Supplementary Materials

Novel Selenoureas Based on Cinchona Alkaloid Skeleton: Synthesis and Catalytic Investigations

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1. Spectral Data

Figure S1. 1H and 13C NMR spectra of $N\{\{8\{5\{S\}\}\}^{-}\{6\}'\cdot$methoxycinchonan-9-yl]-$N'$-phenylselenourea eQN-7a.
Figure S2. IR spectra of N-[(8S,9S)-6'-methoxycinchonan-9-yl]-N'-phenylselenourea cQN-7a.

Figure S3. 1H and 13C NMR spectra of N-[(8S,9S)-6'-methoxycinchonan-9-yl]-N'-[4- methoxyphenyl]selenourea cQN-7b.
Figure S4. IR spectra of \(N'-(8S,9S)-6'-\text{methoxycinchonan-9-yl})-N'-(4\text{-methoxyphenyl})\text{selenourea} \text{e QN-7b.}

Figure S5. 1H and 13C NMR spectra of \(N'-(4\text{-fluorophenyl})-N'-(8S,9S)-6'-\text{methoxycinchonan-9-yl})\text{selenourea} \text{e QN-7c.}
Figure S6. IR spectra of N-[4-fluorophenyl]-N’-(8S,9S)-6’-methoxycinchonan-9-yl]selenourea eQN-7c.

Figure S7. 1H and 13C NMR spectra of N-[4-fluorophenyl]-N’-(8S,9S)-cinchonan-9-yl]selenourea eCD-7d.
Figure S8. IR spectra of $N$-[4-fluorophenyl]-$N'$-[(85,9S)-cinchonan-9-yl]selenourea eCD-7d.

Figure S9. 1H and 13C NMR spectra of $N$-[4-fluorophenyl]-$N'$-[(85,9S)-10,11-dihydro-6- methoxycinchonan-9-yl]selenourea eDHQN-7e.
Figure S10. IR spectra of N-[4-fluorophenyl]-N’-[(8S,9S)-10,11-dihydro-6’-methoxycinchonan-9-yl]selenourea eDHQN-7e.

Figure S11. 1H and 13C NMR spectra of N-4-fluorophenyl]-N’-[8R,9R]-6’-methoxycinchonan-9-yl]selenourea eQD-7f.
Figure S12. IR spectra of N-[4-fluorophenyl]-N'-[(8R,9R)-6'-methoxycinchonan-9-yl]selenourea eQD-7f.

Figure S13. 1H and 13C NMR spectra of N-[4-fluorophenyl]-N'-[(8R,9R)-10,11-dihydro-6'-methoxycinchonan-9-yl]selenourea eDHQD-7g.
Figure S14. IR spectra of N-[4-fluorophenyl]-N’-[(8R,9R)-10,11-dihydro-6’-methoxycinchan-9-y]selenourea eDHQD-7g.

Figure S15. 1H and 13C NMR spectra of N-[(8S,9S)-6’-methoxycinchan-9-y]formamide 8a.
Figure S16. IR spectra of N-[(8S,9S)-6'-methoxycinchonan-9-yl]formamide 8a.

Figure S17. 1H NMR spectra of N,N'-bis[(8S,9S)-6'-metoxycinchonan-9-yl]selenourea 10a.
Figure S18. IR spectra of $N,N'$-bis[(8S,9S)-6'-metoxycinchan-9-yl]selenourea 10a.

Figure S19. 1H and 13C NMR spectra of $N$-[4-fluorophenyl]-$N'$-[(8S,9S)-6'-methoxycinchan-9-yl]thiourea cQN-12a.
Figure S20. IR spectra of $N$-[4-fluorophenyl]-$N'$-[(8S,9S)-6'-methoxycinchonan-9-yl]thiourea \( \epsilon \text{QN}-12a \).

**2. HPLC data**

2.1. Michael addition of nitromethane to trans-chalcone

(Chiralcel AD-H column, hexane/i-PrOH 9:1, flow rate 1.0 mL/min, \( \lambda = 254 \) nm)

Figure S21. HPLC chromatogram for 14: sample obtained with catalyst \( \epsilon \text{QN}-7a \) (81% ee).
Figure S22. HPLC chromatogram for 14: sample obtained with catalyst eQN-7b (70% ee).

Figure S23. HPLC chromatogram for 14: sample obtained with catalyst eQN-7c (95% ee).
Figure S24. HPLC chromatogram for 14: sample obtained with catalyst cCD-7d (91% ee).

Figure S25. HPLC chromatogram for 14: sample obtained with catalyst cDHQN-7e (95% ee).
Figure S26. HPLC chromatogram for 14: sample obtained with catalyst eQD-7f (87% ee).

Figure S27. HPLC chromatogram for 14: sample obtained with catalyst eDHQD-7g (86% ee).
Figure S28. HPLC chromatogram for 14: sample obtained with catalyst eQN-12a (89% ee).

| Ret Time | Area   | Area % | Height | Height % |
|----------|--------|--------|--------|----------|
| 14.563   | 1223536| 53.74  | 53370  | 6.41     |
| 20.018   | 21694987| 94.66  | 786985 | 93.59    |
| **Totals** | **22518525** | **100.00** | **840565** | **100.00** |

Figure S29. HPLC chromatogram for racemic 14 without catalyst 7.

| Peak# | Ret Time | Area  | Area % | Height | Height % |
|-------|----------|-------|--------|--------|----------|
| 1     | 14.241   | 1042789| 49.18  | 41730  | 52.78    |
| 2     | 19.441   | 1014499| 49.67  | 41690  | 52.33    |
| **Total** | **2057288** | **100.00** | **93020** | **100.00** |

2.2. Sulfa-Michael addition of thioacetic acid to trans-chalcone
(Chiralcel AS-H column, hexane/i-PrOH 9:1, flow rate 1.0 mL/min, λ = 254 nm)

Figure S30. HPLC chromatogram for 15: sample obtained with catalyst eQN-7a (13% ee).

Figure S31. HPLC chromatogram for 15: sample obtained with catalyst eQN-7b (3% ee).
Figure S32. HPLC chromatogram for 15: sample obtained with catalyst eQN-7c (21% ee).

Figure S33. HPLC chromatogram for 15: sample obtained with catalyst eCD-7d (17% ee).
Figure S34. HPLC chromatogram for 15: sample obtained with catalyst eDHQN-7e (21% ee).

Figure S35. HPLC chromatogram for 15: sample obtained with catalyst eQD-7f (14% ee).
Figure S36. HPLC chromatogram for 15: sample obtained with catalyst eDHQD-7g (12% ee).

Figure S37. HPLC chromatogram for 15: sample obtained with catalyst eQN-12a (17% ee).
Figure S38. HPLC chromatogram for racemic 15 without catalyst 7.