Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Hydrogen bonding-catalyzed synthesis of 1,4-dioxanes from dehydrative cyclization of vicinal diols in ionic liquids

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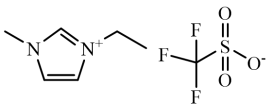
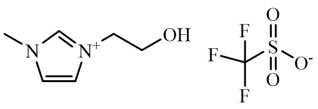
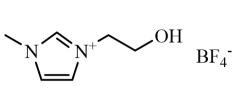


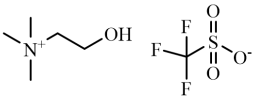
[EtMIm][OTf]



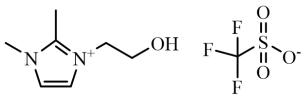
[HO-EtMIm][OTf]



[HO-EtMIm][BF_4]



[HO-EtN_{111}][OTf]



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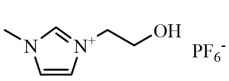
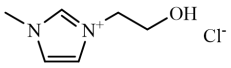
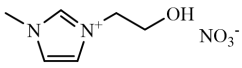


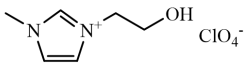
[HO-EtMIm][PF_6]



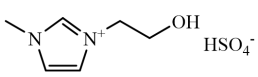
[HO-EtMIm][Cl]



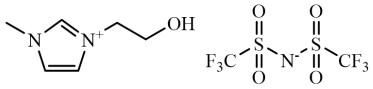
[HO-EtMIm][NO_3]



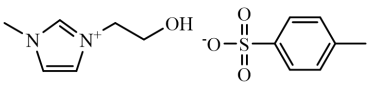
[HO-EtMIm][ClO_4]



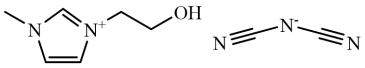
[HO-EtMIm][HSO_4]



[HO-EtMIm][NTf_2]



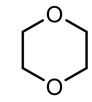
[HO-EtMIm][OTs]

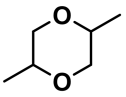


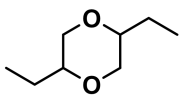
[HO-EtMIm][$N(CN)_2$]

Fig. S1 Chemical structures of ILs in this work

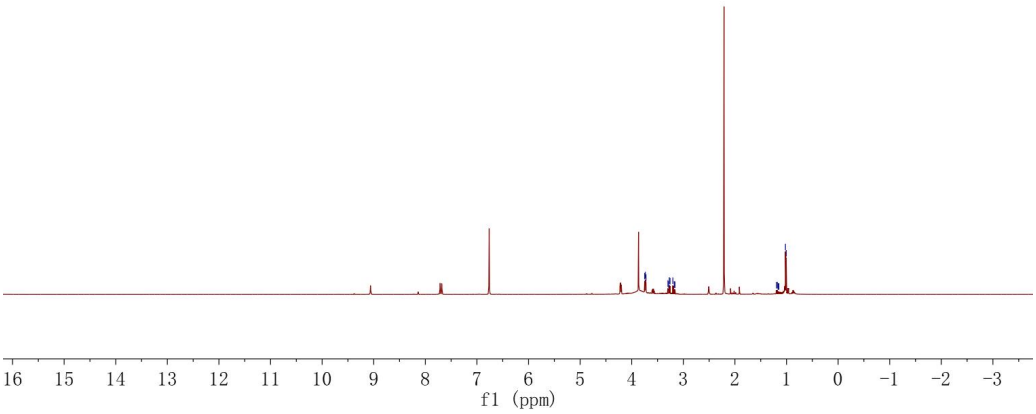
^{1}H NMR Spetra








3.75
3.74
3.72
3.30
3.28
3.27
3.26
3.20
3.18
3.16
1.19
1.18
1.16
1.15
1.02
1.01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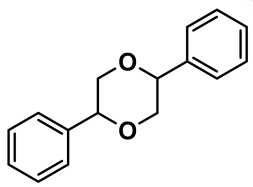


7.72
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7.36
7.36
7.32
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4.95
4.93
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4.20
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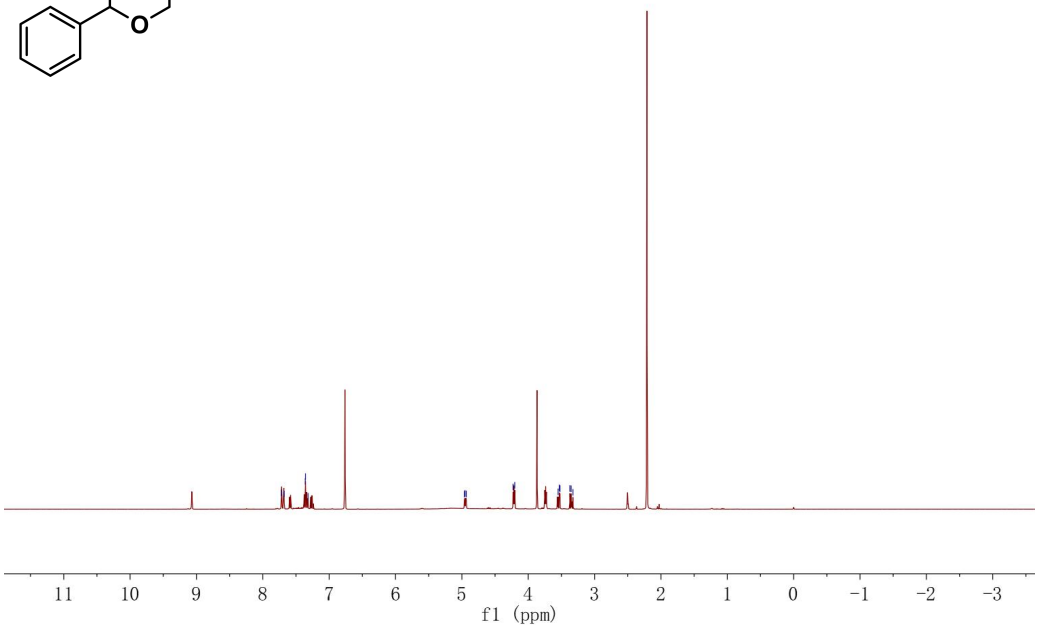
3.35
3.33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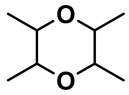
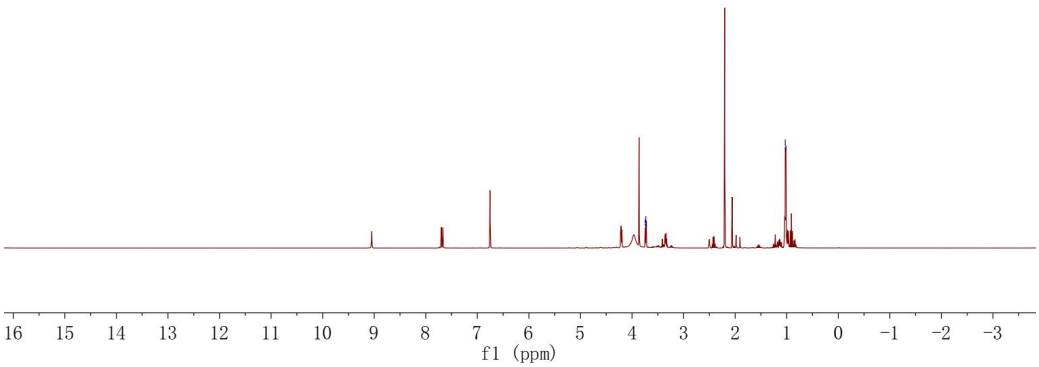



3.74
3.73
3.72

1.03
1.01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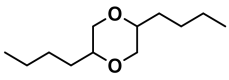

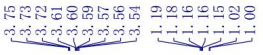
3.75
3.73
3.72
3.61
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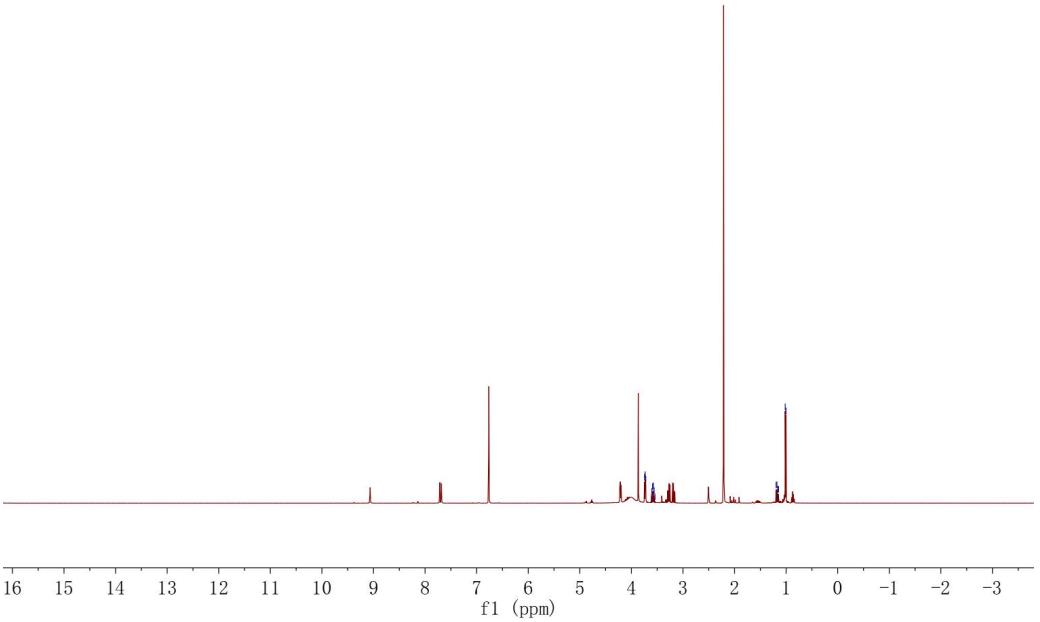
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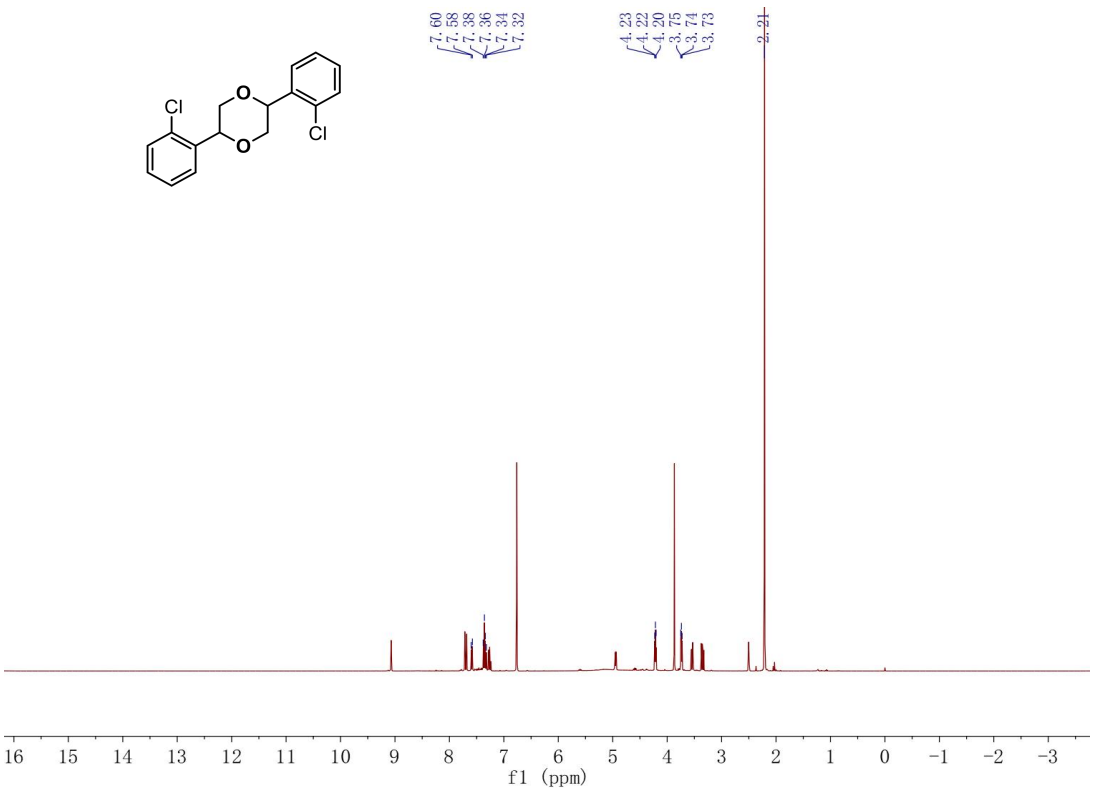

DFT calculations references:

1. Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Scalmani, G., Barone, V., Petersson, G.A., Nakatsuji, H., et al. (2016). Gaussian 16 Rev. C.01.

2. Caldeweyher, E., Bannwarth, C., Grimme, S. (2017). Extension of the D3 dispersion coefficient model. J. Chem. Phys. 147, 034112. (10.1063/1.4993215)

3. Glendening, E.D., Landis, C.R., Weinhold, F. (2012). Natural bond orbital methods. WIREs Computational Molecular Science 2, 1-42. (10.1002/wcms.51)