# **Cryptic Secondary Metabolites from the Sponge-Associated Fungus** *Aspergillus ochraceus*

Marian Frank <sup>1</sup>, Ferhat Can Özkaya <sup>2</sup>, Werner E. G. Müller <sup>3</sup>, Alexandra Hamacher <sup>4</sup>, Matthias U. Kassack <sup>4</sup>, Wenhan Lin <sup>5</sup>, Zhen Liu <sup>1,\*</sup> and Peter Proksch <sup>1,\*</sup>

- <sup>1</sup> Institute of Pharmaceutical Biology and Biotechnology, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany; marian.frank@hhu.de (M.F.)
- <sup>2</sup> Faculty of Fisheries, İzmir Katip Çelebi University, Çiğli, 35620 İzmir, Turkey; fcanozkaya@gmail.com (F.C.Ö.)
- <sup>3</sup> Institute of Physiological Chemistry, Universitätsmedizin der Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany; wmueller@uni-mainz.de (W.E.G.M.)
- <sup>4</sup> Institute of Pharmaceutical and Medicinal Chemistry, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany; alexandra.hamacher@hhu.de (A.H.); matthias.kassack@hhu.de (M.U.K.)
- <sup>5</sup> State Key Laboratory of Natural and Biomimetic Drugs, Peking University, Beijing 100191, People's Republic of China; whlin@bjmu.edu.cn (W.L.)
- \* Correspondence: zhenfeizi0@sina.com (Z.L.); proksch@uni-duesseldorf (P.P.); Tel.: +49-211-81-14163

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#### Figure S1. UV spectrum of compound **1**.



#### Figure S2. HRESIMS of compound 1.





# Figure S3. <sup>1</sup>HNMR (600 MHz, DMSO- $d_6$ ) spectrum of compound **1**.

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# Figure S4. <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **1**.



Figure S5. COSY (600MHz, DMSO- $d_6$ ) spectrum of compound **1**.



Figure S6. HSQC (600MHz/150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **1**.



## Figure S7. HMBC (600MHz/150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **1**.

Figure S8. ROESY (600MHz, DMSO- $d_6$ ) spectrum of compound **1**.





#### Figure S9. UV spectrum of compound **2**.



#### Figure S10. HRESIMS of compound **2**.



## Figure S11. <sup>1</sup>H NMR (600 MHz, MeOH- $d_4$ ) spectrum of compound **2**.



Figure S12. COSY (600 MHz, MeOH- $d_4$ ) spectrum of compound **2**.





# Figure S13. HSQC (600MHz/150 MHz, MeOH- $d_4$ ) spectrum of compound **2**.



## Figure S14. HMBC (600MHz/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of compound **2**.

# Figure S15. UV spectrum of compound **3**.



# Figure S16. HRESIMS of compound **3**.

| and and                    | -                                  | Mass        | Spect                 | rum Sn    | nartFo         | rmula                                 | Repo                       | rt          |               |              |  |
|----------------------------|------------------------------------|-------------|-----------------------|-----------|----------------|---------------------------------------|----------------------------|-------------|---------------|--------------|--|
| Analysis Info              |                                    |             |                       |           |                | Acquisition Date 12/7/2016 9:58:56 AM |                            |             |               |              |  |
| Analysis Name              | ata\spektren 2010                  | 6\Proksch1  | Proksch16HR000289.d   |           |                |                                       |                            |             |               |              |  |
| Method tune low new.m      |                                    |             |                       |           |                |                                       | Operator Peter Tommes      |             |               |              |  |
| Sample Name                | M. Frank MAO-BS-V5-SD4-SP3 (CH3OH) |             |                       |           |                | Instru                                | Instrument maXis 288882.20 |             |               |              |  |
| Comment                    |                                    |             |                       |           |                |                                       |                            |             |               |              |  |
| Acquisition Para           | amete                              | er          |                       |           |                |                                       | J.B. HU                    |             |               | 11.11        |  |
| ource Type                 | E                                  | SI          | Ion Polarity          |           | Positive       |                                       | Set Nebulizer              |             | 0.3 Bar       |              |  |
| ocus                       | us Not active                      |             | Set Capillary         |           | 4000 V         |                                       | Set Dry Heater             |             | 180 °C        |              |  |
| Scan Begin                 | 50 m/z                             |             | Set End Plate Offset  |           | -500 V         |                                       | Set Dry G                  |             | as 4.0 l/min  |              |  |
| ican End                   | 1500 m/z                           |             | Set Collision Cell RF |           | 600.0 vpt      | )                                     | Set Divert Valve           |             |               | Source       |  |
| ntens.                     |                                    |             |                       |           | -              |                                       |                            | +MS, 4.0    | 6-4.8min #271 | 8-288        |  |
| x10 <sup>5</sup>           |                                    |             |                       | 308       | 4127           |                                       |                            |             |               | 1. 1. 1. 1.  |  |
| 1.0-                       |                                    |             |                       | 500       | 1              |                                       |                            |             |               |              |  |
|                            |                                    |             |                       |           | L. Marker L.   |                                       |                            |             |               |              |  |
| 0.8-                       |                                    |             |                       |           |                |                                       |                            |             |               |              |  |
| -                          |                                    |             |                       |           |                |                                       |                            |             |               |              |  |
| 0.6-                       |                                    |             |                       |           | 20415          |                                       |                            |             |               |              |  |
| -                          |                                    |             |                       |           | 330.094        | 7                                     |                            |             |               |              |  |
| 0.4- 150.054               | 9                                  |             |                       |           | 550.054        |                                       |                            |             |               |              |  |
|                            |                                    |             |                       |           |                |                                       |                            |             |               |              |  |
| 0.2-                       |                                    |             |                       |           |                |                                       | 201 2041                   |             |               | 1.           |  |
| 223,2055 255,2681 290,1022 |                                    |             |                       |           |                | 391.2841 4                            | 19.3151                    | 466.0       | 0689          |              |  |
| 0.0 4 4 150                |                                    | 200         | 250                   |           | And the second | 250                                   | 400                        | the free of | 450           | m/7          |  |
| Mana                       |                                    | 200         | 200                   | 500       |                | 300<br># Clama                        | 400                        | rdb         | - Conf        | N Dulo       |  |
| 150.0540                   | #                                  | CRURNO2     | 150.0550              | en [ppin] | moigina        | # moigma                              | 100.00                     | 5.5         | even          | N-Rule<br>ok |  |
| 308 1123                   | 7 1                                | C15H18NO6   | 308 1120              | 0.5       | 5.0            | 4                                     | 100.00                     | 7.5         | even          | ok           |  |
| 330.0947                   | 1                                  | C15H17NN2O6 | 330 0949              | 0.3       | 3.9            | 1                                     | 100.00                     | 75          | even          | ok           |  |
| 550.0541                   | 2                                  | C13H12N7O4  | 330 0945              | -0.5      | 5.4            | 2                                     | 94.52                      | 11.5        | even          | ok           |  |
| 391,2841                   | 1 1                                | C24H39O4    | 391,2843              | 0.5       | 12.9           | 1                                     | 100.00                     | 5.5         | even          | ok           |  |
| 413.2661                   | 1                                  | C24H38NaO4  | 413.2662              | 0.3       | 9.6            | 1                                     | 100.00                     | 5.5         | even          | ok           |  |
|                            | 2                                  | C22H33N6O2  | 413.2660              | -0.4      | 11.0           | 2                                     | 96.76                      | 9.5         | even          | ok           |  |
| 419.3151                   | .1                                 | C26H43O4    | 419.3156              | 1.2       | 13.8           | 1                                     | 100.00                     | 5.5         | even          | ok           |  |
|                            | 2                                  | C25H40N4Na  | 419.3145              | -1.4      | 18.2           | 2                                     | 87.96                      | 7.5         | even          | ok           |  |

# Figure S17. <sup>1</sup>H NMR (600 MHz, MeOH- $d_4$ ) spectrum of compound **3**.



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f1 (ppm)

Figure S18. COSY (600 MHz, MeOH- $d_4$ ) spectrum of compound **3**.



Figure S19. HSQC (600MHz/150 MHz, MeOH- $d_4$ ) spectrum of compound **3**.

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#### Figure S20. HMBC (600MHz/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of compound **3**.

Figure S21. Chromatogram of C<sub>4</sub>-Marfey's L-FDAA adduct of compound  $\mathbf{1}$ .





Figure S22. Chromatogram of  $C_4$ -Marfey's D-FDAA adduct of compound 1.