

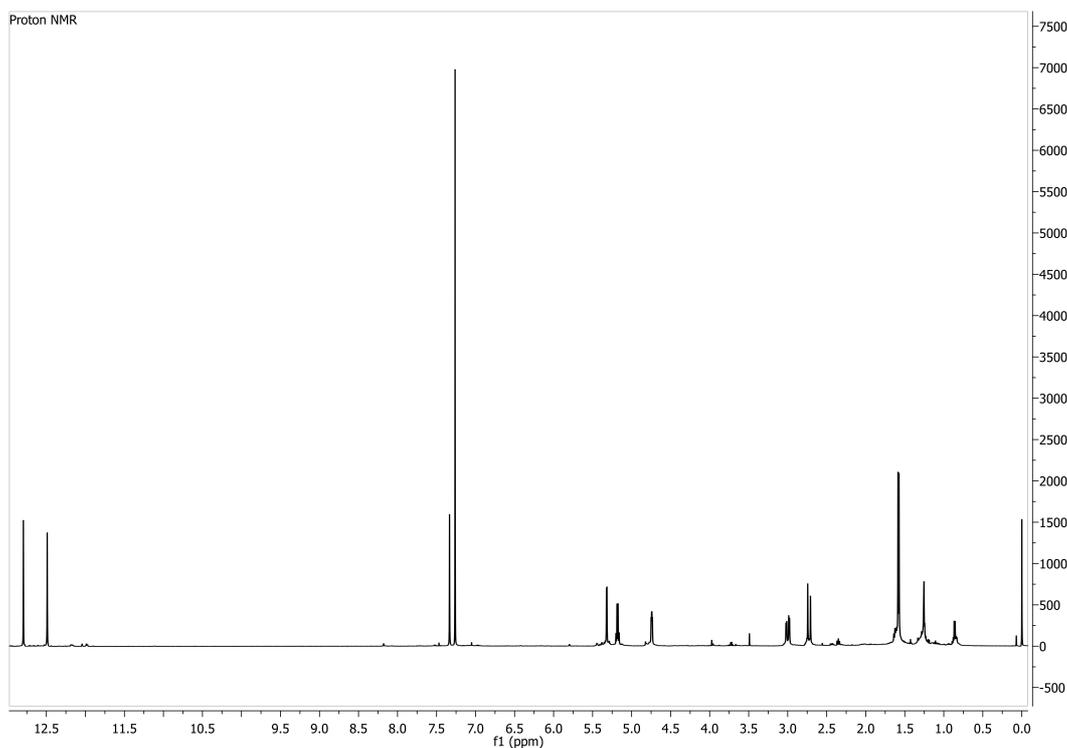
*Supplementary information for:*

**Revisiting unexploited antibiotics in search of new antibacterial drug candidates:  
the case of  $\gamma$ -actinorhodin**

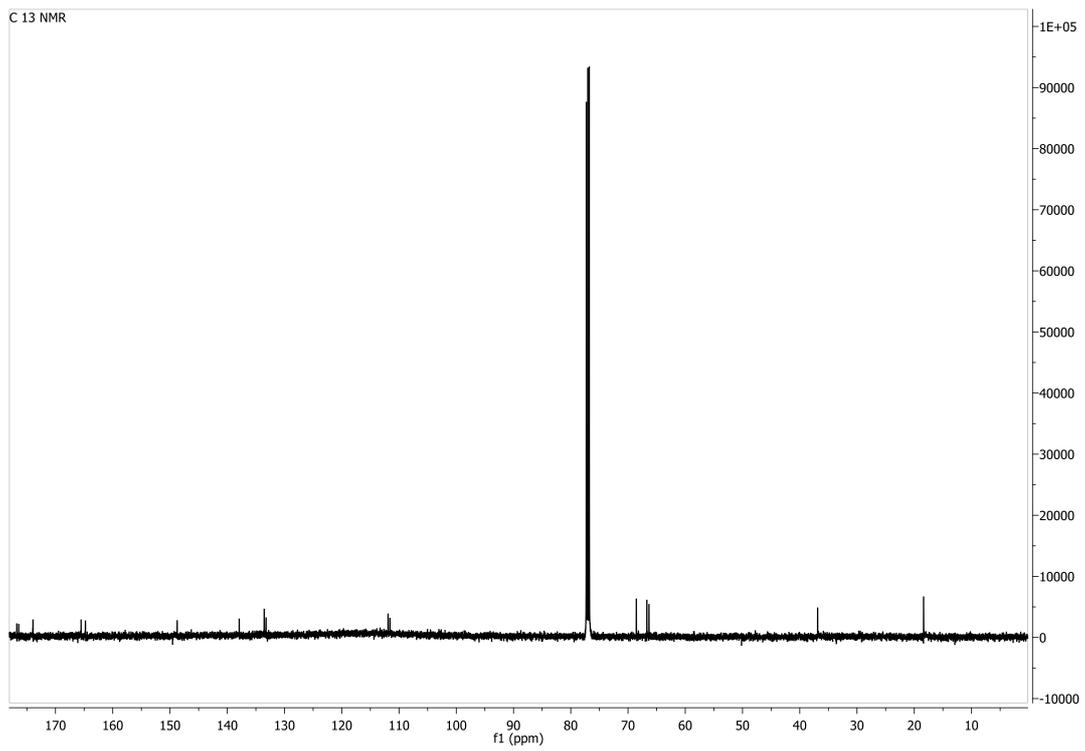
Nada M. Nass, Sannia Farooque, Charlotte Hind, Matthew E. Wand, Christopher P. Randall, J. Mark Sutton, Ryan F. Seipke, Christopher M. Rayner and Alex J. O'Neill

## Identification and characterization of $\gamma$ -actinorhodin

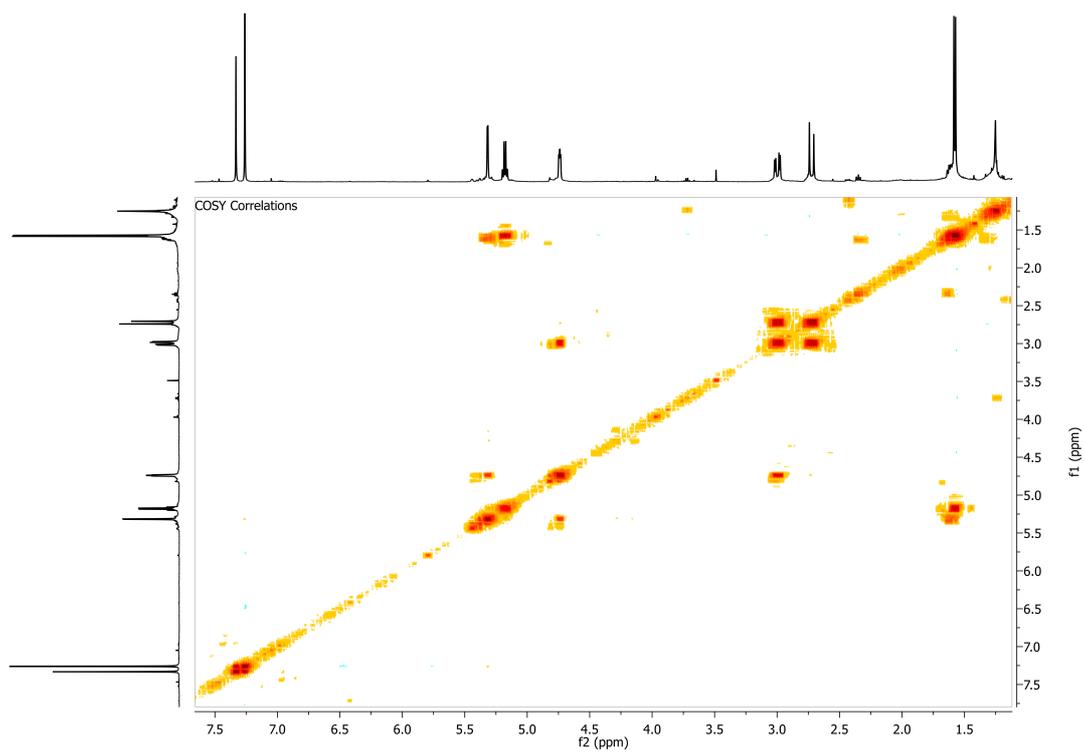
$\gamma$ -actinorhodin was isolated as red precipitate (125 mg, 19% w/w).  $R_f$  0.29 (1% MeOH in dichloromethane);  $\delta_H$  (500 MHz,  $CDCl_3$ ) 12.80 (1H, s, OH-9), 12.50 (1H, s, OH-6), 7.34 (1H, s, H-7), 5.33 (1H, d,  $J$  3.0 Hz, H-4), 5.19 (1H, q,  $J$  7.0 Hz, H-1), 4.74 (1H, m, H-3), 2.99 (1H, dd,  $J$  17.8, 5.3 Hz, H-11), 2.73 (1H, d,  $J$  17.8 Hz, H-11'), 1.59 (3H, d, 7.0 Hz,  $CH_3$ );  $\delta_C$  (125 MHz,  $CDCl_3$ ) 176.90 (C-5), 176.6 (C-10), 174.1 (C-12), 165.67 (C-6), 164.91 (C-9), 148.88 (C-10a), 138.04 (C-8), 133.68 (C-7), 133.35 (C-4a), 112.05 (C-9a), 111.72 (C-5a), 68.68 (C-4), 66.84 (C-1), 66.48 (C-3), 37.02 (C-11), 18.51 ( $CH_3$ ); HRMS (ESI<sup>-</sup>):  $m/z$  calculated for formula  $C_{32}H_{21}O_{14}$  [M-H] 629.0933; found 629.0922; IR ( $\nu_{max}$ , solid,  $cm^{-1}$ ): 3502, 2919, 2850, 1790, 1709, 1613, 1575, 1377, 1260.



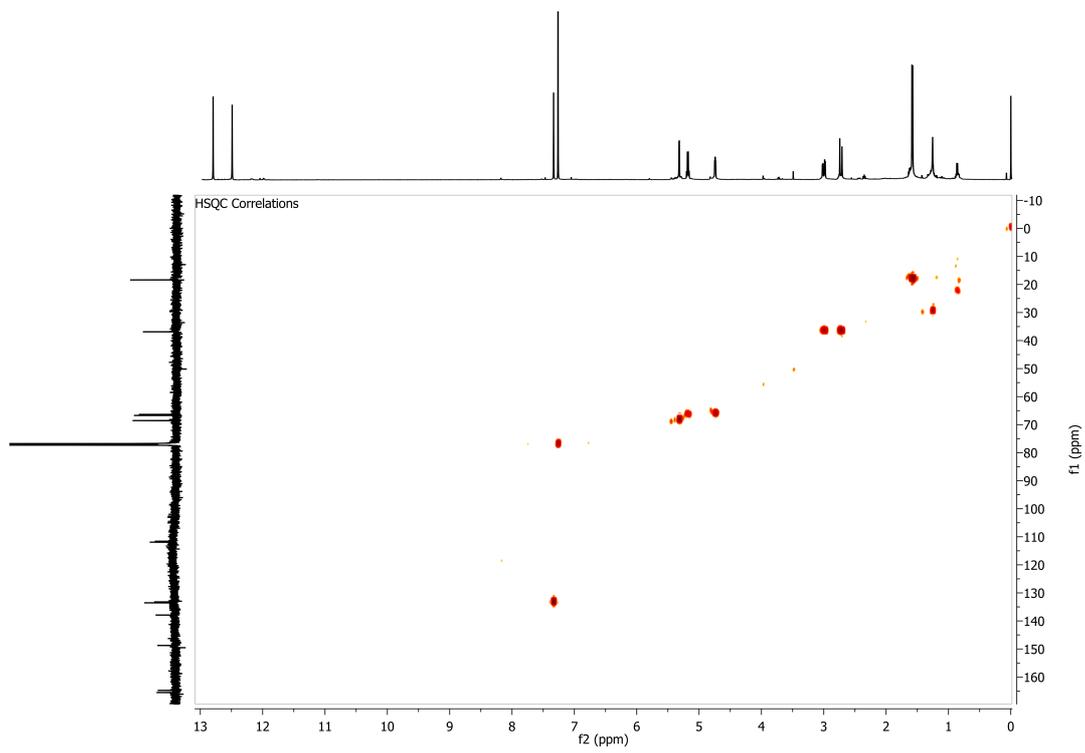
<sup>1</sup>H NMR spectrum for  $\gamma$ -actinorhodin



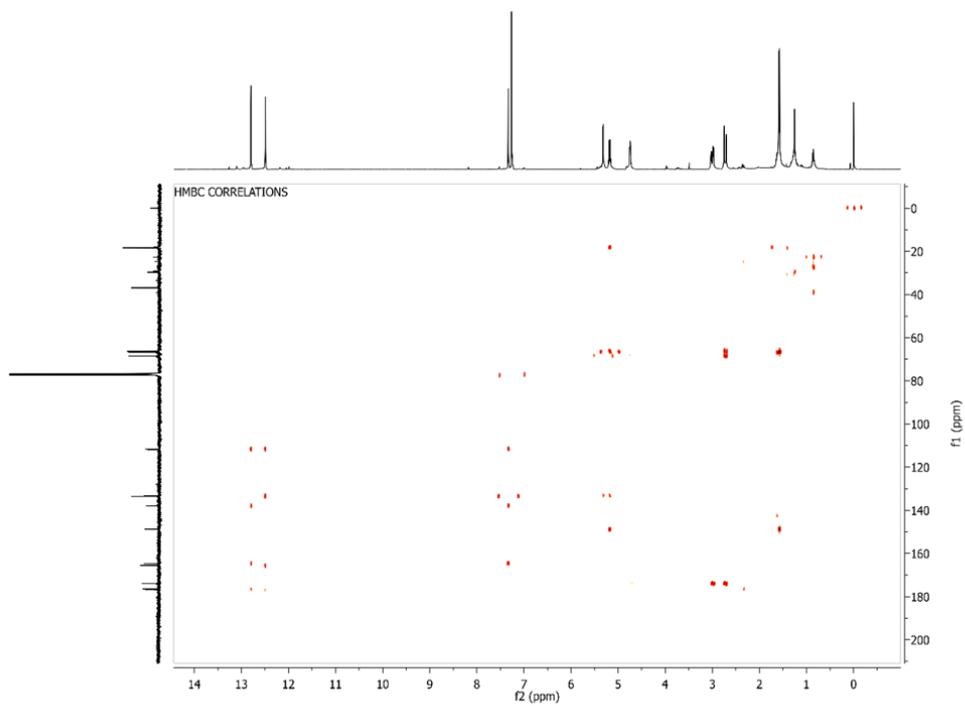
<sup>13</sup>C spectrum for  $\gamma$ -actinorhodin



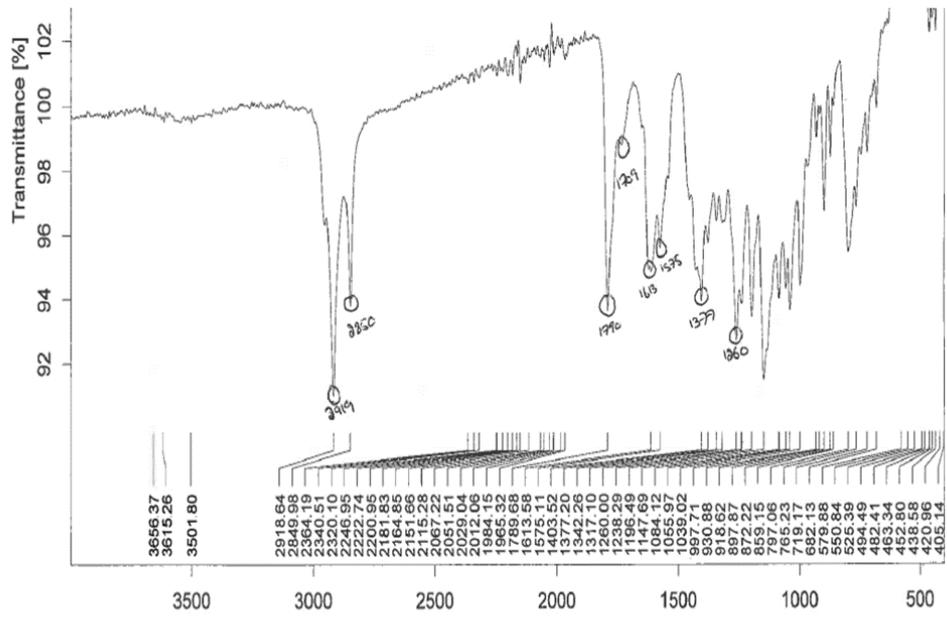
$^1\text{H}$ - $^1\text{H}$  COSY spectrum for  $\gamma$ -actinorhodin



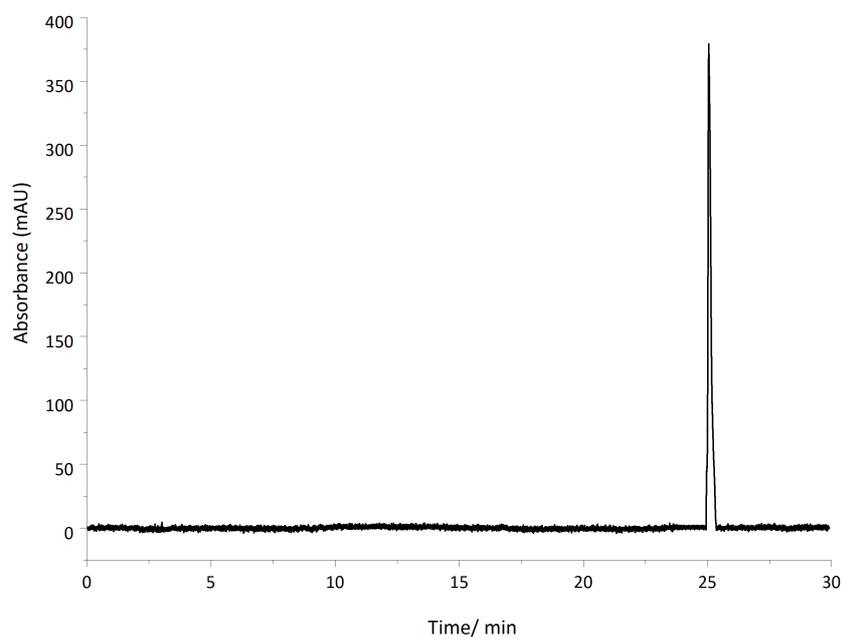
$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum for  $\gamma$ -actinorhodin



$^{13}\text{C}$ - $^1\text{H}$  HMBC spectrum for  $\gamma$ -actinorhodin



IR spectrum for  $\gamma$ -actinorhodin



HPLC chromatogram recorded for  $\gamma$ -actinorhodin in acetone at 520 nm