| 3   | 250.1422  | [M+Na]+| 3.53     | 1.2 | C₈H₁₀N₂O₃   | 138.053                | 3  | Streptenol E          | Acetamide       | *Streptomyces* sp. [5] |     |
| 4   | 239.1261  | [M+H]+ | 3.72     | 2.1 | C₈H₁₀N₂O₃   | 216.0758, 210.1890, 198.0604, 195.1371, 172.0880, 155.0949, 141.9587 | 4  | n.a.                  |                |                 |     |
| 5   | 620.235   | [M+H]+ | 3.96     | 1.1 | C₃₀H₃₈N₃O₁₅ | 142.1230, 98.0971       | 4  | n.a.                  |                |                 |     |
| 6   | 604.2402  | [M+H]+ | 4.04     | 1.3 | C₂₀H₂₄N₂O₁₀ | 572.0979, 142.1230, 124.1113, 98.0970, 79.0555 | 3  | Platensimycin          | Diterpenoid glycoside | *Streptomyces platensis* [6] |     |
| 7   | 366.1893  | [M+Na]+| 4.12     | 0   | C₈H₁₀N₂O₃   | 308.1821, 290.1734, 270.1647, 252.1608, 224.1649, 198.0766, 180.0642, 172.0899, 166.1217, 154.1225, 152.0704, 142.0490, 137.0591, 114.0552, 109.1009 | 3  | Alpinamide A          | Linear polypeptide | *Streptomyces* sp. [7] |     |
| 8   | 253.1415  | [M+H]+ | 4.28     | 0.8 | C₂₀H₂₄N₂O₁₀ | 228.0977, 209.1505, 205.6684, 186.9429, 182.0896, 165.6180 | 4  | n.a.                  |                |                 |     |
| 9   | 253.142   | [M+H]+ | 4.44     | 2.8 | C₂₀H₂₄N₂O₁₀ | 210.0668, 195.9134, 170.9937 | 4  | n.a.                  |                |                 |     |
| 10  | 308.1867  | [M+H]+ | 4.76     | 1.6 | C₂₀H₂₄N₂O₁₀ | 252.1580, 198.0758, 180.0665, 172.0796, 166.1222, 152.0706, 142.0513, 137.0609, 109.1020 | 4  | n.a.                  |                |                 |     |
| 11  | 713.2711  | [M+H]+ | 5.5      | 0.1 | C₂₀H₂₄N₂O₁₀ | 142.1232, 98.0974       | 4  | n.a.                  |                |                 |     |
| 12  | 387.238   | [M+H]+ | 5.7      | -0.8| C₂₀H₂₄N₂O₁₀ | 165.1388, 167.1079, 143.0687, 125.0604, 121.1022, 111.0808, 93.0695 | 2  | Nonactyl nonactoate    | Nonactic acid polypeptide | *Streptomyces* sp. [8] |     |
| 13  | 558.1771  | [M+H]+ | 6.01     | -1.1| C₂₀H₂₄N₂O₁₀ | 174.0918, 162.0919       | 4  | n.a.                  |                |                 |     |
| 14  | 401.254   | [M+H]+ | 6.24     | 0.2 | C₂₀H₂₄N₂O₁₀ | 199.1332, 181.1228, 167.1066, 143.0703, 125.0966, 111.0810, 107.0859 | 2  | Bonactin              | Nonactic acid polypeptide | *Streptomyces* sp. [9] |     |
| 15  | 421.2201  | [M+Na]+| 6.35     | 0.9 | C₂₀H₂₄N₂O₁₀ | 239.1254, 223.0950       | 4  | n.a.                  |                |                 |     |
| 16  | 413.2513  | [M+Na]+| 6.42     | -0.5| C₂₀H₂₄N₂O₁₀ | 227.1261, 209.1144       | 4  | n.a.                  |                |                 |     |
| 17  | 309.1684  | [M+H]+ | 6.62     | 2.9 | C₂₀H₂₄N₂O₁₀ | 265.1174, 221.1151, 207.0990 | 4  | n.a.                  |                |                 |     |
| 18  | 415.2705  | [M+H]+ | 6.82     | 2.2 | C₂₀H₂₄N₂O₁₀ | 199.1374, 181.1226, 163.1117, 143.0700, 139.1125, 135.1168, 125.0959, 107.0853, 81.0709 | 2  | Homononactyl homononactate | Nonactic acid polypeptide | *Streptomyces griseus* [10] |     |
| 19  | 321.1682  | [M+H]+ | 6.89     | 2.2 | C₂₀H₂₄N₂O₁₀ | 221.1566                        | 4  | n.a.                  |                |                 |     |
| No. | m/z value | Adduct      | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern                                      | IC | Putative identification | Chemical family | Biological origin | Ref |
|-----|-----------|-------------|---------------------|-----|-------------|----------------------------------------------------------|----|-------------------------|----------------|-------------------|-----|
| 20  | 312.1967  | [M+H]<sup>+</sup> | 7.49 | 1 | C<sub>20</sub>H<sub>25</sub>NO<sub>2</sub> | 216.1390, 200.1078, 188.1083, 172.1142, 162.0898, 151.1139 | 4  | n.a.                  |                |                  |     |
| 21  | 807.395   | [M+H]<sup>+</sup> | 7.73 | -2.4 | C<sub>46</sub>H<sub>54</sub>N<sub>4</sub>O<sub>9</sub> | 789.3856, 771.2729, 434.1707, 396.1556, 378.1438, 336.1355, 297.1229, 285.1239 | 4  | n.a.                  |                |                  |     |
| 22  | 289.175   | [M+Na]<sup>+</sup> | 7.93 | -1 | C<sub>20</sub>H<sub>25</sub>No | Nf | 4  | n.a.                  |                |                  |     |
| 23  | 585.3634  | [M+H]<sup>+</sup> | 8.12 | -0.9 | C<sub>20</sub>H<sub>25</sub>O<sub>10</sub> | 199.1380, 185.1173, 181.1227, 167.1063, 143.0731, 125.0962, 111.0792, 93.0702 | 4  | n.a.                  |                |                  |     |
| 24  | 352.1552  | [M+H]<sup>+</sup> | 8.4 | 0.9 | C<sub>20</sub>H<sub>25</sub>No | 174.0921, 162.0919 | 4  | n.a.                  |                |                  |     |
| 25  | 807.3981  | [M+H]<sup>+</sup> | 8.56 | 1.5 | C<sub>46</sub>H<sub>54</sub>N<sub>4</sub>O<sub>9</sub> | 789.3876, 771.2750, 434.1710, 396.1559, 378.1448, 365.1138, 336.1154, 297.1230, 285.1233 | 4  | n.a.                  |                |                  |     |
| 26  | 621.3619  | [M+Na]<sup>+</sup> | 8.6 | 0.6 | C<sub>20</sub>H<sub>25</sub>O<sub>10</sub> | 423.2351, 419.2396, 225.1102, 221.1153 | 4  | n.a.                  |                |                  |     |
| 27  | 684.3649  | [M+H]<sup>+</sup> | 8.87 | 0 | C<sub>20</sub>H<sub>25</sub>No | 273.1241, 174.0922, 162.0919 | 4  | n.a.                  |                |                  |     |
| 28  | 560.4683  | [M+H]<sup>+</sup> | 9.06 | 0.7 | C<sub>20</sub>H<sub>25</sub>No | 542.4562, 524.4463 | 4  | n.a.                  |                |                  |     |
| 29  | 546.4896  | [M+H]<sup>+</sup> | 9.87 | 1.8 | C<sub>20</sub>H<sub>25</sub>No | 528.4788, 510.4700 | 4  | n.a.                  |                |                  |     |
| 30  | 783.4903  | [M+H]<sup>+</sup> | 10.09 | 1 | C<sub>20</sub>H<sub>25</sub>O<sub>2</sub> | 199.1337, 185.1174, 181.1226, 167.1068, 143.0703, 125.0961, 111.0809 | 4  | n.a.                  |                |                  |     |
| 31  | 797.5042  | [M+H]<sup>+</sup> | 10.48 | -1.1 | C<sub>20</sub>H<sub>25</sub>O<sub>3</sub> | 199.1342, 181.1236, 167.1073, 143.0718, 125.0973, 107.0860 | 4  | n.a.                  |                |                  |     |
| 32  | 811.5203  | [M+H]<sup>+</sup> | 10.85 | -0.6 | C<sub>20</sub>H<sub>25</sub>O<sub>3</sub> | Nf | 4  | n.a.                  |                |                  |     |
| 33  | 737.4476  | [M+H]<sup>+</sup> | 11.77 | 0 | C<sub>20</sub>H<sub>25</sub>O<sub>2</sub> | MS6: 185.1191, 167.1073, 149.0946, 143.0683, 121.1022, 111.0811 | 2  | Nonactin          | Nonactic acid polyketide | Streptomycetes spp. | [11] |
Table S6. Putatively identified compounds produced by *Micromonospora* sp. extract CKG20-GYM. Putative annotations were based on the accurate mass, the predicted putative molecular formulae (MF), the retention time (Rt), the fragmentation pattern and the biological origin. Different isomers with same m/z value and molecular formula, which cannot be differentiated based on MS/MS data; IC: Identification confidence level [3]; Ref = reference(s).

| No. | m/z value | Adduct | Rt (min) | ppm  | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Ref |
|-----|-----------|--------|----------|------|-------------|----------------------|----|------------------------|----------------|------------------|-----|
| 34  | 243.1348  | [M+H]+ | 2.47     | 1.2  | C11H15N4O6  | 201.1239, 165.1032, 154.0877, 137.1081, 100.0399 | 4  | n.a.                   |                |                  |     |
| 35  | 218.1417  | [M+H]+ | 3.2      | 5    | C11H14N4  | 162.9784, 150.0785   | 4  | n.a.                   |                |                  |     |
| 36  | 280.124   | [M+H]+ | 4.17     | -6.1 | C8H11N4O6  | 262.1132, 196.0661   | 4  | n.a.                   |                |                  |     |
| 37  | 197.118   | [M+H]+ | 5.67     | 1    | C6H11O      | 158.9618, 117.9348, 96.9611  | 4  | n.a.                   |                |                  |     |
| 38  | 420.3119  | [M+H_2O]+ | 6.8     | 1.2  | C7H14NO6    | 378.2967, 332.2931, 315.2679, 229.1942, 203.1753, 175.1504, 149.1352, 135.1159, 107.0873 | 4  | n.a.                   |                |                  |     |
| 39  | 369.218   | [M+H]+ | 7.48     | 0.5  | C6H11N4O6  | 256.0851              | 4  | n.a.                   |                |                  |     |
| 40  | 479.2547  | [M+H]+ | 7.72     | 0.2  | C8H13NO6    | 287.0663, 275.0670, 259.0480 | 4  | n.a.                   |                |                  |     |
| 41  | 466.2933  | [M+H]+ | 7.85     | -0.2 | C7H12NO6P   | 325.2744, 294.2796   | 4  | n.a.                   |                |                  |     |
| 42  | 454.2929  | [M+H]+ | 8.08     | -1.1 | C7H12NO6P   | 313.2740, 282.2794   | 2  | 1-palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine Glycero-phospholipid In cell membranes of all organisms |                |                  |     |
| 43  | 330.2435  | [M+H]+ | 8.11     | 0.6  | C6H11N4O6  | 312.2322              | 4  | n.a.                   |                |                  |     |
| 44  | 463.2597  | [M+H]+ | 8.2      | 0    | C8H13NO6    | 271.0725, 259.0725, 243.0536 | 2  | Diazepinomicin Phenazine alkaloid Micromonospora sp. [12] |                |                  |     |
| 45  | 480.3098  | [M+H]+ | 8.38     | 1.7  | C8H15NO6P   | 339.2955, 308.2907   | 2  | 1-(9Z-octadecenoyl)-sn-glycero-3-phosphoethanolamine Glycero-phospholipid In cell membranes of all organisms |                |                  |     |
| 46  | 479.2547  | [M+H]+ | 8.62     | 0.2  | C8H13NO6    | 258.0409, 240.0301, 146.0241, 112.0401 | 4  | n.a.                   |                |                  |     |
| 47  | 408.0832  | [M+H]+ | 8.78     | 0    | C8H13NO6    | 390.0728, 372.0690, 362.0768, 349.0473, 344.0468, 321.0529, 259.0353, 245.0565, 233.0566, 176.0353 | 4  | n.a.                   |                |                  |     |
| 48  | 411.2281  | [M+H]+ | 8.9      | -0.7 | C8H13NO6    | 393.2157, 383.2320, 285.0869, 271.0714, 259.0710, 243.0767 | 3  | Diazaquinomycin D Phenazine alkaloid Streptomyces sp. [13] |                |                  |     |
| 49  | 619.4077  | [M+H]+ | 8.93     | 1    | C8H15NO6    | 427.3684, 400.3203, 376.3233, 305.2831, 297.1194, 280.0945, 279.1076, 262.0820, 252.0987, 224.1024, 220.0929, 208.1091, 202.0814, 193.0606, 167.0832, 149.0701, 123.0920, 121.0773, 109.1015, 96.0452 | 4  | n.a.                   |                |                  |     |
| No. | m/z value | Adduct | R_t (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Ref |
|-----|-----------|--------|-----------|-----|------------|-----------------------|----|-------------------------|----------------|-------------------|-----|
| 50  | 482.325   | [M+H]^+ | 9.09      | 0.8 | C_23H_48NO_7P | 341.3052, 310.3102 | 2  | 1-stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine | Glycero-phospholipid | In cell membranes of all organisms |     |
| 51  | 607.4077  | [M+H]^+ | 9.27      | 1   | C_32H_54N_4O_7 | 388.3211, 297.1197, 293.2846, 280.0937, 252.0986, 220.0934, 202.0833, 167.0821, 149.0676, 121.0761 | 2  | Rakicidin A | Cyclic depsipeptide | Micromonospora sp. | [14] |
| 52  | 621.4227  | [M+H]^+ | 9.73      | 0   | C_33H_56N_4O_7 | 402.3372, 350.3409, 307.2997, 297.1193, 280.0944, 252.0985, 220.0929, 167.0816, 149.0691, 121.0767 | 2  | Rakicidin B | Cyclic depsipeptide | Micromonospora sp. |     |
| 53  | 635.4383  | [M+H]^+ | 10.19     | -0.2 | C_34H_58N_4O_7 | 416.3523, 364.3604, 321.3148, 297.1199, 280.0939, 252.0980, 220.0930, 202.0839, 167.0817, 149.0708, 121.0757 | 2  | Rakicidin E | Cyclic depsipeptide | Micromonospora sp. | [15] |
| No. | m/z value | Adduct   | R<sub>t</sub> (min) | ppm   | Putative MF                                      | Fragmentation pattern                                                                 | IC | Putative identification | Chemical family | Biological origin | Ref   |
|-----|-----------|----------|---------------------|-------|------------------------------------------------|---------------------------------------------------------------------------------------|----|------------------------|-----------------|------------------|-------|
| 54  | 367.0508  | [M+H]<sup>+</sup> | 3.63               | -1.4  | C<sub>8</sub>H<sub>9</sub>O<sub>3</sub> | 287.0525, 258.0562, 241.9696, 238.0435, 188.0169, 168.9262, 164.9999, 146.9907 | 4  | n.a.                  |                 |                  |       |
| 55  | 424.2082  | [M+H]<sup>+</sup> | 3.71               | -0.5  | C<sub>9</sub>H<sub>10</sub>N<sub>0</sub>O<sub>5</sub> | 407.1817, 390.1540, 330.1343, 274.0708, 250.1446, 232.1337, 215.1069, 195.0942 | 2  | Amicoumacin-A          | Isocoumarin     | Bacillus subtilis   | [16] |
| 56  | 439.2083  | [M+H]<sup>+</sup> | 4.12               | 0.7   | C<sub>10</sub>H<sub>11</sub>N<sub>0</sub>O<sub>5</sub> | 422.1824, 250.1440, 232.1337, 215.1070, 176.0702, 159.0444, 149.0598 | 4  | n.a.                  |                 |                  |       |
| 57  | 255.1207  | [M+H]<sup>+</sup> | 4.25               | 0.4   | C<sub>7</sub>H<sub>6</sub>N<sub>0</sub>O<sub>5</sub> | 195.9121                                                                                     | 4  | n.a.                  |                 |                  |       |
| 58  | 250.1127  | [M+H]<sup>+</sup> | 5.04               | -4.4  | C<sub>9</sub>H<sub>10</sub>N<sub>0</sub>O<sub>5</sub> | 194.0496, 182.0501                                                                          | 4  | n.a.                  |                 |                  |       |
| 59  | 392.1711  | [M+H]<sup>+</sup> | 5.43               | 0.5   | C<sub>10</sub>H<sub>12</sub>N<sub>0</sub>O<sub>5</sub> | 276.1247, 250.1441, 232.1328, 215.1074, 159.0440, 149.0598, 125.0238 | 3  | Bacilloumacin D        | Isocoumarin     | Bacillus sp.       | [17] |
| 60  | 390.1556  | [M+H]<sup>+</sup> | 5.55               | 0.8   | C<sub>10</sub>H<sub>11</sub>N<sub>0</sub>O<sub>5</sub> | 250.1441, 232.1340, 215.1073, 159.0442, 123.0087 | 3  | Antibiotic AI-77-F or -H | Isocoumarin     | Bacillus spp.     | F: [18], H: [19] |
| 61  | 1071.5811 | [M+H]<sup>+</sup> | 6.05               | -2.8  | C<sub>14</sub>H<sub>15</sub>N<sub>0</sub>O<sub>4</sub> | 535.5373, 455.3136, 437.3194, 392.1351, 354.2751, 341.2750, 323.2671, 313.1513, 299.2645, 295.1353, 278.1133, 260.1039, 250.1231, 212.1082, 208.1156, 198.2230, 167.0809, 136.0747 | 3  | Bacillolmycin F2       | Cyclic lipopeptide | Bacillus subtilis | [20], [21] |
| 62  | 1085.5974 | [M+H]<sup>+</sup> | 6.45               | -1.9  | C<sub>14</sub>H<sub>15</sub>N<sub>0</sub>O<sub>4</sub> | 680.4345, 663.4116, 645.3961, 618.3965, 566.3553, 549.3728, 531.3541, 507.3527, 469.3383, 451.3282, 406.1735, 392.1518, 389.1400, 375.1311, 368.2910, 355.2957, 351.2631, 323.1372, 313.2847, 295.1401, 278.1146, 277.1303, 275.1039, 268.2650, 264.0987, 261.0894, 260.1024, 250.1191, 243.1082, 233.0928, 216.0986, 212.2379, 209.0939, 208.1094, 198.0890, 180.1048, 184.1085, 167.0820, 136.0761 | 3  | Bacillolmycin F3       | Cyclic lipopeptide | Bacillus subtilis | [20], [21] |
| 63  | 1099.6122 | [M+H]<sup>+</sup> | 6.88               | -2.7  | C<sub>14</sub>H<sub>15</sub>N<sub>0</sub>O<sub>4</sub> | 694.4479, 677.4232, 660.3998, 632.4120, 580.4044, 563.3820, 545.3659, 483.3513, 465.3430, 406.1723, 392.1563, 389.1466, 382.3062, 375.1307, 369.3107, 365.2799, 351.2957, 337.2988, 327.3002, 323.1351, 313.1502, 299.2888, 295.1408, 278.1149, 275.1031, 264.0986, 261.0898, 250.1187, 233.0918, 226.2534, 212.1035, 209.0947, 188.1048, 184.1090, 167.0815, 136.0763 | 3  | Bacillolmycin F5       | Cyclic lipopeptide | Bacillus subtilis | [20], [21] |
| 64  | 781.4157  | [M+H]<sup>+</sup> | 7.08               | -0.8  | C<sub>7</sub>H<sub>6</sub>O<sub>2</sub> | 557.3537, 539.3503, 419.2196, 405.2093, 401.2106, 399.1993, 389.2074, 373.2114, 371.2022, 367.1888, 365.1761, 359.2000, 351.1960, 349.1813, 343.2067, 341.1881, 335.2000, 333.1837, 331.1708, 323.1975, 321.1785, 305.1885, 303.1775, 209.0880, 188.1048, 184.1090, 167.0815, 136.0763 | 3  | Aurantinin B           | Polyketide glycoside | Bacillus aurantius | [22] |

**Table S7.** Putatively identified compounds produced by *Bacillus* sp. extract CKG24-GYM. Putative annotations were based on the accurate mass, the predicted putative molecular formulae (MF), the retention time (R<sub>t</sub>), the fragmentation pattern and the biological origin. *Parent mass out of detection limit (>1200 Da) and therefore, the ppm error and fragmentation pattern were not determined; *MF with best ppm error displayed; IC: Identification confidence level [3]; Nf: No fragmentation detected or below noise threshold (5e<sup>+</sup>); Ref = reference(s).
| No. | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Ref |
|-----|-----------|--------|---------------------|-----|-------------|-----------------------|----|------------------------|----------------|-------------------|-----|
| 65  | 746.4219  | [M+2H]<sup>+</sup> | 7.14 | n.a.<sup>a</sup> | C<sub>67</sub>H<sub>112</sub>N<sub>22</sub>O<sub>32</sub> | n.a.<sup>a</sup> | 3 | SNA 60-367-5 | Cyclic lipopeptide | Bacillus sp. | [23] |
| 66  | 739.4143  | [M+2H]<sup>+</sup> | 7.14 | n.a.<sup>a</sup> | C<sub>67</sub>H<sub>112</sub>N<sub>22</sub>O<sub>32</sub> | n.a.<sup>a</sup> | 3 | SNA 60-367-6 | Cyclic lipopeptide | Bacillus sp. | [23] |
| 67  | 663.3561  | [M+H]<sup>+</sup> | 7.24 | -0.6 | C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub> or C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub> | 501.3020, 421.1306, 365.1053 | 4 | n.a. | Cyclic lipopeptide | Bacillus sp. | [23] |
| 68  | 753.4296  | [M+2H]<sup>+</sup> | 7.37 | n.a.<sup>a</sup> | C<sub>67</sub>H<sub>112</sub>N<sub>22</sub>O<sub>32</sub> | n.a.<sup>a</sup> | 3 | a: SNA 60-367-12, b: SNA 60-367-13 | Cyclic lipopeptide | Bacillus sp. | [23] |
| 69  | 738.4238  | [M+2H]<sup>+</sup> | 7.56 | n.a.<sup>a</sup> | C<sub>67</sub>H<sub>112</sub>N<sub>22</sub>O<sub>32</sub> | n.a.<sup>a</sup> | 3 | SNA 60-367-17 | Cyclic lipopeptide | Bacillus sp. | [23] |
| 70  | 738.4249  | [M+2H]<sup>+</sup> | 7.64 | n.a.<sup>a</sup> | C<sub>67</sub>H<sub>112</sub>N<sub>22</sub>O<sub>32</sub> | n.a.<sup>a</sup> | 3 | SNA 60-367-18 | Cyclic lipopeptide | Bacillus sp. | [23] |
| 71  | 731.4171  | [M+2H]<sup>+</sup> | 7.64 | n.a.<sup>a</sup> | C<sub>67</sub>H<sub>112</sub>N<sub>22</sub>O<sub>32</sub> | n.a.<sup>a</sup> | 3 | SNA 60-367-19 | Cyclic lipopeptide | Bacillus sp. | [23] |
| 72  | 745.4335  | [M+2H]<sup>+</sup> | 7.82 | n.a.<sup>a</sup> | C<sub>67</sub>H<sub>112</sub>N<sub>22</sub>O<sub>32</sub> | n.a.<sup>a</sup> | 3 | SNA 60-367-23 | Cyclic lipopeptide | Bacillus sp. | [23] |
| 73  | 512.3693  | [M+H]<sup>+</sup> | 8.25 | -1.4 | C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub> or C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub> | 268.2627, 115.0873, 102.0553, 84.0438 | 4 | n.a. | Cyclic lipopeptide | Bacillus sp. | [23] |
| 74  | 1008.6603 | [M+H]<sup>+</sup> | 10.24 | 0.6 | C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub> | 455.3112, 441.2708, 437.3002, 427.3160, 409.3047, 395.2667, 342.2245, 328.1873, 324.2168, 314.2333, 283.2020, 245.1858, 229.1185, 227.1759, 212.2019, 201.1239, 199.1811, 195.1743, 185.1657, 183.1133, 154.1599, 86.0973 | 3 | Anteiso-C<sub>67</sub>-[Leu]<sup>7</sup>-surfactin | Cyclic lipopeptide | Bacillus subtilis | [24] |
| 75  | 1064.5789 | [M+H]<sup>+</sup> | 10.29 | 0.4 | C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub>-Cl or C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub>-CP | NF | 4 | n.a. | Cyclic lipopeptide | Bacillus subtilis | [25] |
| 76  | 994.6426  | [M+H]<sup>+</sup> | 10.41 | -1.4 | C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>2</sub> | 455.3094, 441.2723, 437.2990, 432.2255, 328.1864, 324.2165, 314.2322, 296.2226, 285.1454, 283.2004, 269.1878, 231.1687, 229.1176, 227.1760, 215.1026, 212.2016, 201.1236, 199.1812, 195.1743, 185.1639, 86.0975 | 3 | Lipopeptide NO | Cyclic lipopeptide | Bacillus subtilis | [25] |
| 77  | 1022.6801 | [M+H]<sup>+</sup> | 10.64 | 4.7 | C<sub>67</sub>H<sub>40</sub>N<sub>10</sub>O<sub>3</sub> | 469.3278, 451.3170, 441.2706, 423.3218, 395.2657, 356.2436, 342.2031, 338.2332, 328.1876, 310.2383, 296.1983, 285.1457, 283.2006, 269.1866, 267.2441, 255.1708, 245.1868, 229.1192, 227.1763, 215.1034, 213.1604, 209.1902, 201.1241, 199.1811, 185.1653, 183.1132, 170.1181, 154.1593, 86.0974 | 3 | Iso-C<sub>67</sub>-[Val]<sup>7</sup>-surfactin | Cyclic lipopeptide | Bacillus subtilis | [24] |
| No. | m/z value | Adduct | R<sub>n</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Ref |
|-----|-----------|--------|--------------------|-----|-------------|----------------------|----|------------------------|----------------|------------------|-----|
| 78  | 1078.5947 | [M+H]<sup>+</sup> | 10.66 | 0.5 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>5</sub>C<sub>l</sub> or C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>5</sub>C<sub>l</sub> | NF | 4 | n.a. | | | |
| 79  | 1022.6746 | [M+H]<sup>+</sup> | 10.76 | -0.7 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> | 469.3280, 451.3169, 441.2711, 423.3229, 395.2647, 356.2435, 342.2023, 338.2322, 328.1869, 310.2381, 296.1968, 285.1455, 283.2013, 269.1865, 255.1701, 245.1868, 234.1360, 229.1189, 227.1762, 215.1383, 209.1903, 201.1242, 199.1811, 185.1656, 183.1134, 154.1593, 86.0974 | 3 | n-C<sub>15</sub>-[Leu<sup>7</sup>]-surfactin | Cyclic lipopeptide | Bacillus pumilus | [24] |
| 80  | 1064.5792 | [M+H]<sup>+</sup> | 10.78 | 0.7 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>5</sub>C<sub>l</sub> or C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>5</sub>C<sub>l</sub> | NF | 4 | n.a. | | | | |
| 81  | 1008.6598 | [M+H]<sup>+</sup> | 10.8 | 0.1 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> | 469.3280, 451.3174, 441.2707, 427.3165, 395.2650, 356.2438, 342.2028, 338.2325, 328.1869, 310.2381, 296.1968, 285.1455, 283.2013, 269.1865, 255.1698, 253.2272, 243.1342, 231.1708, 229.1192, 227.1756, 213.1611, 201.1238, 199.1807, 185.1652, 86.0971 | 3 | n-C<sub>15</sub>-[Leu<sup>7</sup>]-surfactin | Cyclic lipopeptide | Bacillus pumilus | [24] |
| 82  | 1036.692 | [M+H]<sup>+</sup> | 10.95 | 1 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> | 483.3431, 465.3328, 455.3480, 441.2714, 437.3377, 395.2664, 370.2592, 352.2489, 342.2029, 328.1875, 324.2541, 311.1967, 296.1978, 285.1458, 283.2004, 269.1868, 267.2441, 255.1722, 253.2282, 245.1872, 240.2331, 229.1195, 227.1764, 215.1037, 213.1607, 210.1243, 199.1815, 185.1657, 183.1137, 170.1186, 154.1597, 86.0977 | 3 | Anteiso-C<sub>14</sub>-[Leu<sup>7</sup>]-surfactin | Cyclic lipopeptide | Bacillus pumilus | [24] |
| 83  | 1092.6073 | [M+H]<sup>+</sup> | 10.97 | 0.1 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>5</sub>C<sub>l</sub> or C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>5</sub>C<sub>l</sub> | NF | 4 | n.a. | | | | |
| 84  | 1022.6751 | [M+H]<sup>+</sup> | 11.16 | -0.2 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> | 483.3442, 465.3320, 441.2701, 395.2653, 370.2591, 356.2491, 342.2023, 328.1870, 324.2528, 296.1963, 285.1446, 283.2008, 269.1873, 255.1707, 240.2331, 231.1708, 229.1192, 227.1765, 215.1028, 213.1597, 210.1245, 199.1814, 185.1651, 183.1138, 154.1593, 86.0979 | 3 | Anteiso-C<sub>15</sub>-[Val<sup>7</sup>]-surfactin | Cyclic lipopeptide | Bacillus pumilus | [24] |
| 85  | 1036.6903 | [M+H]<sup>+</sup> | 11.18 | -1.2 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> | 483.3438, 465.3333, 455.3474, 441.2715, 437.3364, 395.2658, 370.2595, 352.2492, 342.2029, 328.1875, 324.2541, 311.1971, 296.1976, 285.1454, 283.2013, 269.1869, 267.2441, 255.1713, 245.1871, 240.2327, 229.1191, 227.1764, 223.2063, 215.1031, 213.1602, 201.1242, 199.1816, 185.1657, 183.1132, 170.1179, 154.1593, 86.0977 | 3 | n-C<sub>15</sub>-[Leu<sup>7</sup>]-surfactin | Cyclic lipopeptide | Bacillus pumilus | [24] |
| 86  | 1036.687 | [M+H]<sup>+</sup> | 11.48 | -3.8 | C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> | 497.3574, 483.3420, 479.3447, 465.3322, 455.3483, 441.2713, 395.2702, 384.2736, 370.2983, 366.2633, 356.2750, 352.2485, 342.2026, 338.2686, 326.2470, 324.2563, 311.1976, 296.1982, 293.1538, 285.1451, 283.2004, 269.1870, 255.1698, 253.2272, 243.1342, 231.1708, 229.1192, 227.1762, 215.1383, 209.1903, 201.1242, 199.1811, 185.1656, 183.1134, 154.1593, 86.0974 | 3 | Anteiso-C<sub>14</sub>-[Ile<sup>7</sup>]-surfactin | Cyclic lipopeptide | Bacillus pumilus | [24] |
| No. | m/z value | Adduct | R_t (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Ref |
|-----|-----------|---------|-----------|-----|-------------|----------------------|----|-------------------------|----------------|------------------|-----|
| 87  | 1064.7209 | [M+H]^+ | 11.65     | -1.3| CaH_9O_7N_3 | 511.3743, 493.3648, 483.3786, 441.2816, 398.2912, 395.2643, 380.2790, 352.2855, 342.2029, 328.1868, 296.1967, 285.1422, 283.2024, 268.2642, 255.1717, 245.1867, 233.2294, 229.1197, 227.1754, 215.1038, 201.1240, 199.1813, 185.1668, 183.1134, 154.1599, 86.0986 | 3   | KMM 1364E | Cyclic lipopeptide | Bacillus pumilus | [26] |
Table S8. Putatively identified compounds produced by *Trichoderma* sp. extracts CHG34-CAG and CHG34-PDA. Putative annotations were based on the accurate mass, the predicted putative molecular formulae (MF), the retention time (Rt), the fragmentation pattern and the biological origin.  

- Different isomers with same m/z value and molecular formula, which cannot be differentiated based on MS/MS data;  
- Parent mass out of detection limit (>1200 Da) and therefore, the ppm error and fragmentation pattern were not determined;  
- *MF with best ppm error displayed; IC: Identification confidence level [3]; Nf: No fragmentation detected or below noise threshold (5e-1); Ref = reference(s).

| No. | m/z value | Adduct | Rt (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|----------|------|-------------|-----------------------|----|------------------------|----------------|------------------|--------|-----|
| 88  | 237.132   | [M+H]^+ | 4.51     | 2.1  | C_{13}H_{16}O_{4} | 195.9131, 167.4925, 165.0561, 141.9551, 139.0753, 125.0237, 123.0437, 113.0982 | 3  | Trichosorbidin E | Sorbicillinoid | * | CAG, PDA | [27] |
| 89  | 410.218   | [M+H]^+ | 5.22     | 0.2  | C_{21}H_{31}O_{7} | 242.0663, 224.0546, 124.0363 | 4  | n.a. | CAG | |
| 90  | 562.3585  | [M+Na]^+ | 5.23     | 0.7  | C_{27}H_{49}N_{5}O_{6} | 320.1957 | 4 | n.a. | CAG | |
| 91  | 473.1602  | [M+H]^+ | 5.42     | 0.4  | C_{25}H_{38}O_{7} | 455.1462, 445.1667, 399.1955, 371.1277, 367.1292, 353.1223, 343.1312, 325.1264, 321.1159, 315.1418, 301.1224, 293.1167, 279.0644, 277.1200, 275.0994, 269.0819, 265.1256, 253.0858, 247.1097 | 4  | n.a. | CAG | |
| 92  | 451.2694  | [M+H]^+ | 5.52     | -0.4 | C_{28}H_{24}O_{7} | 289.2172, 271.2065, 217.1958, 215.1443, 205.1220, 197.1335, 187.1477, 185.1332, 182.1101, 171.1170, 169.1024, 159.1187, 157.1004, 155.0854, 151.1133, 147.1177, 145.1024, 137.0966, 133.1015, 131.0863, 127.0398, 119.0860, 105.0706, 99.0446 | 4  | n.a. | PDA | |
| 93  | 473.1603  | [M+H]^+ | 5.69     | 0.6  | C_{25}H_{38}O_{7} | 455.1467, 445.1640, 427.1577, 399.1955, 381.1467, 371.1253, 353.1160, 343.1339, 325.1219, 321.1107, 303.1307, 293.1172, 279.0655, 275.1062, 269.0769, 265.1217, 253.0830, 247.1122, 243.0975, 241.0873, 231.1372, 224.0547, 195.9114, 143.0857, 129.0681 | 4  | n.a. | CAG | |
| 94  | 391.2457  | [M+Na]^+ | 5.96     | -0.8 | C_{16}H_{20}O_{4} | 359.219 | 4 | n.a. | CAG | |
| 95  | 259.1335  | [M-H2O]^+ | 6.36     | 0.4  | C_{16}H_{20}O_{4} | 241.1224, 223.1130, 213.1285, 197.1323, 195.1142, 185.1317, 180.0920, 171.1167, 169.1014, 167.0865, 165.0684, 157.1010, 155.0842, 145.1008, 143.0855, 141.0714, 129.0699, 105.0713 | 4  | n.a. | CAG | |
| 96  | 277.144   | [M+H]^+ | 6.6      | 0    | C_{16}H_{20}O_{4} | 231.1372, 201.0457, 195.9114, 143.0857, 129.0681 | 4  | n.a. | CAG |
| No. | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|-------------------|-----|-------------|-----------------------|----|------------------------|----------------|-------------------|--------|-----|
| 97  | 331.1521  | [M+H]<sup>+</sup> | 6.76 | 0.6 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>3</sub> | 299.1237, 211.1088, 189.1274, 133.0657 | 4 | n.a. |  | CAG |  |
| 98  | 588.39    | [M+H]<sup>+</sup> | 6.86 | 0 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 423.2950, 253.1597, 251.1447, 235.1489, 225.1640, 223.1465, 148.0973, 130.0874, 102.0919 | 4 | n.a. |  | CAG, PDA |  |
| 99  | 189.1278  | [M+H]<sup>+</sup> | 6.87 | 0.5 | C<sub>6</sub>H<sub>10</sub>O | 171.1169, 147.1166, 145.1010, 133.0649, 105.0698 | 4 | n.a. |  | CAG |  |
| 100 | 439.3324  | [M+H]<sup>+</sup> | 7.11 | -0.2 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub> | 279.2345, 209.1549, 173.1328, 161.1080, 149.1325, 137.1328, 109.1021, 95.0867, 81.0709 | 4 | n.a. |  | CAG, PDA |  |
| 101 | 344.3164  | [M+H]<sup>+</sup> | 7.4  | -0.3 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 344.3129, 300.2899, 282.2793, 270.2758, 264.2762, 252.2674, 88.0771 | 4 | n.a. |  | CAG, PDA |  |
| 102 | 345.1677  | [M+Na]<sup>+</sup> | 7.76 | -0.3 | C<sub>6</sub>H<sub>10</sub>O<sub>*</sub> | Nf | 4 | n.a. |  | CAG |  |
| 103 | 770.5386  | [M+H]<sup>+</sup> | 7.79 | -0.8 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 453.3084, 354.2396, 326.2451, 300.2278, 241.1562, 184.1345, 143.1185, 86.0972 | 4 | n.a. |  | CAG, PDA |  |
| 104 | 1197.756  | [M+Na]<sup>+</sup> | 7.93 | -2.3 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>3</sub> | 983.5846, 955.5931, 897.5527, 870.5408, 843.5667, 757.4554, 730.4795, 645.4308, 547.3153, 489.2869, 462.2697, 403.2706 | 3 | Trichoderminde C Peptaibol | Trichoderma viride | CAG, PDA | [28] |
| 105 | 754.5424  | [M+H]<sup>+</sup> | 8.12 | -2.4 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 453.2956, 354.2416, 326.2400, 241.1605, 184.1328, 86.0979 | 3 | n.a. |  | CAG, PDA |  |
| 106 | 498.379   | [M+H]<sup>+</sup> | 8.29 | -1 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 480.3684, 236.1504 | 4 | n.a. |  | CAG, PDA |  |
| 107 | 751.9497  | [M+2Na]<sup>+</sup> | 8.29 | -0.7 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>3</sub> | n.a.<sup>*</sup> | 3 | Tv29-145-Vc Peptaibol | Trichoderma viridus | CAG, PDA | [29] |
| 108 | 836.4872  | [M+H]<sup>+</sup> | 8.29 | 0.5 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>3</sub> | 369.2141, 256.1304 | 4 | n.a. |  | CAG, PDA |  |
| 109 | 623.4496  | [M+H]<sup>+</sup> | 8.29 | 0 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 324.2295, 215.1763, 211.1452, 183.1501 | 4 | n.a. |  | CAG, PDA |  |
| 110 | 1197.7583 | [M+Na]<sup>+</sup> | 8.39 | -0.3 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>3</sub> | 1179.7465, 955.5943, 897.5522, 870.5408, 757.4554, 645.4308, 547.3153, 489.2869, 462.2697, 403.2706 | 3 | Trichorizin-II Peptaibol | Trichoderma harzianum | CAG, PDA | [30] |
| 111 | 553.3351  | [M+H]<sup>+</sup> | 8.41 | 0.2 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 355.1985, 256.1306, 228.1352, 128.0710, 102.0919 | 4 | n.a. |  | PDA |  |
| 112 | 623.4495  | [M+H]<sup>+</sup> | 8.41 | -0.2 | C<sub>6</sub>H<sub>10</sub>N<sub>4</sub>O<sub>*</sub> | 324.2296, 215.1762, 211.1454, 183.1503 | 4 | n.a. |  | CAG, PDA |  |
| No. | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|-------------------|-----|------------|----------------------|----|-------------------------|----------------|-------------------|--------|----|
| 113 | 961.6072  | [M+H]<sup>+</sup> | 8.41              | -0.1| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> or C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 355.1985, 256.1304 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 114 | 345.168   | [M+Na]<sup>+</sup> | 8.45              | 0.6 | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> | n.a. | 4  | n.a.                   |                |                  | CAG    |    |
| 115 | 623.4493  | [M+H]<sup>+</sup> | 8.45              | -0.5| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 324.2290, 215.1765, 211.1449, 183.1499 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 116 | 553.335   | [M+H]<sup>+</sup> | 8.45              | 0   | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 355.1923, 256.1304, 228.1354, 128.0707, 101.0713 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 117 | 837.4725  | [M+H]<sup>+</sup> | 8.45              | 0.4 | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> or C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 370.1981, 257.1146, 128.0712 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 118 | 623.4493  | [M+H]<sup>+</sup> | 8.52              | -0.5| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 324.2288, 215.1760, 211.1449, 183.1497 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 119 | 758.9578  | [M+2Na]<sup>+</sup> | 8.52             | -0.4| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> | n.a. | 3  | Tv29-145-VI Peptaibol  | Trichoderma virens | CAG, PDA |    |
| 120 | 850.5023  | [M+H]<sup>+</sup> | 8.52              | -0.2| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> or C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 383.2293, 270.1457, 142.0862 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 121 | 874.5392  | [M+2H]<sup>+</sup> | 8.59              | 1.7 | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> | n.a. | 3  | Trichorzin MA-2 Peptaibol | Trichoderma harzianum | CAG, PDA | [31]|
| 122 | 1136.6675 | [M+H]<sup>+</sup> | 8.59              | -0.4| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> or C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 397.1981, 257.1146, 128.0712 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 123 | 623.4504  | [M+H]<sup>+</sup> | 8.67              | -0.8| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 324.2294, 215.1759, 211.1451, 183.1497 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 124 | 975.6241  | [M+H]<sup>+</sup> | 8.67              | -0.2| C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> or C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 369.2148, 270.1460 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 125 | 874.5398  | [M+2H]<sup>+</sup> | 8.78              | 1.7 | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> | n.a. | 3  | Trichokindin Ia Peptaibol | Trichoderma harzianum | CAG, PDA | [32]|
| 126 | 1136.6686 | [M+H]<sup>+</sup> | 8.78              | 0.6 | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> or C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 697.3896, 484.2784, 399.2252, 286.1411, 268.1303 197.0926 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 127 | 623.4493  | [M+H]<sup>+</sup> | 8.85              | -1  | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 324.2296, 215.1763, 211.1452, 183.1502 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| 128 | 975.6257  | [M+H]<sup>+</sup> | 8.85              | 0.1 | C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub> or C<sub>9</sub>H<sub>12</sub>N<sub>3</sub>O<sub>6</sub>* | 369.2148, 256.1304 | 4  | n.a.                   |                |                  | CAG, PDA |    |
| No. | m/z value | Adduct       | R<sub>t</sub> (min) | ppm   | Putative MF                                                                 | Fragmentation pattern                                           | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------------|---------------------|-------|----------------------------------------------------------------------------|-----------------------------------------------------------------|----|------------------------|-----------------|-------------------|--------|-----|
| 129 | 976.6094  | [M+H]<sup>+</sup> | 8.96               | -0.2  | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | 370.1984, 342.2027, 257.1147                                   | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 130 | 623.4506  | [M+H]<sup>+</sup> | 8.98               | -0.5  | C₃₀H₅₄N₁₀O₂<sup>*</sup>                                                   | 324.2290, 296.1980, 215.1765, 211.1454, 183.1500                | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 131 | 867.5361  | [M+2H]<sup>+</sup> | 8.98               | n.a.<sup>+</sup> | n.a.<sup>+</sup> | n.a.<sup>+</sup> | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 132 | 892.5373  | [M+H+Na]<sup>+</sup> | 8.98               | n.a.<sup>+</sup> | n.a.<sup>+</sup> | n.a.<sup>+</sup> | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 133 | 892.5372  | [M+H+Na]<sup>+</sup> | 9.04               | n.a.<sup>+</sup> | n.a.<sup>+</sup> | n.a.<sup>+</sup> | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 134 | 909.527   | [M+2H]<sup>+</sup> | 9.04               | -0.9  | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | n.a.<sup>+</sup>                                                | 3  | Trichobrachin B-I     | Peptaibol       | Trichoderma longibrachiatum | CAG,   |
| 135 | 989.6424  | [M+H]<sup>+</sup> | 9.04               | 1.1   | C₈₀H₇₇N₁₃O₈ or C₈₀H₇₇N₁₃O₈<sup>*</sup>                                   | 383.2299, 270.1472                                            | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 136 | 623.4505  | [M+H]<sup>+</sup> | 9.04               | -0.6  | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | 324.2296, 211.1455, 183.1503                                   | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 137 | 623.4506  | [M+H]<sup>+</sup> | 9.08               | -0.3  | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | 324.2294, 211.1452, 183.1503                                   | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 138 | 892.5372  | [M+H+Na]<sup>+</sup> | 9.08               | n.a.<sup>+</sup> | n.a.<sup>+</sup> | n.a.<sup>+</sup> | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 139 | 989.6392  | [M+H]<sup>+</sup> | 9.08               | 0.6   | C₈₀H₇₇N₁₃O₈ or C₈₀H₇₇N₁₃O₈<sup>*</sup>                                   | 383.2303, 270.1464                                            | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 140 | 892.5383  | [M+H+Na]<sup>+</sup> | 9.15               | n.a.<sup>+</sup> | n.a.<sup>+</sup> | n.a.<sup>+</sup> | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 141 | 623.4499  | [M+H]<sup>+</sup> | 9.21               | 0.5   | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | 324.2297, 215.1770, 211.1457, 183.1502                         | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 142 | 990.6248  | [M+H]<sup>+</sup> | 9.21               | 0.9   | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | 384.2148, 356.2190, 271.1308, 142.0871                         | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| 143 | 874.5402  | [M+2H]<sup>+</sup> | 9.25               | 1.7   | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | n.a.<sup>+</sup>                                                | 3  | Trichokindin Ib       | Peptaibol       | Trichoderma harzianum   | CAG,   |
| 144 | 874.5392  | [M+2H]<sup>+</sup> | 9.38               | 1.7   | C₈₀H₇₇N₁₃O₈<sup>*</sup>                                                   | n.a.<sup>+</sup>                                                | 3  | Trichokindin Ia       | Peptaibol       | Trichoderma harzianum   | CAG,   |
| 145 | 1136.6674 | [M+H]<sup>+</sup> | 9.38               | -0.4  | C₈₀H₇₇N₁₃O₈ or C₈₀H₇₇N₁₃O₈<sup>*</sup>                                   | 697.3872, 484.2768, 399.2243, 286.1408, 268.1303, 197.0931 | 4  | n.a.                   |                 |                  | CAG,   | PDA |
| No. | m/z value | Adduct          | R<sub>t</sub> (min) | ppm  | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref  |
|-----|-----------|-----------------|---------------------|------|-------------|-----------------------|----|------------------------|----------------|------------------|--------|------|
| 146 | 1164.6991 | [M+H]<sup>+</sup> | 9.41                | -0.1 | C<sub>28</sub>H<sub>42</sub>O<sub>5</sub> or C<sub>26</sub>H<sub>36</sub>N<sub>2</sub>O<sub>3</sub> | 498.2934, 399.2248, 286.1414, 268.1305, 197.0930 | 4  | n.a.                  | Peptaibol       | Trichoderma harzianum | CAG, PDA |      |
| 147 | 881.5459  | [M+2H]<sup>+</sup> | 9.5                 | 0.4  | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Trichokindin IIb       | Peptaibol       | Trichoderma harzianum | CAG, PDA | [32] |
| 148 | 844.5923  | [M+2H]<sup>+</sup> | 9.57                | n.a.<sup>a</sup> | n.a.<sup>a</sup> | n.a.<sup>a</sup> | 4  | n.a.                  | Peptaibol       | Trichoderma harzianum | CAG, PDA |      |
| 149 | 873.55    | [M+2H]<sup>+</sup> | 9.57                | 2.2  | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Neoatroviridin B       | Peptaibol       | Trichoderma atroviride | CAG, PDA | [34] |
| 150 | 881.5432  | [M+2H]<sup>+</sup> | 9.57                | 0.4  | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Trichokindin IIIa/b   | Peptaibol       | Trichoderma harzianum | CAG, PDA | [32] |
| 151 | 881.547   | [M+2H]<sup>+</sup> | 9.61                | 0.4  | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Trichokindin IV       | Peptaibol       | Trichoderma harzianum | CAG, PDA | [32] |
| 152 | 902.5486  | [M+2H]<sup>+</sup> | 9.61                | n.a.<sup>a</sup> | n.a.<sup>a</sup> | n.a.<sup>a</sup> | 4  | n.a.                  | Peptaibol       | Trichoderma harzianum | CAG, PDA |      |
| 153 | 913.543   | [M+2Na]<sup>2+</sup> | 9.61              | n.a.<sup>a</sup> | n.a.<sup>a</sup> | n.a.<sup>a</sup> | 4  | n.a.                  | Peptaibol       | Trichoderma harzianum | CAG, PDA |      |
| 154 | 881.5477  | [M+2H]<sup>+</sup> | 9.74                | 0.4  | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Trichokindin Va/b     | Peptaibol       | Trichoderma harzianum | CAG, PDA | [32] |
| 155 | 888.5443  | [M+2H]<sup>+</sup> | 9.99                | -0.8 | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Trichokindin VI       | Peptaibol       | Trichoderma harzianum | CAG, PDA | [32] |
| 156 | 891.5471  | [M+H+Na]<sup>2+</sup> | 9.99              | n.a.<sup>a</sup> | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Neoatroviridin D      | Peptaibol       | Trichoderma atroviride | CAG, PDA | [34] |
| 157 | 888.555   | [M+2H]<sup>+</sup> | 10.14              | -0.8 | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Trichokindin VII      | Peptaibol       | Trichoderma harzianum | CAG, PDA | [32] |
| 158 | 916.5155  | [M+2H]<sup>+</sup> | 10.14              | n.a.<sup>a</sup> | n.a.<sup>a</sup> | n.a.<sup>a</sup> | 4  | n.a.                  | Peptaibol       | Trichoderma harzianum | CAG, PDA |      |
| 159 | 481.2935  | [M+Na]<sup>+</sup> | 10.33, 10.39       | 1    | C<sub>14</sub>H<sub>12</sub>O<sub>5</sub> | 423.2865, 355.2252 | 3  | Ergokonin B           | Ergosterol      | Trichoderma koningii | CAG, PDA | [35] |
| 160 | 873.5497  | [M+2H]<sup>+</sup> | 10.33              | 2.2  | C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub> | n.a.<sup>a</sup> | 3  | Neoatroviridin C      | Peptaibol       | Trichoderma atroviride | CAG, PDA | [34] |
| 161 | 895.5413  | [M+2H]<sup>+</sup> | 10.39              | n.a.<sup>a</sup> | n.a.<sup>a</sup> | n.a.<sup>a</sup> | 4  | n.a.                  | Peptaibol       | Trichoderma atroviride | CAG, PDA |      |
Table S9. Putatively identified compounds produced by *Fusarium* sp. extracts CHG38-CAG and CHG38-PDA. Putative annotations were based on the accurate mass, predicted putative molecular formulae (MF), the retention time (R_t), the fragmentation pattern and the biological origin. *MF with best ppm error; IC: Identification confidence level [3]; Nf: No fragmentation detected or below noise threshold (5e); Ref = reference(s). 

| No. | m/z value | Adduct | R_t (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|-----------|-----|-------------|----------------------|----|------------------------|----------------|-----------------|--------|-----|
| 162 | 235.0614  | [M+H]^+| 2.97      | 3.4 | C5H7O3N  | 217.0504, 193.0493, 189.0548, 175.0385, 161.0598, 151.0394, 149.0594, 125.0603, 111.0084 | 3  | Diploquinone A         | Naphthoquinone | *Diploodia mutila* | PDA    | [36]|
| 163 | 277.0715  | [M+H]^+| 3.09      | 1.1 | C5H7O3N  | 259.0608, 235.0603, 231.0657, 217.0498, 193.0496, 191.0697, 123.0438 | 3  | Norjavanicin           | Naphthoquinone | *Fusarium sp.* | PDA    | [37]|
| 164 | 235.0977  | [M+H]^+| 3.52      | 3   | C5H7O3N  | 217.0866, 191.0711, 176.0474, 163.0749, 151.0393, 135.0808 | 2  | Aloesol                | Chromone      | *Fusarium sp.* | PDA    | [38]|
| 165 | 233.0820  | [M+H]^+| 3.63      | 2.6 | C5H7O3N  | 217.0872, 191.0711, 151.0393 | 2  | Macrocarpone C        | Chromone      | *Fusarium tricinctum* | PDA    | [39]|
| 166 | 279.0881  | [M+H]^+| 3.7       | 4.3 | C5H7O3N  | 261.0784, 243.0665, 219.0644, 201.0530, 191.0708, 177.0186, 173.0605, 163.0770 | 3  | (-)-Citreoisocoumarin | Isocoumarin   | *Fusarium tricinctum* | PDA    | [39]|
| 167 | 191.0710  | [M+H]^+| 3.97      | 1   | C5H7O3N  | 176.0488, 151.0390, 149.9310, 135.0444, 110.0086 | 4  | n.a.                  |              |                | PDA    |     |
| 168 | 359.1109  | [M+Na]^+| 4.37      | 0.6 | C5H7O3N  | 324.5316, 322.0607, 291.0259, 271.0585, 253.8915, 252.3335 | 3  | 3-O-Ethylidihydrofusarubin A or B | Naphthoquinone | *Fusarium solani* | PDA    | [40]|
| 169 | 339.1803  | [M+H]^+| 4.58      | -1.5| C5H7O3N  | 303.1549, 285.1486, 267.1371, 259.1721, 257.1524, 229.0869, 217.0846, 215.0682, 189.0564, 177.0592, 175.0392, 167.0347, 161.0622, 149.0613, 135.1176 | 2  | 2'-hydroxyzearalanol  | Zearalenone (Macrolide) | *Penicillium sp.* | CAG    | [41]|
| 170 | 249.0768  | [M+H]^+| 5.46      | 2   | C5H7O3N  | 217.0504, 192.0427, 153.0183 | 4  | n.a.                  |              |                | PDA    |     |
| 171 | 259.0615  | [M+H]^+| 5.66      | 3.5 | C5H7O3N  | 244.0369, 231.0674, 213.0604, 191.0726 | 3  | Huperxanthone B       | Xanthone      | *Aspergillus versicolor* | PDA    | [42]|
| 172 | 384.3954  | [M+H]^+| 5.96      | 0   | C5H7O3N  | 367.3683, 296.2959 | 4  | n.a.                  |              |                | PDA    |     |
| 173 | 629.3642  | [M+Na]^+| 6.23      | 0.6 | C5H7O3N  | 557.3420, 387.2336 | 4  | n.a.                  |              |                | CAG, PDA |     |
| 174 | 690.2125  | [M+H]^+| 6.56      | 1.6 | C5H7O3N  | 373.0741, 355.0630 | 4  | n.a.                  |              |                | CAG    |     |
| 175 | 412.4270  | [M+H]^+| 6.59      | 0.7 | C5H7O3N  | 324.3275 | 4  | n.a.                  |              |                | PDA    |     |
| 176 | 319.1553  | [M+H]^+| 6.63      | 2.5 | C5H7O3N  | 301.1441, 283.1342, 265.1237, 255.1386, 241.0873, 231.0662, 229.0860, 227.0712, 217.0859, 215.0706, 213.0561, 205.0868 | 2  | Zearalenone            | Zearalenone (Macrolide) | *Fusarium graminearum* | CAG    | [43]|

**Medium**: PDA, CAG; **Ref**: reference(s).
| No.  | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|------|-----------|--------|-------------------|-----|------------|-----------------------|----|-------------------------|----------------|-------------------|--------|-----|
| 177  | 575.1199  | [M+H]<sup>+</sup> | 7.32              | 1.6 | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub> | 287.0563, 274.0464, 259.0613 | 4  | n.a.                    | Zearalanone (Macrolide) | Fusarium spp. | CAG, PDA | |
| 178  | 273.0771  | [M+H]<sup>+</sup> | 7.43              | 2.9 | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub> | 258.0524, 255.0665, 230.0581, 227.0702 | 3  | n.a.                    | Fusarium equiseti | PDA [44]   | |
| 179  | 303.1605  | [M-H<sub>2</sub>O]<sup>+</sup> | 7.47             | 3   | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub> | 285.1493, 229.0855, 215.0695, 205.0511, 191.0348, 163.0399 | 2  | n.a.                    | Zearalanone | Fusarium equiseti | PDA [45] | |
| 180  | 289.1786  | [M+Na]<sup>+</sup> | 7.91              | 2.1 | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub> | Nf | 4  | n.a.                    | | | PDA | |
| 181  | 691.4647  | [M+H]<sup>+</sup> | 8.95              | 0.1 | C<sub>19</sub>H<sub>12</sub>O<sub>4</sub>* | 659.4388, 482.3079, 377.3063, 359.2942, 331.2989, 313.2980, 303.2622, 263.2337, 235.2063, 232.1362, 220.1098, 181.0634, 172.1087, 164.0696, 155.0792, 147.0751, 130.0498, 121.1051 | 4  | n.a.                    | | | CAG | |
| 182  | 659.4385  | [M+H]<sup>+</sup> | 9.07              | 0.2 | C<sub>19</sub>H<sub>12</sub>O<sub>4</sub>* | 428.3166, 377.3065, 359.2950, 331.2991, 303.2691, 263.2368, 232.1301, 215.1033, 185.0930, 172.1086, 164.0710, 155.0815, 147.0771, 130.0506 | 3  | n.a.                    | Fusaristatin A | Fusarium sp. | CAG, PDA | [46] |
| 183  | 695.3956  | [M+H]<sup>+</sup> | 9.52              | 1.2 | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub> | 379.3360, 309.2571, 295.2407, 253.1958, 239.1786, 213.1648, 201.1647, 199.1482, 187.1492, 185.1322, 173.1342, 171.1174, 161.1311, 159.1167, 157.1026, 149.1328, 147.1171, 145.1016, 143.0850, 133.1014, 131.0849 | 4  | n.a.                    | | | PDA | |
| 184  | 437.3425  | [M+H]<sup>+</sup> | 10.67             | 1.1 | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub> | 401.3213, 381.2794, 367.2639, 353.2500, 341.2487, 339.2319, 327.2321, 315.2170, 307.2427, 267.2122, 225.1645, 211.1495, 197.1337, 183.1170, 169.1021, 157.1024 | 4  | n.a.                    | | | CAG, PDA | |
| 185  | 737.4779  | [M-H<sub>2</sub>O]<sup>+</sup> | 10.82            | -0.3 | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub>* | 701.4548, 593.3277, 575.3162, 567.3481, 441.2057, 381.2049, 263.1950, 215.1449, 295.1334, 293.1901, 275.1901, 267.1755, 249.1637, 225.1637, 209.1335, 201.0553, 199.0755, 195.1171, 183.1152 | 4  | n.a.                    | | | CAG | |
| 186  | 468.3607  | [M+H]<sup>+</sup> | 11.44             | 0.8 | C<sub>9</sub>H<sub>6</sub>O<sub>4</sub> | 437.3426, 393.2792, 365.2496, 352.2406, 339.2327, 337.2165, 319.2072, 307.2425, 293.2269, 265.1950, 251.1812, 249.1646, 237.1648, 235.1481, 223.1490, 211.1495 | 4  | n.a.                    | | | CAG | |
| No. | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|---------------------|-----|------------|-----------------------|----|------------------------|----------------|------------------|--------|-----|
| 187 | 793.5020  | [M+H]<sup>+</sup> | 11.54 | 0.5 | C<sub>47</sub>H<sub>64</sub>N<sub>6</sub>O<sub>5</sub> | 761.4775, 743.4667, 651.4027 | 4 | n.a. | CAG |  |
| 188 | 755.4899  | [M+H]<sup>+</sup> | 11.54 | 1.6 | C<sub>48</sub>H<sub>66</sub>O<sub>7</sub> | n.a. | 4 | n.a. | CAG |  |
| 189 | 437.3420  | [M+H]<sup>+</sup> | 11.59 | 0 | C<sub>48</sub>H<sub>66</sub>O<sub>7</sub> | 419.3311, 401.3185, 381.2783, 357.1451, 335.2753, 313.2141, 299.2004, 275.1782, 259.1690, 223.1484, 211.1479, 195.1165, 183.1165, 169.1019, 159.1168, 145.0999 | 4 | n.a. | PDA |  |
| 190 | 436.3340  | [M+H]<sup>+</sup> | 11.68 | -0.2 | C<sub>48</sub>H<sub>66</sub>O<sub>7</sub> | 421.3112, 385.2896, 365.2484, 337.2177, 323.2018, 317.2274, 311.2021, 301.1965, 297.1866, 261.1650, 235.1489, 209.1336, 195.1180 | 4 | n.a. | CAG, PDA |  |
| 191 | 437.3424  | [M+H]<sup>+</sup> | 11.69 | 0.9 | C<sub>48</sub>H<sub>66</sub>O<sub>7</sub> | 421.3102, 419.3308, 401.3206, 385.2891, 337.2167, 323.2014, 317.2267, 313.2159, 311.2007, 301.1959, 297.1853, 275.1794, 263.1789, 261.1641, 259.1678, 253.1947, 249.1632, 235.1488, 223.1482, 221.1327, 211.1463, 209.1327, 197.1323, 195.1172, 183.1167, 169.1006 | 4 | n.a. | PDA |  |
| 192 | 753.4741  | [M+H]<sup>+</sup> | 11.82 | -0.4 | C<sub>49</sub>H<sub>60</sub>N<sub>4</sub>O<sub>3</sub> | 735.4622, 656.3732, 638.3626, 623.3362, 605.3292, 587.3196, 565.3297, 523.2813, 521.2742, 509.2715, 497.2628, 495.2540, 481.2378, 477.2425, 469.2356, 467.2224, 463.2249, 459.2343, 455.2342, 421.1327, 201.0557, 199.0752, 195.1175 | 4 | n.a. | CAG |  |
| 193 | 436.3335  | [M+H]<sup>+</sup> | 11.93 | -1.3 | C<sub>48</sub>H<sub>66</sub>O<sub>7</sub> | 421.3098, 403.2995, 393.2770, 385.2880, 340.2391, 325.2155, 323.2359, 321.2568, 319.2407, 307.2062, 293.2261, 279.2098, 265.1939, 251.1783, 249.1631, 237.1637, 235.1479, 225.1630, 223.1380, 211.1479, 208.1323, 197.1318, 195.1164, 184.1246, 169.1005, 155.0851 | 4 | n.a. | CAG, PDA |  |
Table S10. Putatively identified compounds produced by *Penicillium* sp. extracts CKG23-CAG and CKG23-PDA. Putative annotations were based on the accurate mass, the predicted putative molecular formulae (MF), the retention time (Rt), the fragmentation pattern and the biological origin. *Different isomers with same m/z value and molecular formula, which cannot be differentiated based on MS/MS data; *MF with best ppm error displayed; IC: Identification confidence level [3]; Nf: No fragmentation detected or below noise threshold (5e-4); Ref = reference(s).

| No. | m/z value | Adduct | Rt (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|----------|-----|-------------|-----------------------|----|------------------------|----------------|------------------|--------|----|
| 194 | 245.082   | [M+H]+  | 1.24     | 2.4 | C₈H₁₀O₅    | 227.071, 217.0888, 209.0590, 199.0762, 189.0916, 185.0596, 181.0651, 175.0771, 173.0607, 171.0809, 161.0699, 157.0655, 153.0705, 151.0388, 147.0443, 143.0853, 135.0447, 123.0446, 107.0495 | 3  | 3-methylbisnoryangonin | Styrylpyrone | Penicillium glabrum | CAG, PDA | [47] |
| 195 | 157.0059  | [M+H]+  | 2.14     | 1.9 | C₈H₅O₆Cl   | 129.0107, 121.0266, 101.0160, 94.0412 | 4  | n.a.                  |                |                 |        | CAG |
| 196 | 233.082   | [M+H]+  | 2.84     | 2.6 | C₈H₁₀O₅    | 194.9339, 191.0710, 187.0742, 173.0589, 149.0604, 147.0451, 123.0438, 121.0669, 183.0296, 165.0552 | 4  | n.a.                  |                |                 |        | PDA |
| 197 | 325.1292  | [M+H]+  | 3.46     | 1.5 | C₈H₁₀O₅    | 289.1072, 247.0972, 233.0819, 231.0644, 227.1076, 213.0559, 191.0341, 189.0549, 183.0296, 165.0552 | 3  | 11,12-Dihydroxycurvularin | Zearalenone (Macrolide) | Penicillium citreus-viride | PDA | [48] |
| 198 | 327.1235  | [M+H]+  | 3.9      | 0.9 | C₈H₁₀O₅    | 309.1131, 294.0894, 285.0765 | 3  | 1,7-Dihydroxy-2-methoxy-3-prenylxanthone | Xanthone | Phomopsis sp. | CAG | [49] |
| 199 | 309.1345  | [M+H]+  | 4        | 2.3 | C₈H₁₀O₅    | 273.1129, 255.1038, 231.1031, 229.1228, 215.0716, 213.0914, 201.0553, 189.0924, 187.0768, 177.0551, 173.0400, 173.0602, 161.0605, 149.0605 | 3  | (3S,7S)-7-hydroxyresorcylic acid | Zearalenone (Macrolide) | Penicillium sp. | PDA | [50] |
| 200 | 273.0409  | [M+H]+  | 4.12     | 3.7 | C₈H₁₀O₅    | 245.0457, 227.0340, 217.0508, 199.0397 | 3  | 2,8-dihydroxy-9-oxo-9H-xanthene-6-carboxylic acid | Xanthone | Arthrinium arundinis | PDA | [51] |
| 201 | 399.1813  | [M+H]+  | 4.55, 4.875 | 1.3 | C₈H₁₀O₅    | 381.1706, 363.1587, 355.1514, 352.1281, 348.1369, 339.1246, 327.1208, 311.0899 | 3  | Sceo-penicitrolin A | Xanthone | Penicillium citrinum | CAG | [52] |
| 202 | 289.0717  | [M+H]+  | 4.57     | 1.7 | C₈H₁₀O₅    | 274.0483, 270.0526, 246.0534, 243.0657, 204.0488 | 3  | Drimiopsin I | Xanthone | Penicillium sp. | PDA | [53] |
| 203 | 511.2927  | [M+H]+  | 4.96     | 1.4 | C₈H₁₀O₅    | 265.1557, 247.1459, 219.1503, 199.1437, 171.1505, 166.0866, 120.0811, 72.0825 | 2  | Bilaid A | Tetrapeptide | Penicillium sp. | PDA | [54] |
| 204 | 447.2936  | [M+Na]+ | 5.22     | 0.4 | C₈H₁₀O₅    | Nf | 4  | n.a. | CAG | PDA | [50] |
| 205 | 309.1343  | [M+H]+  | 5.25     | 1.6 | C₈H₁₀O₅    | 291.1229, 273.1129, 255.1022, 245.1183, 231.0663, 227.1073, 217.0497, 213.0556, 207.0497, 195.0292, 193.0501, 191.0343, 183.0296, 165.0552, 149.0605 | 3  | (3S,7R)-7-hydroxyresorcylic acid | Zearalenone (Macrolide) | Penicillium sp. | PDA | [50] |
| No. | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|------------------|-----|-------------|----------------------|----|------------------------|----------------|-------------------|--------|-----|
| 206 | 457.2601  | [M+H]<sup>+</sup> | 5.47            | -0.7| C<sub>3</sub>H<sub>7</sub>N<sub>2</sub>O<sub>5</sub> | 440.2370, 439.2495, 399.2179, 385.2024, 382.1911, 381.1940, 368.1750, 340.1801, 326.1655, 323.1541, 309.1378, 299.1517, 297.1387, 255.1489, 238.1450, 210.1285, 198.1156, 197.1081, 185.0918, 181.0893, 168.0813, 159.0927 | 2 | Communesin A | Indole alkaloid | *Penicillium* sp. | CAG | [55] |
| 207 | 427.1757  | [M+H]<sup>+</sup> | 5.47            | 0  | C<sub>4</sub>H<sub>9</sub>O<sub>3</sub> | 381.1703, 363.1595, 354.1459, 348.1355, 339.1234, 326.1150, 321.1122, 311.0921, 308.1045, 297.0759 | 4 | n.a. | | | CAG | |
| 208 | 293.1393  | [M+H]<sup>+</sup> | 5.97            | 1.4| C<sub>3</sub>H<sub>7</sub>O<sub>3</sub> | 275.1283, 257.1166, 239.1059, 231.1375, 229.1258, 215.0709, 205.0494, 201.0546, 189.0547, 187.0414, 179.0341, 177.0546, 175.0888, 173.0599, 163.0749, 161.0593, 151.0390, 149.0599, 99.0811, 81.0702 | 3 | Dihydroresorcylide | Zearealenone (Macrolide) | *Penicillium expansum* | CAG, PDA | [56] |
| 209 | 529.2708  | [M+H]<sup>+</sup> | 6              | 1.1| C<sub>7</sub>H<sub>11</sub>N<sub>2</sub>O<sub>3</sub> | 331.1811, 201.1068, 185.0722, 130.0658 | 3 | Chaetoglobosin D | Cytochalasin alkaloid | *Penicillium expansum* | CAG | [57] |
| 210 | 509.2773  | [M+H]<sup>+</sup> | 6.11            | -0.8| C<sub>7</sub>H<sub>11</sub>N<sub>2</sub>O<sub>5</sub> | 311.1388, 283.1449, 263.1399, 247.1446, 235.1447, 219.1502, 199.1440, 171.1498, 136.0762, 120.0815 | 4 | n.a. | | | PDA | |
| 211 | 357.1341  | [M+H]<sup>+</sup> | 6.22            | 0.8 | C<sub>7</sub>H<sub>11</sub>O<sub>3</sub> | 342.1103, 327.0872, 315.0868, 313.0717, 301.0714, 286.0481, 257.0454, 229.0506 | 4 | n.a. | | | PDA | |
| 212 | 529.27    | [M+H]<sup>+</sup> | 6.29            | -0.4| C<sub>7</sub>H<sub>11</sub>O<sub>3</sub> | 200.1071, 198.0916, 185.0718, 174.0925, 174.1057, 170.1037 | 2 | Chaetoglobosin A | Cytochalasin alkaloid | *Penicillium chrysogenum* | CAG | [58] |
| 213 | 307.1551  | [M+H]<sup>+</sup> | 6.38            | 2  | C<sub>7</sub>H<sub>11</sub>O<sub>3</sub> | 265.1435, 201.1277, 155.0864, 135.0807, 133.1008, 131.0864, 105.0695 | 3 | Expansolide A or B | Sesquiterpenoid | *Penicillium expansum* | CAG | [59] |
| 214 | 707.2095  | [M+H]<sup>+</sup> | 6.42            | -1 | C<sub>7</sub>H<sub>11</sub>N<sub>2</sub>O<sub>5</sub> | 668.0617, 602.0138, 584.0034, 573.0614, 365.0998, 296.0298, 275.0551 | 4 | n.a. | | | PDA | |
| 215 | 313.1084  | [M+H]<sup>+</sup> | 6.64            | 2.6| C<sub>7</sub>H<sub>11</sub>O<sub>3</sub> | 297.0678, 271.0612, 257.0456, 229.0503 | 4 | n.a. | | | PDA | |
| 216 | 289.0716  | [M+H]<sup>+</sup> | 6.72            | 1.4| C<sub>7</sub>H<sub>11</sub>O<sub>3</sub> | 274.0482, 270.0525, 265.0518, 243.0680, 232.0370, 228.0296, 200.0479 | 3 | Drimiopsin H | Xanthone | *Penicillium* sp. | PDA | [53] |
| 217 | 305.1296  | [M+H]<sup>+</sup> | 6.72            | 2  | C<sub>7</sub>H<sub>11</sub>N<sub>2</sub>O<sub>5</sub> | 277.1343, 254.1274, 220.1120, 187.0869, 152.0810 | 4 | n.a. | | | CAG | |
| 218 | 339.0871  | [M+H]<sup>+</sup> | 6.85            | 0.6| C<sub>7</sub>H<sub>11</sub>O<sub>3</sub> | 324.0636, 321.0758, 311.0922, 296.0687, 293.0815, 283.0966, 269.0456, 265.0869, 249.0918 | 4 | n.a. | | | PDA | |
| No.  | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|------|-----------|--------|-------------------|-----|------------|----------------------|----|-------------------------|----------------|------------------|--------|-----|
| 219  | 509.2922  | [M+H]<sup>+</sup> | 7.04 | 1 | C<sub>22</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub> | 491.2809, 451.2503, 437.2342, 381.1972, 367.1808, 357.2074, 343.1924, 340.1916, 326.1661, 323.1545, 309.1391, 255.1501, 253.1346, 197.1083, 185.1085, 183.0922, 159.0922, 95.0501 | 2 | Communesin B | Indole alkaloid | Penicillium sp. | CAG | [55] |
| 220  | 357.1341  | [M+H]<sup>+</sup> | 7.05 | 0.8 | C<sub>21</sub>H<sub>19</sub>O<sub>6</sub> | 341.1023, 327.0877, 313.1076, 311.0921, 301.0721, 286.0482, 273.0771, 258.0528, 247.0608, 230.0600 | n.a. | PDA |
| 221  | 359.1135  | [M+H]<sup>+</sup> | 7.22, 7.71<sup>a</sup> | 1.1 | C<sub>22</sub>H<sub>24</sub>O<sub>5</sub> | 341.1030, 326.0796, 323.0922, 313.1078, 302.0749, 271.0614, 257.0455 | 3 | Penixanthone D | Xanthone | Penicillium sp. | PDA | [60] |
| 222  | 487.27    | [M+H]<sup>+</sup> | 7.22 | 0.8 | C<sub>21</sub>H<sub>19</sub>O<sub>6</sub> | 395.2227, 377.2127, 367.2277, 349.2178, 243.1752, 225.1640, 215.1806, 185.1337, 183.1183, 175.1487, 171.1180, 161.1338, 151.0396 | n.a. | PDA |
| 223  | 319.1455  | [M+H]<sup>+</sup> | 7.28 | 2.5 | C<sub>21</sub>H<sub>24</sub>O<sub>5</sub> | 291.1506, 234.1290, 201.1029, 188.0718, 132.0817, 91.0551 | 4 | n.a. | CAG |
| 224  | 307.1552  | [M+H]<sup>+</sup> | 7.42 | 2.1 | C<sub>20</sub>H<sub>18</sub>O<sub>5</sub> | 289.1434, 271.1339, 243.1392, 229.0860, 193.0503, 191.0710, 189.0561, 175.0766, 165.0543, 163.0751 | 3 | a: 5-oxolasiodiplodin, b: 7-oxolasiodiplodin | Zearalenone (Macrolide) | a: Lasiodiplodia theobromae, b: Lasiodiplodia sp. | PDA | [62], [63] |
| 225  | 355.1188  | [M+H]<sup>+</sup> | 7.54 | 1.7 | C<sub>20</sub>H<sub>18</sub>O<sub>5</sub>* | 339.0874, 325.0719, 311.0926 | 4 | n.a. | PDA |
| 226  | 357.1346  | [M+H]<sup>+</sup> | 8 | 2.2 | C<sub>20</sub>H<sub>18</sub>O<sub>5</sub> | 342.1128, 327.0954, 315.0874, 313.0724, 301.0730, 286.0486, 281.0819, 273.0769, 258.0534, 255.0661, 247.0605 | 4 | n.a. | PDA |
| 227  | 711.2451  | [M+H]<sup>+</sup> | 8.12 | -0.6 | C<sub>21</sub>H<sub>24</sub>N<sub>2</sub>O<sub>5</sub>* | 679.2186, 636.2005, 356.1266, 341.1040, 327.1239, 232.0929 | 4 | n.a. | PDA |
| 228  | 367.2253  | [M+Na]<sup>+</sup> | 8.13 | 1.1 | C<sub>20</sub>H<sub>18</sub>O<sub>5</sub> | 320.1843, 252.0905, 242.1019, 234.1131, 224.0923, 198.1151, 149.0231, 138.0189 | 4 | n.a. | CAG |
| 229  | 389.2327  | [M+H]<sup>+</sup> | 8.39 | -0.3 | C<sub>20</sub>H<sub>18</sub>O<sub>5</sub> | Nf | 4 | n.a. | CAG |
| 230  | 865.5916  | [M+H]<sup>+</sup> | 8.8 | 0.1 | C<sub>21</sub>H<sub>24</sub>N<sub>2</sub>O<sub>5</sub>* | 594.4034, 526.3393, 481.3192, 413.2555, 408.3224, 368.2338, 340.2582, 300.1718, 295.2392, 272.1769, 267.2441, 227.1761, 199.1817, 159.0919 | 4 | n.a. | CAG |
| 231  | 500.3957  | [M+H]<sup>+</sup> | 8.95 | 1.2 | C<sub>21</sub>H<sub>24</sub>N<sub>2</sub>O<sub>5</sub>* | 482.3847, 256.1509, 144.1026 | n.a. | PDA |
| 232  | 371.1132  | [M+H]<sup>+</sup> | 9.49 | 0.3 | C<sub>20</sub>H<sub>18</sub>O<sub>5</sub> | 339.0872, 329.1029, 311.0927, 296.0686, 287.0599, 283.0973, 273.0402, 269.0455, 265.0868, 255.0296, 241.0500 | 3 | Chaetoxanthone A | Xanthone | Chaetomium sp. | PDA | [64] |
| No. | m/z value | Adduct | R<sub>t</sub> (min) | ppm | Putative MF | Fragmentation pattern | IC | Putative identification | Chemical family | Biological origin | Medium | Ref |
|-----|-----------|--------|---------------------|-----|-------------|-----------------------|----|------------------------|----------------|-------------------|--------|-----|
| 233 | 467.0751  | [M+H]<sup>+</sup> | 9.49 | -0.4 | C<sub>24</sub>H<sub>6</sub>N<sub>10</sub>O<sub>2</sub> | 426.0487, 423.0406, 421.0434, 412.9966, 405.0294, 403.0327, 390.0050, 388.0096, 385.0206, 371.9950, 369.9992 | 4 | n.a. | | | PDA |
| 234 | 279.233   | [M+H]<sup>+</sup> | 9.66 | 2.1 | C<sub>18</sub>H<sub>30</sub>O<sub>2</sub> | 261.2221, 223.1700, 209.1532, 201.0458, 195.1395, 191.1436, 187.1490, 177.1271, 173.1328, 163.1481, 159.1174, 151.1479, 149.1330, 147.1175, 145.1004, 137.1334, 135.1168, 131.0853, 123.1168, 121.1018, 109.1015, 107.0859, 95.0860, 93.0696, 81.0707 | 4 | n.a. | | | PDA |
| 235 | 279.2333  | [M+H]<sup>+</sup> | 9.74 | 3.2 | C<sub>18</sub>H<sub>30</sub>O<sub>2</sub> | 261.2222, 223.1702, 209.1537, 201.0462, 195.1386, 191.1434, 187.1488, 177.1286, 173.1329, 163.1490, 159.1176, 151.1487, 149.1335, 147.1167, 145.1022, 137.1334, 135.1173, 133.1024, 131.0863, 123.1177, 121.1020, 109.1017, 107.0863, 95.0861, 93.0698, 81.0708, 79.0556 | 4 | n.a. | | | PDA |
| 236 | 343.1188  | [M+H]<sup>+</sup> | 9.82 | 1.7 | C<sub>19</sub>H<sub>18</sub>O<sub>6</sub> | 327.0860, 313.0720, 301.0718, 287.0565, 275.0558, 259.0612, 233.0453, 213.0556 | 3 | Umbilicaxanthone A | Xanthone | Umbilicaria proboscidea | | |
| 237 | 843.3354  | [M+H]<sup>+</sup> | 9.82 | 0 | C<sub>44</sub>H<sub>34</sub>N<sub>20</sub>O<sub>5</sub> or C<sub>46</sub>H<sub>46</sub>N<sub>6</sub>O<sub>10</sub> | 364.0936 | 4 | n.a. | | | PDA |
| 238 | 714.4153  | [M+H]<sup>+</sup> | 10.44 | -0.7 | C<sub>46</sub>H<sub>46</sub>N<sub>6</sub>O<sub>10</sub> | 696.4050, 571.2720 | 4 | n.a. | | | PDA |
| 239 | 850.4537  | [M+H]<sup>+</sup> | 10.93 | 0.8 | C<sub>46</sub>H<sub>46</sub>N<sub>6</sub>O<sub>10</sub> | 377.3211, 341.1031, 326.0794, 313.1082 | 4 | n.a. | | | PDA |
References

1. Wang, M.; Carver, J.J.; Phelan, V.V.; Sanchez, L.M.; Garg, N.; Peng, Y.; Nguyen, D.D.; Watrous, J.; Kapono, C.A.; Luzzatto-Knaan, T.; et al. Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. Nat. Biotechnol. 2016, 34, 828-837, doi:10.1038/nbt.3597.

2. Altschul, S.F.; Gish, W.; Miller, W.; Myers, E.W.; Lipman, D.J. Basic local alignment search tool. J. Mol. Biol. 1990, 215, 403-410, doi:10.1016/S0022-2836(05)80360-2.

3. Sumner, L.W.; Amberg, A.; Barrett, D.; Beale, M.H.; Beger, R.; Daykin, C.A.; Fan, T.W.; Fiehn, O.; Goodacre, R.; Griffin, J.L.; et al. Proposed minimum reporting standards for chemical analysis Chemical Analysis Working Group (CAWG) Metabolomics Standards Initiative (MSI). Metabolomics 2007, 3, 211-221, doi:10.1007/s11306-007-0082-2.

4. Drautz, H.; Zähner, H.; Kupfer; Keller-Schierlein, W. 164. Stoffwechselprodukte von Mikroorganismen, 205. Mitteilung. Isolierung und Struktur von Streptazolin. Helv. Chim. Acta 1981, 64, 1752-1765, doi:10.1002/hlca.19810640605.

5. Puder, C.; Loya, S.; Hizi, A.; Zeeck, A. New co-metabolites of the streptazolin pathway. J. Nat. Prod. 2001, 64, 42-45, doi:10.1021/np000377i.

6. Paulus, C.; Rebets, Y.; Zapp, J.; Ruckert, C.; Kalinowski, J.; Luzhetskyy, A. New alpiniamides from Streptomyces sp. IB2014/011-12 assembled by an unusual hybrid non-ribosomal peptide synthetase Trans-AT polyketide synthase enzyme. Front. Microbiol. 2018, 9, 1959, doi:10.3389/fmicb.2018.01959.

7. Fleck, W.F.; Ritzau, M.; Heinze, S.; Gräfe, U. Isolation of dimeric nonactic acid from the nonactin-producing Streptomyces spec. JA 5909-1. J. Basic Microbiol. 1996, 36, 235-238, doi:10.1002/jobm.3620360405.

8. Schumacher, R.W.; Talmage, S.C.; Miller, S.A.; Sarris, K.E.; Davidson, B.S.; Goldberg, A. Isolation and structure determination of an antimicrobial ester from a marine sediment-derived bacterium. J. Nat. Prod. 2003, 66, 1291-1293, doi:10.1021/np020594e.

9. Huang, H.; Lan, X.; Wang, Y.; Tian, L.; Fang, Y.; Zhang, L.; Zhang, K.; Zheng, X. New bioactive derivatives of nonactic acid from the marine Streptomyces griseus derived from the plant Salicornia sp. Phytochem. Lett. 2015, 12, 190-195, doi:10.1016/j.phytol.2015.04.001.

10. Jeong, S.Y.; Shin, H.J.; Kim, T.S.; Lee, H.S.; Park, S.K.; Kim, H.M. Streptokordin, a new cytotoxic compound of the methylpyridine class from a marine-derived Streptomyces sp. KORDI-3238. J. Antibiot. 2006, 59, 234-240, doi:10.1038/ja.2006.33.

11. Charan, R.D.; Schlingmann, G.; Janso, J.; Bernan, V.; Feng, X.; Carter, G.T. Diazepinomicin, a new antimicrobial alkaloid from a marine Micromonospora sp. J. Nat. Prod. 2004, 67, 1431-1433, doi:10.1021/np040042r.

12. Maskey, R.P.; Grun-Wollny, I.; Laatsch, H. Isolation and structure elucidation of diazaquinomycin C from a terrestrial Streptomyces sp. and confirmation of the akashin structure. Nat. Prod. Res. 2005, 19, 137-142, doi:10.1080/14786410410001704741.

13. McBrien, K.D.; Berry, R.L.; Lowe, S.E.; Neddermann, K.M.; Bursuker, I.; Huang, S.; Klohr, S.E.; Leet, J.E. Rakicidins, new cytotoxic lipopeptides from Micromonospora sp. fermentation, isolation and characterization. J. Antibi. 1995, 48, 1446-1452, doi:10.7164/antibiotics.48.1446.

14. Oku, N.; Matoba, S.; Yamazaki, Y.M.; Shimasaki, R.; Miyanaga, S.; Igarashi, Y. Complete stereochemistry and preliminary structure-activity relationship of rakicidin A, a hypoxia-selective cytotoxin from Micromonospora sp. J. Nat. Prod. 2014, 77, 2561-2565, doi:10.1021/np500276c.
Iida, A.; Sanekata, M.; Wada, S.; Fujita, T.; Tanaka, H.; Enoki, A.; Fuse, G.; Kanai, M.; Asami, K. Fungal metabolites. XVIII. New membrane-modifying peptides, trichorozins I-IV, from the fungus Trichoderma harzianum. Chem. Pharm. Bull. 1995, 43, 392-397, doi:10.1248/cpb.43.392.

Goulard, C.; Hlimi, S.; Rebuffat, S.; Bodo, B. Trichorozins HA and MA, antibiotic peptides from Trichoderma harzianum. I. Fermentation, isolation and biological properties. J. Antibiot. 1995, 48, 1248-1253, doi:10.7164/antibiotics.48.1248.

Iida, A.; Sanekata, M.; Fujita, T.; Tanaka, H.; Enoki, A.; Fuse, G.; Kanai, M.; Rudewicz, P.J.; Tachikawa, E. Fungal metabolites. XVI. Structures of new peptaibols, trichokinds I-VII, from...
the fungus *Trichoderma harzianum*. *Chem. Pharm. Bull.* **1994**, *42*, 1070-1075, doi:10.1248/cpb.42.1070.

33. Mohamed-Benkada, M.; Montagu, M.; Biard, J.F.; Mondeguer, F.; Verite, P.; Dalgalarondon, M.; Bissett, J.; Pouchus, Y.F. New short peptaibols from a marine *Trichoderma* strain. *Rapid Commun. Mass Spectrom.* **2006**, *20*, 1176-1180, doi:10.1002/rcm.2430.

34. Oh, S.U.; Yun, B.S.; Lee, S.J.; Kim, J.H.; Yoo, I.D. Atroviridins A-C and neotroviridins A-D, novel peptaibol antibiotics produced by *Trichoderma atroviride* F80317. *I. Taxonomy, fermentation, isolation and biological activities. J. Antibiot.* **2002**, *55*, 557-564, doi:10.7164/antibiotics.55.557.

35. Augustiniak, H.; Forche, E.; Reichenbach, H.; Wray, V.; Gräfe, U.; Höfle, G. Isolierung und Strukturaufklärung von Ergokonin A und B; zwei neue antifungische Sterol-Antibiotika aus *Trichoderma koningii*. *Liebigs Ann. Chem.* **1991**, *1991*, 361-366, doi:10.1002/jlac.199119910163.

36. Reveglia, P.; Savocchia, S.; Billones-Baaijens, R.; Masi, M.; Cimmino, A.; Evidente, A. Diploquinones A and B, two new phytotoxic tetrasubstituted 1,4-naphthoquinones from *Diplodia mutila*, a causal agent of grapevine trunk disease. *J. Agr. Food Chem.* **2018**, *66*, 11968-11973, doi:10.1021/acs.jafc.8b05004.

37. Chilton, W.S. Isolation and structure of norjavanicin. *J. Org. Chem.* **1968**, *33*, 4299-4300, doi:10.1021/jo01275a074.

38. Trisuwan, K.; Khamthong, N.; Rukachaisirikul, V.; Phongpaichit, S.; Preedanon, S.; Sakayaroj, J. Anthraquinone, cyclopentanone, and naphthoquinone derivatives from the sea fan-derived fungi *Fusarium* spp. *PSU-F14 and PSU-F135*. *J. Nat. Prod.* **2010**, *73*, 1507-1511, doi:10.1021/np100282k.

39. Ola, A.R.; Thomy, D.; Lai, D.; Brotz-Oesterhelt, H.; Proksch, P. Inducing secondary metabolite production by the endophytic fungus *Fusarium tricinctum* through coculture with *Bacillus subtilis*. *J. Nat. Prod.* **2013**, *76*, 2094-2099, doi:10.1021/np400589h.

40. Kurobane, I.; Vining, L.C.; McInnes, A.G.; Gerber, N.N. Metabolites of *Fusarium solani* related to dihydrofusarubin. *J. Antibiot.* **1980**, *33*, 1376-1379, doi:10.7164/antibiotics.33.1376.

41. Yang, X.; Khong, T.T.; Chen, L.; Choi, H.D.; Kang, J.S.; Son, B.W. 8'-hydroxyzearalanone and 2'-hydroxyzearalanol: Resorcylic acid lactone derivatives from the marine-derived fungus *Penicillium* sp. *Chem. Pharm. Bull.* **2008**, *56*, 1355-1356, doi:10.1248/cpb.56.1355.

42. Ma, T.-T.; Shan, W.-G.; Ying, Y.-M.; Ma, L.-F.; Liu, W.-H.; Zhan, Z.-J. Xanthones with α-glucosidase inhibitory activities from *Aspergillus versicolor*, a fungal endophyte of *Huperzia serrata*. *Helv. Chim. Acta* **2015**, *98*, 148-152, doi:10.1002/hlca.201400165.

43. Stob, M.; Baldwin, R.S.; Tuite, J.; Andrews, F.N.; Gillette, K.G. Isolation of an anabolic, uterotrophic compound from corn infected with *Gibberella zeae*. *Nature* **1962**, *196*, 1318, doi:10.1038/1961318a0.

44. Hawas, U.W.; Farrag, A.R.H.; Ahmed, E.F.; Abou El-Kassem, L.T. Cytotoxic effect of *Fusarium equiseti* fungus metabolites against N-Nitrosodimethylamine- and CCL4-induced hepatocarcinogenesis in rats. *Pharm. Chem. J.* **2018**, *52*, 326-333, doi:10.1007/s11094-018-1816-3.

45. Richardson, K.E.; Hagler, W.M.; Mirocha, C.J. Production of zearalenone, α- and β-zearalenol, and α- and β-zearalanol by *Fusarium* spp. in rice culture. *J. Agr. Food Chem.* **1985**, *33*, 862-866, doi:10.1021/jf00065a024.

46. Shiono, Y.; Tsuchinari, M.; Shimanuki, K.; Miyajima, T.; Murayama, T.; Koseki, T.; Laatsch, H.; Funakoshi, T.; Takanami, K.; Suzuki, K. Fusaristatins A and B, two new cyclic lipopeptides from an endophytic *Fusarium* sp. *J. Antibiot.* **2007**, *60*, 309-316, doi:10.1038/ja.2007.39.

47. Hammerschmidt, L.; Wray, V.; Lin, W.; Kamilova, E.; Proksch, P.; Aly, A.H. New styrylpyrones from the fungal endophyte *Penicillium glabrum* isolated from *Punica granatum*. *Phytochemistry.* **2012**, *5*, 600-603, doi:10.1016/j.phytochem.2012.06.003.

48. Lai, S.; Shizuri, Y.; Yamamura, S.; Kawai, K.; Furukawa, H. New curvularin-type metabolites from the hybrid strain ME 0005 derived from *Penicillium citreo-viride* B. *IFO 4692 and 6200*. *Bull. Chem. Soc. Jpn.* **1991**, *64*, 1048-1050, doi:10.1246/bcsj.64.1048.
49. Huang, Z.; Yang, R.; Yin, X.; She, Z.; Lin, Y. Structure elucidation and NMR assignments for two xanthone derivatives from a mangrove endophytic fungus (No. ZH19). Magn. Reson. Chem. 2010, 48, 80-82, doi:10.1002/mrc.2539.

50. Li, F.; Sun, W.; Zhang, S.; Gao, W.; Lin, S.; Yang, B.; Chai, C.; Li, H.; Wang, J.; Hu, Z.; et al. New cyclopiane diterpenes with anti-inflammatory activity from the sea sediment-derived fungus Penicillium sp. TJ403-2. Chin. Chem. Lett. 2020, 31, 197-201, doi:10.1016/j.cclet.2019.04.036.

51. Liao, Z.-J.; Tian, W.-J.; Liu, X.-X.; Jiang, X.; Wu, Y.; Lin, T.; Chen, H.-F. A new xanthone from an endophytic fungus of Anoectochilus roxburghii. Chem. Nat. Compd. 2018, 54, 267-269, doi:10.1007/s10600-018-2320-4.

52. Yang, S.-Q.; Li, X.-M.; Li, X.; Li, H.-L.; Meng, L.-H.; Wang, B.-G. New citrinin analogues produced by coculture of the marine algal-derived endophytic fungal strains Aspergillus sydowii EN-534 and Penicillium citrinum EN-535. Phytochem. Lett. 2018, 25, 191-195, doi:10.1016/j.phytol.2018.04.023.

53. Zhuang, Y.-B.; Yin, H.; Zhang, X.-W.; Zhou, W.; Liu, T. Three new xanthones from the fungus Penicillium sp. NH-7-1. Helv. Chim. Acta 2015, 98, 699-703, doi:10.1002/hlca.201400296.

54. Dekan, Z.; Sianati, S.; Yousf, A.; Sutcliffe, K.J.; Gillis, A.; Mallet, C.; Singh, P.; Jin, A.H.; Wang, A.M.; Mohammadi, S.A.; et al. A tetrapeptide class of biased analogues from an Australian fungus targets the micro-opioid receptor. Proc. Natl. Acad. Sci. USA 2019, 116, 22353-22358, doi:10.1073/pnas.1908662116.

55. Numata, A.; Takahashi, C.; Ito, Y.; Takada, T.; Kawai, K.; Usami, Y.; Matsumura, E.; Imachi, M.; Ito, T.; Hasegawa, T. Communesins, cytotoxic metabolites of a fungus isolated from a marine alga. Tetrahedron Lett. 1993, 34, 2355-2358, doi:10.1016/s0040-4039(00)77612-x.

56. Zhang, P.; Meng, L.-H.; Mándi, A.; Li, X.-M.; Kurthán, T.; Wang, B.G. Structure, absolute configuration, and conformational study of resorcylic acid derivatives and related congeners from the fungus Penicillium brocae. RSC Adv. 2015, 5, 39870-39877, doi:10.1039/c5ra02203g.

57. Andersen, B.; Smedsgaard, J.; Frisvad, J.C. Penicillium expansum: Consistent production of patulin, chaetoglobosins, and other secondary metabolites in culture and their natural occurrence in fruit products. J. Agr. Food Chem. 2004, 52, 2421-2428, doi:10.1021/jf035406k.

58. Huang, S.; Chen, H.; Li, W.; Zhu, X.; Ding, W.; Li, C. Bioactive chaetoglobosins from the mangrove endophytic fungus Penicillium chrysogenum. Mar. Drugs 2016, 14, 172, doi:10.3390/md14100172.

59. Massias, M.; Rebuffat, S.; Molho, L.; Chiaroni, A.; Riche, C.; Bodo, B. Expansolides A and B: Tetra cyclic sesquiterpene lactones from Penicillium expansum. J. Am. Chem. Soc. 1990, 112, 8112-8115, doi:10.1021/ja00178a039.

60. Huang, J.; She, J.; Yang, X.; Liu, J.; Zhou, X.; Yang, B. A new macrolide and two new polycyclic chromones from the fungus Penicillium sp. SCSIO041218. Molecules 2019, 24, 1686, doi:10.3390/molecules24091686.

61. Cheng, Z.; Xu, W.; Wang, Y.; Bai, S.; Liu, L.; Luo, Z.; Yuan, W.; Li, Q. Two new meroterpenoids and two new monoterpenoids from the deep sea-derived fungus Penicillium sp. YPGA11. Fitoterapia 2019, 133, 120-124, doi:10.1016/j.fitote.2018.12.022.

62. Matsuura, H.; Nakamori, K.; Omer, E.A.; Hatakeyama, C.; Yoshihara, T.; Ichihara, A. Three lasiodiplodins from Lasiodiplodia theobromae IFO 31059. Phytochemistry 1998, 49, 579-584, doi:10.1016/s0031-9422(98)00267-2.

63. Li, J.; Xue, Y.; Yuan, J.; Lu, Y.; Zhu, X.; Lin, Y.; Liu, L. Lasiodiplodins from mangrove endophytic fungus Lasiodiplodia sp. 318. Nat. Prod. Res. 2016, 30, 755-760, doi:10.1080/14786419.2015.1062762.

64. Pontius, A.; Krick, A.; Kehraus, S.; Brun, R.; Konig, G.M. Antiprotozoan activities of heterocyclic-substituted xanthones from the marine-derived fungus Chaetomium sp. J. Nat. Prod. 2008, 71, 1579-1584, doi:10.1021/np800294q.

65. Řezanka, T.; Jáchymová, J.; Dembitsky, V.M. Prenylated xanthone glucosides from Ural’s lichen Umbilicaria proboscidea. Phytochemistry 2003, 62, 607-612, doi:10.1016/s0031-9422(02)00539-3.