Supporting Information

Chiroptical Inversion Induced by Rotation of a C–C Single Bond: An Experimental and Theoretical Study

Wei Lu, Ganhong Du, Keyuan Liu, Liming Jiang,* Jun Ling,* Zhiquan Shen

MOE Key Laboratory of Macromolecular Synthesis and Functionalization;

Department of Polymer Science and Engineering,

Zhejiang University, Hangzhou 310027, China

cejlm@zju.edu.cn; junling@zju.edu.cn

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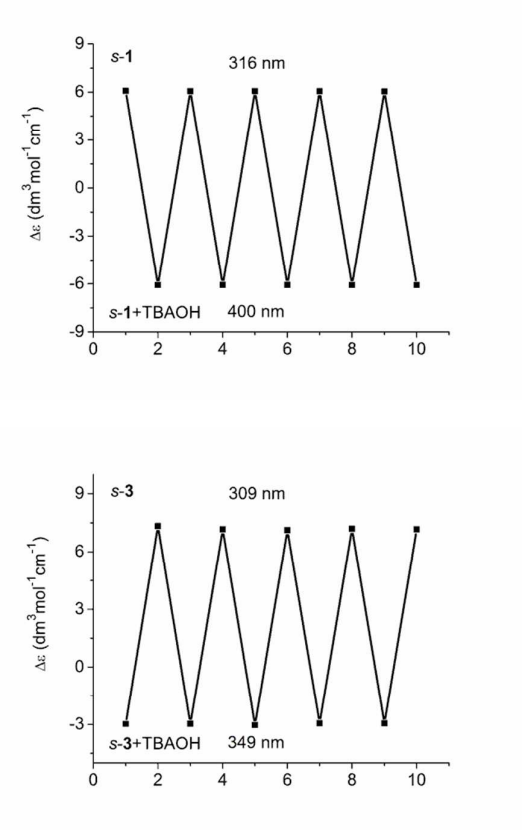

Figure S1. Illustration of the switchable behavior with Cotton effect as "output signal" after sequential addition of 2.0 equiv of TBAOH and HCl in DMSO for *s*-**1** (top) and *s*-**3** (bottom).

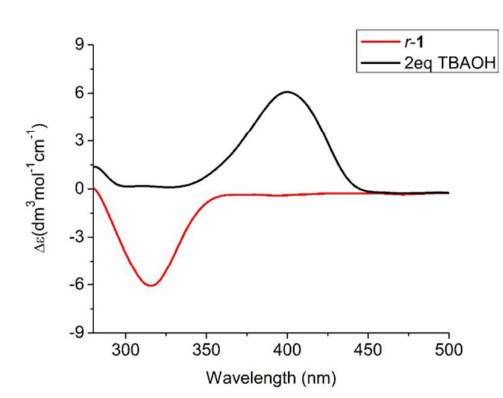

Figure S2. CD spectra of *r*-**1** (1×10^{-4} mol/L) in DMSO before and after addition of 2.0 equiv of TBAOH.

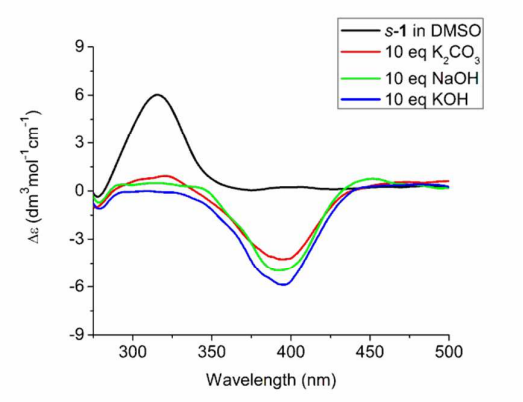

Figure S3. CD spectra of *s*-**1** (1×10^{-4} mol/L) upon the addition of different kinds of bases (including K_2CO_3, NaOH and KOH, 10 equiv).

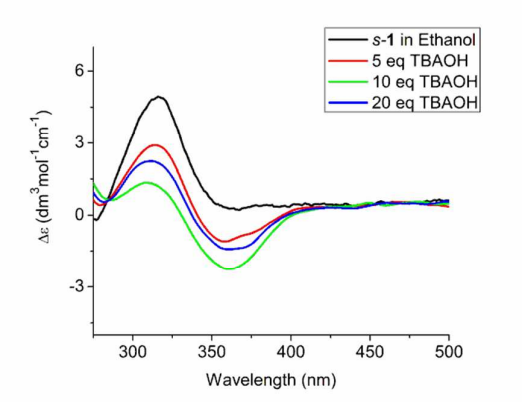

Figure S4. CD titration spectra of *s*-**1** (1×10^{-4} mol/L) upon addition of different amounts of TBAOH in ethanol (containing 10% THF).

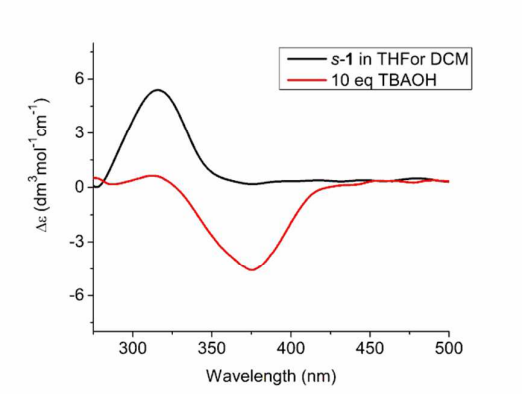

Figure S5. CD spectra of *s*-**1** (1×10^{-4} mol/L) in THF or in CH_2Cl_2 before and after addition of 2.0 equiv of TBAOH.

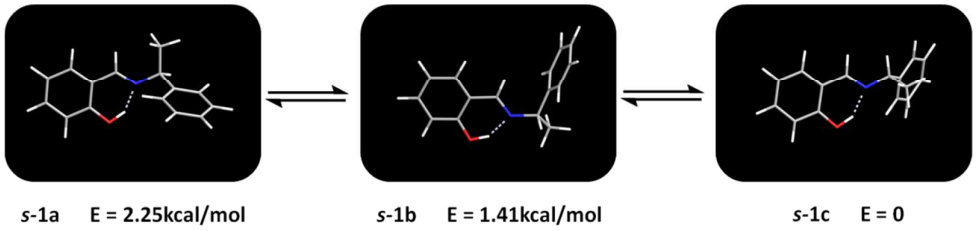

Figure S6. Stick representation of the B3LYP/6-311++G**-optimized conformation of ***s*-1a**, ***s*-1b** and ***s*-1c** in vacuum. The intramolecular hydrogen bond is denoted as white dotted line; O–H···N distance: 1.74 Å (***s*-1a**), 1.73 Å (***s*-1b**), 1.74 Å (***s*-1c**).

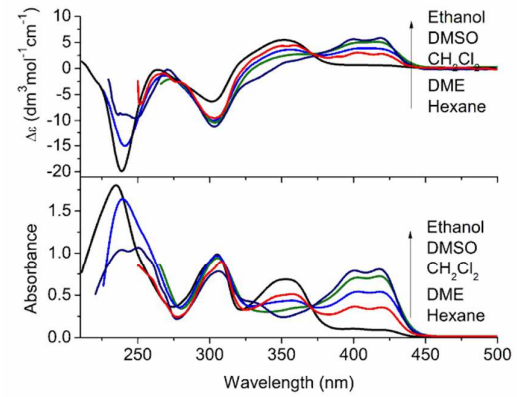

Figure S7. UV-Vis and CD spectra of ***s*-2** (1×10^{-4} mol/L) in various solvents.

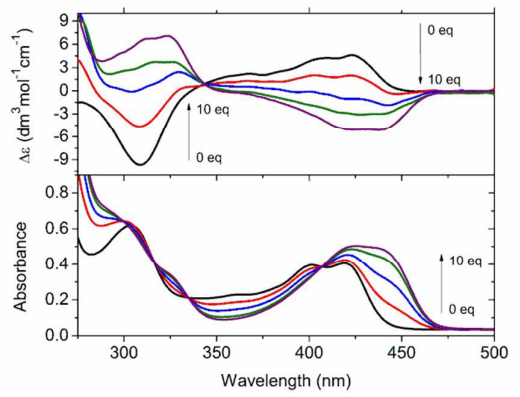

Figure S8. CD and UV-Vis titration spectra of ***s*-2** (1×10^{-4} mol/L) in DMSO with increasing amount of TBAOH (0–1.0 equiv).

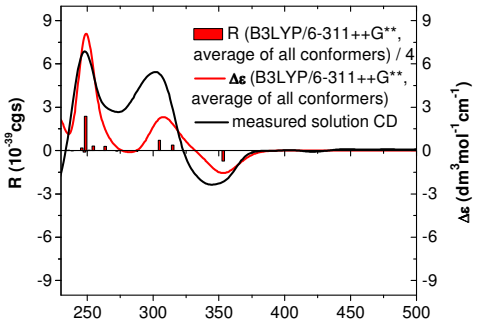

Figure S9. Experimental (in hexane:THF = 4:1) and Boltzmann-averaged ECD solution spectra of Et-*s*-**2** optimized at B3LYP/6-311++G**/IEFPCM (hexane) level of theory. Bars represent the calculated rotational strength values.

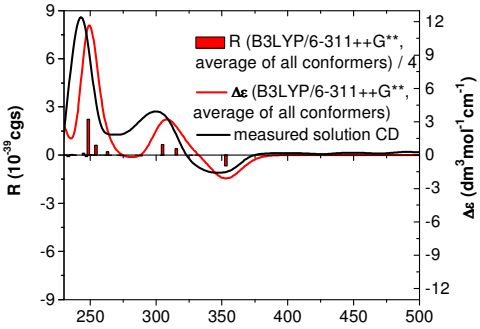

Figure S10. Experimental (in hexane:THF = 4:1) and Boltzmann-averaged ECD solution spectra of Me-*s*-**2** optimized at B3LYP/6-311++G**/IEFPCM (hexane) level of theory. Bars represent the calculated rotational strength values.

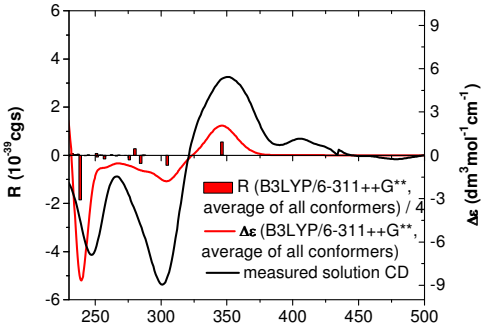

Figure S11. Experimental (in hexane:THF = 4:1) and Boltzmann-averaged ECD solution spectra of *s*-**2** optimized at B3LYP/6-311++G**/IEFPCM (hexane) level of theory. Bars represent the calculated rotational strength values.

2. Determination of optical rotation values for *s*-1 and *s*-3

Optical rotaion was measured at 20℃ in DMSO on a polarimeter using sodium lamp (λ = 589 nm) as the light source. The specific optical rotaion $[\alpha]^{20}_{589}$ = +121° (0.01g/mL, DMSO) for free ***s*-1**; after addition of 2 eq of TBAOH (0.8 mol/L in methanol), $[\alpha]^{20}_{589}$ = −250°. $[\alpha]^{20}_{589}$ = +15° (0.01 g/mL, DMSO) for free ***s*-3**; after addition of 2 eq of TBAOH (0.8 mol/L in methanol), $[\alpha]^{20}_{589}$ = +150°.

3. Copies of NMR and MS-ESI spectra of the compounds.

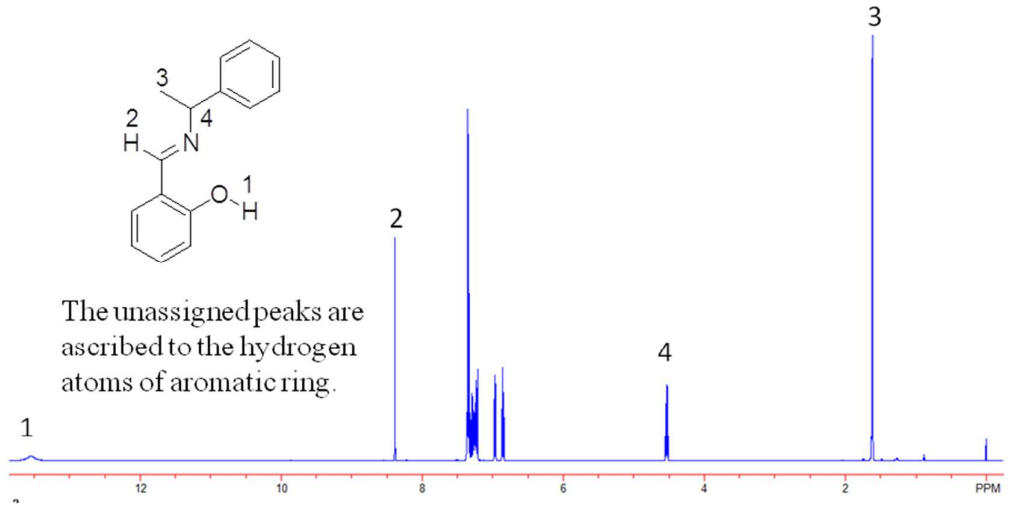

Figure S12. ^{1}H NMR of *s*-**1** (in $CDCl_3$).

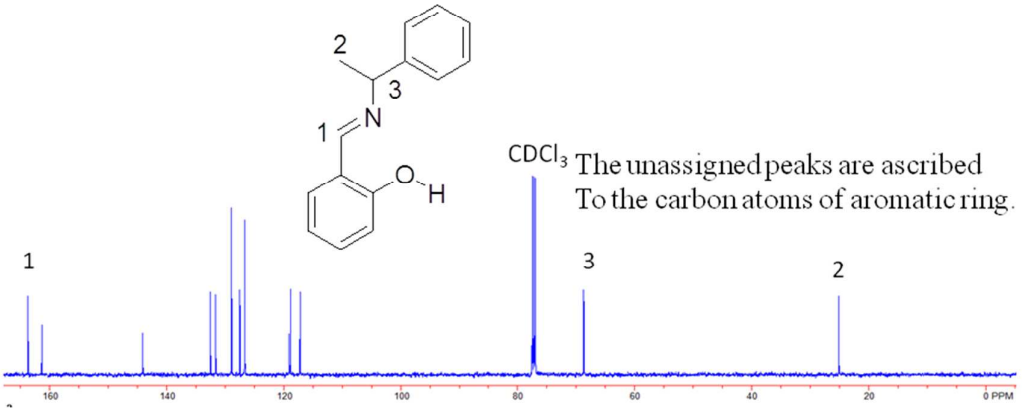

Figure S13. ^{13}C NMR of *s*-**1** (in $CDCl_3$).

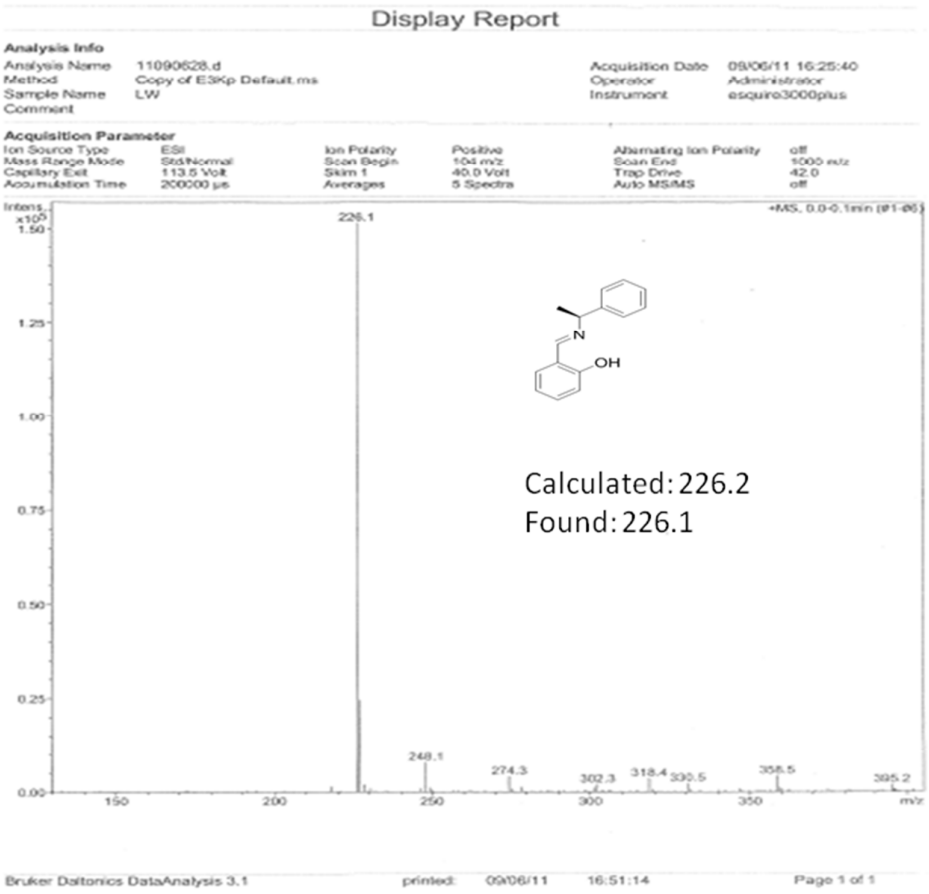

Figure S14. MS of *s*-**1**.

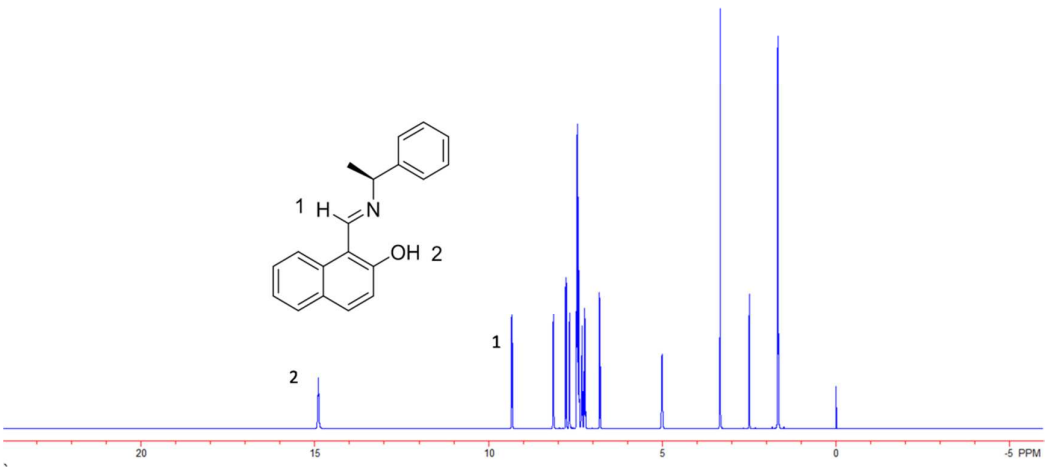

Figure S15. ^{1}H NMR of *s*-**2** (in $CDCl_3$).

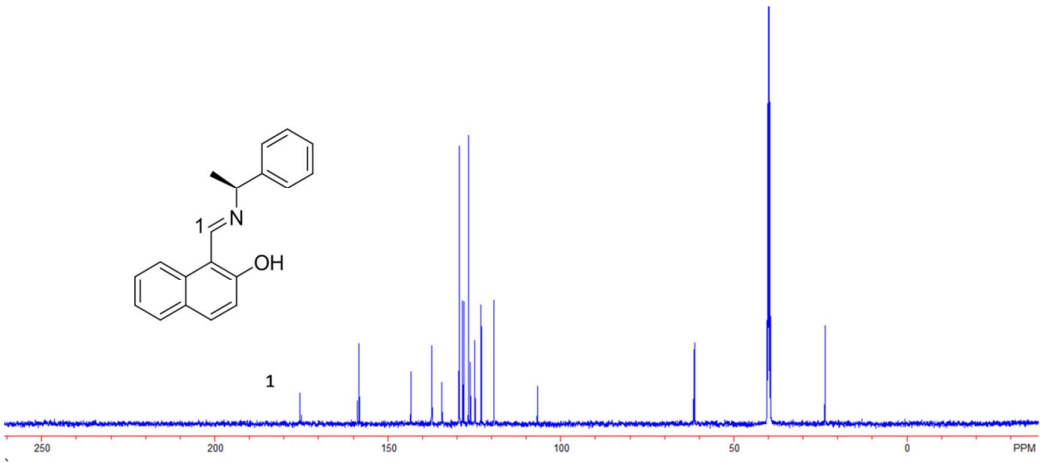

Figure S16. ^{13}C NMR of *s*-**2** (in $CDCl_3$).

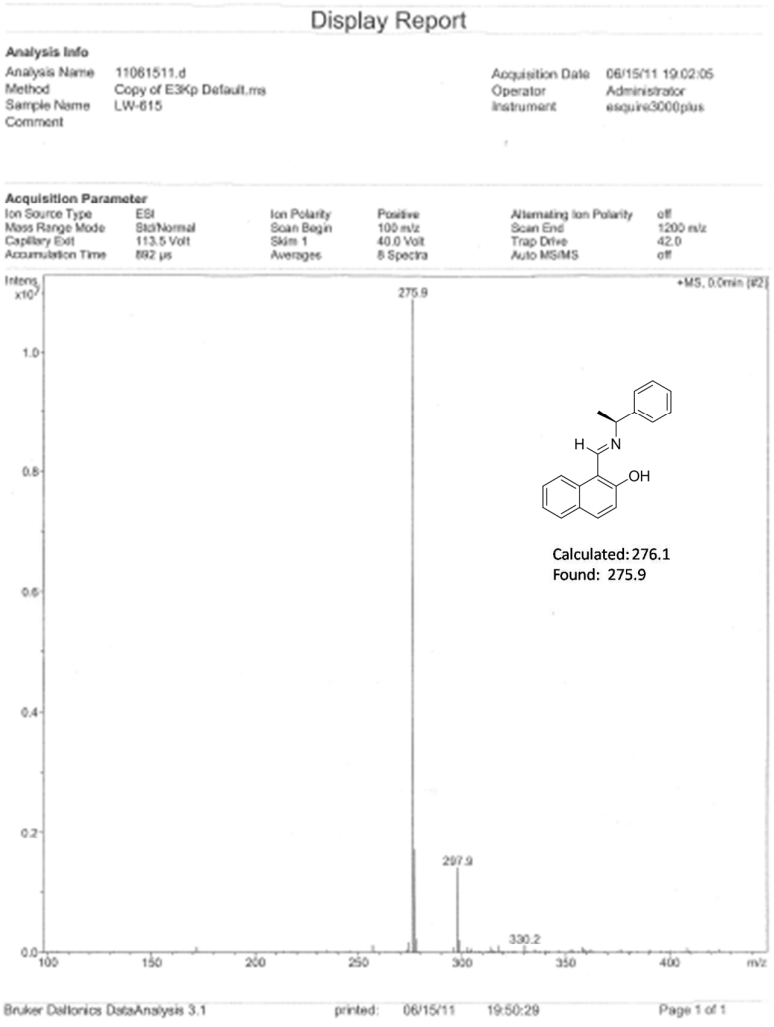

Figure S17. MS of *s*-**2**.

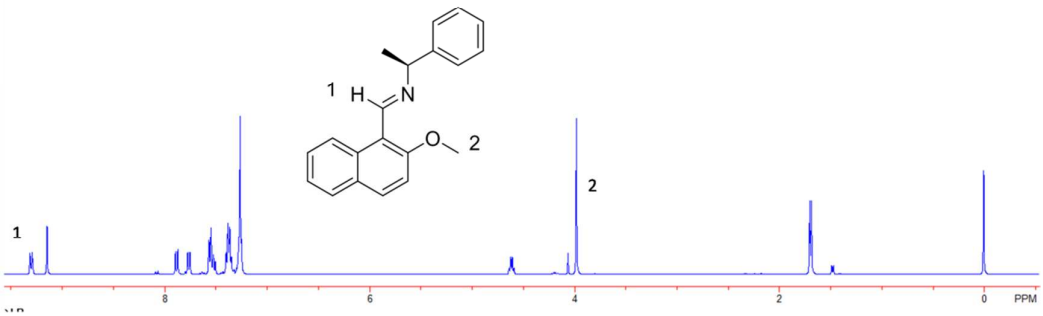

Figure S18. ^{1}H NMR of Me-*s*-**2** (in $CDCl_3$).

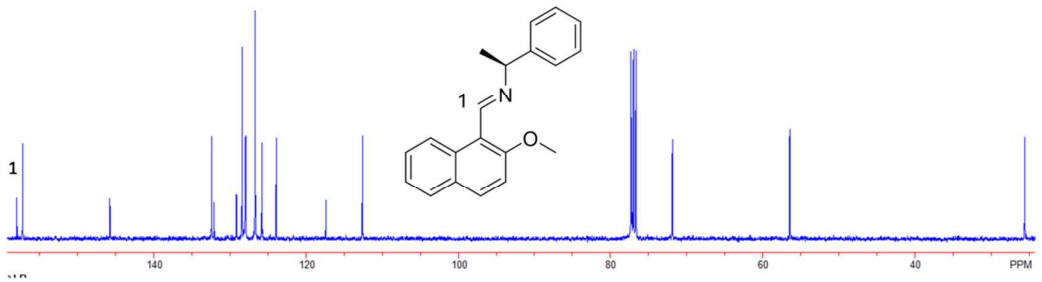

Figure S19. ^{13}C NMR of Me-*s*-**2** (in $CDCl_3$).

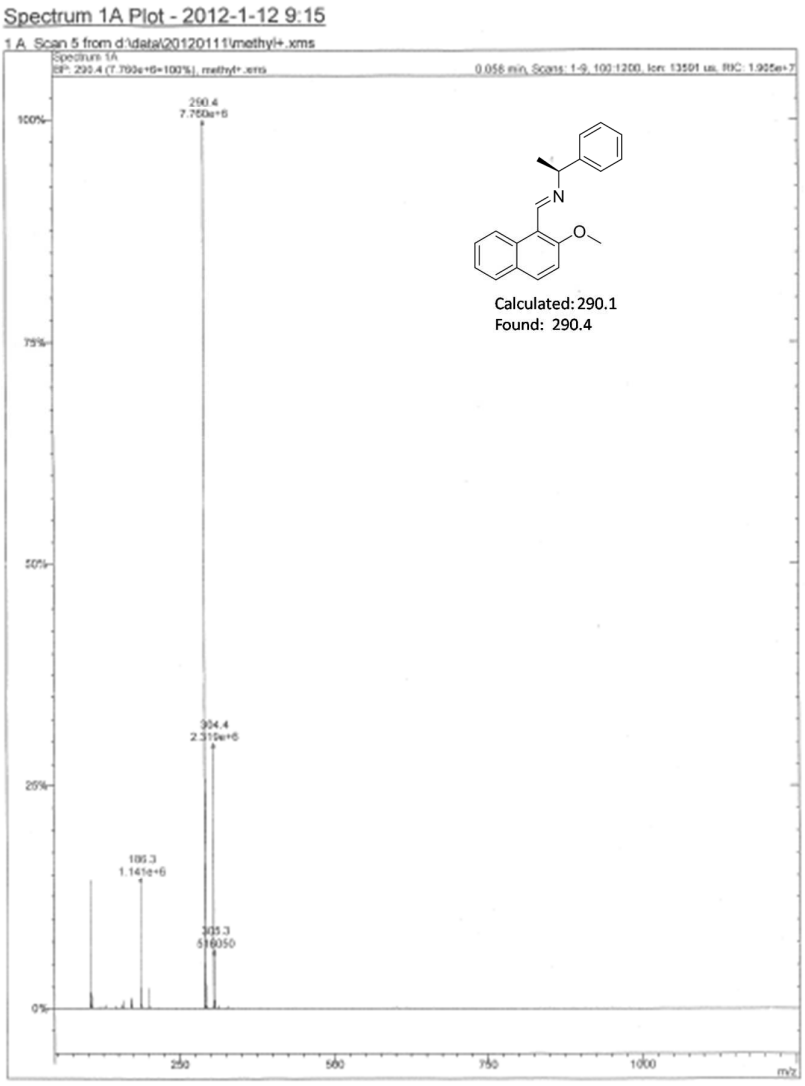

Figure S20. MS of Me-*s*-**2**.

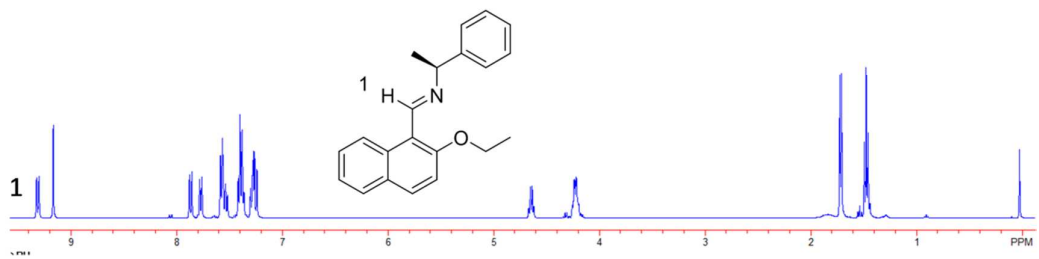

Figure S21. ^{1}H NMR of Et-*s*-**2** (in $CDCl_3$).

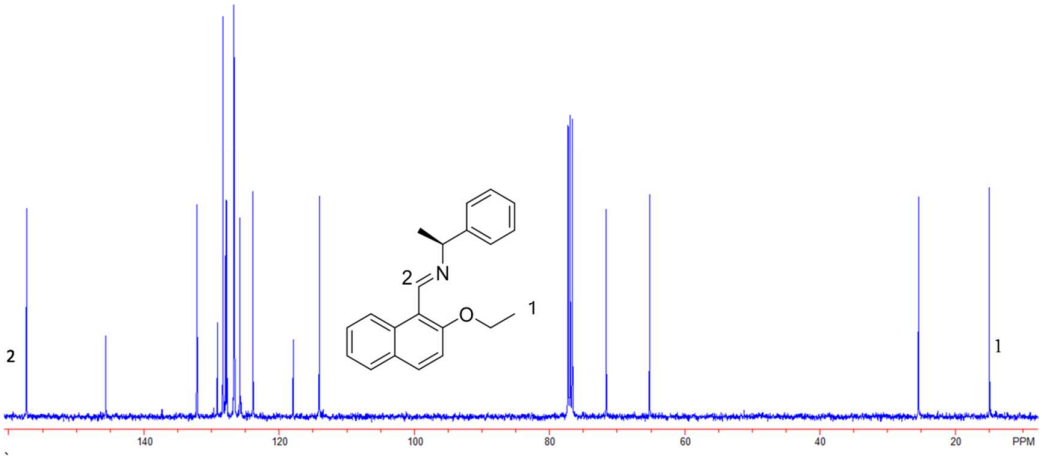

Figure S22. ^{13}C NMR of Et-*s*-**2** (in $CDCl_3$).

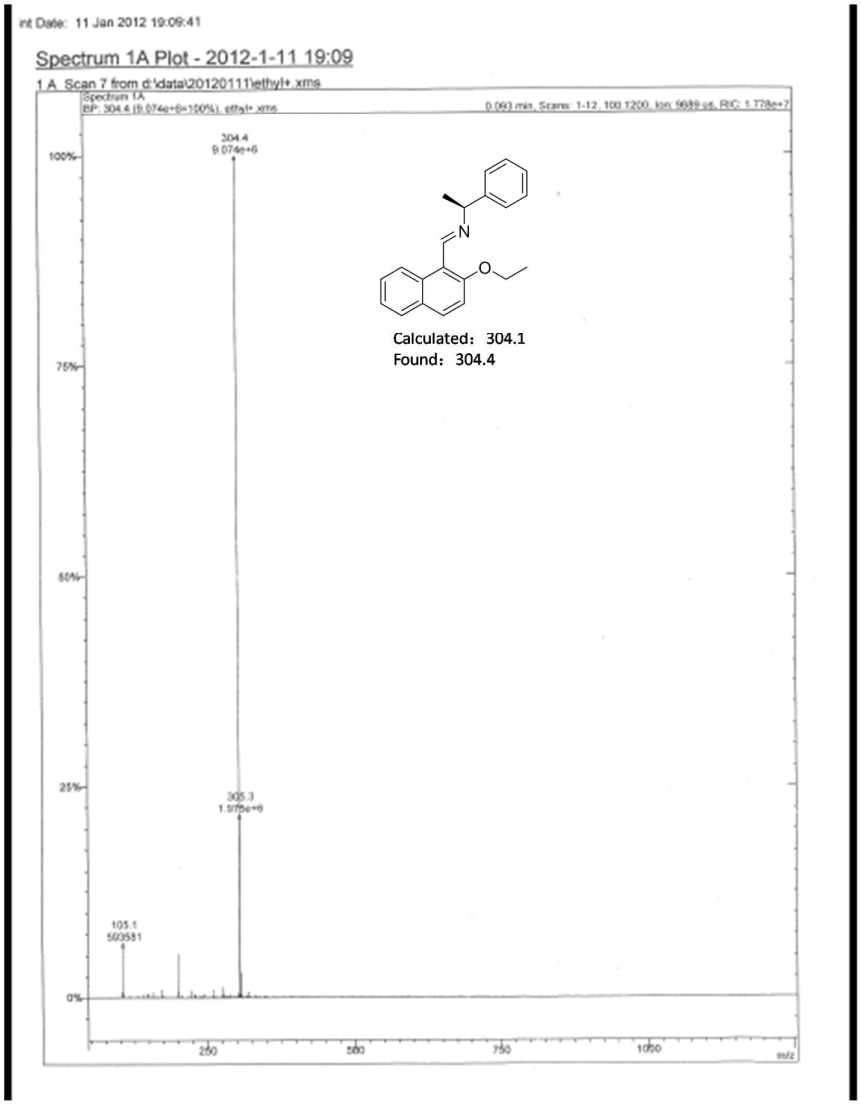

Figure S23. MS of Et-*s*-**2**.

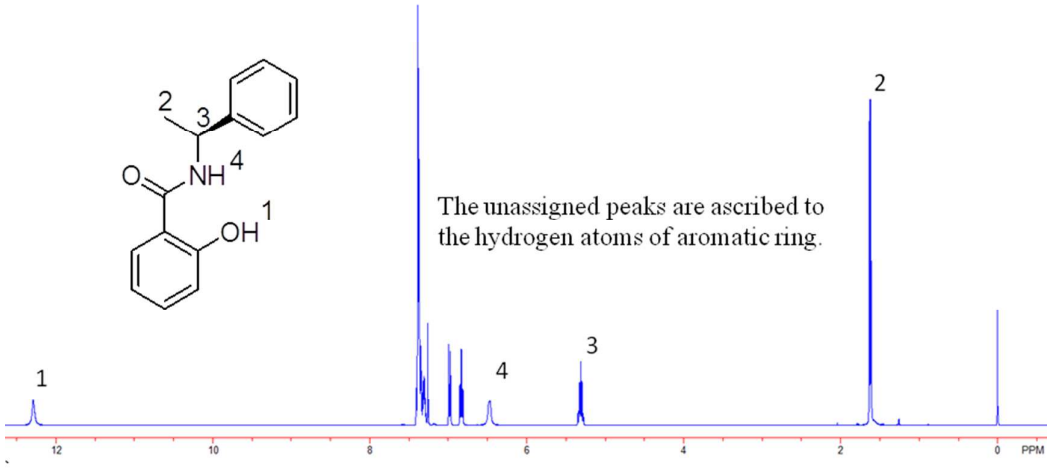

Figure S24. ^{1}H NMR of *s*-**3** (in $CDCl_3$).

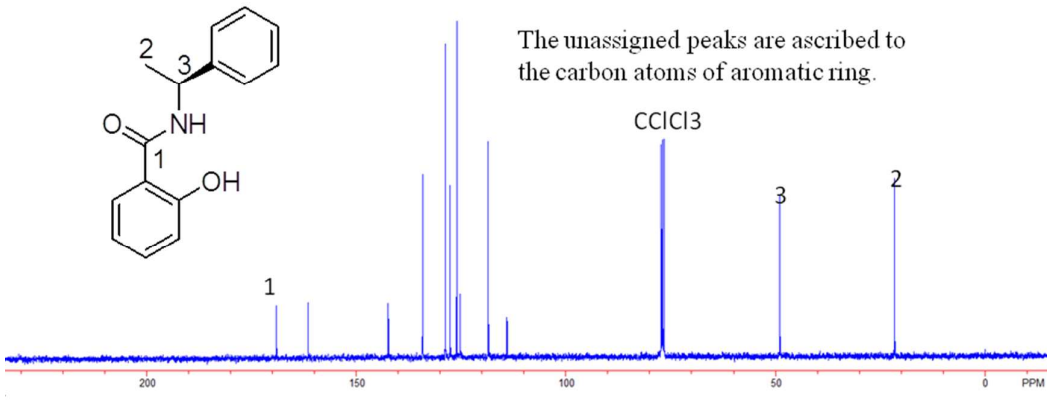

Figure S25. ^{13}C NMR of *s*-**3** (in $CDCl_3$).

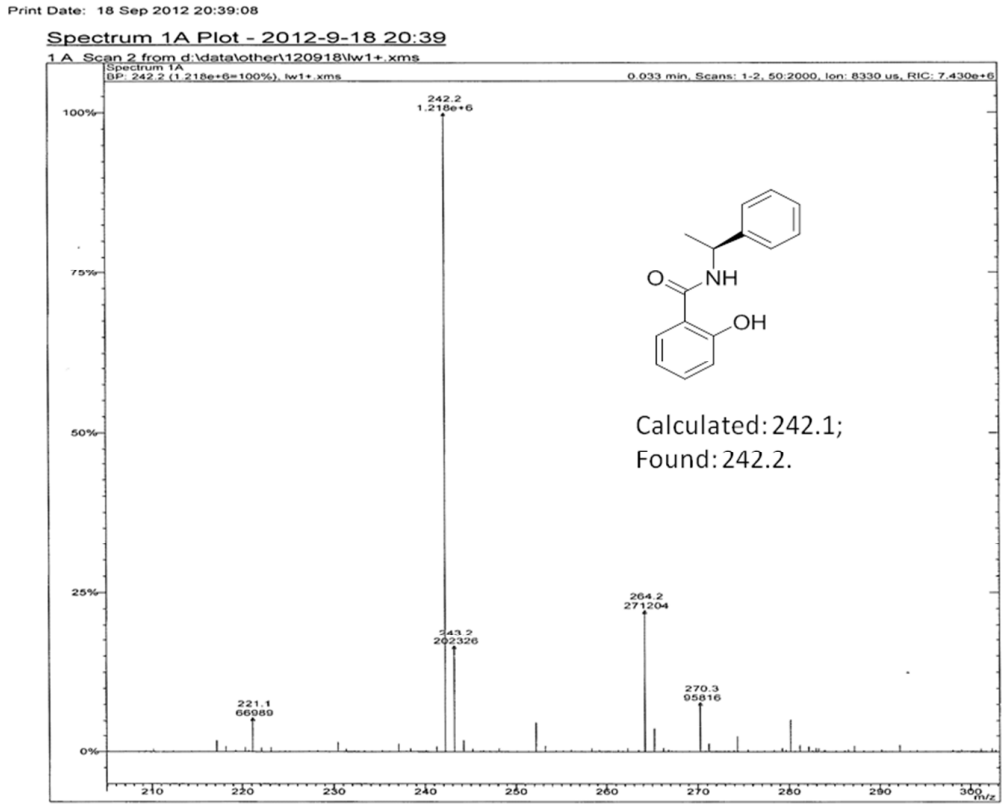

Figure S26. MS of *s*-**3**.