

Supplementary Materials

Antibacterial isoquinoline alkaloids from the fungus *Penicillium spathulatum* Em19

Christina Nord ¹, Jolanta J. Levenfors ^{1,2}, Joakim Bjerketorp ^{1,2}, Christer Sahlberg ³, Bengt Guss ⁴, Bo Öberg ^{2,5}, and Anders Broberg ^{1,*}

¹ Department of Molecular Sciences, Uppsala BioCentrum, Swedish University of Agricultural Sciences, P.O. Box 7015, SE-750 07 Uppsala, Sweden; Christina.Nord@slu.se (C.N.), Jolanta.Levenfors@slu.se (J.J.L.), Joakim.Bjerketorp@slu.se (J.B.), Anders.Broberg@slu.se (A.B.)

² Ultupharma AB, Södra Rudbecksgatan 13, SE-752 36 Uppsala, Sweden. bo.oberg1@gmail.com

³ Medivir AB, P.O. Box 1086, SE-141-22 Huddinge, Sweden; christer.sahlberg@gmail.com

⁴ Department of Biomedical Sciences and Veterinary Public Health, Swedish University of Agricultural Sciences, P.O. Box 7036, SE-750 07 Uppsala, Sweden; Bengt.Guss@slu.se

⁵ Department of Medicinal Chemistry, Uppsala University, P.O. Box 574, SE-751 23 Uppsala, Sweden

* Correspondence: Anders.Broberg@slu.se; Tel.: +46 18 672217.

Contents

Figure S1: ¹ H NMR (acetone- <i>d</i> ₆ , 600 MHz) spectrum of 1	3
Figure S2: ¹³ C NMR (acetone- <i>d</i> ₆ , 150 MHz) spectrum of 1	4
Figure S3: COSY NMR (acetone- <i>d</i> ₆) spectrum of 1	5
Figure S4: HSQC NMR (acetone- <i>d</i> ₆) spectrum of 1	6
Figure S5: HMBC NMR (acetone- <i>d</i> ₆) spectrum of 1	7
Figure S6: ¹ H NMR (acetone- <i>d</i> ₆ , 600 MHz) spectrum of 2	8
Figure S7: ¹³ C NMR (acetone- <i>d</i> ₆ , 150 MHz) spectrum of 2	9
Figure S8: COSY NMR (acetone- <i>d</i> ₆) spectrum of 2	10
Figure S9: HSQC NMR (acetone- <i>d</i> ₆) spectrum of 2	11
Figure S10: HMBC NMR (acetone- <i>d</i> ₆) spectrum of 2	12
Figure S11: ¹ H NMR (acetone- <i>d</i> ₆ , 600 MHz) spectrum of 3 . Integral values shown for signals from compound 3, the other signals belong to compound 1 , the solvent or residual amounts of methanol....	13
Figure S12: ¹³ C NMR (acetone- <i>d</i> ₆ , 150 MHz) spectrum of 3 . Shift values shown for carbons from compound 3, remaining signals belong to compound 1	14
Figure S13: COSY NMR (acetone- <i>d</i> ₆) spectrum of 3	15
Figure S14: HSQC NMR (acetone- <i>d</i> ₆) spectrum of 3	16

Figure S15: HMBC NMR (acetone- d_6) spectrum of 3	17
Figure S16: HRMS base peak chromatogram of the mixture of compound 3 (2.6 min – m/z 242.0451) and compound 1 (3.0 min – m/z 246.0762).	18
Figure S17: HR mass spectrum of compound 1 , m/z 246.0762 [M+H] ⁺ (calcd. for C ₁₃ H ₁₂ NO ₄ , 246.0761).	18
Figure S18: HR mass spectrum of compound 2 , m/z 202.0861 [M+H] ⁺ (calcd. for C ₁₂ H ₁₂ NO ₂ , 202.0863).	18
Figure S17: HR mass spectrum of compound 3 , m/z 242.0451 [M+H] ⁺ (calcd. for C ₁₃ H ₈ NO ₄ , 242.0448).	18

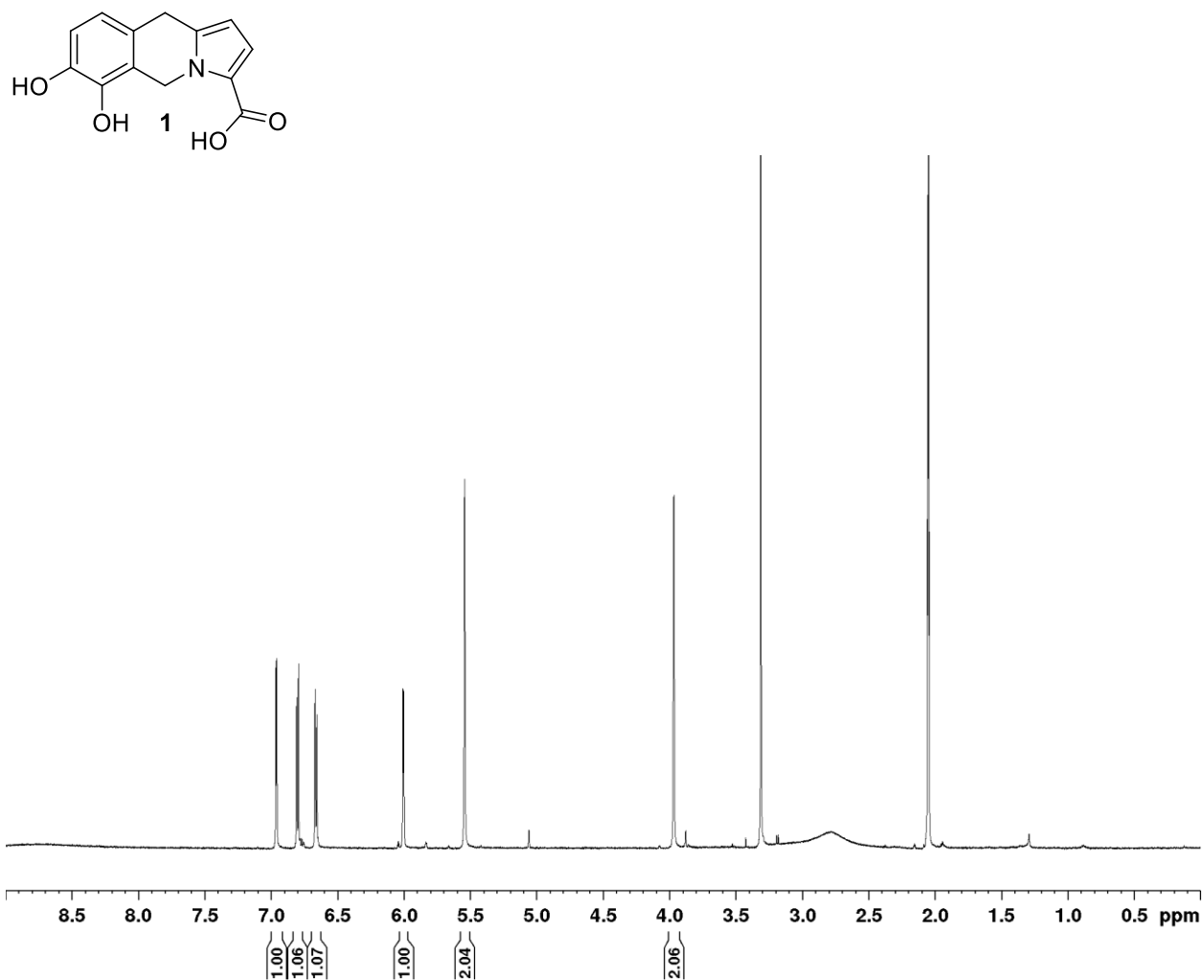


Figure S1: ¹H NMR (acetone-*d*₆, 600 MHz) spectrum of **1**. Signal at δ_{H} 2.05 is acetone-*d*₅ and the signal at δ_{H} 3.31 is methanol.

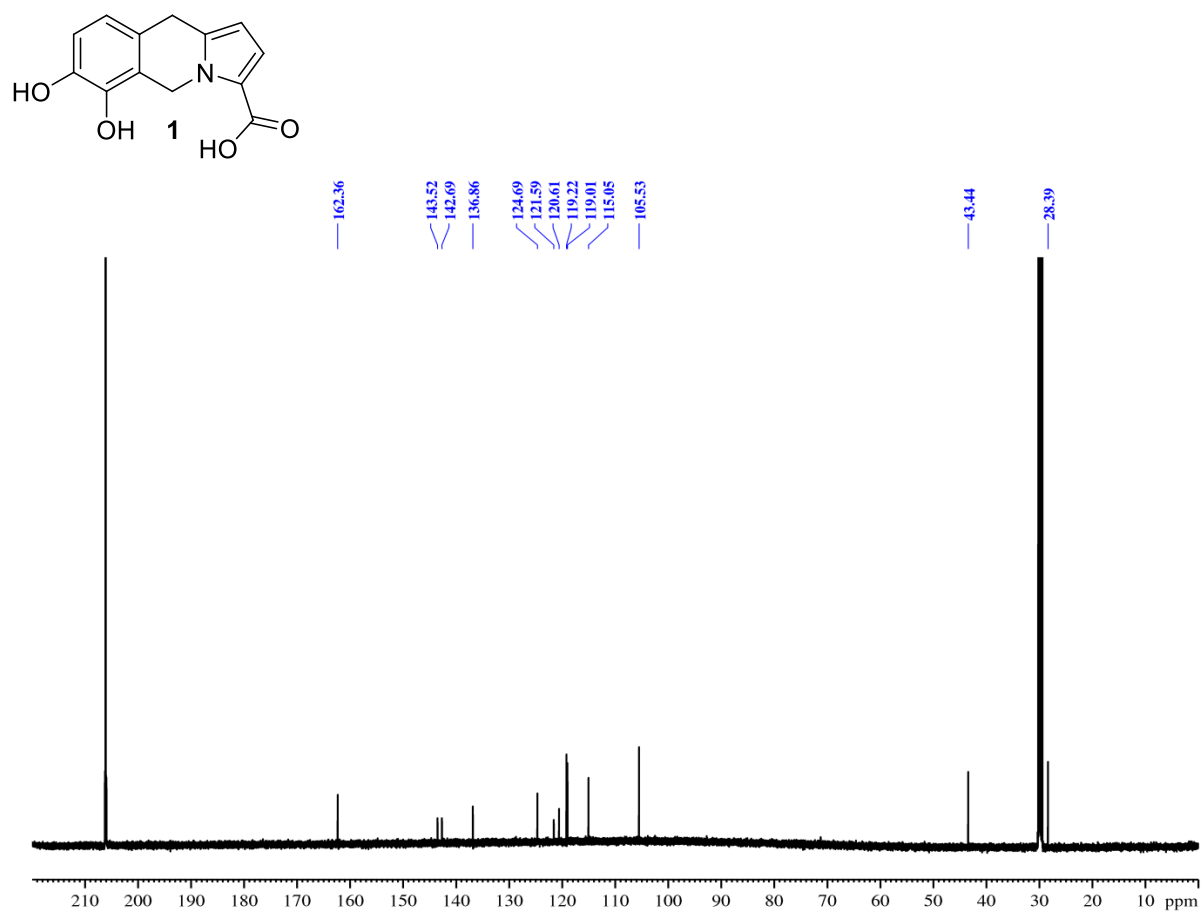


Figure S2: ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of **1**.

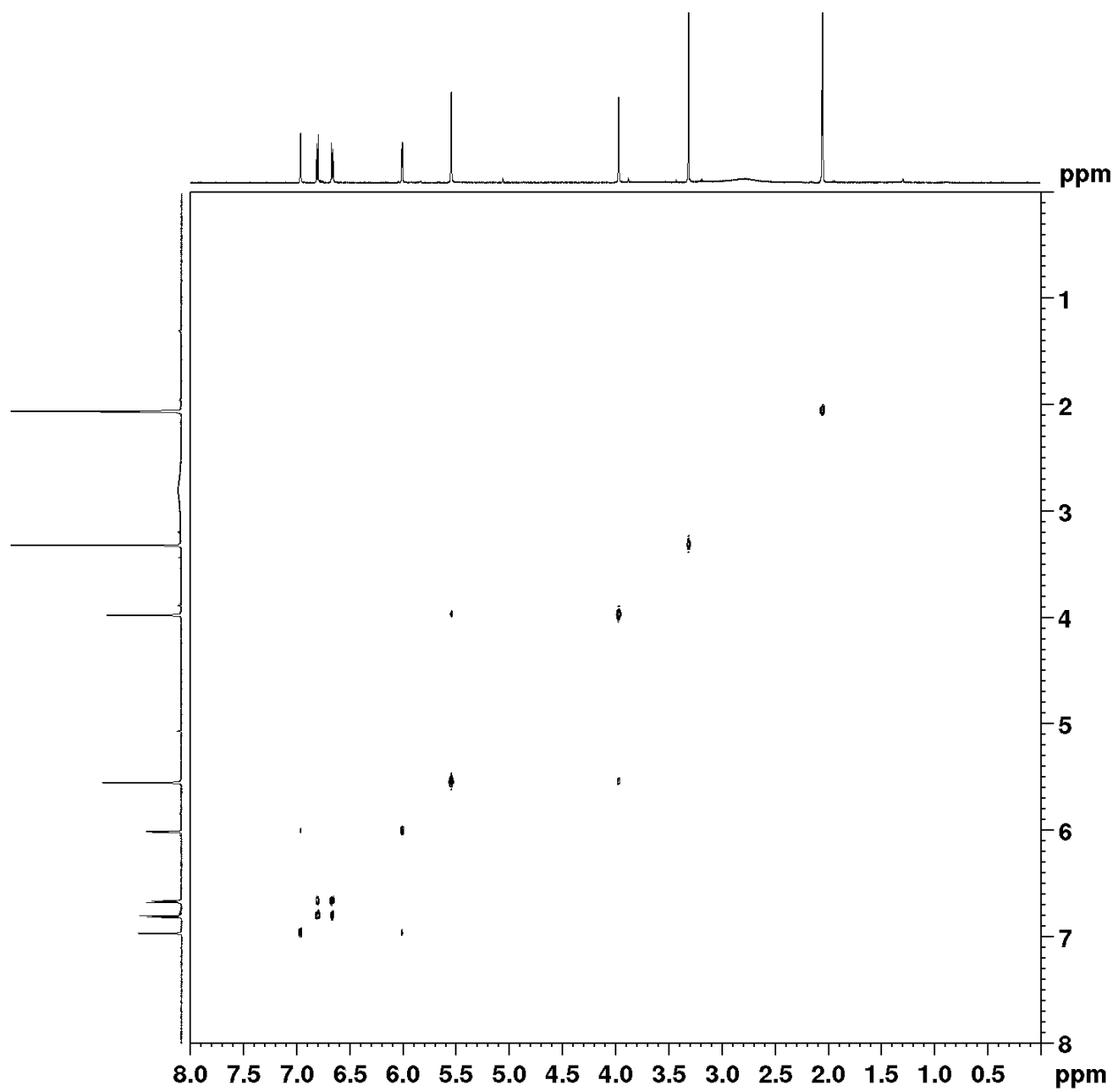
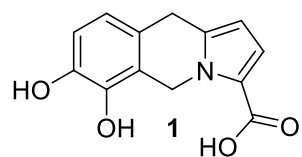


Figure S3: COSY NMR (acetone- d_6) spectrum of **1**. Signal at δ_H 2.05 is acetone- d_5 and the signal at δ_H 3.31 is methanol.

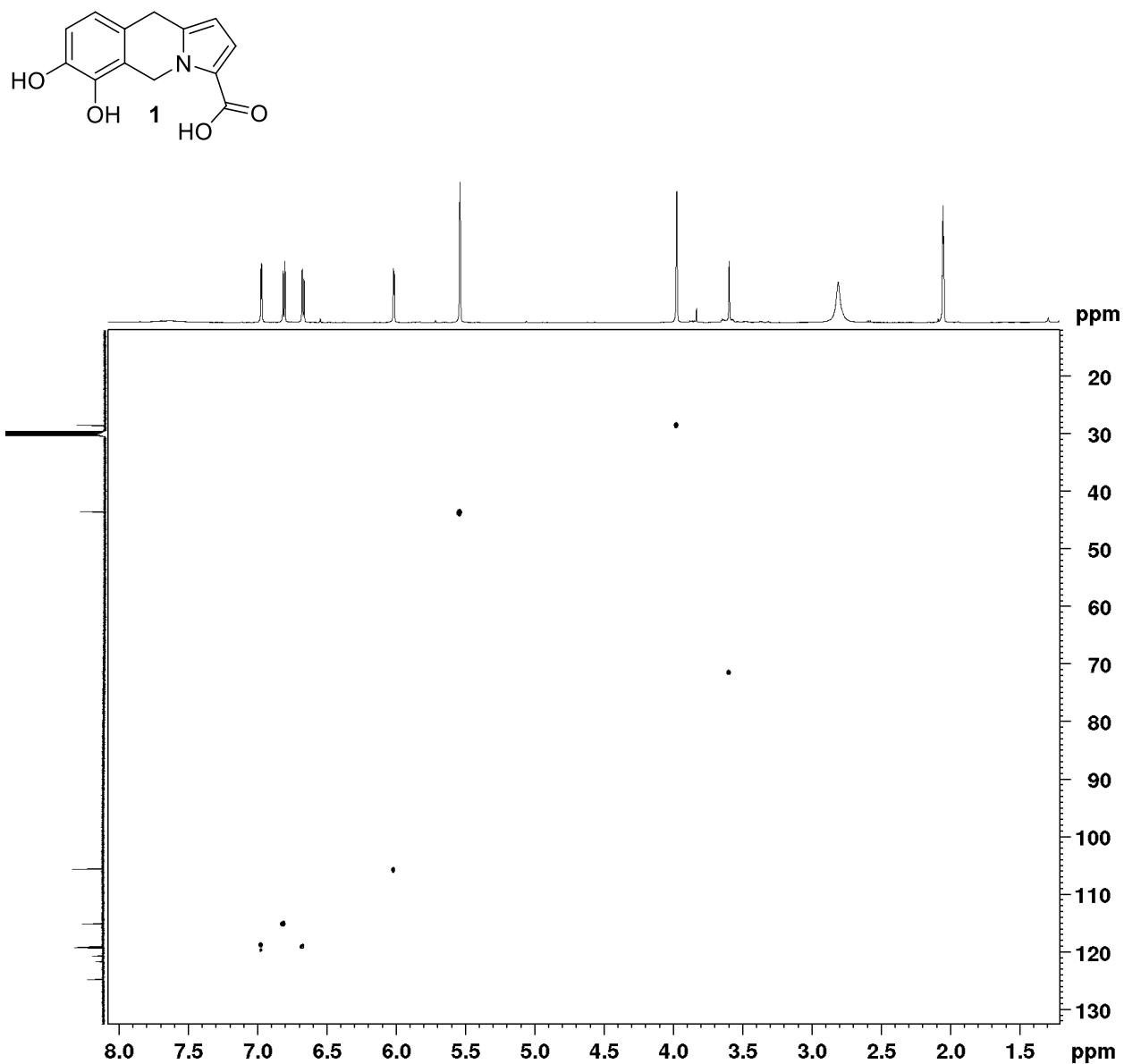


Figure S4: HSQC NMR (acetone- d_6) spectrum of **1**. Signal at $\delta_{\text{H}} 3.59 / \delta_{\text{C}} 71.4$ is from a polyethylene glycol type contaminant.

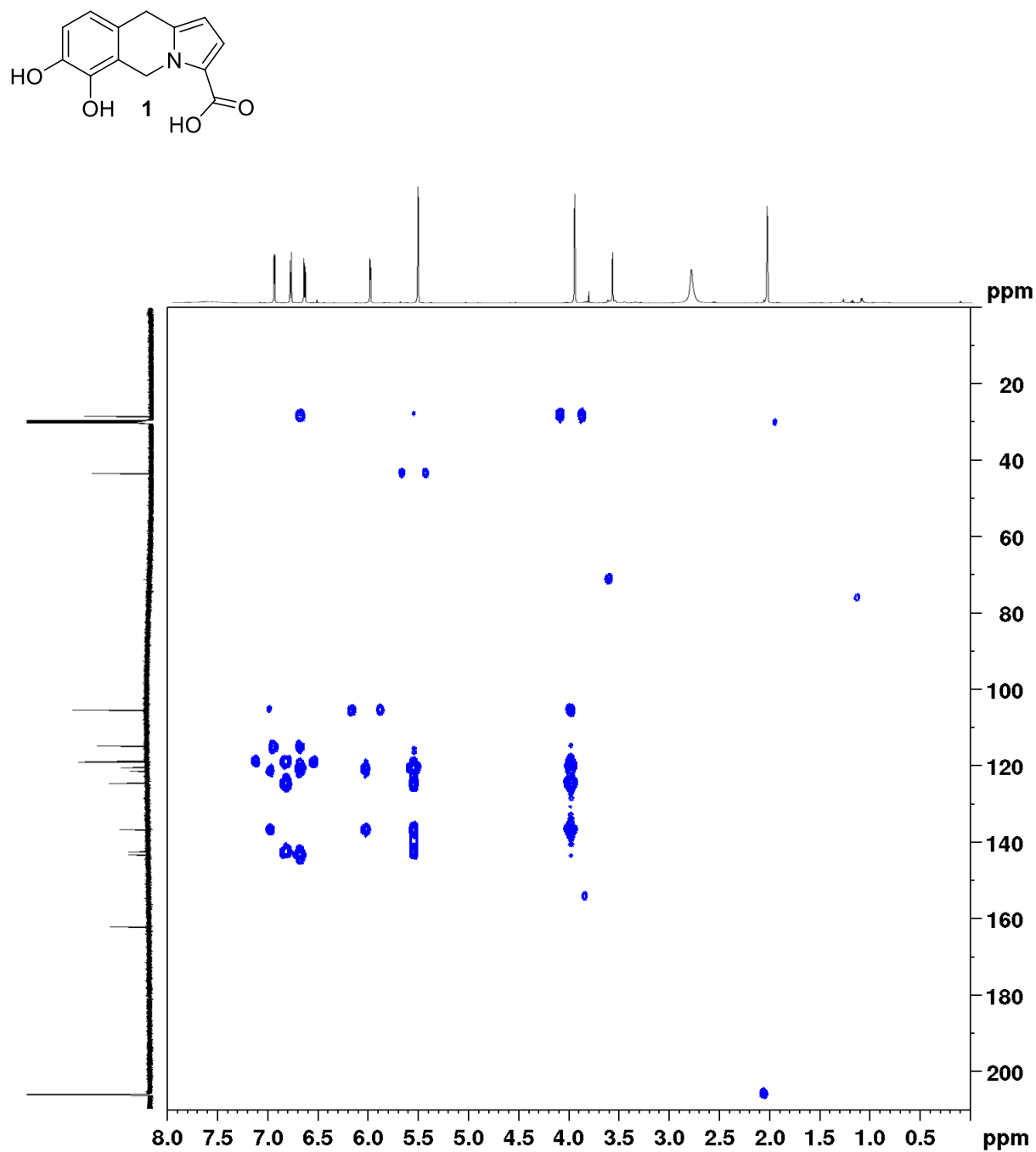


Figure S5: HMBC NMR (acetone- d_6) spectrum of **1**. Signal at δ_H 3.59/ δ_C 71.4 is from a polyethylene glycol type contaminant.

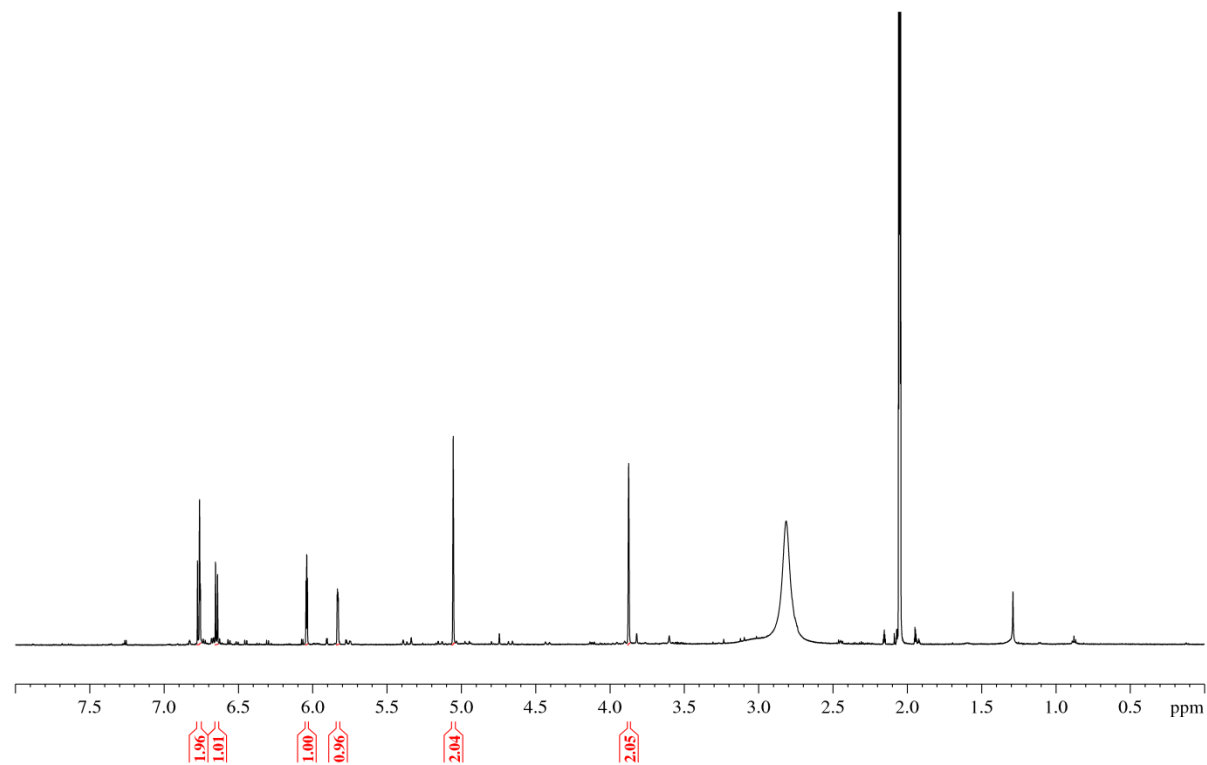
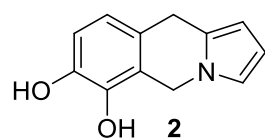


Figure S6: ^1H NMR (acetone- d_6 , 600 MHz) spectrum of **2**. Signal at δ_{H} 2.05 from acetone- d_5 .

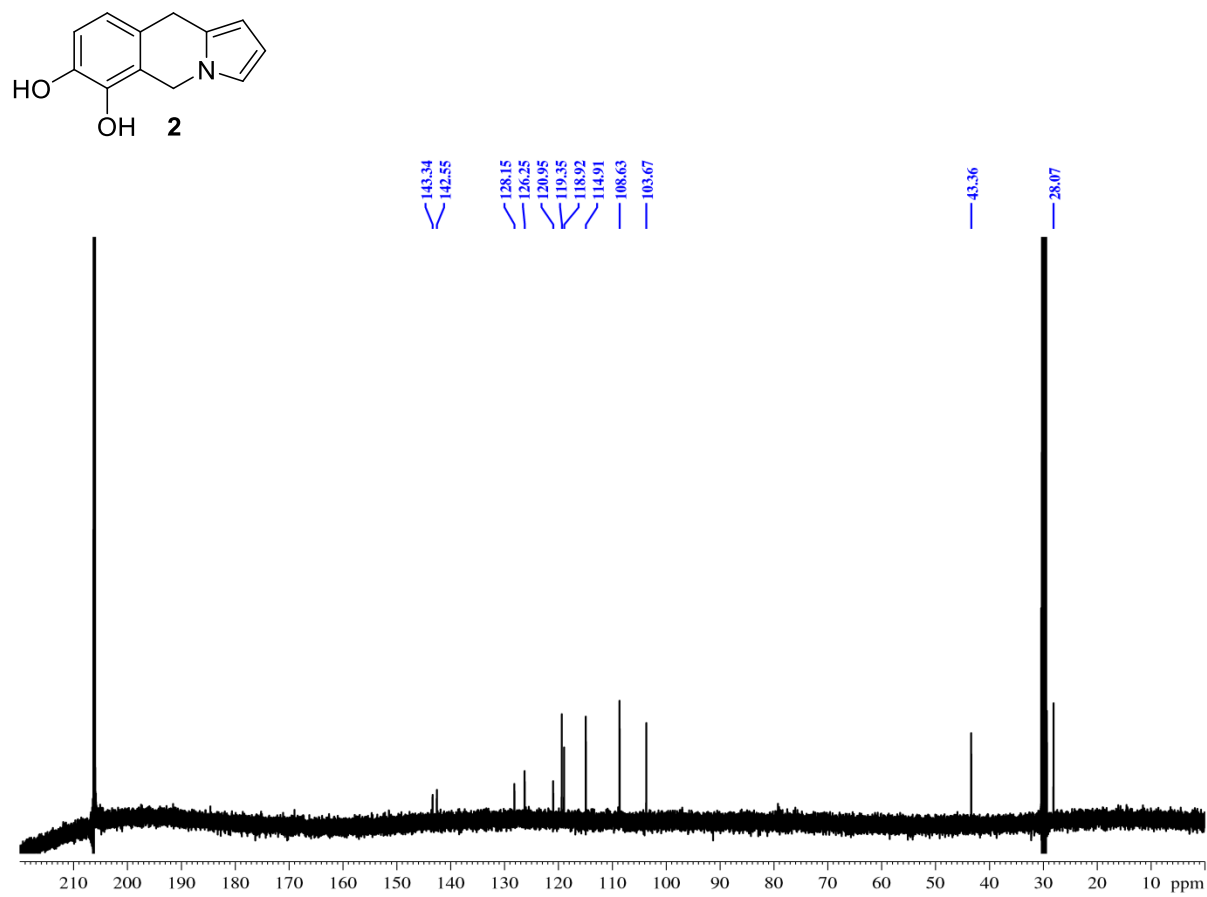


Figure S7: ¹³C NMR (acetone-*d*₆, 150 MHz) spectrum of **2**.

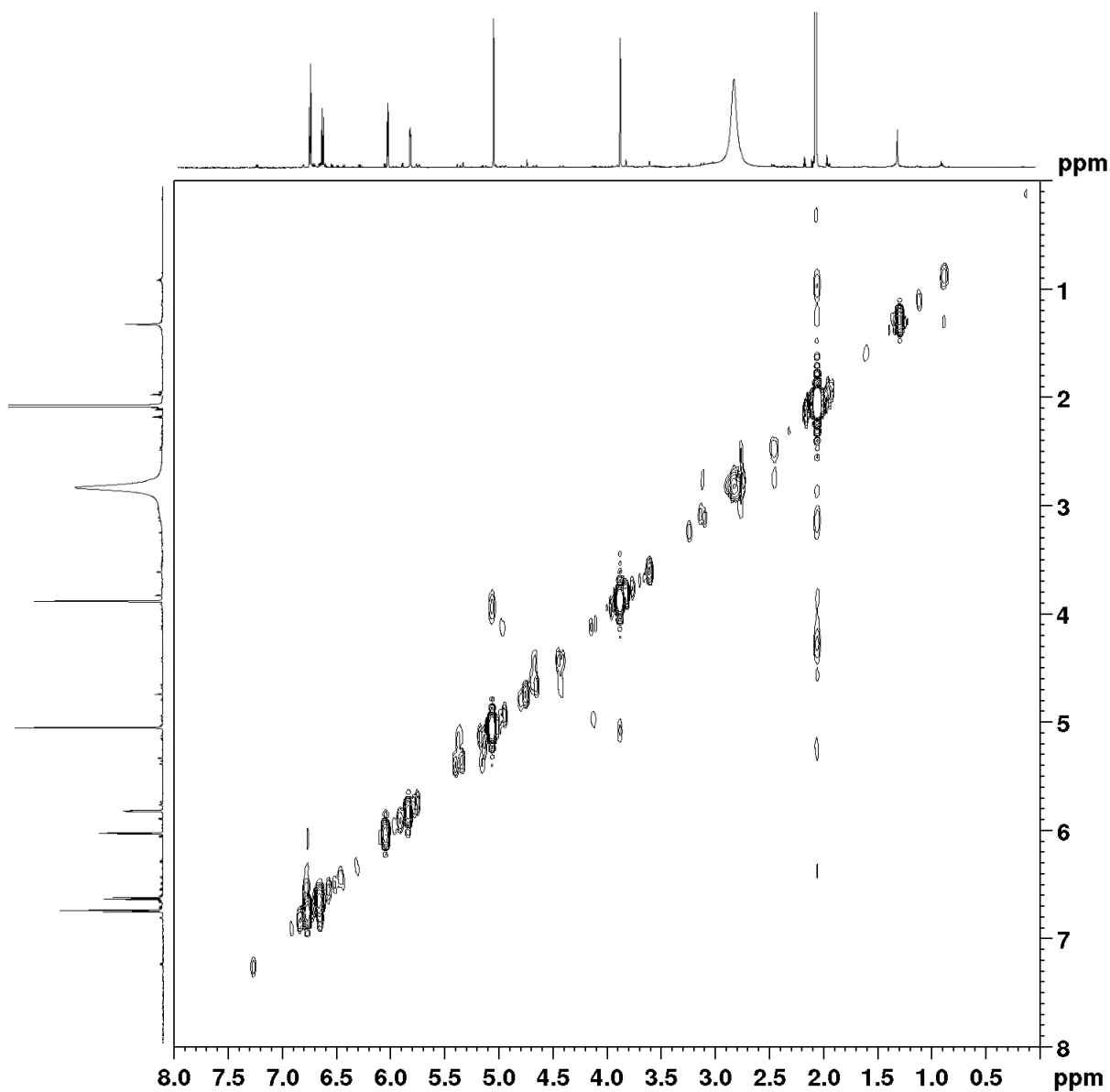
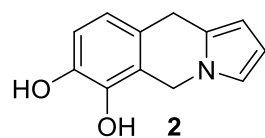


Figure S8: COSY NMR (acetone- d_6) spectrum of **2**.

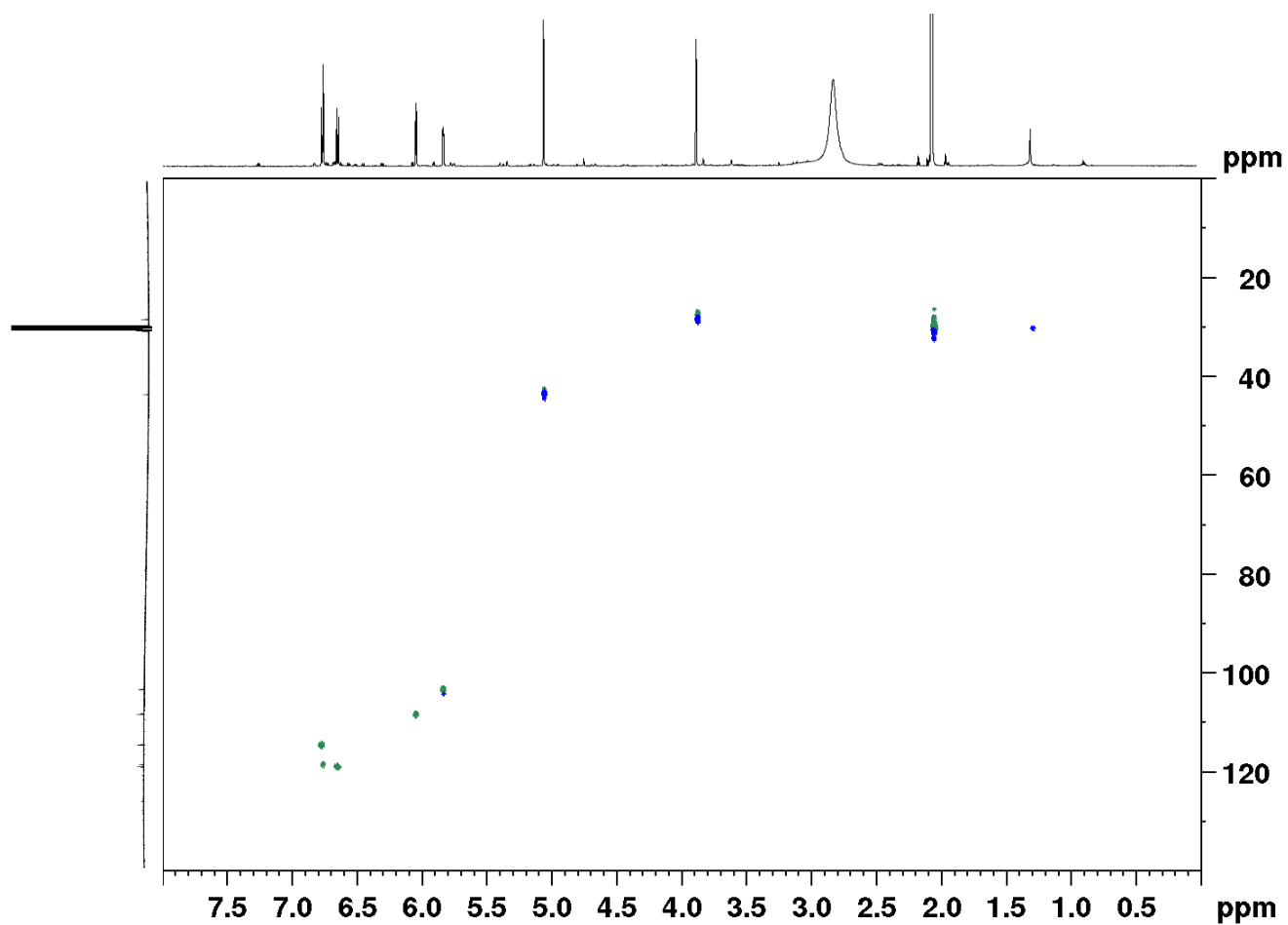
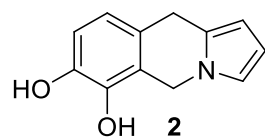


Figure S9: HSQC NMR (acetone- d_6) spectrum of 2.

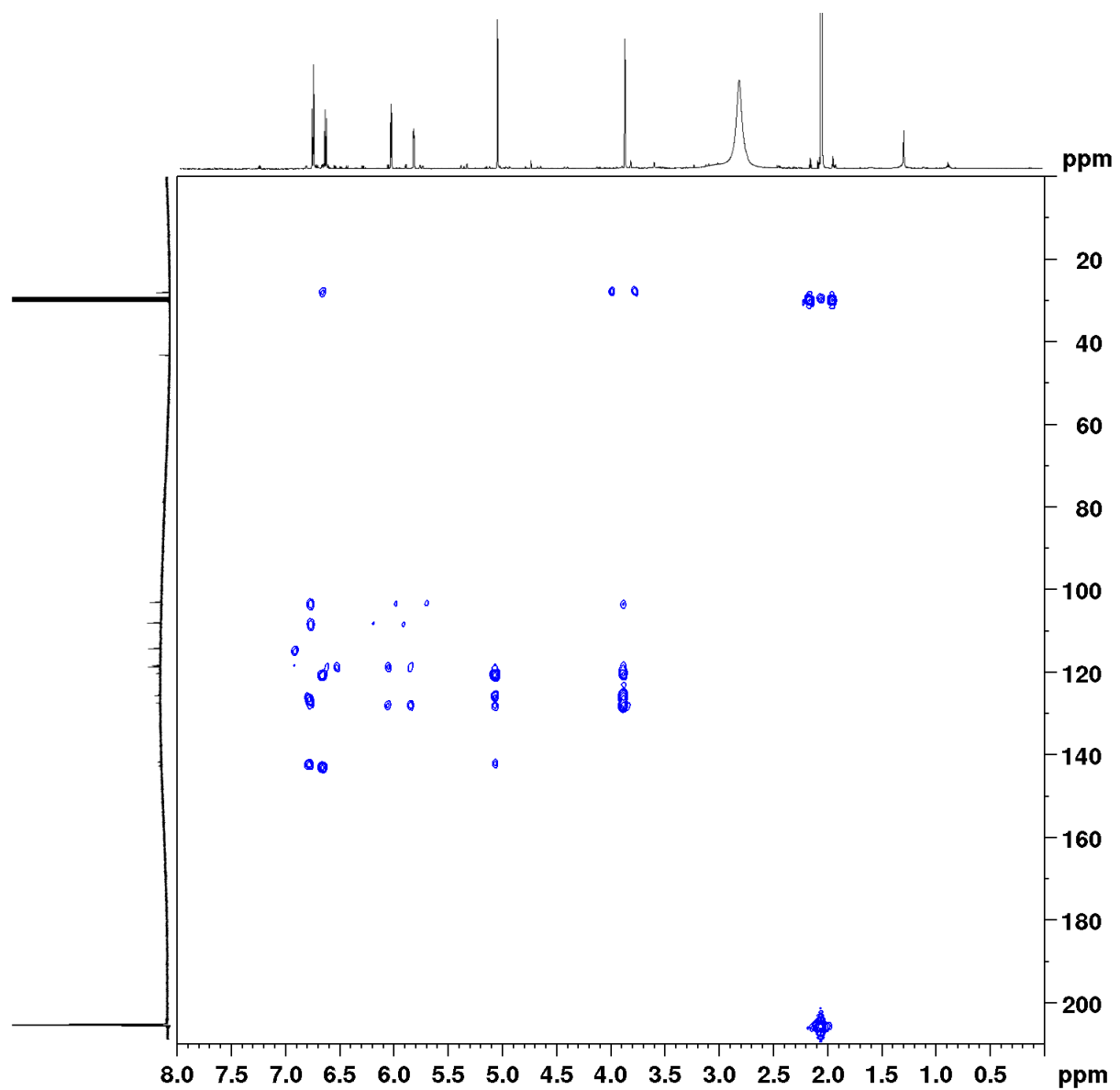
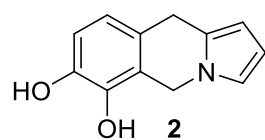


Figure S10: HMBC NMR (acetone- d_6) spectrum of **2**.

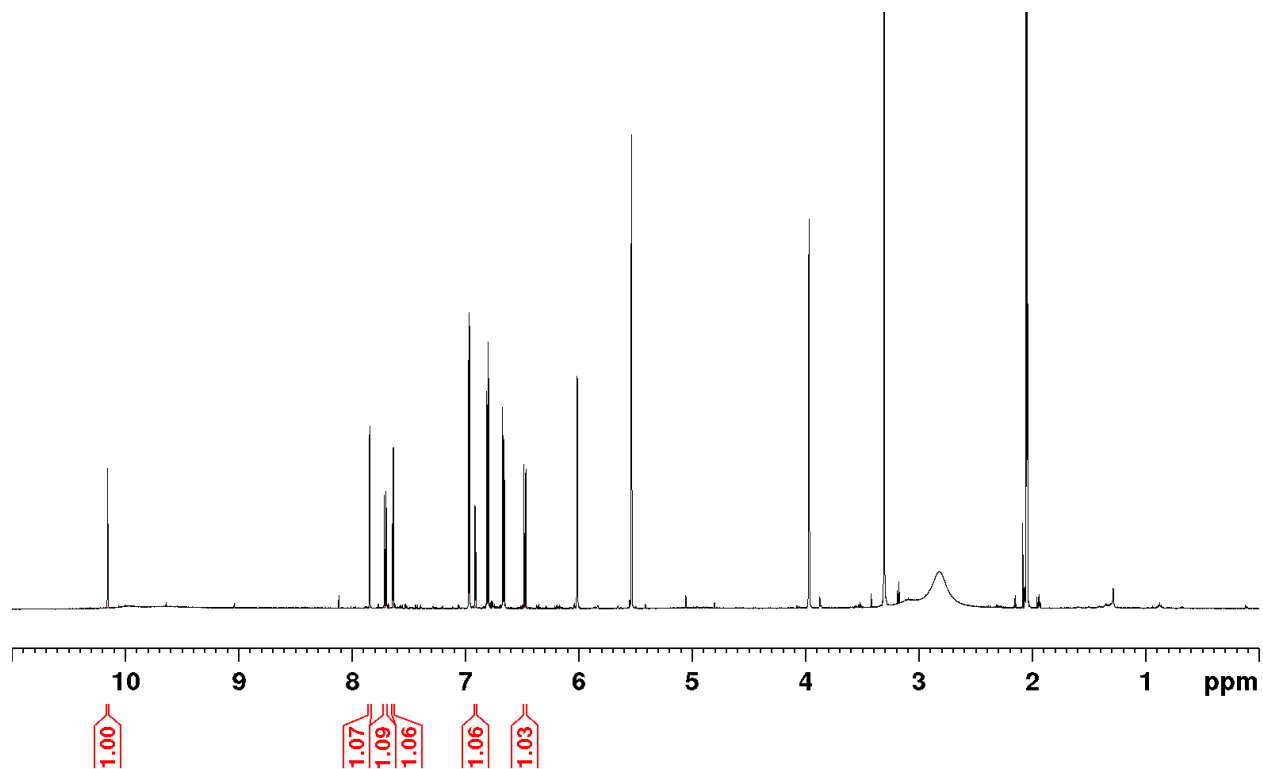
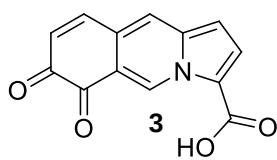


Figure S11: ^1H NMR (acetone- d_6 , 600 MHz) spectrum of **3**. Integrals are shown for signals from compound **3**, the other signals belong to compound **1**, acetone- d_5 (δ_{H} 2.05) or residual methanol (δ_{H} 3.31).

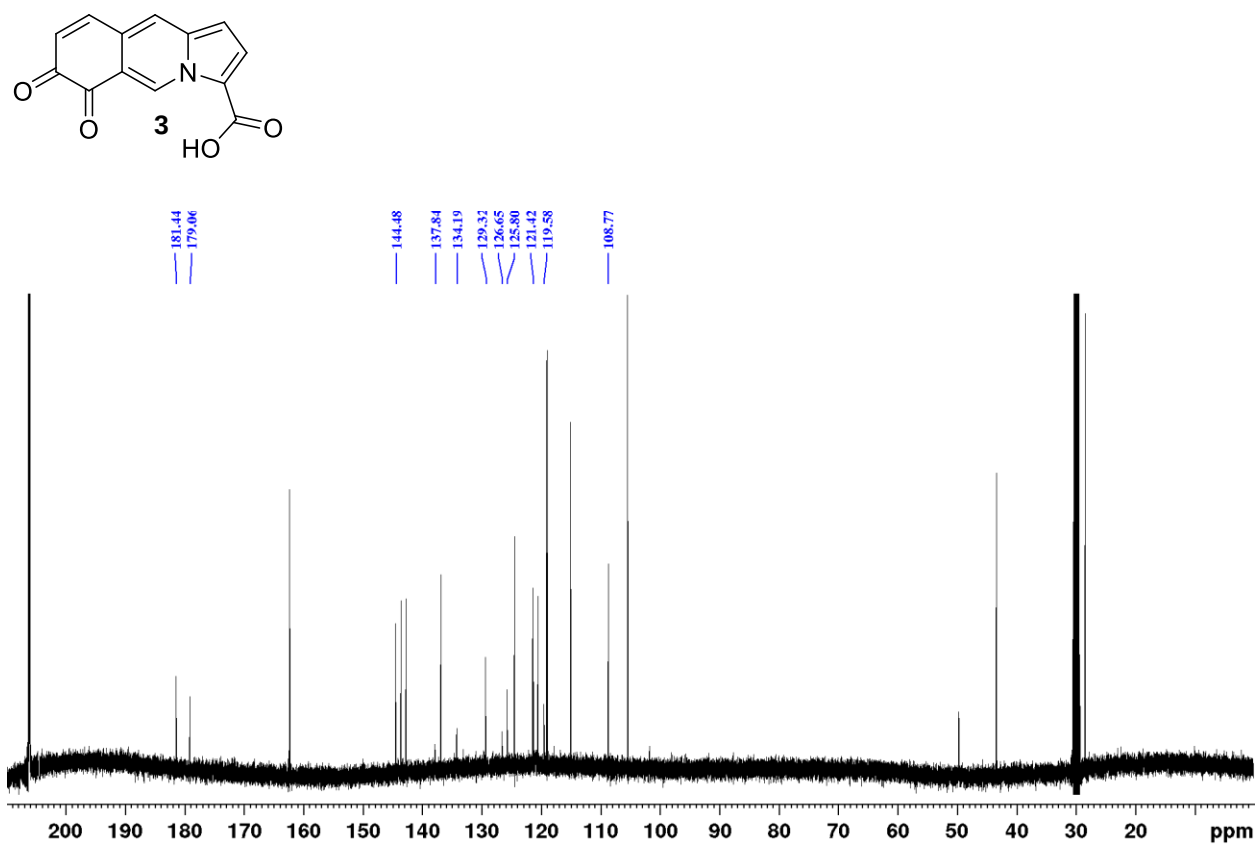


Figure S12: ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of **3**. Chemical shifts are shown for carbons from compound **3**, and remaining signals belong to compound **1**.

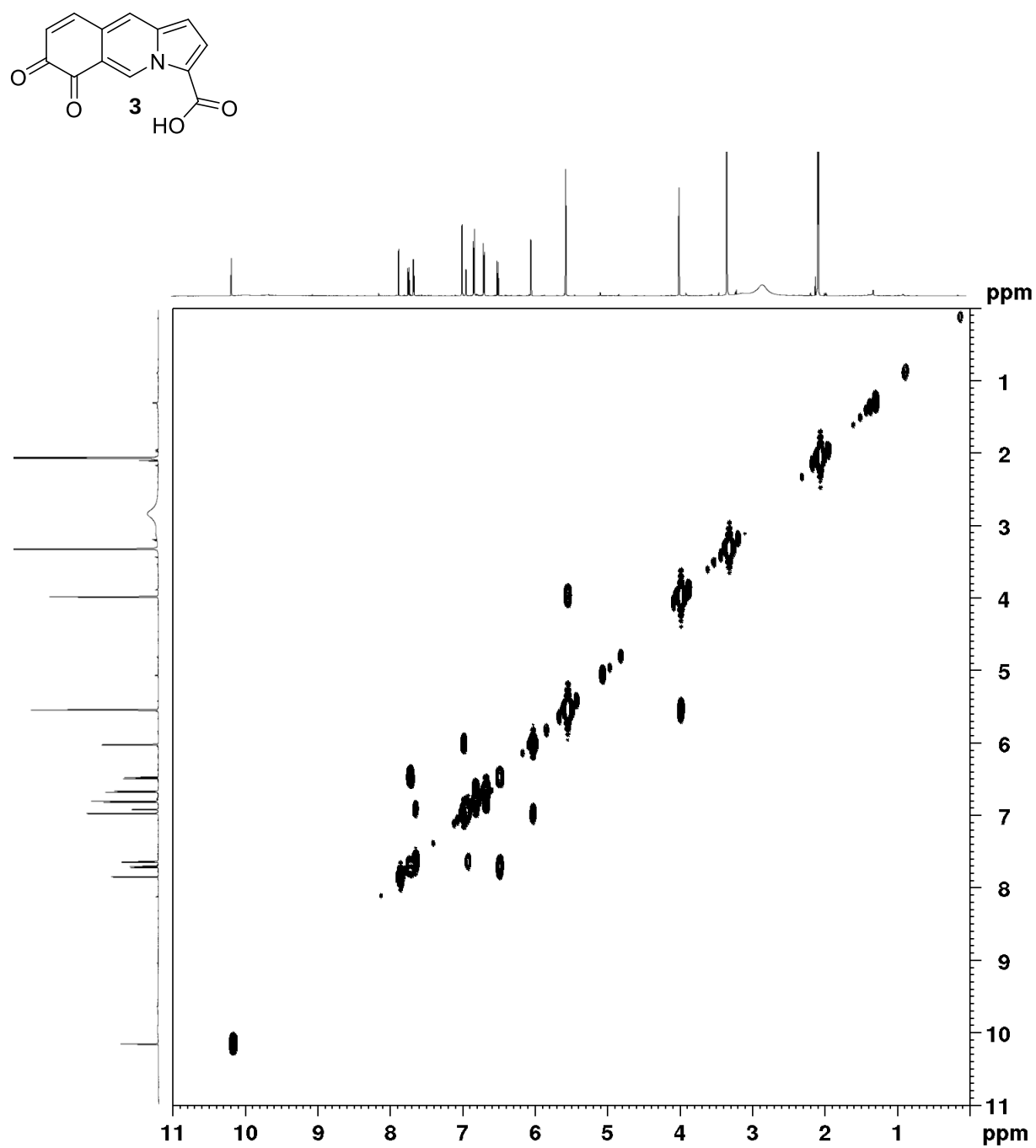


Figure S13: COSY NMR (acetone- d_6) spectrum of **3**.

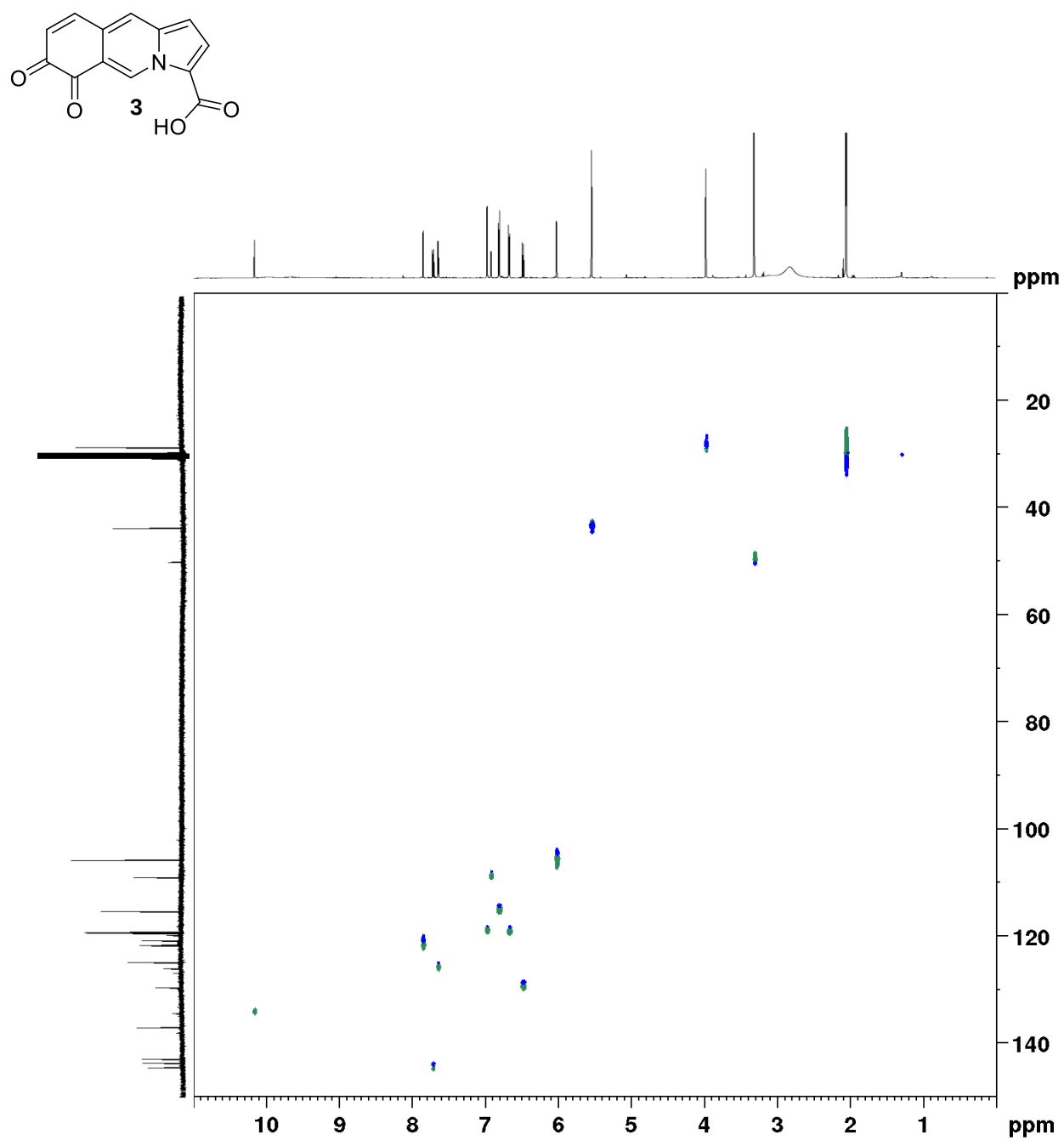


Figure S14: HSQC NMR (acetone- d_6) spectrum of **3**.

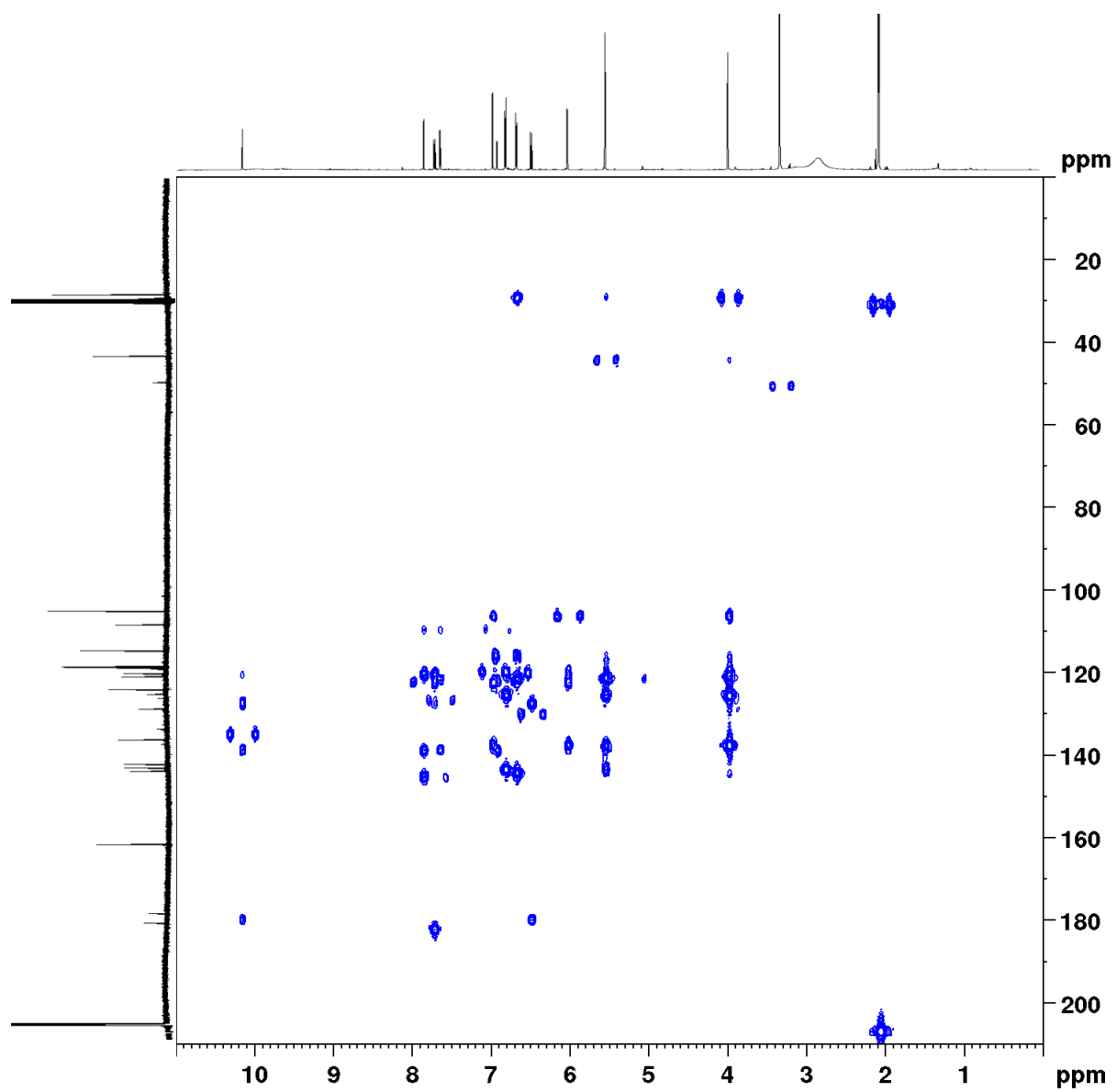
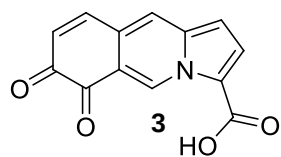


Figure S15: HMBC NMR (acetone- d_6) spectrum of 3.

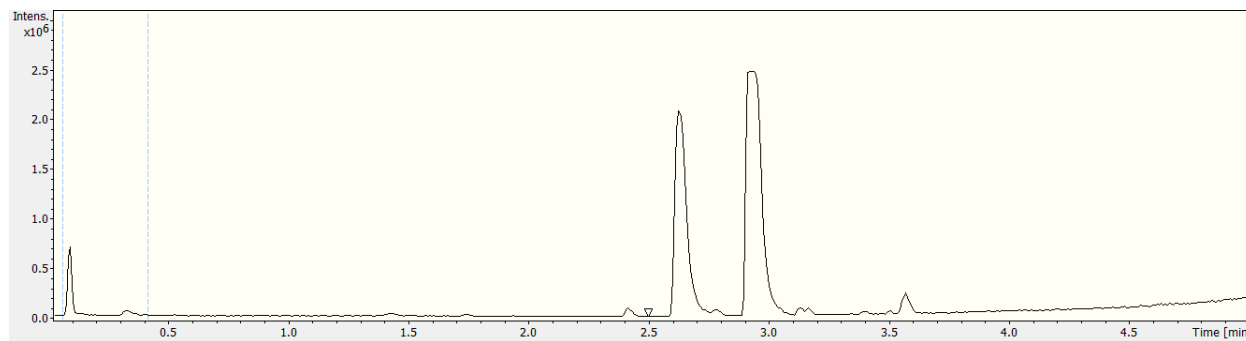


Figure S16: HRMS base peak chromatogram of the mixture of compound **3** (2.6 min – m/z 242.0451) and compound **1** (3.0 min – m/z 246.0762).

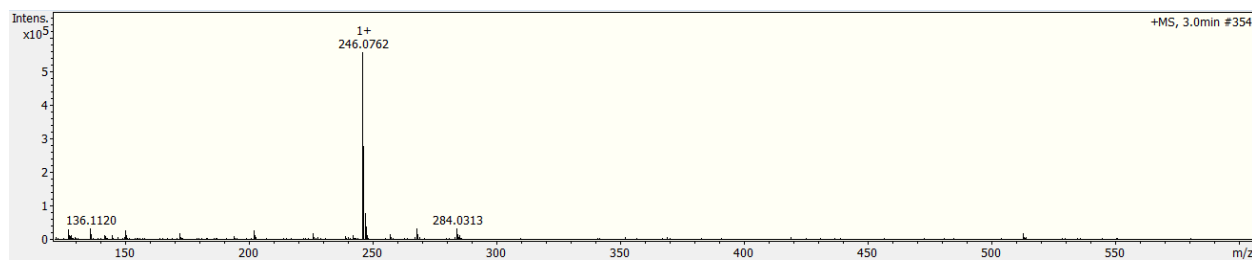


Figure S17: HR mass spectrum of compound **1**, m/z 246.0762 $[M+H]^+$ (calcd. for $C_{13}H_{12}NO_4$, 246.0761).

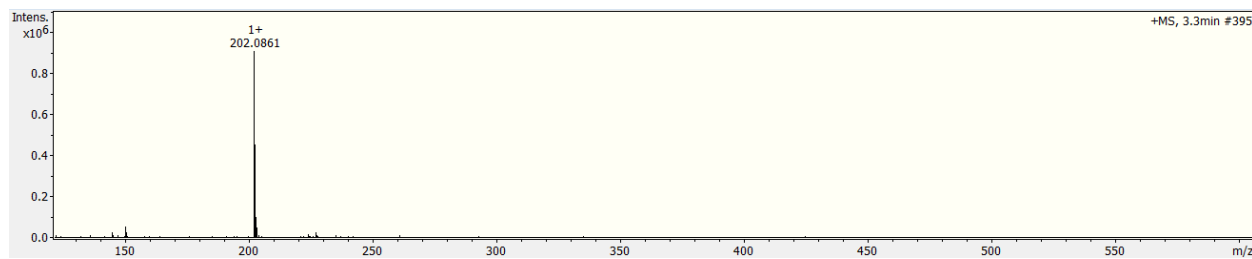


Figure S18: HR mass spectrum of compound **2**, m/z 202.0861 $[M+H]^+$ (calcd. for $C_{12}H_{12}NO_2$, 202.0863).

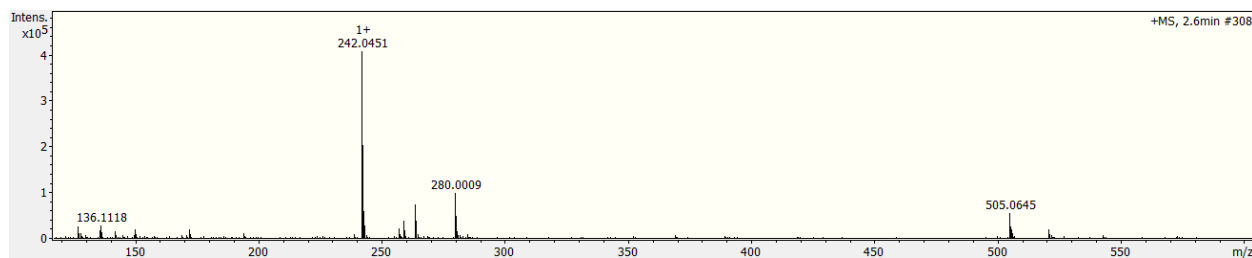


Figure S19: HRMS spectrum of compound **3**, m/z 242.0451 $[M+H]^+$ (calcd. for $C_{13}H_8NO_4$, 242.0448).