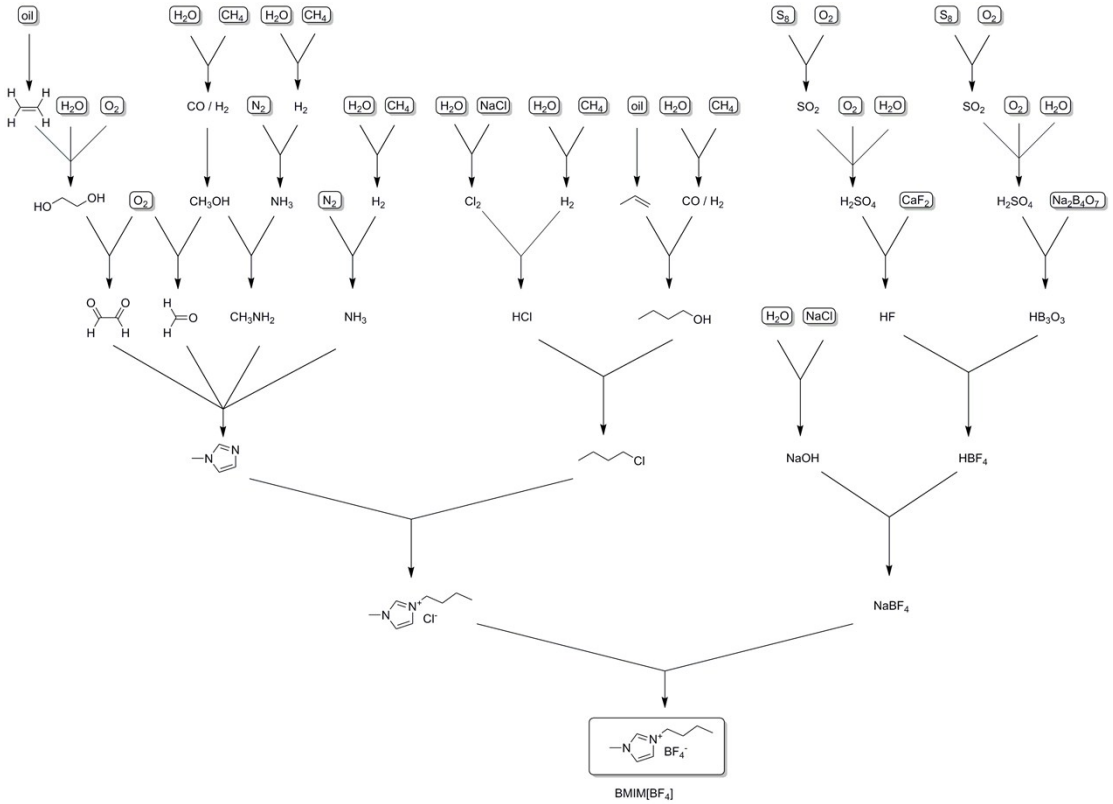
Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Chemoenzymatic epoxidation of alkenes with *Candida antarctica* lipase B and hydrogen peroxide in deep eutectic solvents

Pengfei Zhou,[a] Xuping Wang,[b] Bo Yang,[a] Frank Hollmann[c] and Yonghua Wang[b,*]

[a]*School of Bioscience and Bioengineering, South China University of Technology, Guangzhou 510006, P.R China.*
[b]*School of Food Science and Engineering, South China University of Technology, Guangzhou 510640, P.R China. E-Mail: yonghw@scut.edu.cn, Tel/fax: 0086 (0)20 8711 3842*
[c]*Department of Biotechnology, Delft University of Technology, Van der Maasweg 9, 2629HZ, Delft, The Netherlands*



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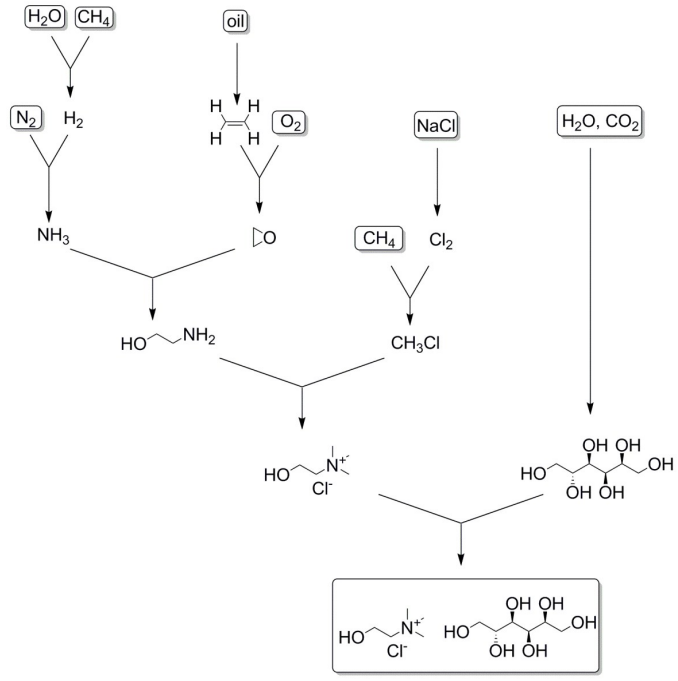

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33 **Fig. S1.** Comparison of the synthesis trees for BMIM[BF_4] (upper)[1] and ChCl/sorbitol (lower).

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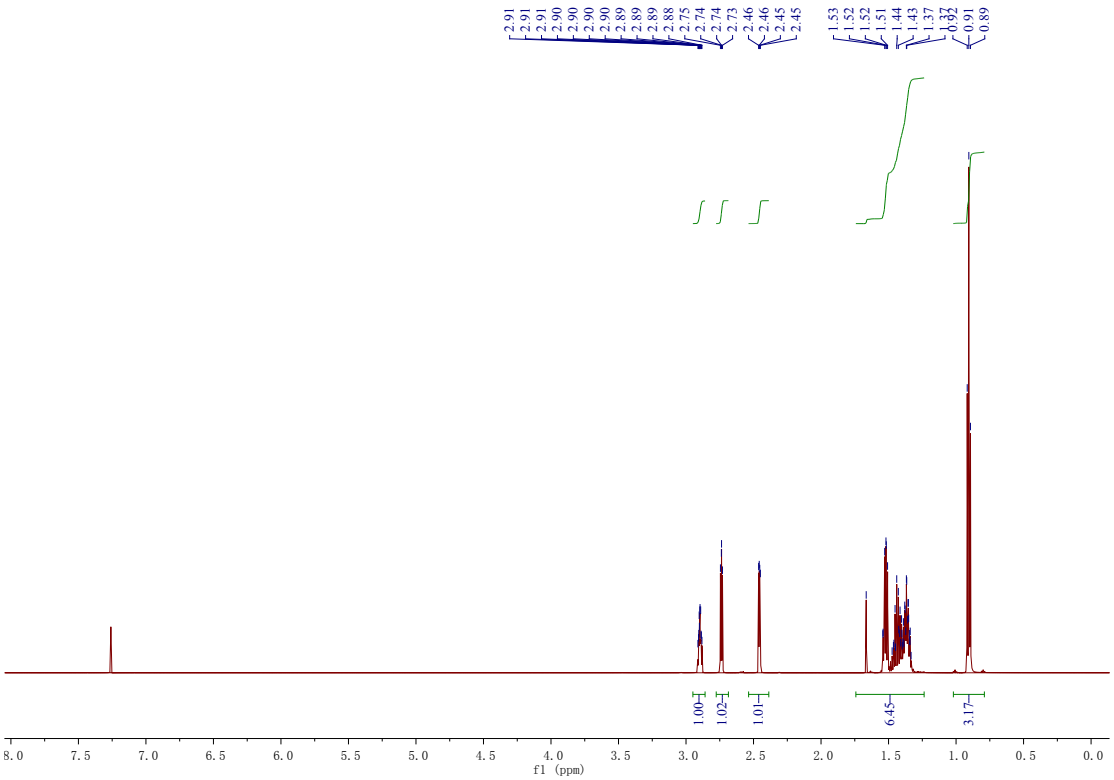

Fig. S2. ^{1}H NMR ($C_6H_{12}O$ in $CDCl_3$)

^{1}H NMR ($CDCl_3$): δ 2.95 – 2.84 (m, 1H), 2.74 (dd, *J* = 4.9, 4.1 Hz, 1H), 2.46 (dd, *J* = 5.0, 2.7 Hz, 1H), 1.75 – 1.23 (m, 6H), 0.91 (t, *J* = 7.2 Hz, 3H).

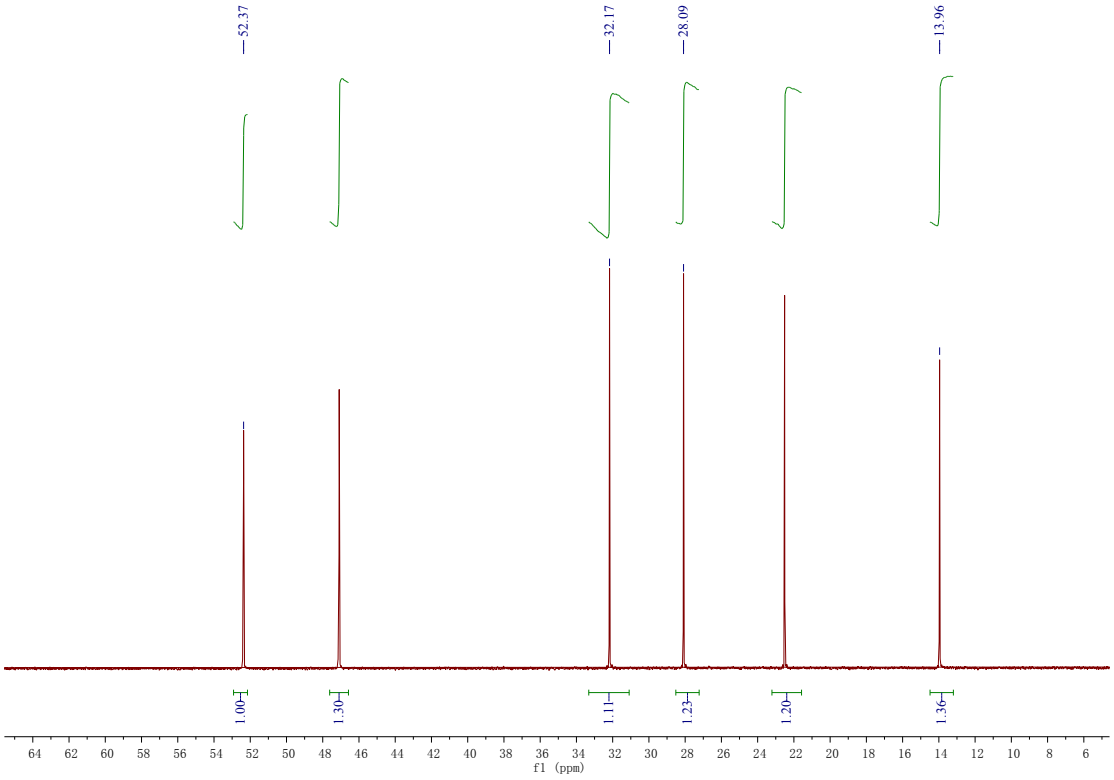

Fig. S3. ^{13}C NMR ($C_6H_{12}O$ in $CDCl_3$)

^{13}C NMR ($CDCl_3$): δ 52.37 (CH), 47.09 (CH_2), 32.17 (CH_2), 28.09 (CH_2), 22.51 (CH_2), 13.96 (CH_3).

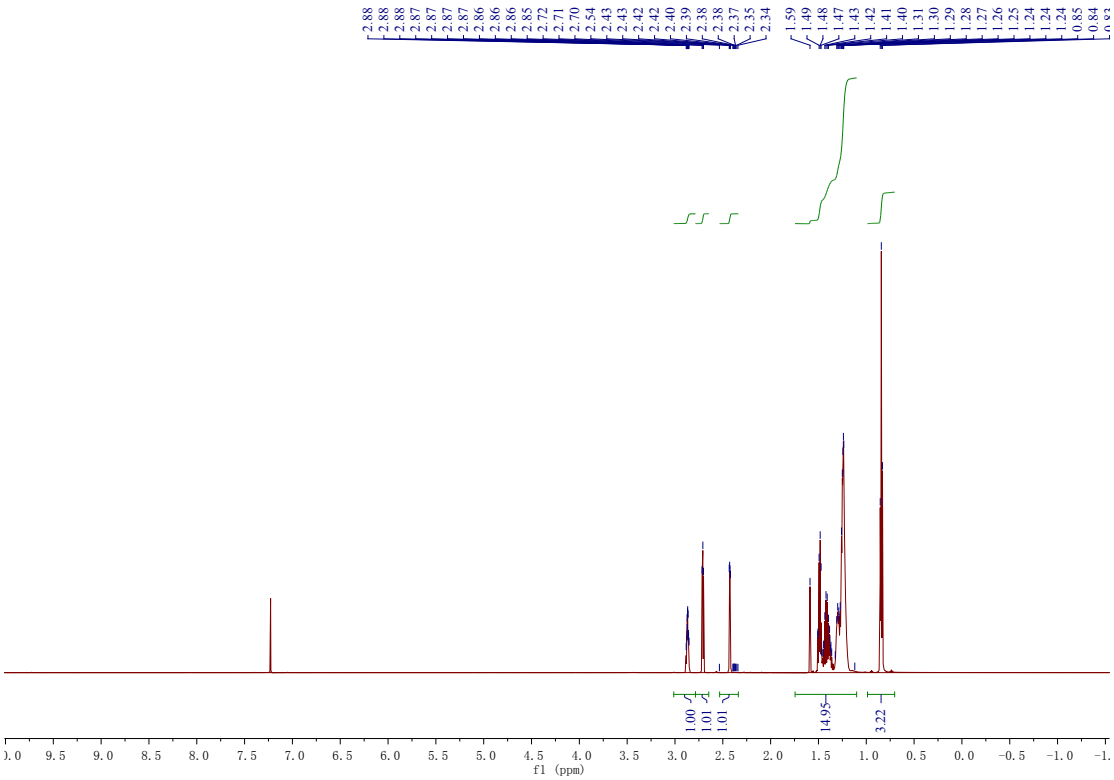

Fig. S4. ^{1}H NMR ($C_{10}H_{20}O$ in $CDCl_3$)

^{1}H NMR ($CDCl_3$): δ 3.04 – 2.79 (m, 1H), 2.76 – 2.62 (m, 1H), 2.43 (dd, *J* = 5.0, 2.7 Hz, 1H), 1.72 – 1.13 (m, 14H), 0.84 (t, *J* = 7.0 Hz, 3H).

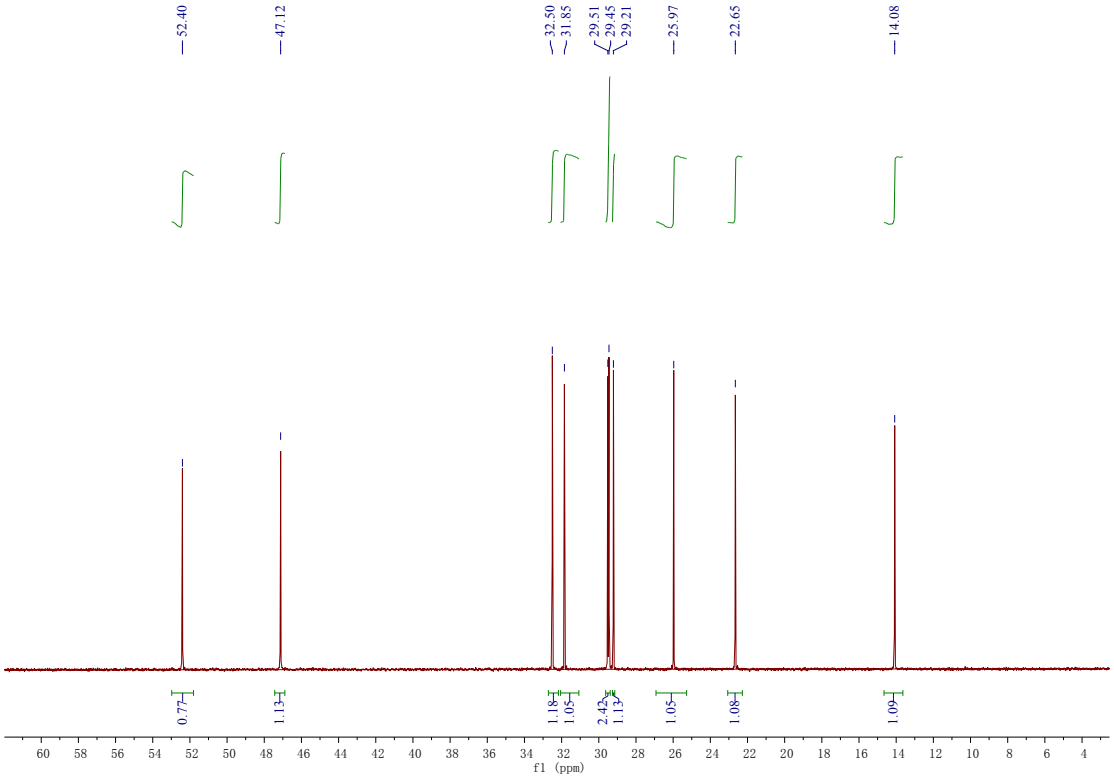

Fig. S5. ^{13}C NMR ($C_{10}H_{20}O$ in $CDCl_3$)

^{13}C NMR ($CDCl_3$): δ 52.40 (CH), 47.12 (CH_2), 32.50 (CH_2), 31.85 (CH_2), 29.48 (d, *J* = 9.3 Hz, 2CH_2), 29.21 (CH_2), 25.97 (CH_2), 22.65 (CH_2), 14.08 (CH_3).

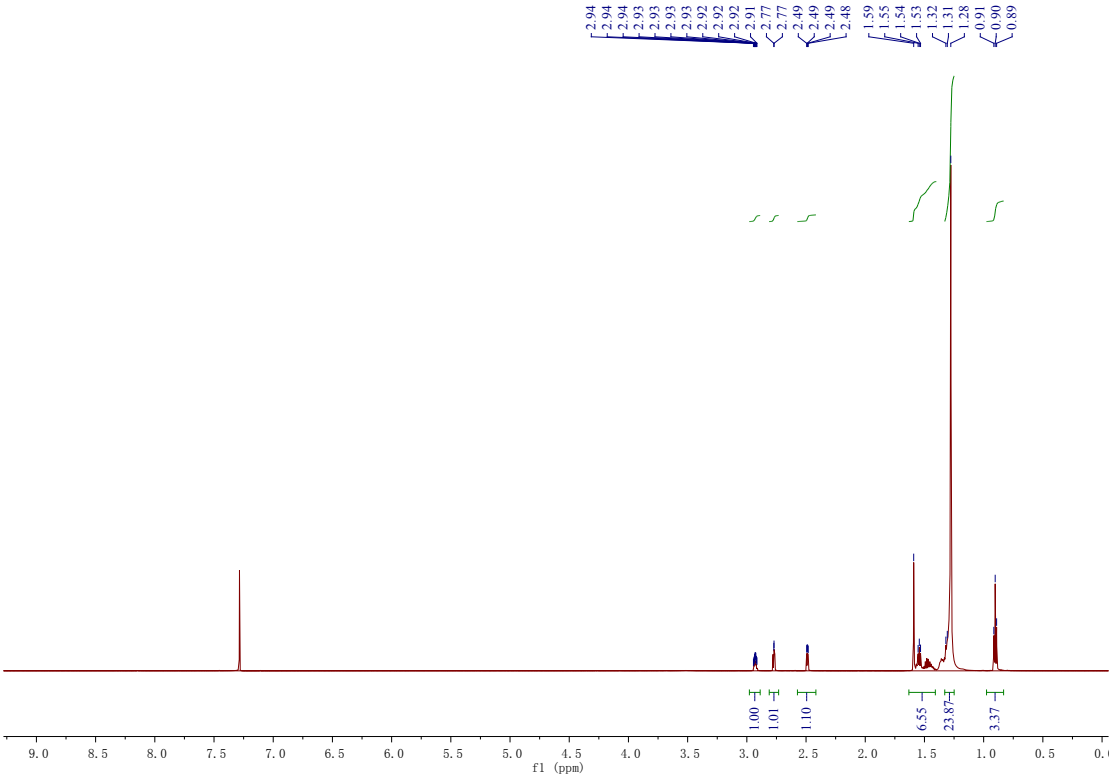

Fig. S6. ^{1}H NMR ($C_{18}H_{36}O$ in $CDCl_3$)

^{1}H NMR ($CDCl_3$): δ 2.99 – 2.86 (m, 1H), 2.77 (dd, *J* = 4.9, 4.1 Hz, 1H), 2.49 (dd, *J* = 5.0, 2.7 Hz, 1H), 1.70 – 1.42 (m, 6H), 1.39 – 1.16 (m, 24H), 0.90 (t, *J* = 7.0 Hz, 3H).

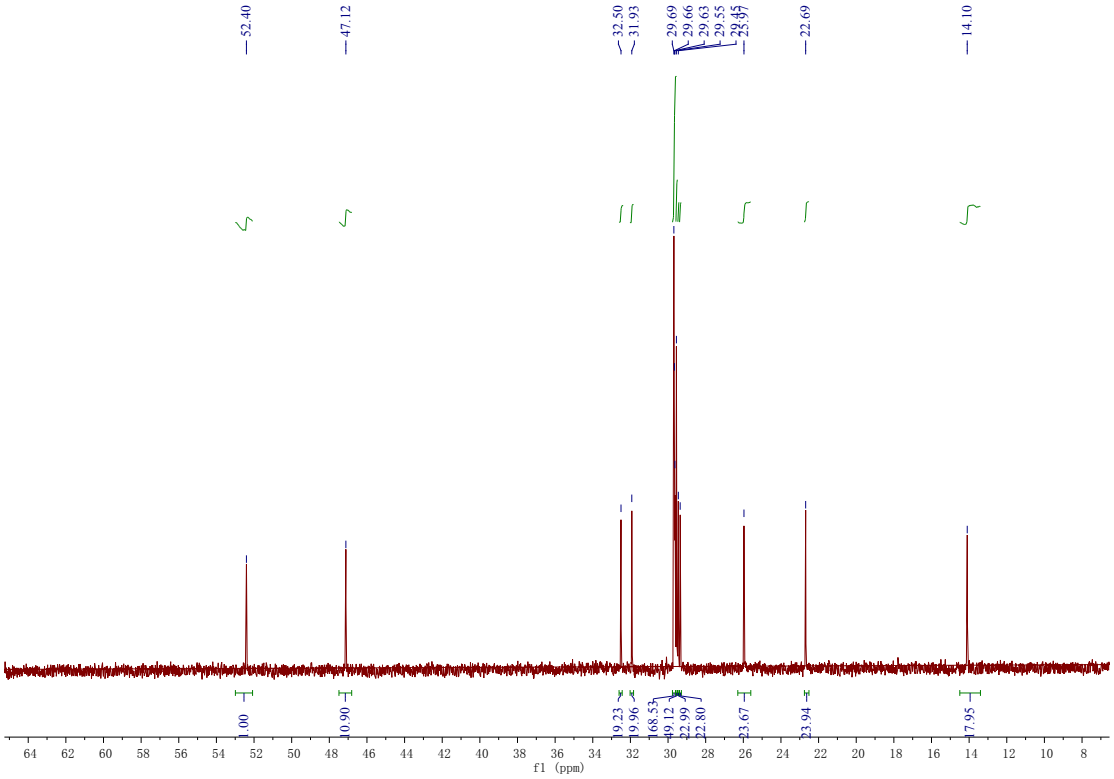

Fig. S7. ^{13}C NMR ($C_{18}H_{36}O$ in $CDCl_3$)

^{13}C NMR ($CDCl_3$): δ 52.40 (CH), 47.12 (CH_2), 32.50 (CH_2), 31.93 (CH_2), 29.76 – 29.59 (8CH_2), 29.55 (CH_2), 29.45 (CH_2), 29.36 (CH_2), 25.97 (CH_2), 22.69 (CH_2), 14.10 (CH_3).

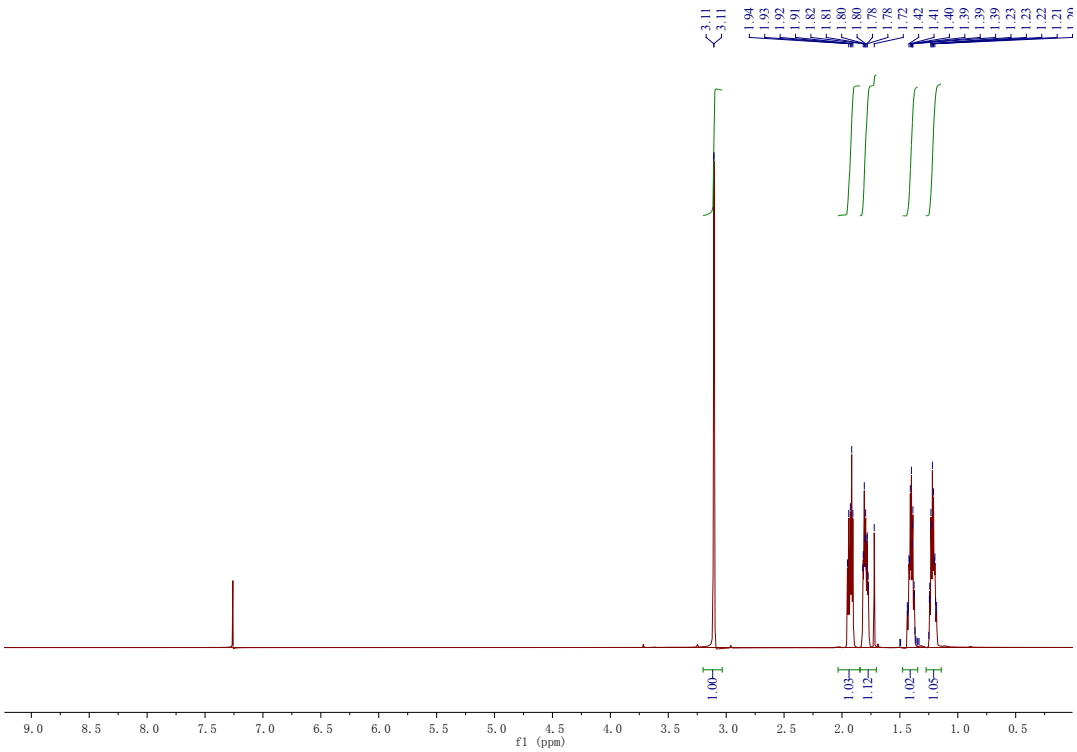

Fig. S8. ^{1}H NMR (C_6H_6O in $CDCl_3$)

^{1}H NMR ($CDCl_3$): δ 3.11 (d, *J* = 1.1 Hz, 2H), 2.00 – 1.87 (m, 1H), 1.86 – 1.69 (m, 1H), 1.45 – 1.33 (m, 1H), 1.27 – 1.13 (m, 1H).

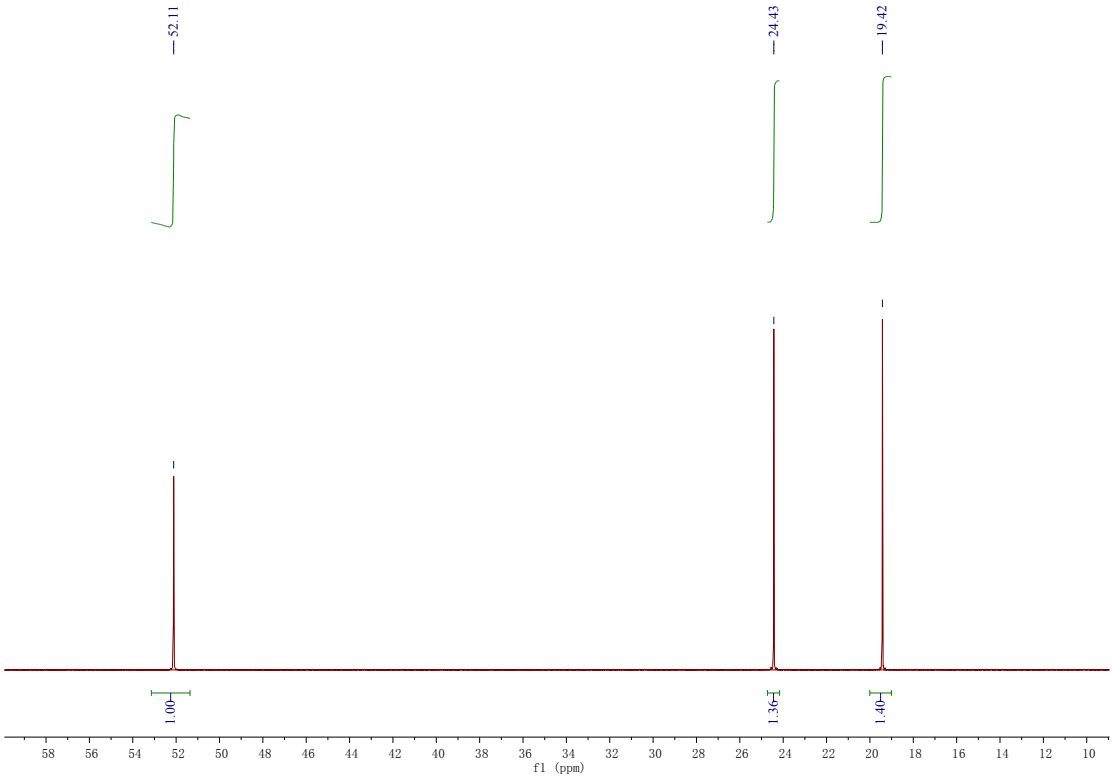

Fig. S9. ^{13}C NMR (C_6H_6O in $CDCl_3$)

^{13}C NMR ($CDCl_3$): δ 52.11 (2CH), 24.43 ($2CH_2$), 19.42 ($2CH_2$).

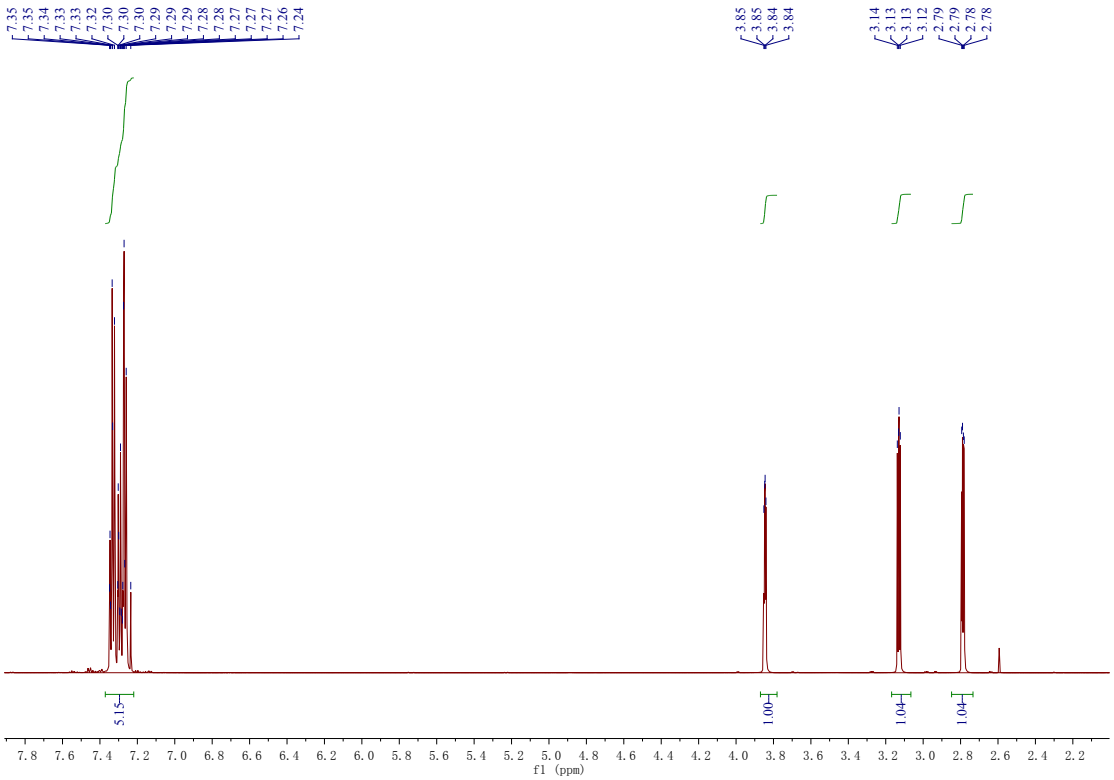

Fig. S10. ^{1}H NMR (C_8H_8O in $CDCl_3$)

^{1}H NMR ($CDCl_3$): δ 7.36 – 7.27 (m, 5H), 3.85 (dd, *J* = 3.9, 2.7 Hz, 1H), 3.13 (dd, *J* = 5.5, 4.1 Hz, 1H), 2.79 (dd, *J* = 5.5, 2.6 Hz, 1H).

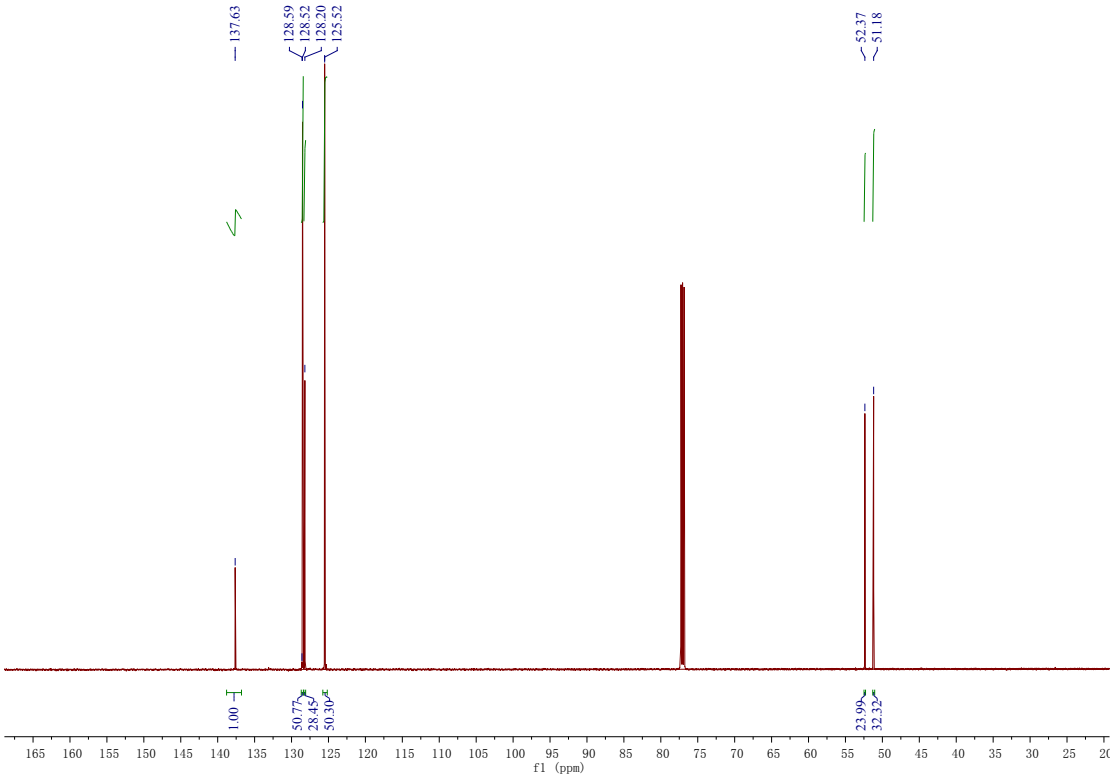

Fig. S11. ^{13}C NMR (C_8H_8O in $CDCl_3$)

^{13}C NMR ($CDCl_3$): δ 137.63 (C), 128.52 (2CH), 128.20 (CH), 125.52 (2CH), 52.37 (CH), 51.18 (CH_2).

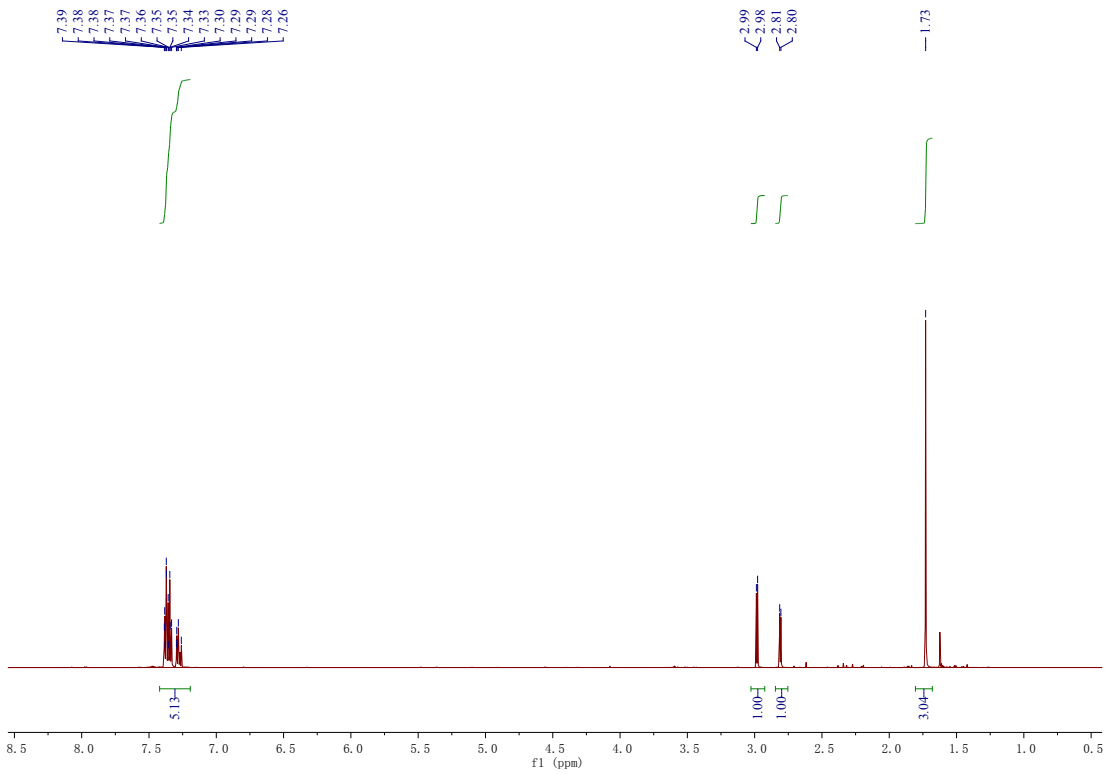

Fig. S12. ^{1}H NMR ($C_9H_{10}O$ in $CDCl_3$)

^{1}H NMR ($CDCl_3$): δ 7.46 – 7.17 (m, 5H), 2.98 (d, *J* = 5.4 Hz, 1H), 2.81 (d, *J* = 5.4 Hz, 1H), 1.73 (s, 3H).

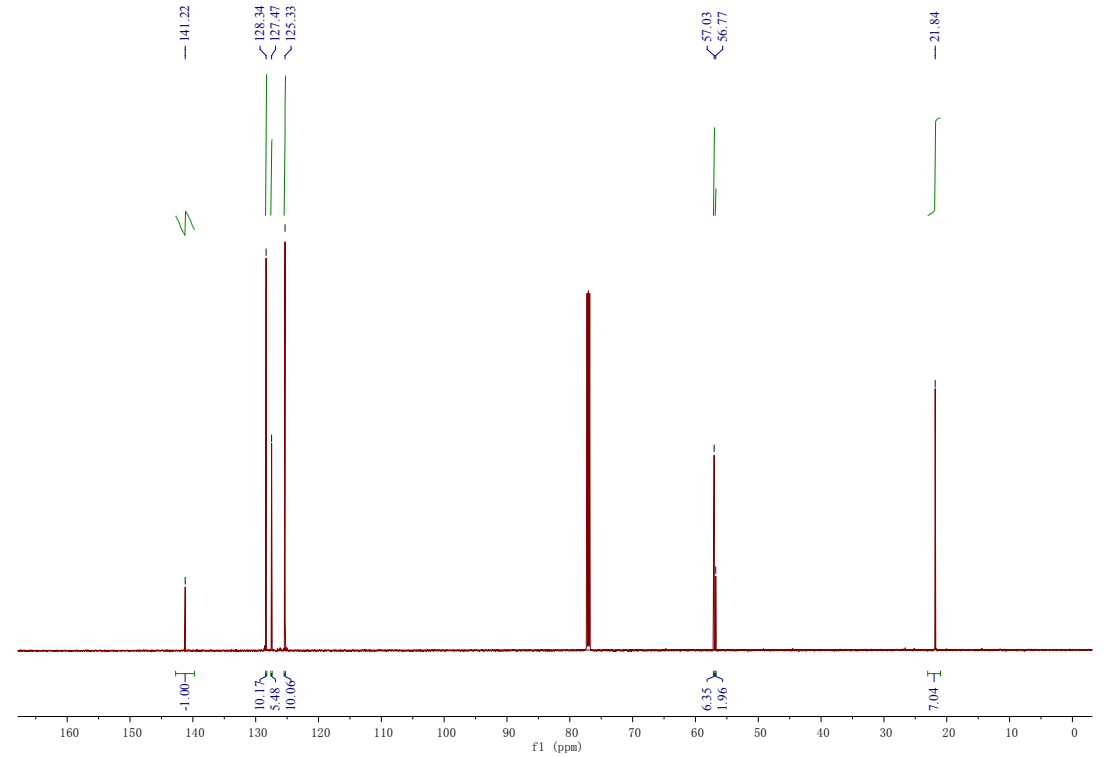

Fig. S13. ^{13}C NMR ($C_9H_{10}O$ in $CDCl_3$)

^{13}C NMR ($CDCl_3$): δ 141.22 (C), 128.34 (2CH), 127.47 (CH), 125.33 (2CH), 57.03 (CH), 56.77 (CH), 21.84 (CH_3).

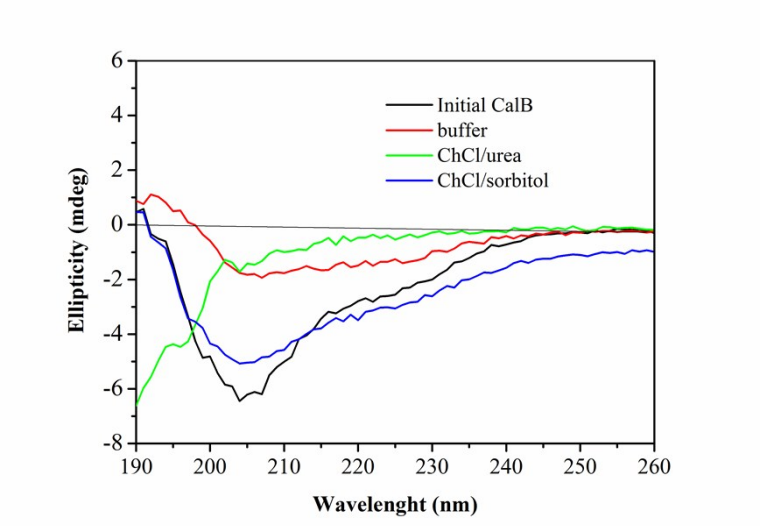

Fig. S14. CD spectra of CalB in different solvents.

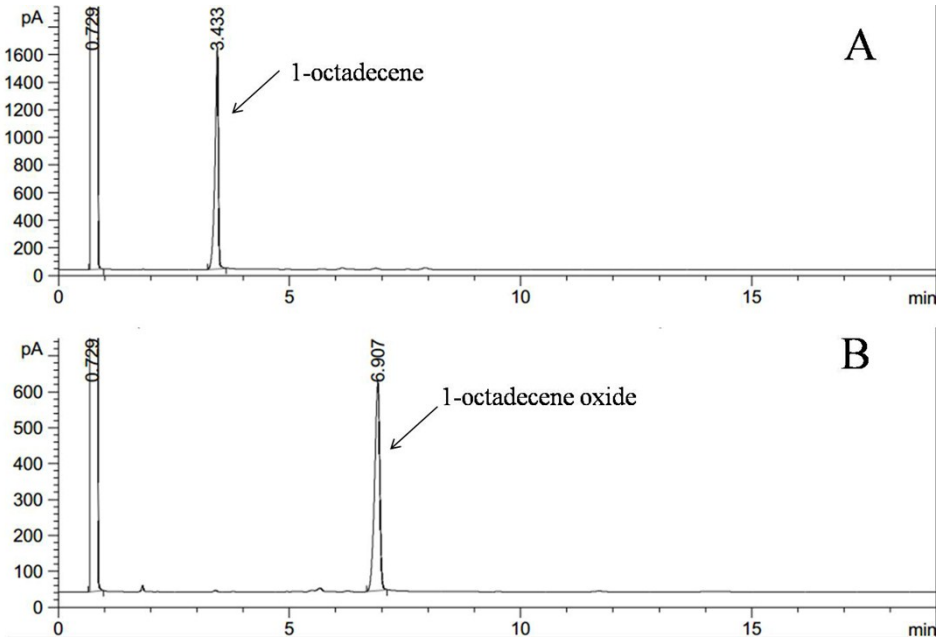

Fig. S15. GC graph of 1-octadecene (A) and 1- octadecene oxide (B).

References

1 P. G. Jessop, *Green Chem.*, 2011, **13**, 1391–1398.