

Supplementary Information for

Guanine crystal formation by bacteria

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Additional file 2

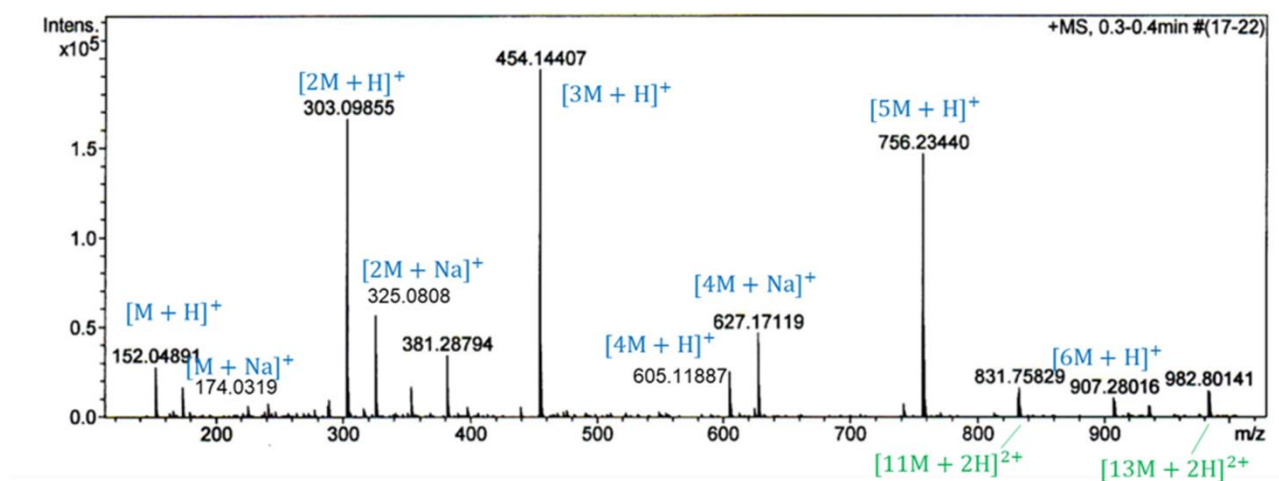


Fig. S3. ESI-MS experimental results for guanine produced by 34mel. The spectrum shows guanine association in solution. Solvent: methanol: DMSO 80:20.

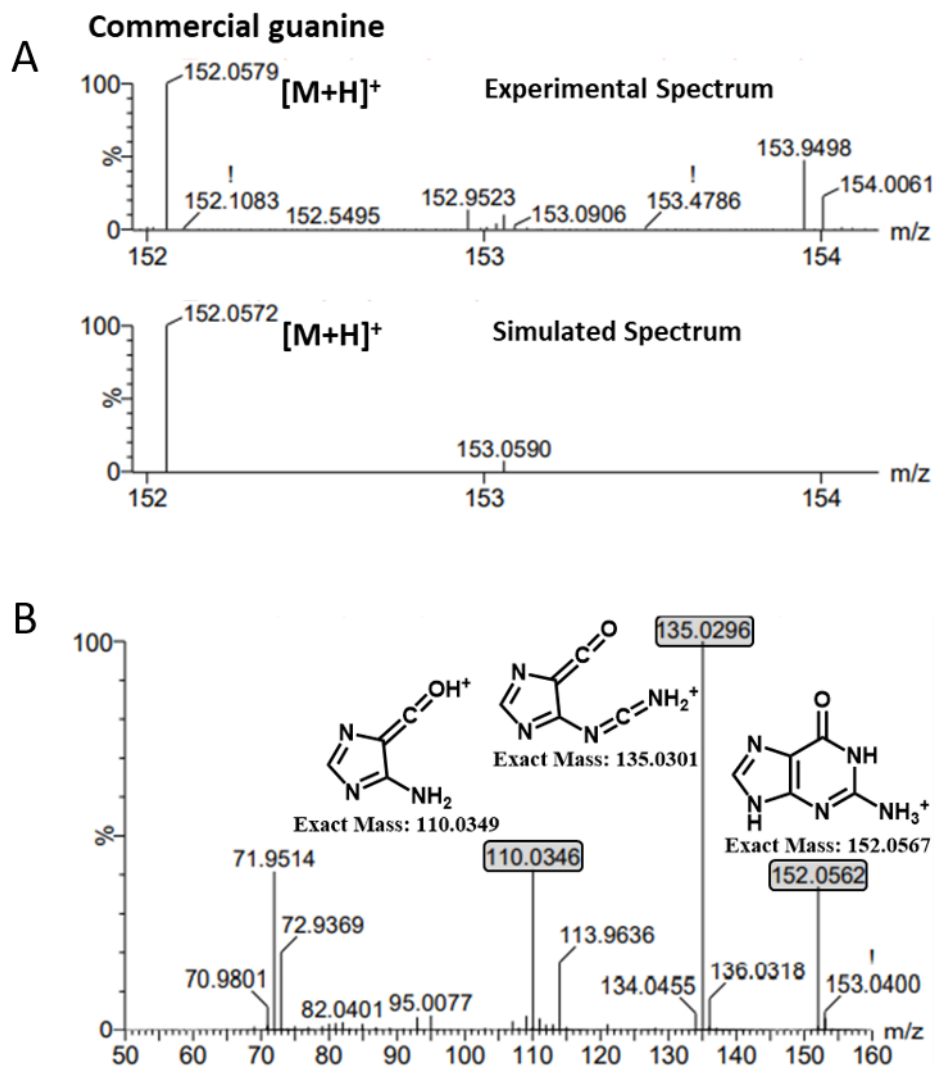


Fig. S4. ESI-MS and MS/MS experiments for commercial guanine. A ESI-MS experimental result compared with the simulated spectrum; $[M+H]^+$ ion (m/z 152.0579) is indicated. **B** MS/MS experimental results using $[M+H]^+$ ion (m/z 152.0579) as the parent ion. Solvent: methanol: H_2O .

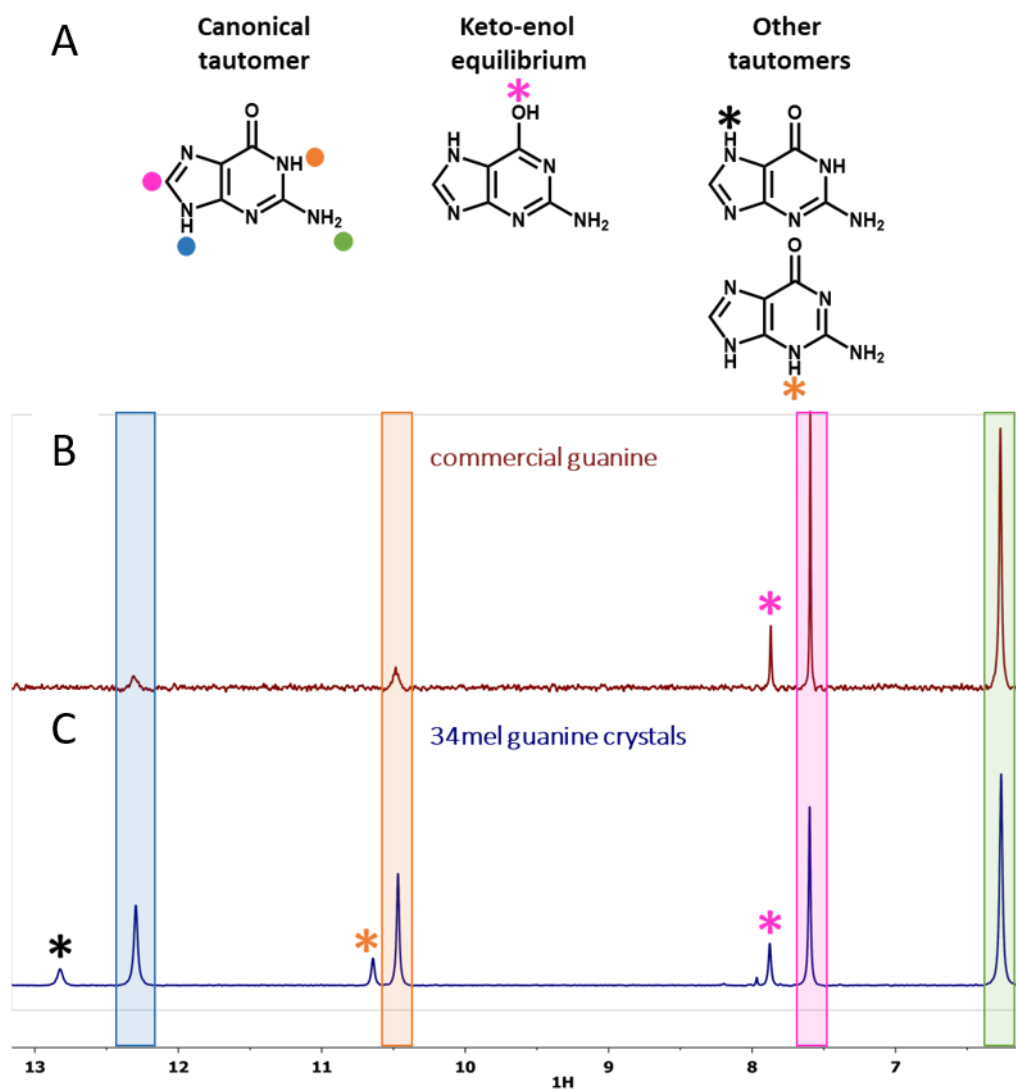


Fig. S5. $^1\text{H-NMR}$ characterization of 34mel crystals. **A** Scheme of some of the expected tautomeric forms of guanine. **B-C** $^1\text{H-NMR}$ spectra for commercial guanine (**B**) and guanine crystals produced by 34mel (**C**). In color, signal assignment for guanine hydrogens and proposed signal assignment that may be produced from tautomers in solution.

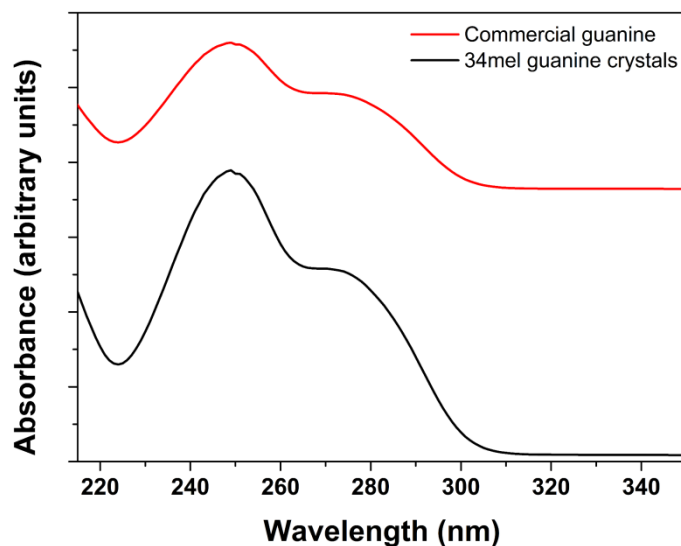


Fig. S6. UV-vis spectra for commercial and 34mel guanine in acid solution.

Additional data 1. Elemental analysis of crystals purified from 34mel.

The presence of biogenic melanin and water molecules were taken into account in the calculated values of C% H% and N% for the guanine samples. Biogenic melanin was represented using a pyromelanin monomer which corresponds to a homogentisic acid unit with two hydrogen atoms removed $[(C_8H_4O_4)_n]$. A good agreement was obtained when considering 6% of the monomer and 14% of water $[(C_5H_5N_5O)_{15}(C_8H_4O_4) \cdot 22H_2O]$.