Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting Information

Synthesis of Oxygenated Fuel Additive from Waste Biomass Derived Aldehyde using Green Catalyst: An Experimental and DFT Study

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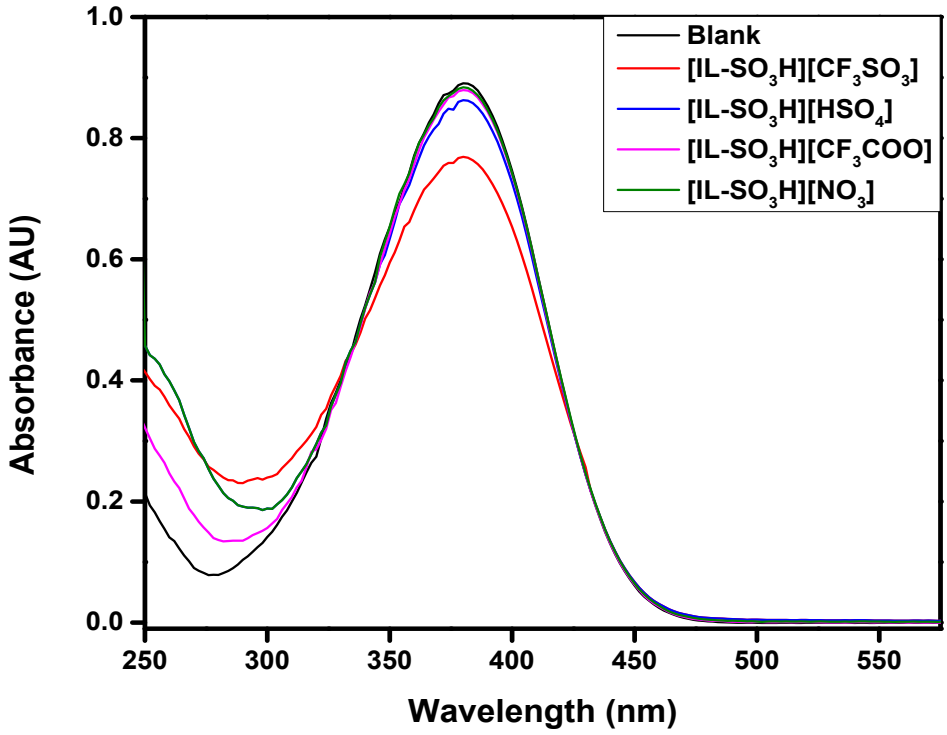

Fig. S1. Absorption spectra of 4-nitroaniline with the 30 mM concentrations of different protic ionic liquid catalyst in H_2O.

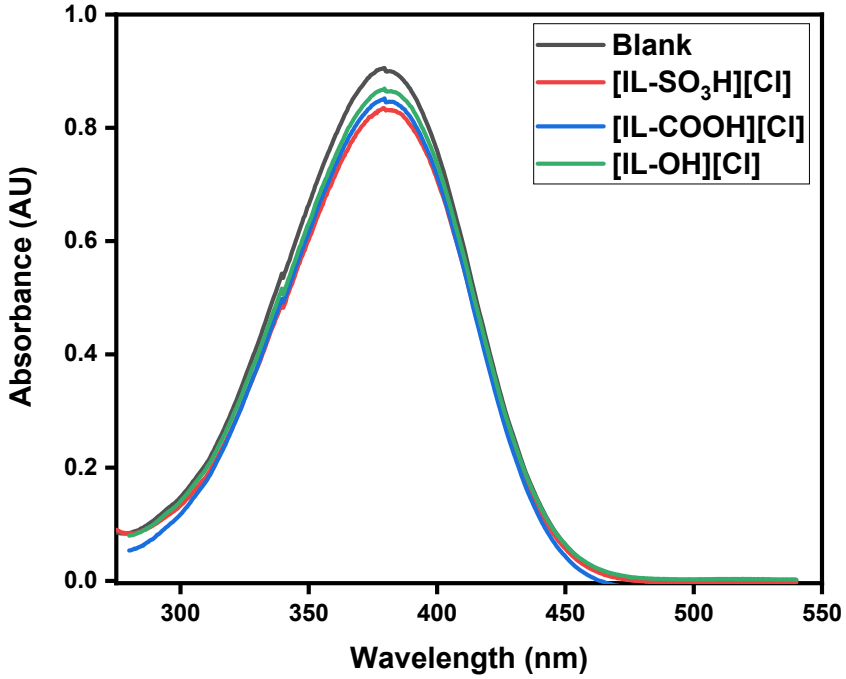

Fig. S2. Absorption spectra of 4-nitroaniline with the 25 mM concentrations of different protic ionic liquid catalyst in H_2O.

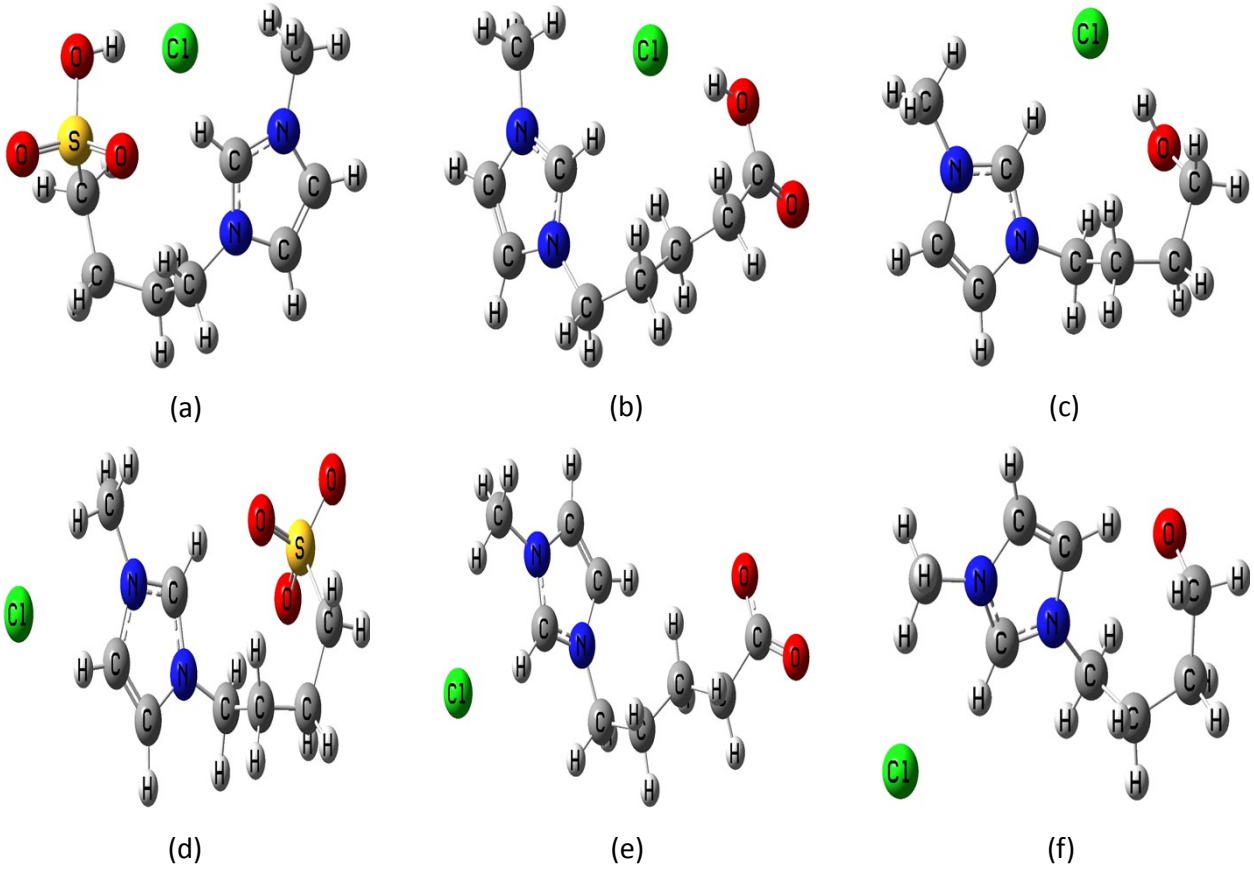

Fig. S3.Optimized structures of ionic liquid (a) [IL-SO_3H][Cl] (b) [IL-COOH][Cl] (c) [IL-OH][Cl] and (d-f) shows their conjugate base respectively.

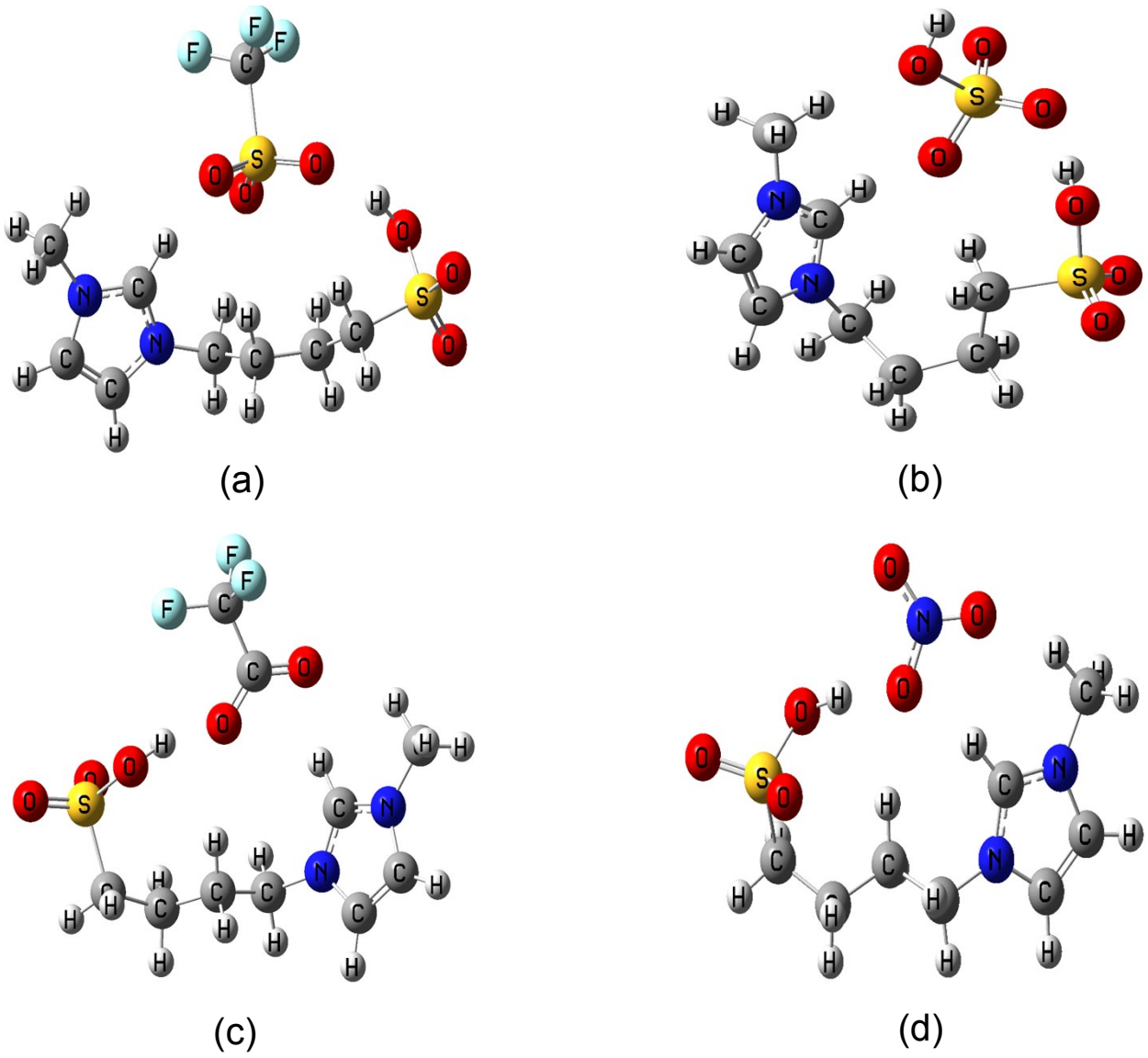

Fig. S4. Optimized structures of ionic liquid (a) [IL-SO_3H][CF_3SO_3] (b) [IL-SO_3H][HSO_4] (c) [IL-SO_3H][CF_3COO] and (d) [IL-SO_3H][NO_3].

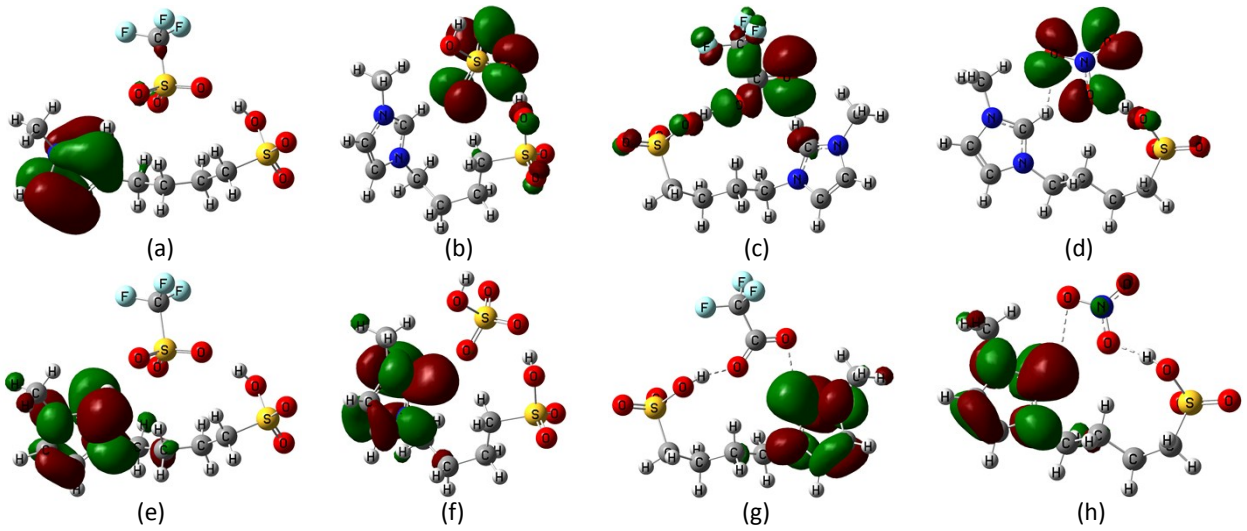

Fig. S5. Frontier Orbital diagram (a-d) are the HOMOs and (e-h) are the LUMOs of protic ionic liquid [IL-SO_3H][CF_3SO_3], [IL-SO_3H][HSO_4], [IL-SO_3H][CF_3COO], and [IL-SO_3H][NO_3] respectively. (isovalue = 0.03 a.m.u.)

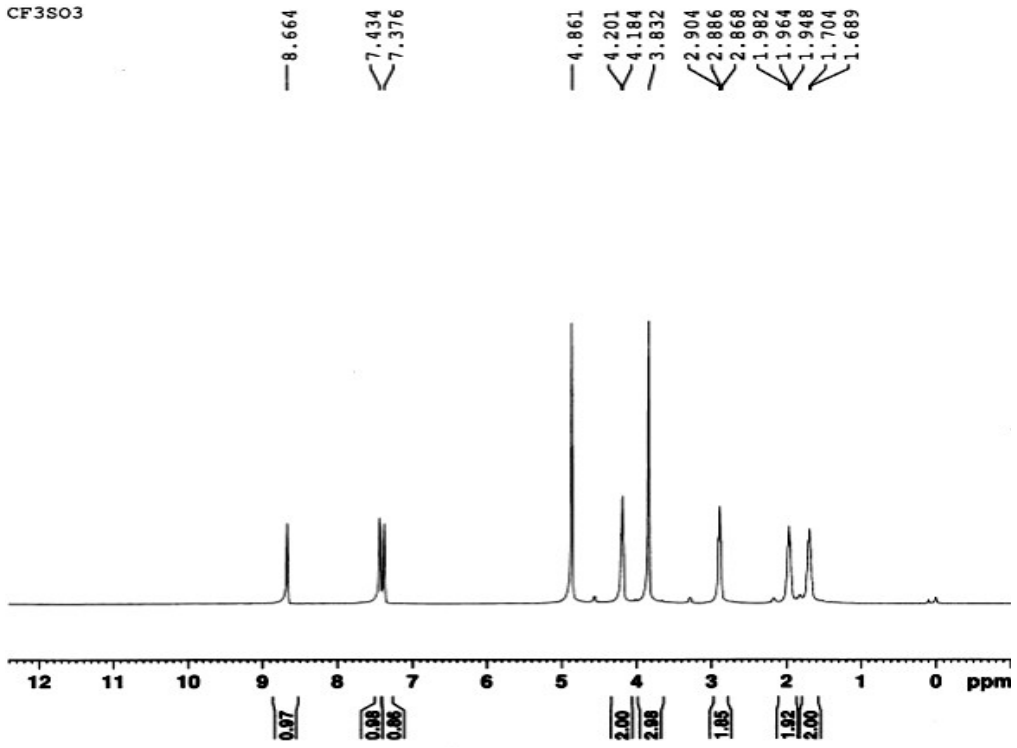

Fig. S6. ^1H NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][CF_3SO_3] catalyst.

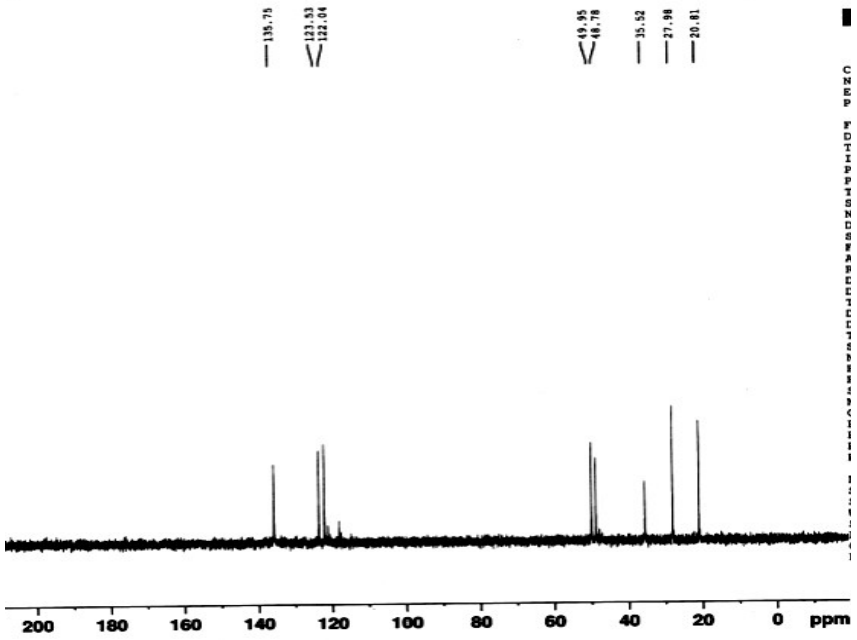

Fig. S7. ^{13}C NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][CF_3SO_3] catalyst.

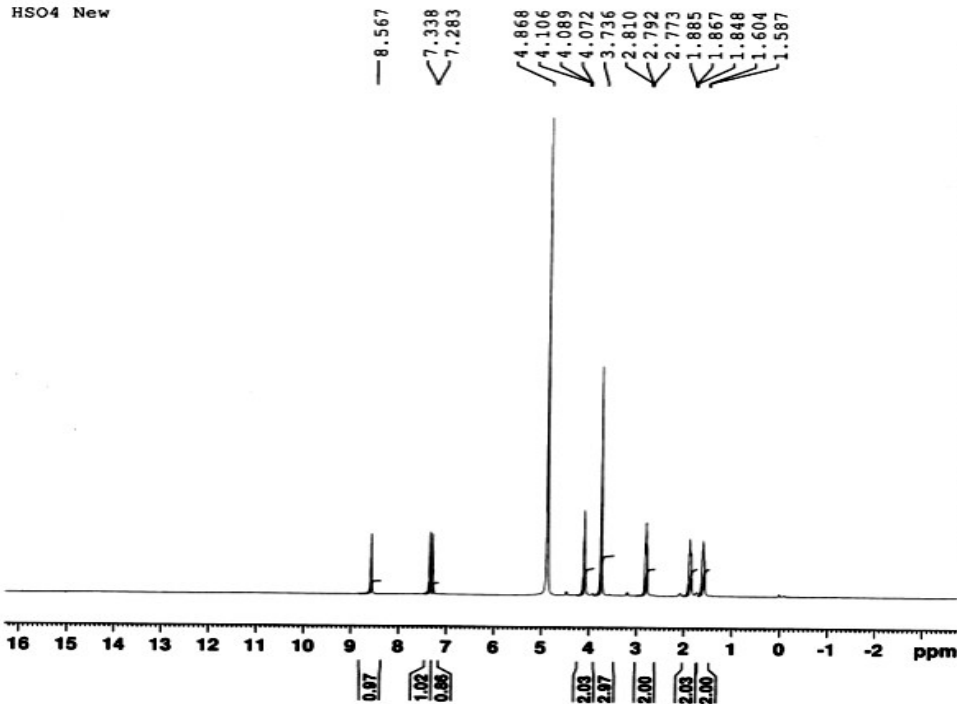

Fig. S8. ^{1}H NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][HSO_4] catalyst.

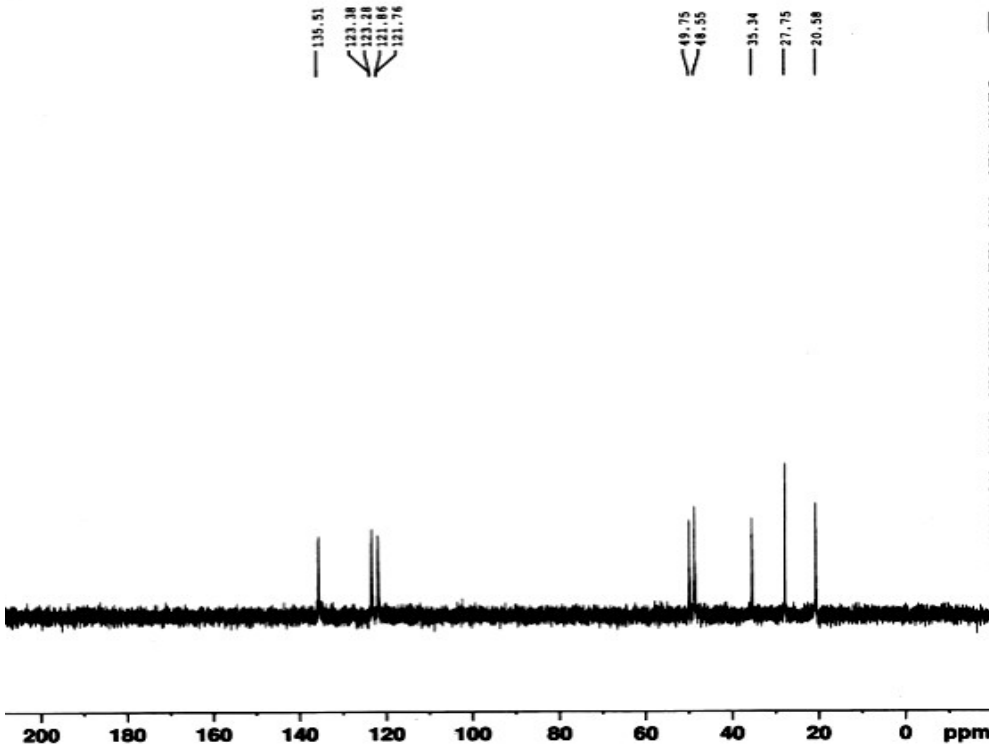

Fig. S9. ^{13}C NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][HSO_4] catalyst.

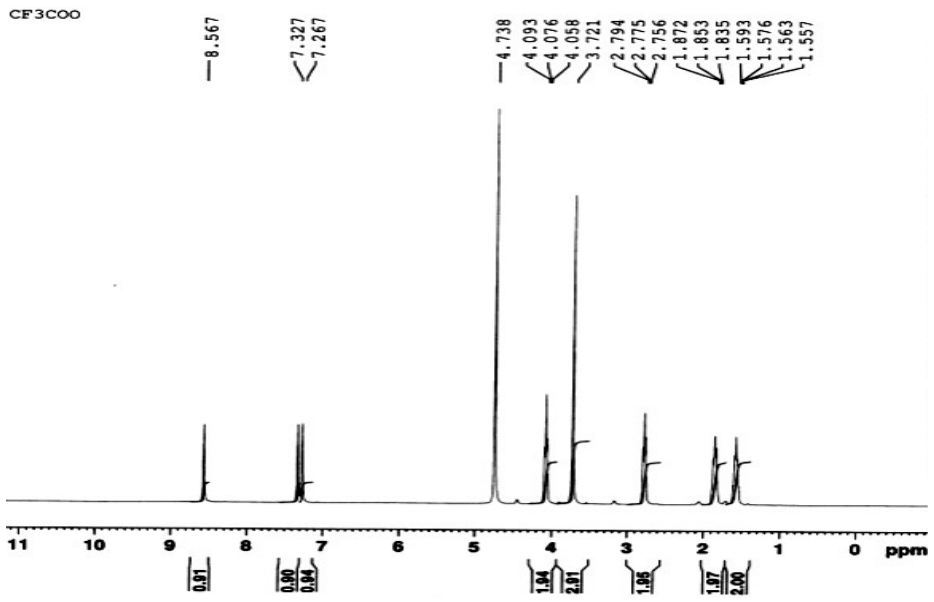

Fig. S10. ^{1}H NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][CF_3COO] catalyst.

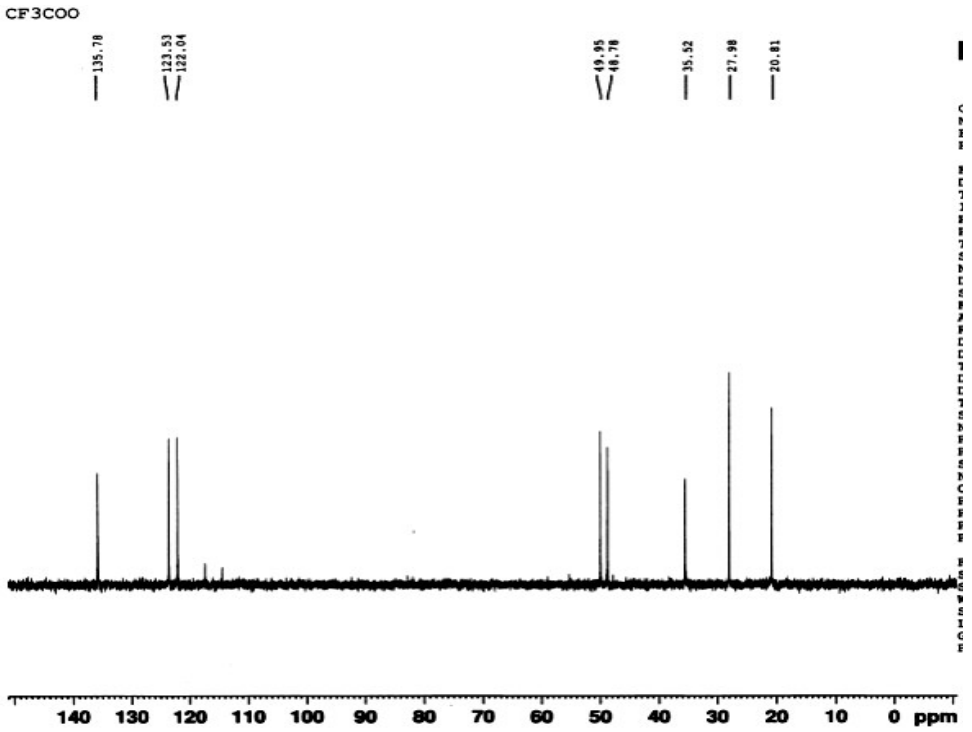

Fig. S11. ^{13}C NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][CF_3COO] catalyst.

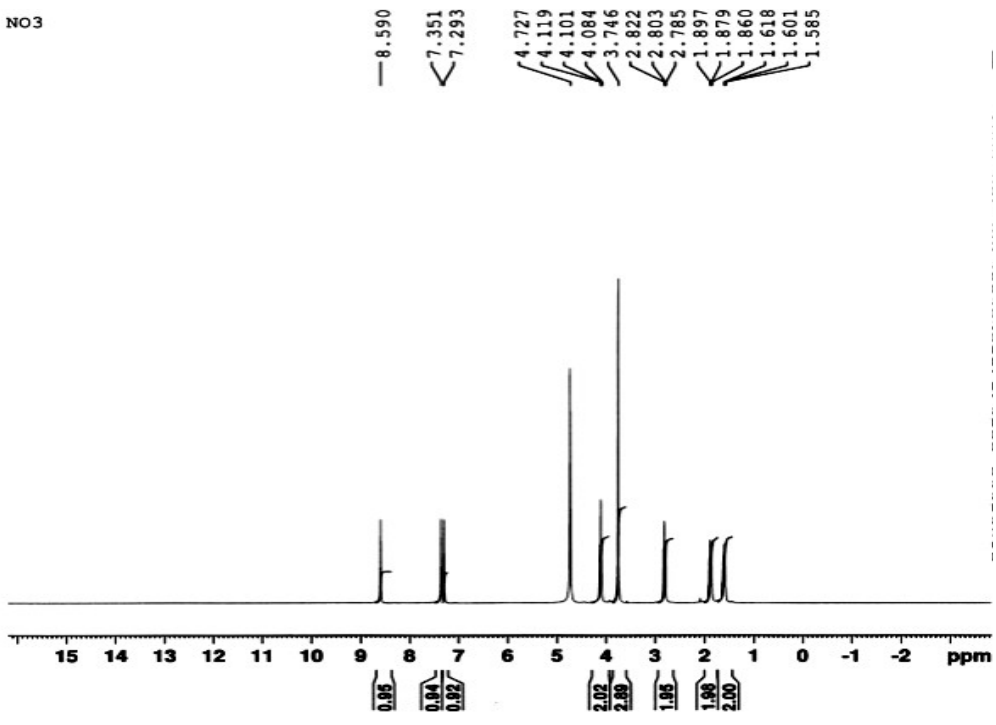

Fig. S12. ^{1}H NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][NO_3] catalyst.

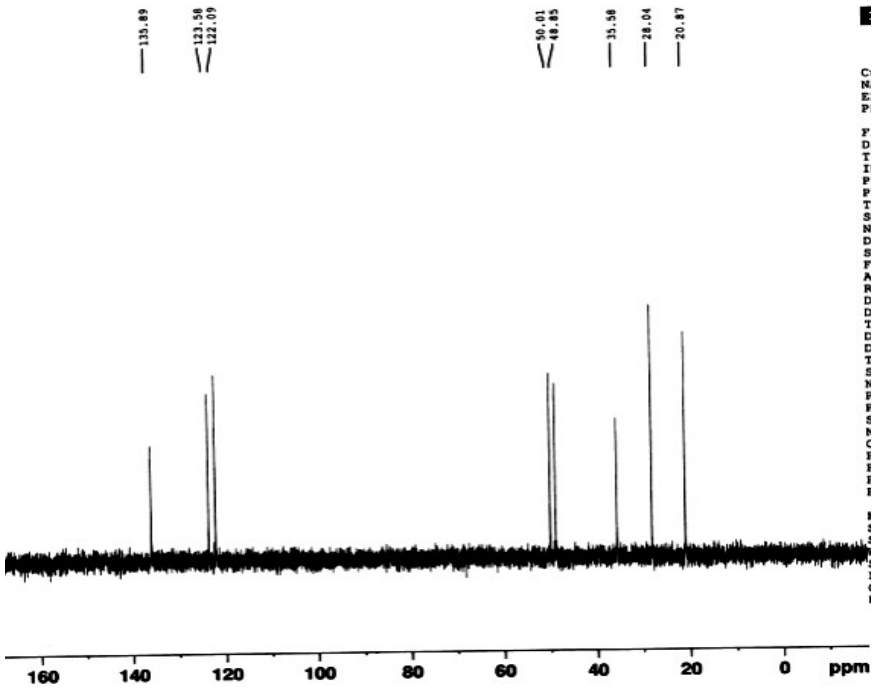

Fig. S13. ^{13}C NMR spectrum of the synthesized protic ionic liquid [IL-SO_3H][NO_3] catalyst.

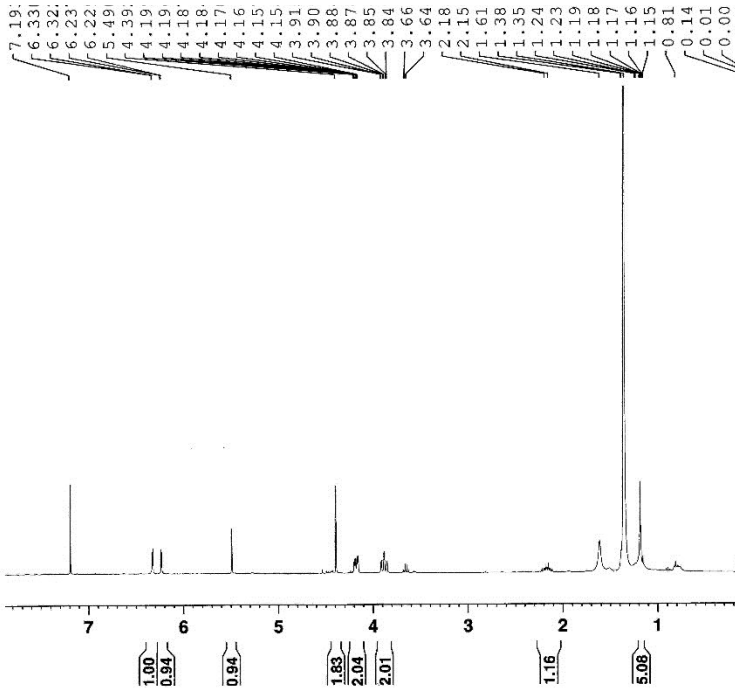

Fig. S14. ^{1}H NMR spectrum of the synthesized product.

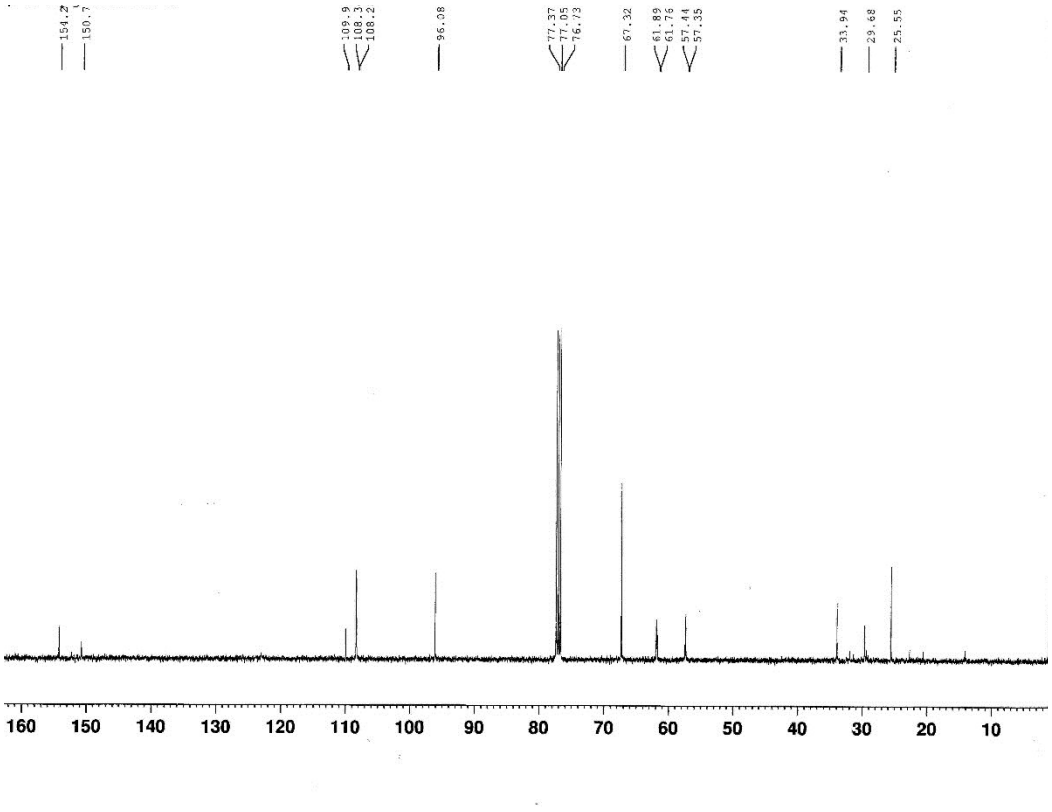

Fig. S15. ^{13}C NMR spectrum of the synthesized product.