## Thiophene enantiomers from the aerial parts of Eclipta prostrata

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Number	Conformer	Energy (hartree)	Energy (kcal/mol)	Proportion (%)
1		-2100.2458634	-1317925.28174213	4.89
2	مهر می	-2100.245943	-1317925.33169193	5.32
3		-2100.2467351	-1317925.8287426	12.32
4		-2100.2458657	-1317925.28318541	4.90
5		-2100.2458729	-1317925.28770348	4.94
6		-2100.2468504	-1317925.9010945	13.92

 Table S1. Re-optimized conformers, energies and proportions for (S)-Ac-1.

7	-2100.2469006	-1317925.93259551	14.68
8	-2100.2468638	-1317925.90950314	14.12
9	-2100.2458418	-1317925.26818792	4.78
10	-2100.2471992	-1317926.11996999	20.15

Number	Conformer	Energy (hartree)	Energy (kcal/mol)	Proportion (%)
1		-1715.1674619	-1076284.73401687	7.83
2		-1715.1674619	-1076284.73401687	7.83
3		-1715.1674619	-1076284.73401687	7.83
4		-1715.1681003	-1076285.13461925	15.4
5		-1715.1680505	-1076285.10336926	14.6
6		-1715.1680505	-1076285.10336926	15.4
7		-1715.1681003	-1076285.13461925	15.4

 Table S2. Re-optimized conformers, energies and proportions for (S)-Ac-3

3

8		-1715.1674619	-1076284.73401687	7.83
9		-1715.1669432	-1076284.40852743	4.52
10	Jag He waa aa ge de ge je	-1715.1668708	-1076284.36309571	4.18

Figure S1. Structures of thiophenes 4–10 from *Eclipta prostrata*.



Figure S2. <sup>1</sup>H NMR spectrum of 1 in CDCl<sub>3</sub>





Figure S3. <sup>13</sup>C and DEPT NMR spectra of 1 in CDCl<sub>3</sub>



**Figure S4.**  $^{1}H^{-1}H$  COSY spectrum of **1** in CDCl<sub>3</sub>



Figure S5. HSQC spectrum of 1 in CDCl<sub>3</sub>



Figure S6. HMBC spectrum of 1 in CDCl<sub>3</sub>



Figure S7. (+)-ESIMS spectrum of 4



Figure S8. (+)-HR-ESIMS spectrum of 1



Figure S9. <sup>1</sup>H NMR spectrum of 2 in CDCl<sub>3</sub>



Figure S10. <sup>13</sup>C and DEPT NMR spectra of 2 in CDCl<sub>3</sub>



**Figure S11.** <sup>1</sup>H–<sup>1</sup>H COSY spectrum of **2** in CDCl<sub>3</sub>



Figure S12. HSQC spectrum of 2 in CDCl<sub>3</sub>



Figure S13. HMBC spectrum of 2 in CDCl<sub>3</sub>



Figure S14. (+)-ESIMS spectrum of 2



Figure S15. (+)-HR-ESIMS spectrum of 2



Figure S16. <sup>1</sup>H NMR spectrum of Ac-1 in CDCl<sub>3</sub>



Figure S17. <sup>1</sup>H NMR spectrum of Ac-3 in CDCl<sub>3</sub>



Figure S18. Chiral HPLC chromatogram of Ac-6