Supplementary Figures and Tables

Supplementary Table 1. Processed table from the LC-MS/MS data analyzed using MZmine 2.

| row ID* | row m/z      | row retention time | BE93_R2A.mz ML Peak area | BE93_NB.mz ML Peak area | BE93_LB.mz ML Peak area | BE93_TSB.mz ML Peak area |
|---------|--------------|---------------------|--------------------------|-------------------------|-------------------------|--------------------------|
| 2       | 197.0541697  | 14                  | 5.05E+08                 | 3.31E+08                | 9.58E+08                | 4.83E+08                 |
| 3       | 211.1000061  | 18                  | 1.22E+09                 | 1.41E+09                | 2.28E+09                | 2.64E+09                 |
| 5       | 261.0514594  | 13                  | 6.57E+08                 | 2.44E+08                | 5.10E+08                | 1.92E+09                 |
| 6       | 340.2874908  | 24                  | 2.55E+08                 | 2.66E+08                | 2.49E+08                | 2.65E+08                 |
| 7       | 371.1000061  | 25                  | 4.29E+08                 | 7.79E+07                | 1.01E+08                | 2.02E+08                 |
| 8       | 385.1000061  | 29                  | 6.22E+08                 | 1.20E+08                | 2.33E+08                | 3.94E+08                 |
| 9       | 453.25       | 20                  | 3.35E+08                 | 3.34E+08                | 3.38E+08                | 3.36E+08                 |
| 10      | 679.3499756  | 24                  | 2.54E+08                 | 2.61E+08                | 2.48E+08                | 2.83E+08                 |
| 11      | 235.0479196  | 3.6                 | 1.65E+08                 | 2.12E+07                | 4.99E+08                | 6.84E+08                 |
| 12      | 245.0625038  | 20                  | 3.13E+08                 | 4.05E+08                | 5.21E+08                | 2.74E+09                 |
| 13      | 243.0077386  | 24                  | 3.17E+08                 | 1.66E+08                | 3.65E+08                | 1.95E+08                 |
| 14      | 138          | 20                  | 6.15E+08                 | 2.70E+08                | 9.59E+08                | 1.18E+09                 |
| 15      | 347.0499878  | 22                  | 2.31E+08                 | 2.78E+07                | 2.97E+08                | 4.37E+08                 |
| 16      | 701.3499756  | 24                  | 2.13E+08                 | 1.98E+08                | 2.42E+08                | 2.43E+08                 |
| 17      | 219.0750046  | 25                  | 2.13E+08                 | 2.01E+07                | 1.09E+07                | 4.54E+07                 |
| 18      | 279.0624924  | 13                  | 4.91E+08                 | 8.82E+07                | 6.92E+08                | 3.44E+08                 |
| 19      | 383.1000061  | 27                  | 4.11E+08                 | 2.24E+08                | 1.16E+08                | 1.96E+08                 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 20 | 283.0499878 | 14 | 2.95E+08 | 824787 | 6.81E+08 | 5.38E+08 |
| 21 | 475.2000122 | 20 | 1.76E+08 | 1.92E+08 | 2.01E+08 | 2.55E+08 |
| 22 | 147.0500031 | 14 | 4.87E+08 | 8.23E+08 | 6.91E+07 | 3.06E+08 |
| 23 | 419.0499878 | 30 | 1.76E+08 | 2.71E+07 | 7339755 | 1.67E+07 |
| 25 | 804.3279597 | 44 | 1.56E+09 | 1.59E+08 | 1.77E+08 | 3.45E+09 |
| 27 | 440.1535666 | 43 | 3.82E+08 | 3.31E+08 | 1.75E+07 | 1.27E+08 |
| 28 | 426.1499939 | 41 | 2.13E+08 | 1.42E+08 | 3.06E+08 | 3.90E+07 |
| 30 | 401.1499939 | 29 | 9.55E+07 | 9.23E+07 | 8.33E+07 | 9.81E+07 |
| 31 | 220.0592623 | 22 | 1.21E+08 | 3.06E+08 | 2.01E+07 | 3.44E+08 |
| 37 | 343.0624924 | 17 | 1.25E+08 | 3094458 | 3.19E+07 | 3.90E+07 |
| 38 | 239       | 21 | 6.30E+07 | 1.39E+08 | 4.23E+08 | 3.44E+08 |
| 41 | 229.0355169 | 15 | 1.19E+08 | 9.21E+07 | 7.15E+08 | 4.16E+08 |
| 42 | 267.0437393 | 30 | 7.43E+07 | 4459639 | 6904997 | 3642243.07 |
| 43 | 227.1000061 | 13 | 9.28E+07 | 1.10E+08 | 7.77E+07 | 8.26E+07 |
| 44 | 164.0468779 | 7.3 | 7.99E+07 | 6.94E+07 | 2.30E+08 | 1.68E+08 |
| 45 | 298       | 11 | 8.43E+07 | 7.42E+07 | 6.49E+07 | 1.98E+08 |
| 51 | 266.0472124 | 35 | 6.98E+07 | 8.61E+07 | 1873981.63 |
| 52 | 250.0500031 | 34 | 9.93E+07 | 1.01E+08 | 2.16E+08 | 5.49E+08 |
| 58 | 282.2187576 | 54 | 7.07E+07 | 1.12E+08 | 3.76E+07 | 1.86E+07 |
| 60 | 382.0812492 | 34 | 4.92E+07 | 1.39E+07 | 4.10E+07 | 4.33E+07 |
| 77 | 256.2000122 | 54 | 6.98E+07 | 4.29E+07 | 4.82E+07 | 5.82E+07 |
|    |         |     |    |    |    |    |    |
|----|---------|-----|----|----|----|----|----|
| 78 | 213.1000061 | 22  | 7.90E+07 | 1.20E+08 | 7.49E+08 | 8.23E+08 |
| 80 | 146.0250015 | 24  | 7.15E+07 | 1.95E+08 | 9.61E+07 | 6.28E+07 |
| 86 | 284.0875015 | 23  | 3.84E+07 | 4.18E+08 | 4.39E+08 | 4.80E+08 |
| 94 | 280.1985402 | 52  | 6.76E+07 | 7.86E+07 | 6.59E+07 | 3.97E+07 |
| 96 | 242.1999969 | 52  | 6.47E+07 | 2.82E+07 | 1.50E+07 | 1709740.65 |
| 100| 227.1000061 | 26  | 3.24E+07 | 5.28E+07 | 2.01E+08 | 9.17E+08 |
| 102| 137      | 4.7 | 3.52E+07 | 6.63E+08 | 2.18E+08 | 2.13E+08 |
| 105| 261.0624924 | 27  | 3.06E+07 | 8.59E+07 | 3.86E+08 | 9.20E+08 |
| 120| 169.0125008 | 15  | 8.17E+07 | 6.76E+07 | 1.78E+08 | 1.99E+08 |
| 125| 185.0708373 | 15  | 3.22E+07 | 3.75E+07 | 1.05E+08 | 4.61E+08 |
| 129| 169.0500031 | 8.5 | 3.00E+07 | 6.42E+07 | 3.77E+08 | 4.51E+08 |
| 135| 110.0874996 | 3.6 | 6279400  | 1.44E+08 | 1.07E+08 | 5.84E+08 |
| 139| 340.1000061 | 27  | 1.30E+07 | 1.40E+08 | 1.73E+08 |
| 142| 166.0125008 | 8.3 | 2.36E+07 | 2.37E+08 | 4.98E+08 | 2.56E+08 |
| 144| 195.0500031 | 11  | 2.25E+07 | 7.66E+07 | 1.92E+08 | 1.26E+08 |
| 148| 171.0553062 | 12  | 1.95E+07 | 1.54E+08 | 1.23E+08 | 1.38E+08 |
| 151| 155.0500031 | 7   | 2.34E+07 | 7.76E+08 | 7.42E+07 | 1.40E+08 |
| 154| 226.9187508 | 2.9 | 4084656  | 1.09E+08 | 3.10E+07 | 5935563.94 |
| 170| 295.0499878 | 29  | 1.27E+07 | 1.85E+07 | 6.49E+07 | 3.51E+08 |
| 171| 229.064586  | 15  | 1.98E+07 | 1.19E+07 | 3.59E+08 | 1.57E+09 |
| 175| 227.0583369 | 15  | 1.64E+07 | 6.82E+08 | 1673810.66 |
|   |                   |   |      |      |      |      |
|---|-------------------|---|------|------|------|------|
| 181 | 319.2000122      | 52 | 2.67E+07 | 2.56E+07 | 2.26E+07 | 2.25E+07 |
| 187 | 199.0500031      |  7.8 | 1.59E+07 | 3.28E+07 | 9.23E+07 | 2.34E+08 |
| 188 | 201.05417        |  9.8 | 1.43E+07 | 1.22E+08 | 1.93E+08 | 6.33E+07 |
| 191 | 169.0498046      |  12 | 1.58E+07 | 4696578  | 1.39E+08 | 2.32E+08 |
| 192 | 120.0625019      |  8.3 | 1.45E+07 | 1.22E+08 | 1.93E+08 | 6.33E+07 |
| 198 | 277.1000061      |  17 | 1.42E+07 | 1.71E+07 | 1.84E+08 | 3.83E+08 |
| 201 | 275.183936       |  52 | 2.18E+07 | 2.05E+07 | 2.45E+07 | 7.049855.63 |
| 219 | 387.2000122      |  52 | 3.01E+07 | 7536653  | 3.75E+07 | 8563853.26 |
| 242 | 336.2375031      |  52 | 1.64E+07 | 1.46E+07 | 1.69E+07 | 1.53E+07 |
| 244 | 306.0499878      |  23 | 1.18E+07 | 1.51E+08 | 1.79E+08 | 2.37E+08 |
| 274 | 765.3729261      |  53 | 4.38E+07 | 7.19E+07 | 1.25E+07 | 1.72247.461 |
| 277 | 414.2140675      |  51 | 2.09E+07 | 303989.7 | 475987  | 488828.925 |
| 322 | 277.0812492      |  19 | 3320808  | 5027876  | 4.28E+07 | 3.02E+08 |
| 350 | 285.0624924      |  9.9 | 3607384  | 3.09E+07 | 6.33E+07 | 2.64E+08 |
| 380 | 284.0750008      |  21 | 4900168  | 8.87E+07 | 2.07E+07 | 1.57E+08 |
| 457 | 663.2916565      |  55 | 1.04E+07 | 2940666  | 4887182  | 110466.492 |
| 559 | 213.1000023      |  40 | 878417.5 | 1071069  | 7.51E+07 | 3.09E+08 |
| 566 | 313.0875015      |  49 | 4193142  | 8087895  | 1.04E+07 | 3.15E+07 |
| 582 | 251.125          |  55 | 5114305  | 6375429  | 2043587  | 979266.614 |
| 665 | 531.3187408      |  56 | 2447589  | 192899.5 | 478222  | 2154981.07 |
| 672 | 269.1281261      |  51 | 4660973  | 5046578  | 1101521  | 4.77E+07 |
|   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 705 | 496.3291673 | 55 | 2408563 | 2205758 | 267373 | 1301236.4 |
| 719 | 295.1124954 | 51 | 1965950 | 2140326 | 6114477 | 2.43E+07 |
| 765 | 148.9749985 | 55 | 1275250 | 1634210 | 1208511 | 171465.248 |
| 816 | 391.2000122 | 59 | 1715697 | 547297 | 1093476 | 839303.685 |
| 870 | 284.2250061 | 57 | 1557755 | 2353089 | 1923939 | 2644702.9 |
| 911 | 391.244165  | 55 | 1465034 | 1299297 | 984571 | 332950.241 |
| 979 | 584.3270683 | 53 | 403892.9 | 143668.2 | 8408356 | 9661979.71 |
| 987 | 391.2708276 | 55 | 812510.6 | 465231.8 | 452035 | 149478.551 |
| 1000| 309.1573003 | 55 | 456356.5 | 206284.4 | 1208691 | 122530.136 |
| 1006| 663.299998  | 56 | 136079.2 | 1143140 | 75204.5 | 93493.0295 |
| 1189| 422.1750031 | 37 | 3.38E+08  | 2709619.52 |
| 1194| 369.125     | 37 | 2.32E+08  | 798204.451 |
| 1212| 147.0895882 | 2.8 | 5.72E+07  | 6864018.04 |
| 1246| 146.0250015 | 12 | 1.90E+07  | 1.48E+08  | 9.25E+07 |
| 1270| 261.0493934 | 13 | 5.48E+08  | 2.11E+09  | 8.46E+08 |
| 1277| 181.048753  | 16 | 3.33E+07  | 5.72E+08  | 7.15E+08 |
| 1312| 249.0944485 | 3.5 | 8304105 | 808995 | 4.42E+07 |
| 1402| 199.0805605 | 18 | 566908.7 | 6882961 | 8718170 | 4.85E+07 |
| 1418| 231.0416692 | 19 | 1.30E+07  | 3.53E+07  | 1.40E+08 |
| 1619| 279.0333252 | 24 | 1467297 | 2.24E+07 | 1.18E+08 |
| 1655| 423.1770871 | 51 | 231500.9 | 8338574 | 320880 | 355950.234 |
| ID  | Row ID     | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 |
|-----|------------|---------|---------|---------|---------|---------|
| 1770| 283.2000122| 53      | 684822.9| 9091966 | 1.85E+07| 1.47E+08|
| 1901| 515.329243 | 59      | 14505.49| 160496.5| 165493  | 4826    |
| 1991| 393.247945 | 55      | 156825.3| 271198.4| 458076  | 4339737.84|
| 2061| 251.086463 | 3.6     | 1.78E+07| 913971.7| 1.04E+08| 9.83E+07|
| 2062| 267.049978 | 21      |         |         | 1.87E+08| 2.95E+08|
| 2064| 203.003335 | 12      | 2267657 |         | 1.03E+08| 1.86E+08|
| 2069| 284.100061 | 27      |         |         | 8.02E+07| 1.20E+08|
| 2071| 822.302076 | 42      | 9561268 | 4.92E+07| 9.60E+08| 1.30E+09|
| 2131| 276.072511 | 13      | 9084312 |         | 1.93E+07| 1.66E+08|

* Note: The row ID numbers presented here were “raw” and were not changed to numbers 1 to 110 to represent the 110 spectral features.
Supplementary Figure 1. Molecular network of ions ranging from 211.10 to 261.05 m/z (circled), representing compounds of the diketopiperazines family.
Supplementary Figure 2. MS/MS spectral data of koranimine from the GNPS library (bottom) matching with the MS/MS spectrum of the detected compound in the *P. frigoritolerans* culture extracts (top).
Supplementary Figure 3. ERRAT plot showing that the generated 3D model has a good resolution as the regions of the modelled structure that can be rejected at the 95% and 99% of confidence is very low with overall quality factor of 92.136%. Figures a-e represent each chain of the modelled protein.