

Supporting information

Mechanism studies on the VO(acac)₂-catalyzed oxidative cleavage of lignin model compounds in acetic acid

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Additional results

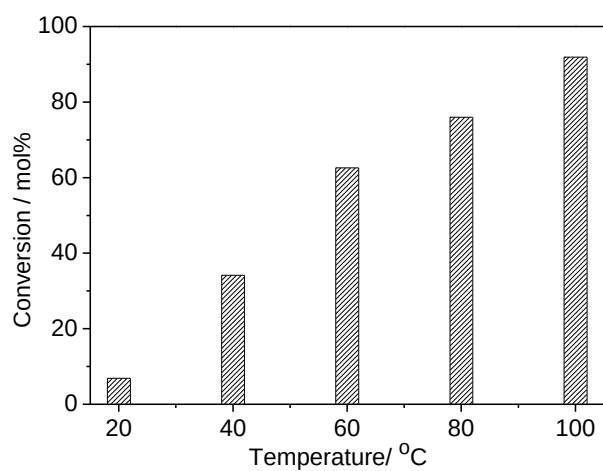


Figure S1 VO(acac)₂-catalyzed oxidation of **1** in acetic acid under different reaction temperatures.

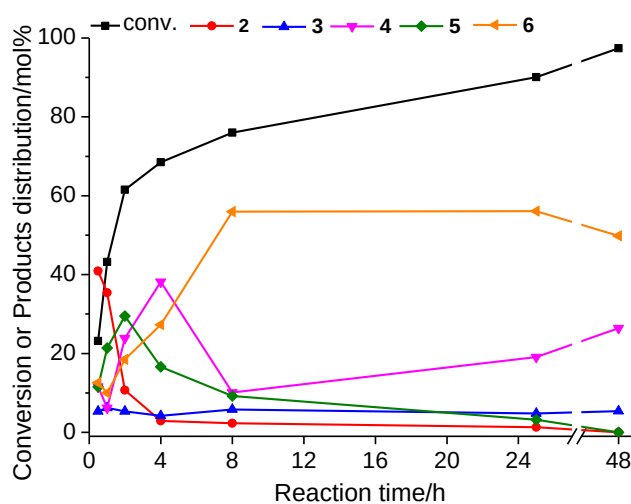
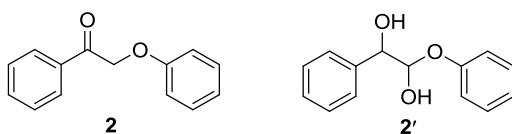


Figure S2 Time course of VO(acac)₂-catalyzed oxidation of **1** in acetic acid. Reaction conditions: 0.25 mmol model compound **1**, 0.025 mmol VO(acac)₂, 0.5 mL solvent, 80 °C, 8 h, 1 atm O₂.



Scheme S1 The supposed reaction intermediates in the VO(acac)₂-catalysed oxidation of 2-phenoxy-1-phenylethanol in acetic acid.

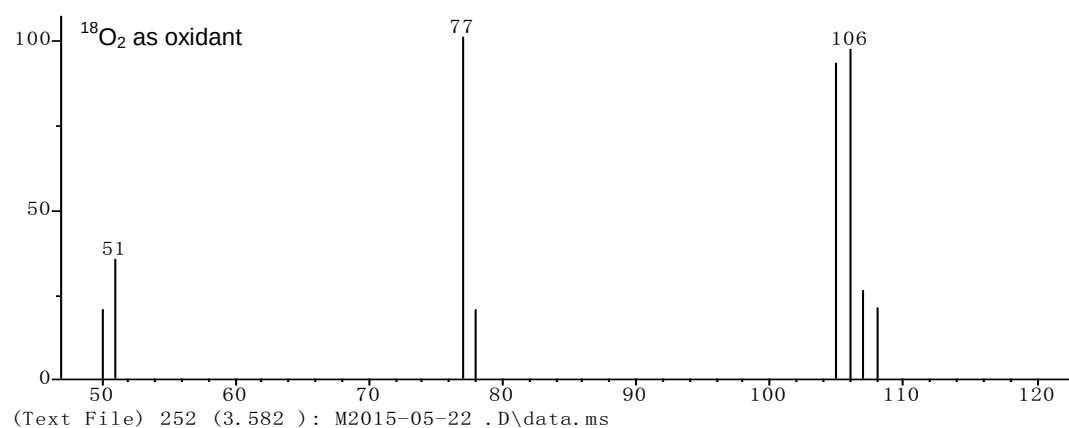
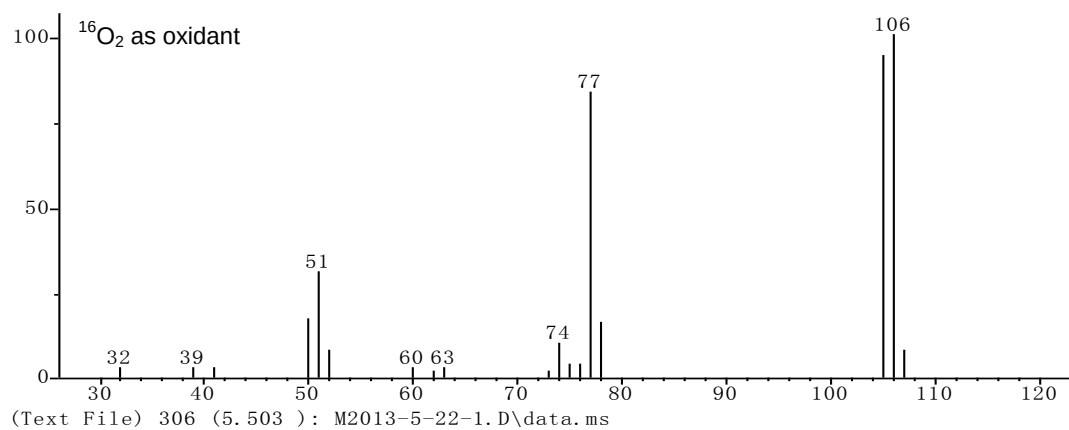


Figure S3 Mass spectra of benzaldehyde.

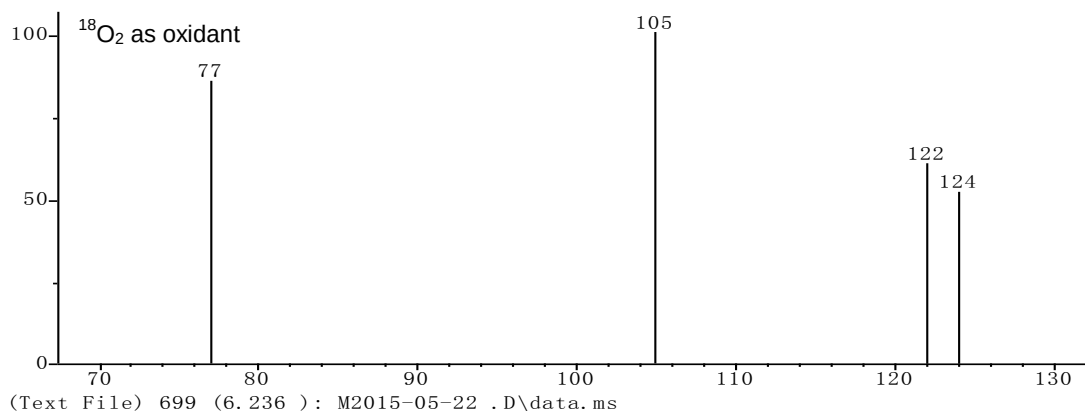
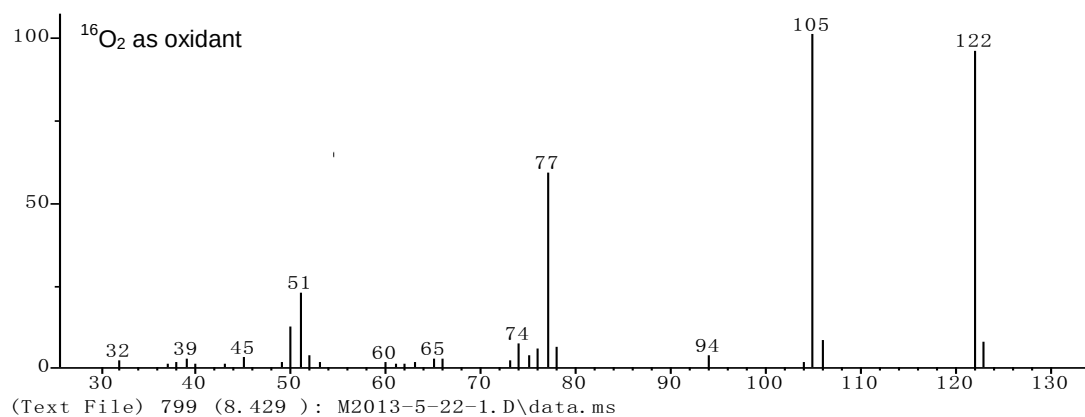


Figure S4 Mass spectra of benzoic acid.

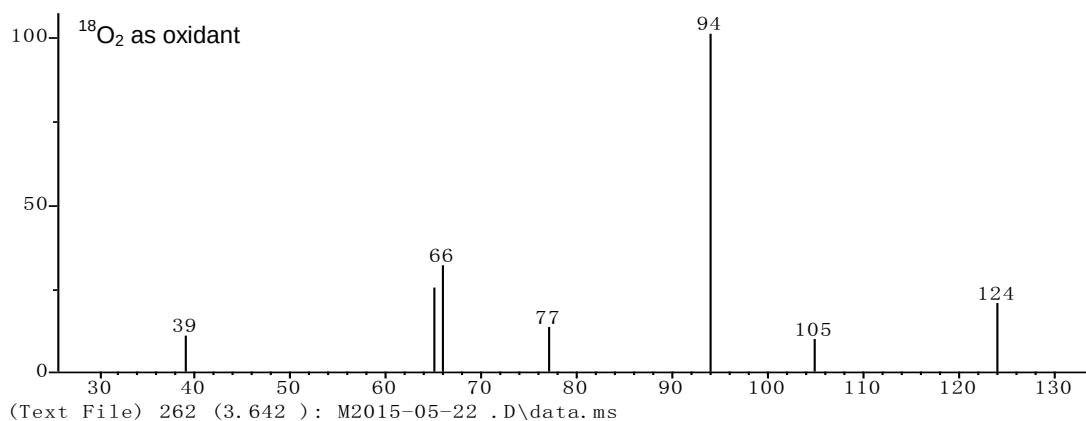
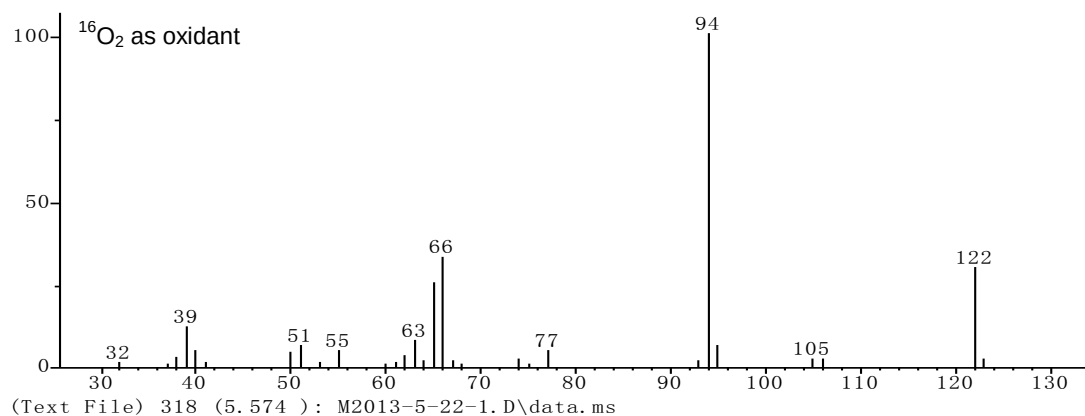


Figure S5 Mass spectra of phenyl formate.

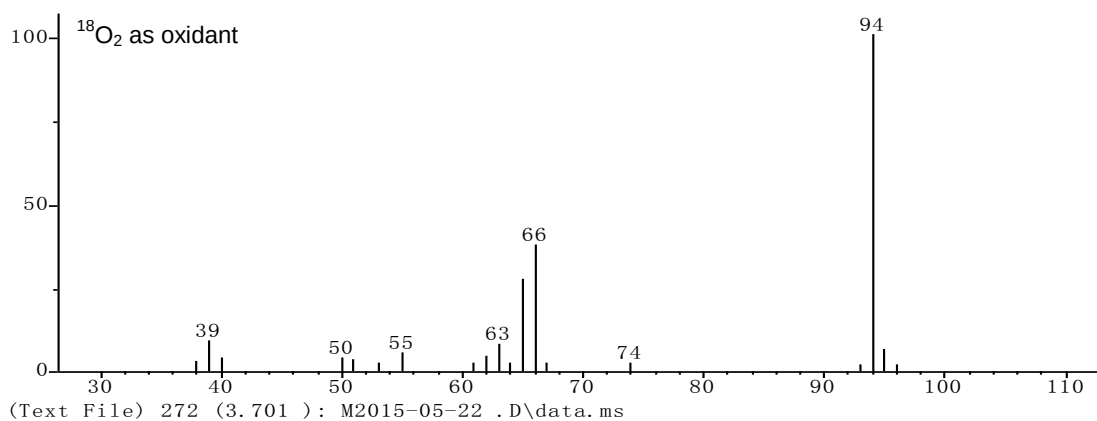
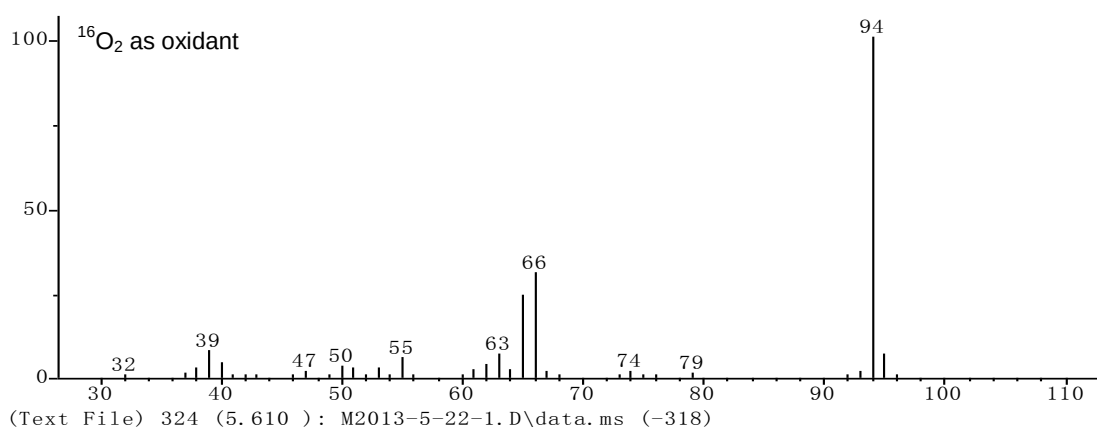


Figure S6 Mass spectra of phenol.

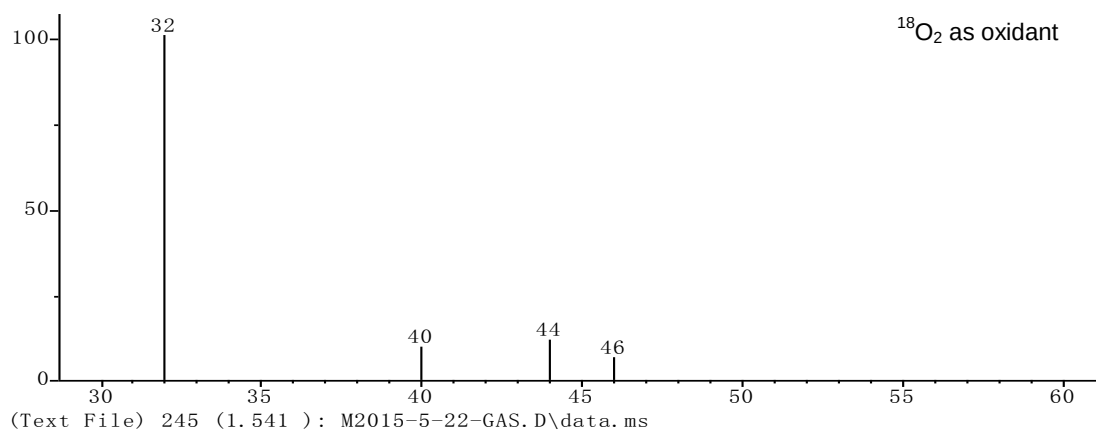
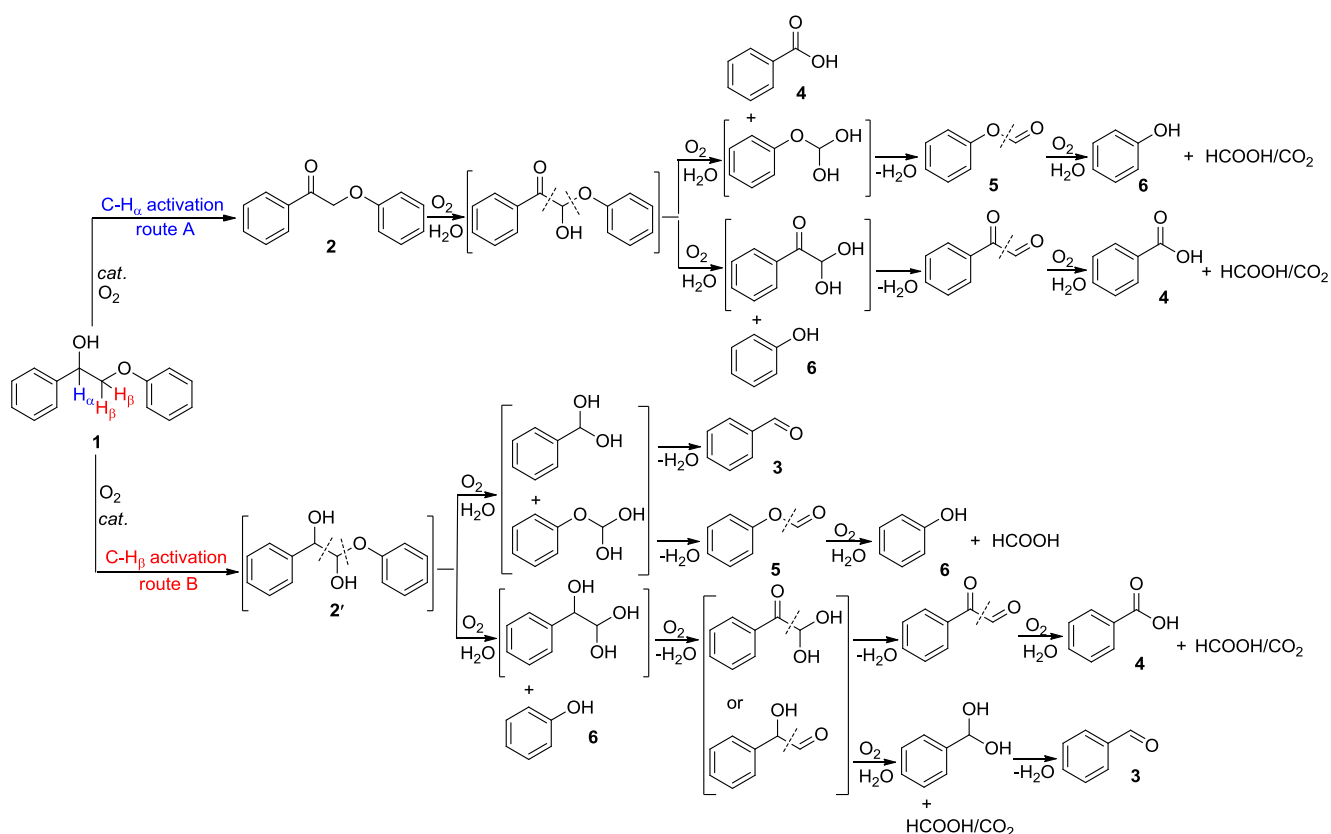


Figure S7 Mass spectra for carbon oxide detected in VO(acac)₂-catalyzed oxidation of 2-phenoxy-1-phenylethanol in acetic acid when employing ¹⁸O₂ as the oxidant.



Scheme S2 The proposed detailed reaction pathways for VO(acac)₂-catalyzed oxidative cleavage of 2-phenoxy-1-phenylethanol in acetic acid.

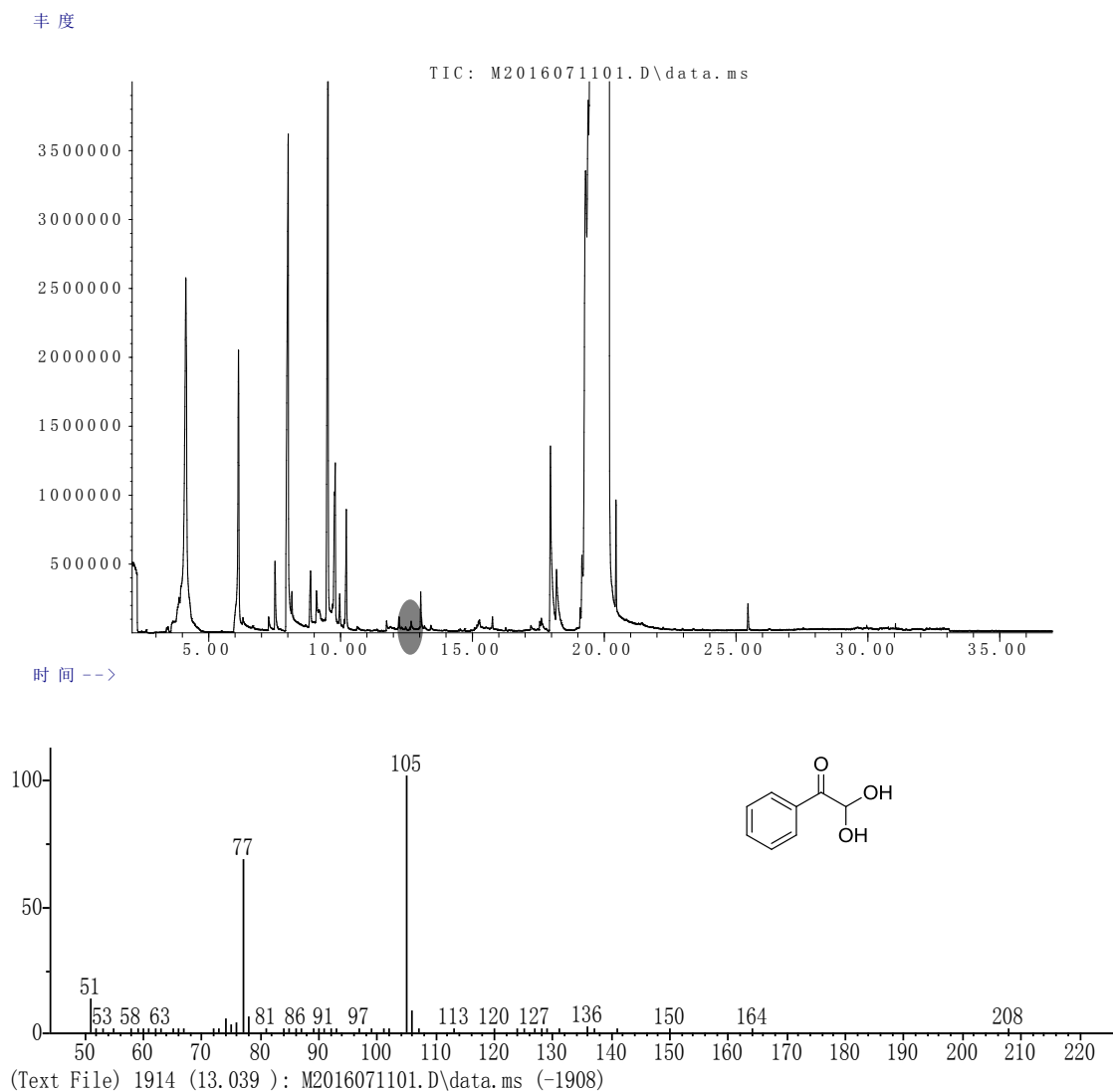


Figure S8 Mass spectra for reaction products in VO(acac)₂-catalyzed oxidation of lignin model compound **1** in acetonitrile. Reaction condition: 0.25 mmol model compound **1**, 0.025 mmol VO(acac)₂, 0.5 mL solvent, 80 °C, 1 atm O₂, 1 h.

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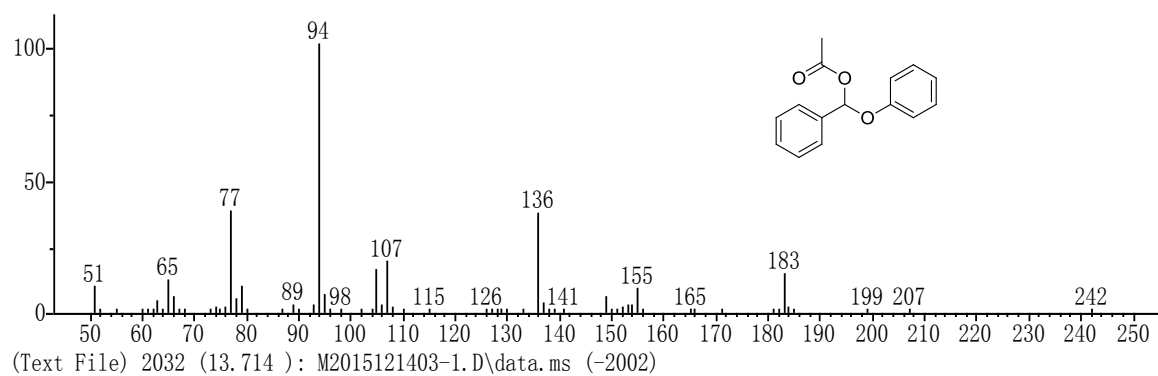
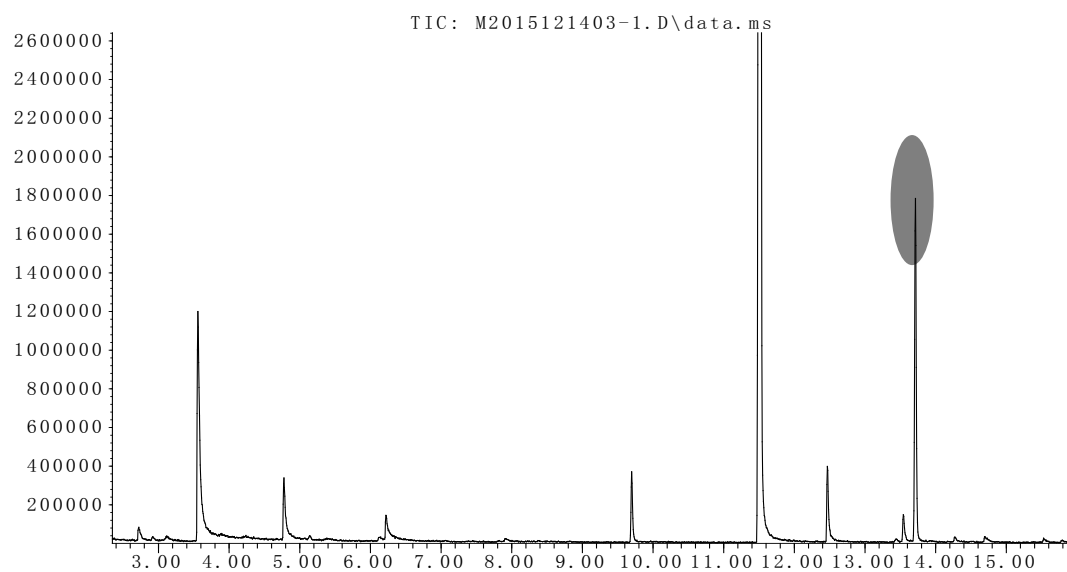


Figure S9 Mass spectra for reaction products in VO(acac)₂-catalyzed oxidation of benzyl phenyl ether in the mixture of acetic acid and acetic anhydride (v/v=1:1).