Steric Factors Directed Baylis–Hillman and Aldol Reactions in Titanium Tetrachloride Mediated Coupling Between α -Keto Esters and Cyclohex-2-enone Derivatives

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Supporting Information

¹³C NMR Spectra of the compounds

- S1. Ethyl 2-hydroxy-2-phenyl-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4a**)
- S2. Ethyl 2-hydroxy-2-(4-methylphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4b**)
- S3. Ethyl 2-hydroxy-2-(4-ethylphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4c**)
- S4. Ethyl 2-hydroxy-2-(4-methoxyphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4d**)
- S5. Ethyl 2-hydroxy-2-(2-methylphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4e**)
- S6. Methyl 2-hydroxy-2-phenyl-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4f**)
- S7. Methyl 2-hydroxy-2-(3-methoxyphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4g**)
- S8. Methyl 2-hydroxy-2-(2-methylphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4h**)
- S9. Methyl 2-hydroxy-2-(2-methoxyphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4i**)
- S10. Isopropyl 2-hydroxy-2-(4-methylphenyl)-2-(5,5-dimethylcyclohex-2-en-1-on-2-yl)ethanoate (**4j**)
- S11. 2-[Hydroxy(4-nitrophenyl)methyl]cyclohex-2-en-1-one (**3**)
- S12. 2-[Hydroxy(phenyl)methyl]cyclohex-2-en-1-one (**3a**)
- S13. Ethyl *syn*-2-hydroxy-2-phenyl-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**5**)
- S14. Ethyl 2-hydroxy-2-phenyl-2-(cyclohex-2-en-1-on-2-yl)ethanoate (**4**)
- S15. Ethyl *syn*-2-hydroxy-2-(4-methylphenyl)-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**6**)
- S16. Ethyl *syn*-2-hydroxy-2-(4-methoxyphenyl)-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**7**)
- S17. Methyl *syn*-2-hydroxy-2-phenyl-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**8**)
- S18. Isopropyl *syn*-2-hydroxy-2-(4-methylphenyl)-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**9**)
- S19. Ethyl *syn*-2-hydroxy-2-(4-bromophenyl)-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**10**)
- S20. Ethyl *syn*-2-hydroxy-2-(naphth-1-yl)-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**11**)
- S21. Methyl *syn*-2-hydroxy-2-(4-methylphenyl)-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**12**)
- S22. Methyl *syn*-2-hydroxy-2-(4-ethylphenyl)-2-(cyclohex-5-en-1-on-2-yl)ethanoate (**13**)
- S23. Ethyl *syn*-2-hydroxy-2-phenyl-2-(cyclopent-4-en-1-on-2-yl)ethanoate (**14**)
- S24. Cyclohex-2-enone and it's TiCl₄ complex
- S25. Cyclohex-2-enone and 3-chlorocyclohexanone
- S26. 5,5-Dimethylcyclohex-2-enone and it's TiCl₄ complex
- S27. 5,5-Dimethylcyclohex-2-enone and 3-chloro-5,5-dimethylcyclohexanone