A cost-effective synthesis of enantiopure ovothiol A from L-histidine, its natural precursor

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NMR spectra
In all NMR spectra analyses the $^1$H and $^{13}$C peaks of the solvent (CD$_2$OD, D$_2$O) was adjusted to its ppm value downstream of tetramethylsilane (TMS) or sodium 3-trimethylsilylpropane-1-sulfonate (DSS)$^1$.

Supplementary Figure S1. The $^1$H NMR spectrum of (2), with residual solvent peaks (triethylamine, water, methanol).
Supplementary Figure S2. The $^{13}$C NMR spectrum of (2), with residual solvent peaks (triethylamine, methanol).

Supplementary Figure S3. The $^1$H NMR spectrum of (3), with residual solvent peaks (ethyl acetate, water).
Supplementary Figure S4. The $^{13}$C NMR spectrum of (3), with residual solvent peaks (ethyl acetate).

Supplementary Figure S5. The NOESY NMR spectrum of (3). Mixing time was set to 500 ms.
Supplementary Figure S6. The expanded region of N‘CH of the NOESY NMR spectrum of (3).

Supplementary Figure S7. The $^1$H-$^{15}$N HMBC NMR spectrum of (3). Coupling constant parameter was set to 8 Hz.
Supplementary Figure S8. The $^1$H NMR spectrum of (4), with residual solvent peaks (methanol, water) and residual succinimide.

Supplementary Figure S9. The $^{13}$C NMR spectrum of (4), with residual solvent peaks (methanol, water) and residual succinimide.
Supplementary Figure S10. The $^1$H NMR spectrum of (5), with residual solvent peaks (water, methanol).

Supplementary Figure S11. The $^{13}$C NMR spectrum of (5).
Supplementary Figure S12. The $^1$H NMR spectrum of L-ovothiol A (6), with residual solvent peaks (water) and supplementary in situ pH indicators: imidazole, dichloroacetic acid, sarcosine.

Supplementary Figure S13. The $^{13}$C NMR spectrum of L-ovothiol A (6).
Supplementary Figure S14. The $^1$H NMR spectrum of L-ovothiol A disulfide (7), with residual solvent peaks (water) and supplementary in situ NMR pH indicators\textsuperscript{[3]}: imidazole, dichloroacetic acid, sarcosine.

References