# Hydrogen Bonds in Precursor Solution：The Origin of the Anomalous *J-V* Curves in Perovskite Solar Cells from Gas-quenching Process

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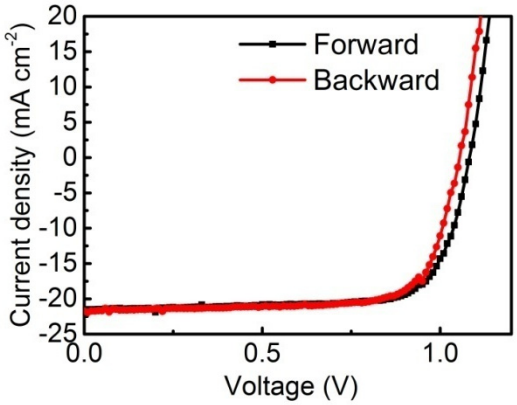



Figure S 1 DMSO/A=2.0 anti-solvent method.

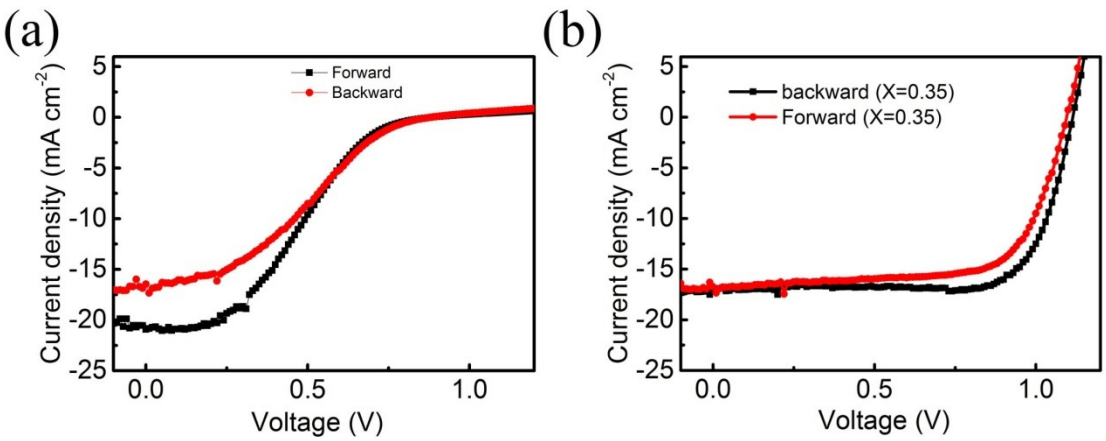



Figure S2 NMP/A =1.4 (a) and 0.35 (b).

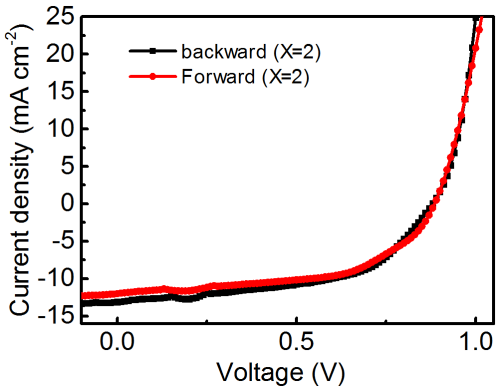



Figure S3 *J-V* curve of p-i-n device with $Cs_{0.5}MA_{0.95}PbI_3$ perovskite, which was prepared from precursor solution containing 2.0 molar equivalent of NMP to A cations.

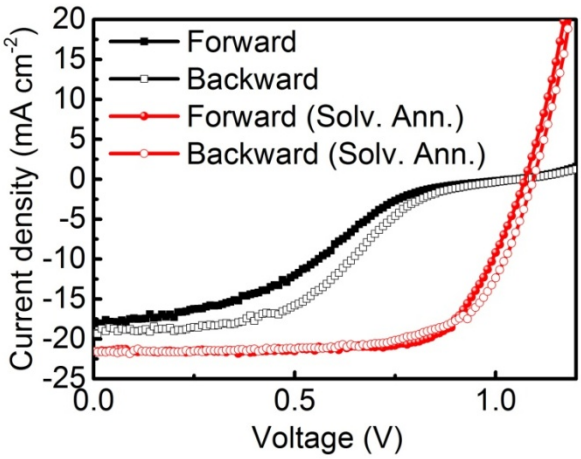



Figure S4 DMSO solvent post annealing can eliminate the weak S-shape.

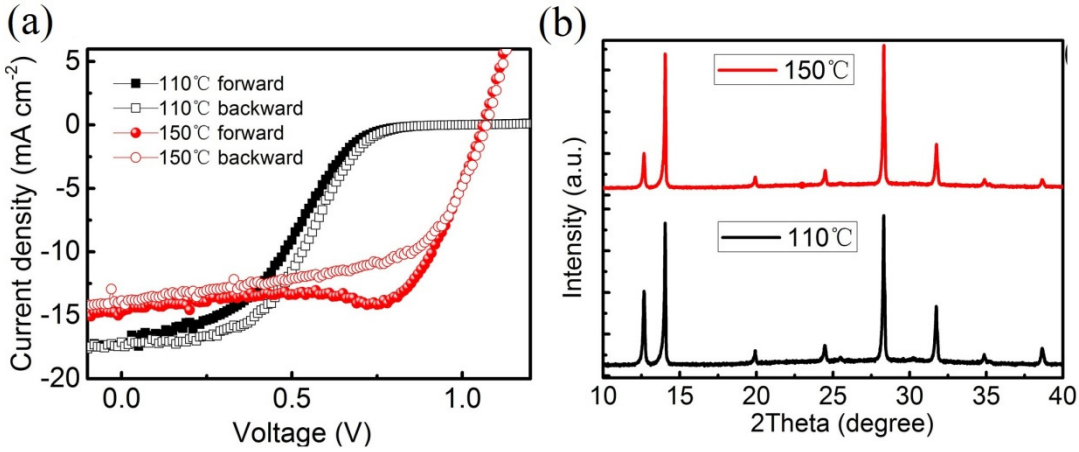



Figure S5 (a) X-ray diffractograms of $Cs_{0.05}(FA_{0.85}MA_{0.15})_{0.95}Pb(I_{0.85}Br_{0.15})_3$ perovskite layers annealed at 110 and 150 ℃. (b) *J-V* curves of solar cells with perovskite layers obtained under different annealing temperature. Here the NMP/A molar ratio in the precursor solution is 1.0.

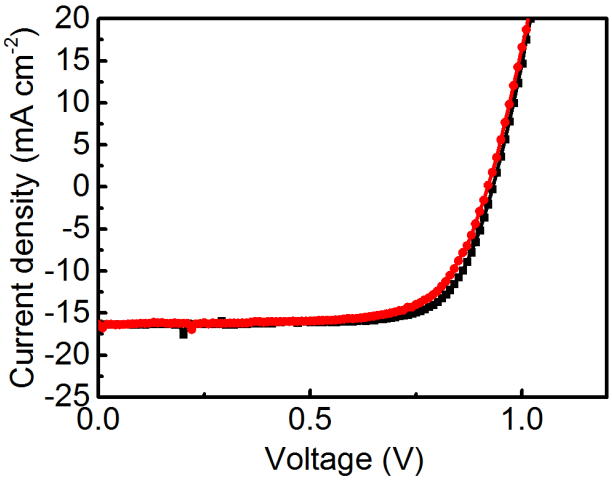



Figure S6 *J-V* curves of devices prepared with ultra dry lead halides (DMSO/A = 0.7, thiourea / A = 0.1).

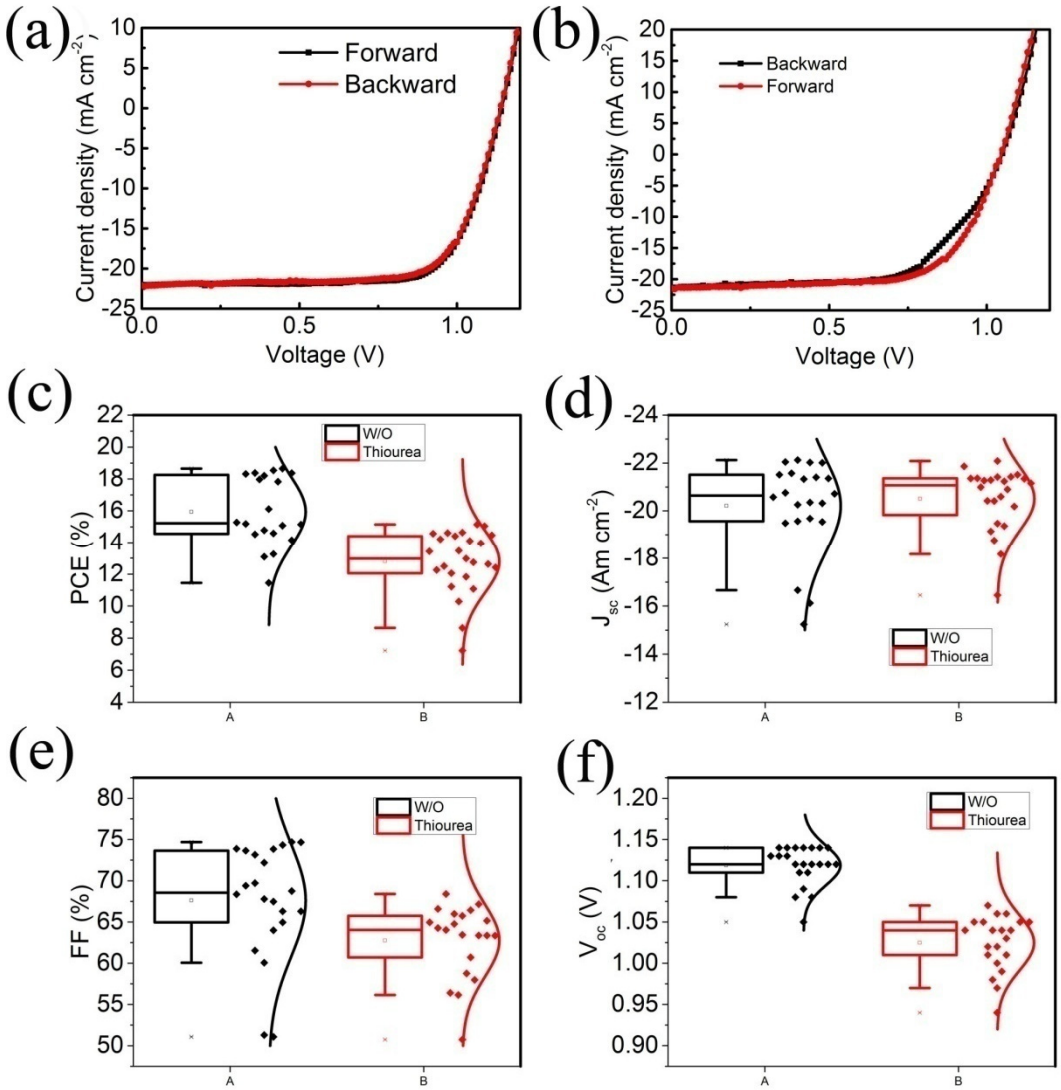



Figure S7 (a)Non ultra dry Pb source. 0.7 DMSO without thiourea. (b) Non ultra dry Pb source. 0.7 DMSO with thiourea (molar ratio = 0.06). （c）~（f）the historical results of two groups of devices.

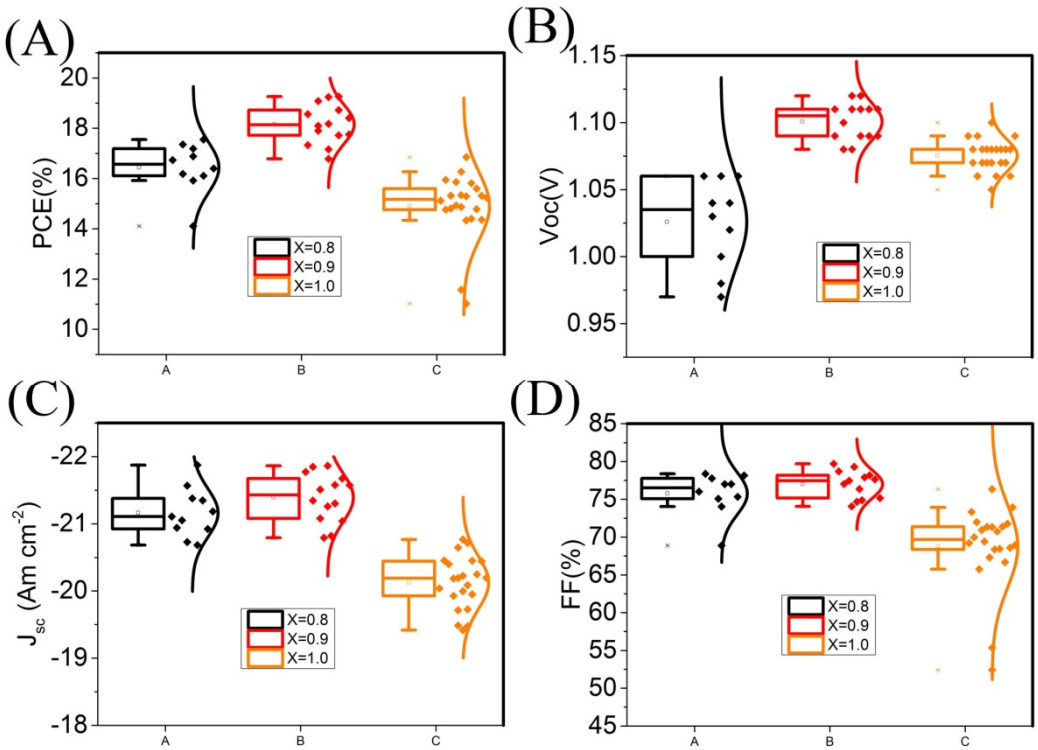



Figure S8 Historical results for the devices prepared from another bottle of non-ultra dry $PbI_2$ opened in the glove box. X is the molar ratio between DMSO and A cation and no thiourea was used.

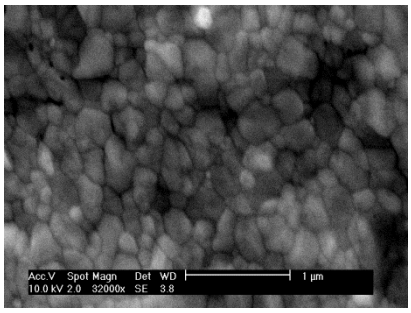



Figure S9 The SEM images of the perovskite layers from non-ultra dry $PbI_2$ using DMSO as LBM (X=0.9).

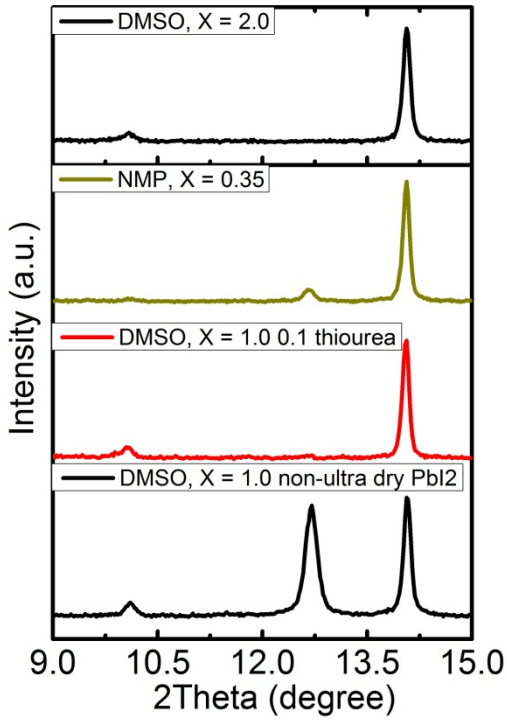



Figure S10 X-ray diffractograms of $Cs_{0.05}(FA_{0.85}MA_{0.15})_{0.95}Pb(I_{0.85}Br_{0.15})_3$ perovskite layers.

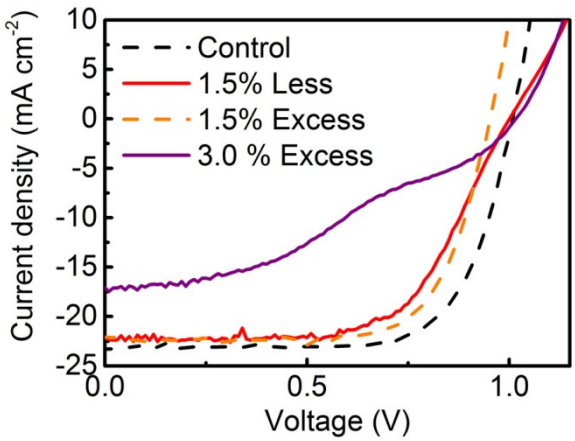



Figure S11 *J-V* curves of control device, and devices based on perovskite with -1.5~3.0% more $PbI_2$ than the control composition.

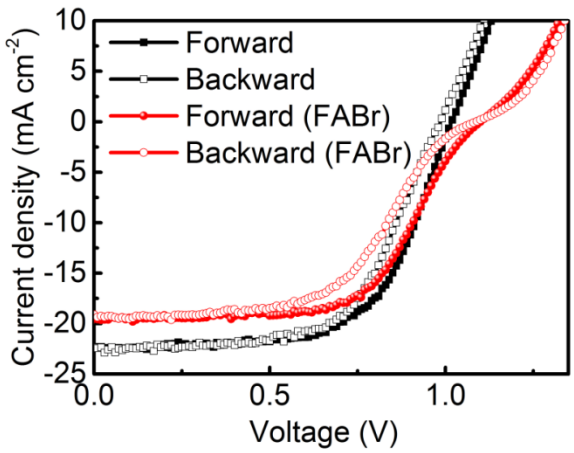
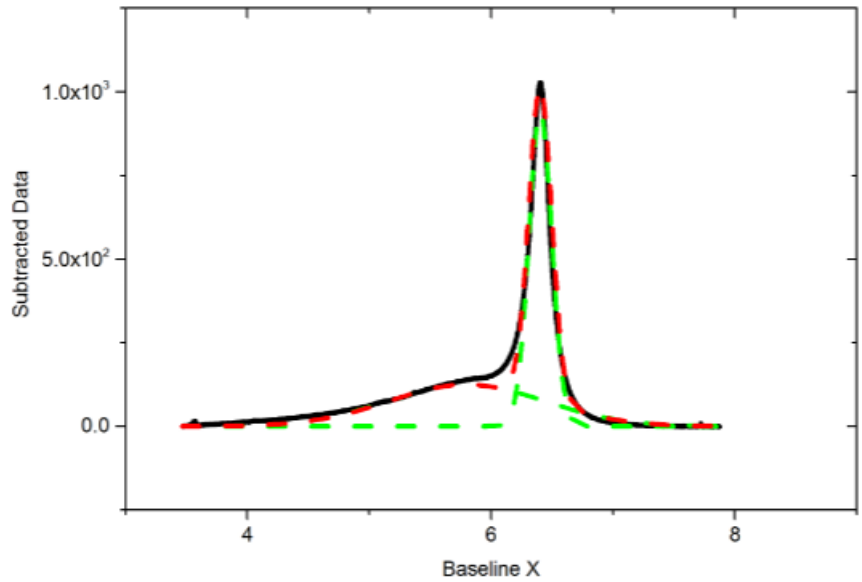



Figure S12 FA salt isopropanol solution post treatment the perovskite layer to introduced more FA salts.




Fitting Results

| Peak Index | Peak Type | Area Intg | FWHM | Max Height | Center Grvty | Area IntgP |
|---|---|---|---|---|---|---|
| 1. | Gaussian | 199.86174 | 1.5 | 125.2583 | 5.8 | 47.6018 |
| 2. | Gaussian | 220 | 0.22 | 939.43728 | 6.40295 | 52.3982 |

Figure S13 normalized $^1$H NMR spectra of MAI and thiourea.

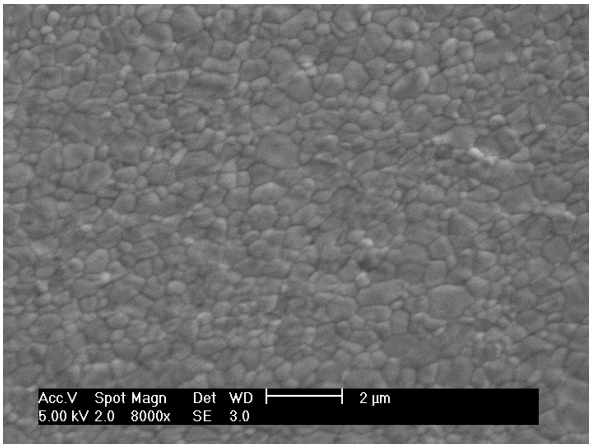



Figure S14 SEM of perovskite layer from Anti-solvent technology, where DMSO was used as LBS and 0.06 molar ratio of thiourea was used. Toluene is the anti-solvent here.

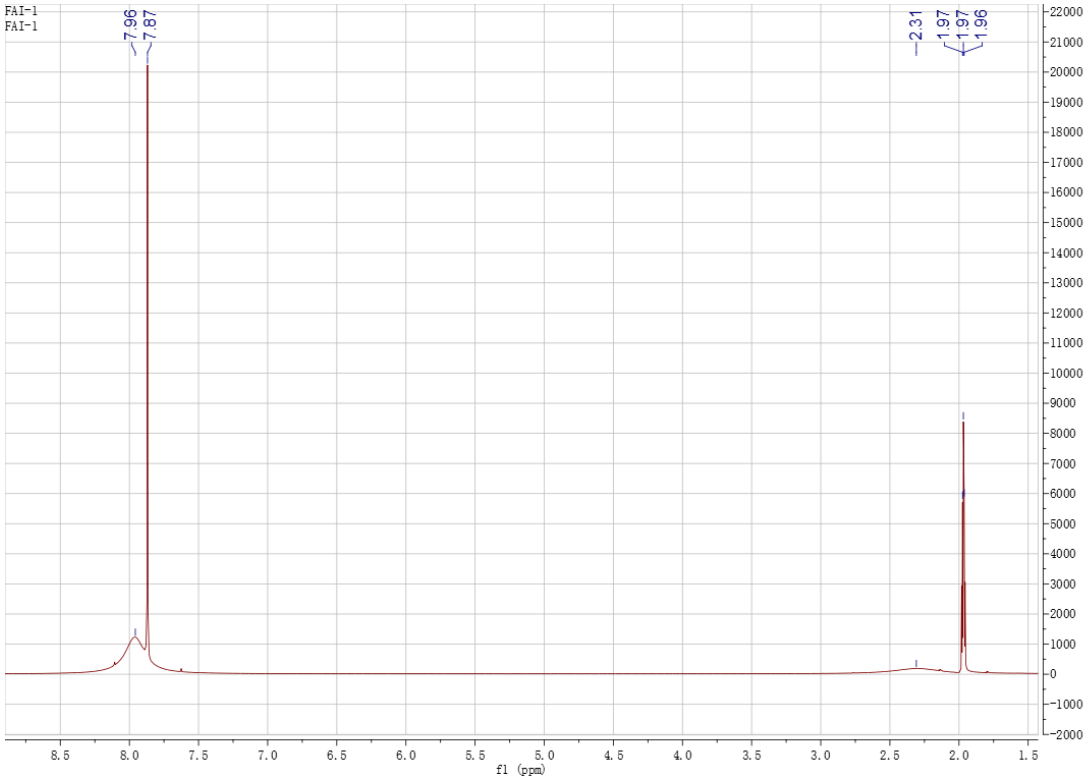



Figure S15 The $^{1}H$ NMR of pure FAI in acetonitrile-$D_3$.

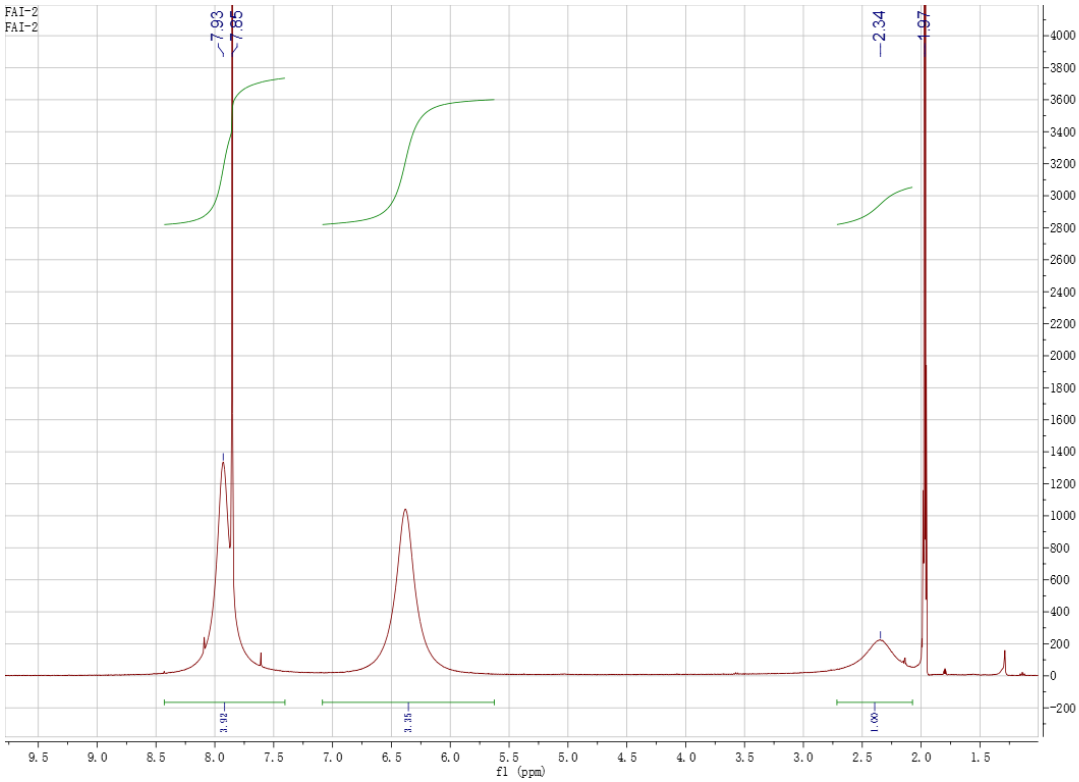



Figure S16 The $^{1}$H NMR of FAI with equivalent thiourea in acetonitrile-$D_3$.

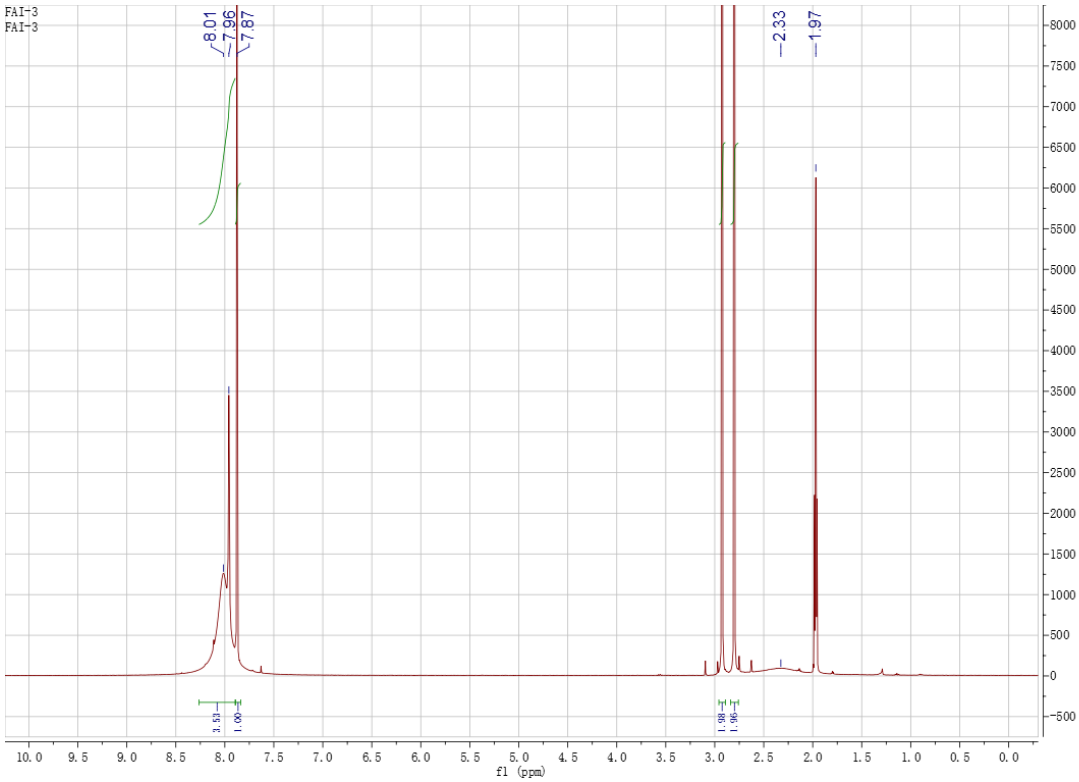



Figure S17 The $^{1}$H NMR of FAI with equivalent DMF in acetonitrile-$D_3$.

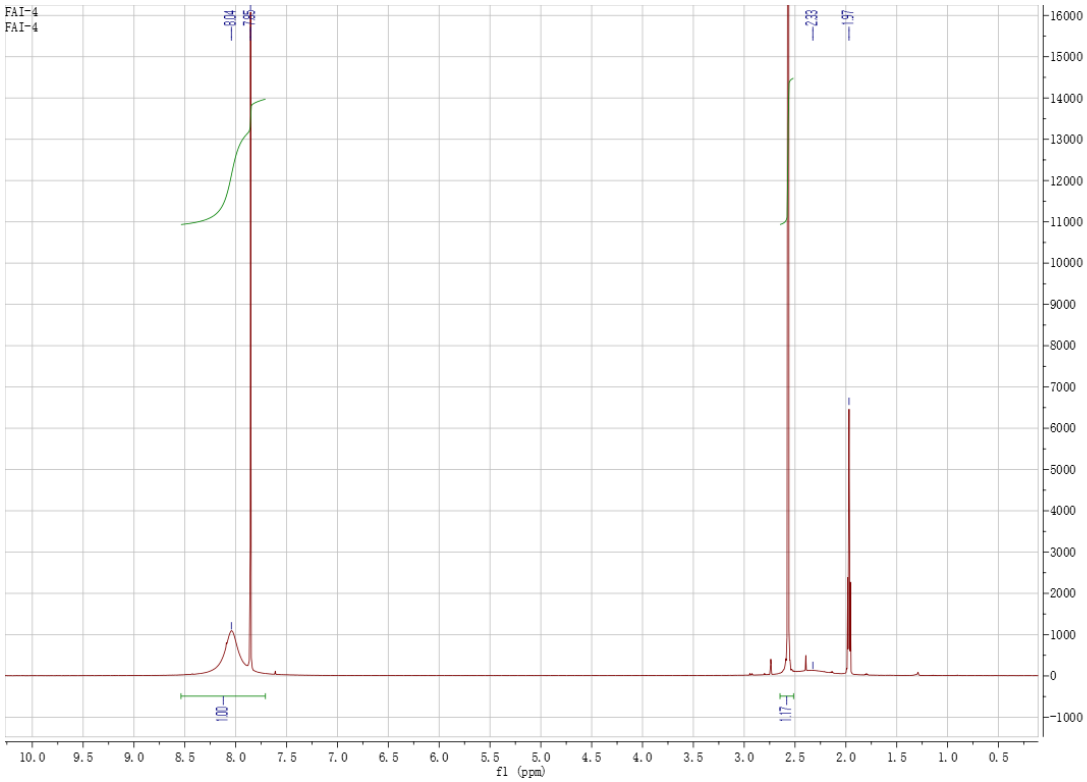



Figure S18 The $^{1}$H NMR of FAI with equivalent DMSO in acetonitrile-$D_3$.

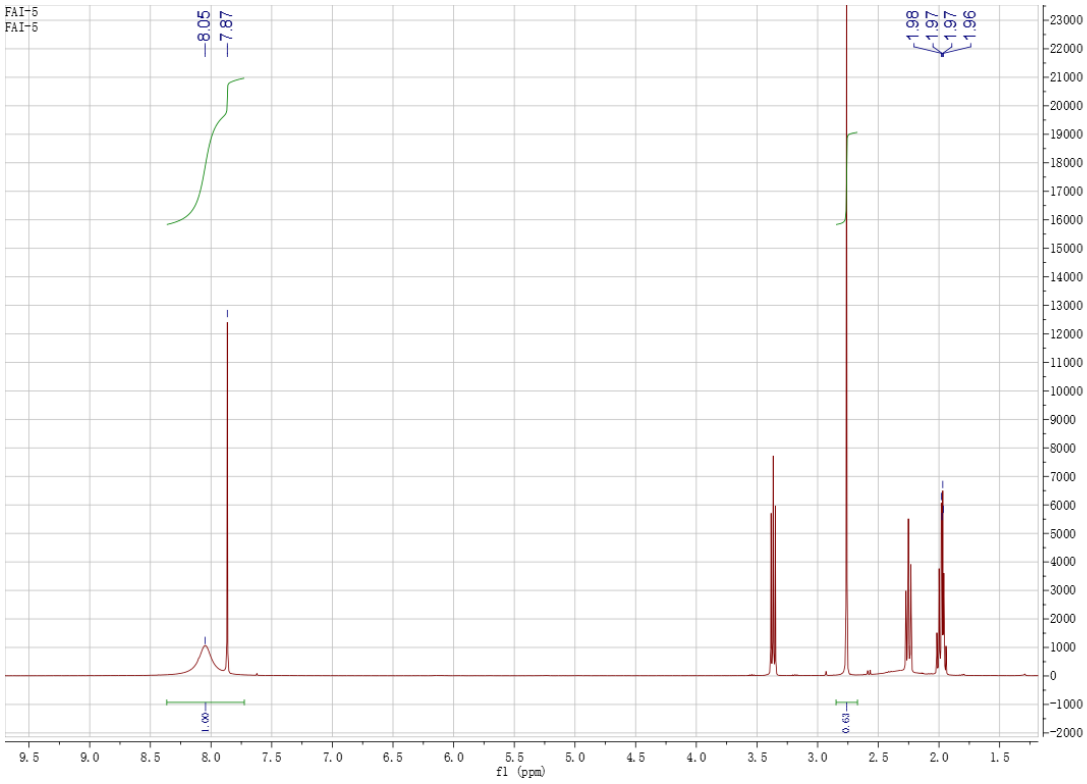



Figure S19 The $^{1}$H NMR of FAI with equivalent NMP in acetonitrile-$D_3$.

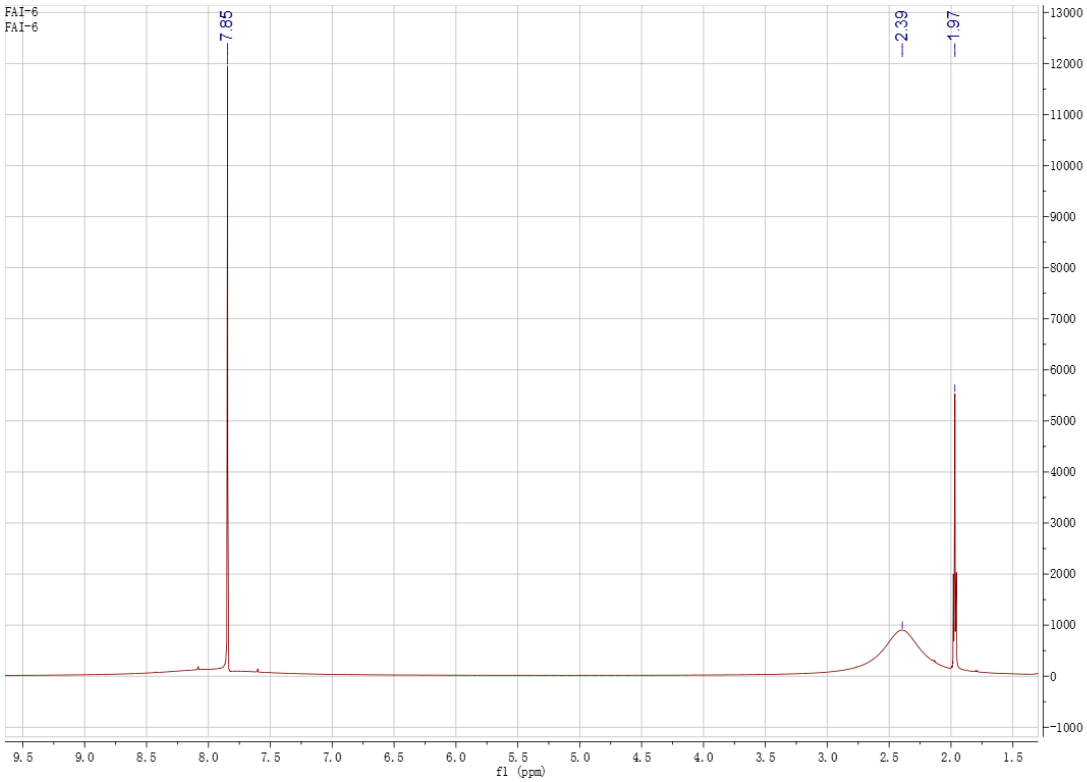



Figure S20 The $^{1}$H NMR of FAI with $H_2O$ in acetonitrile-$D_3$.

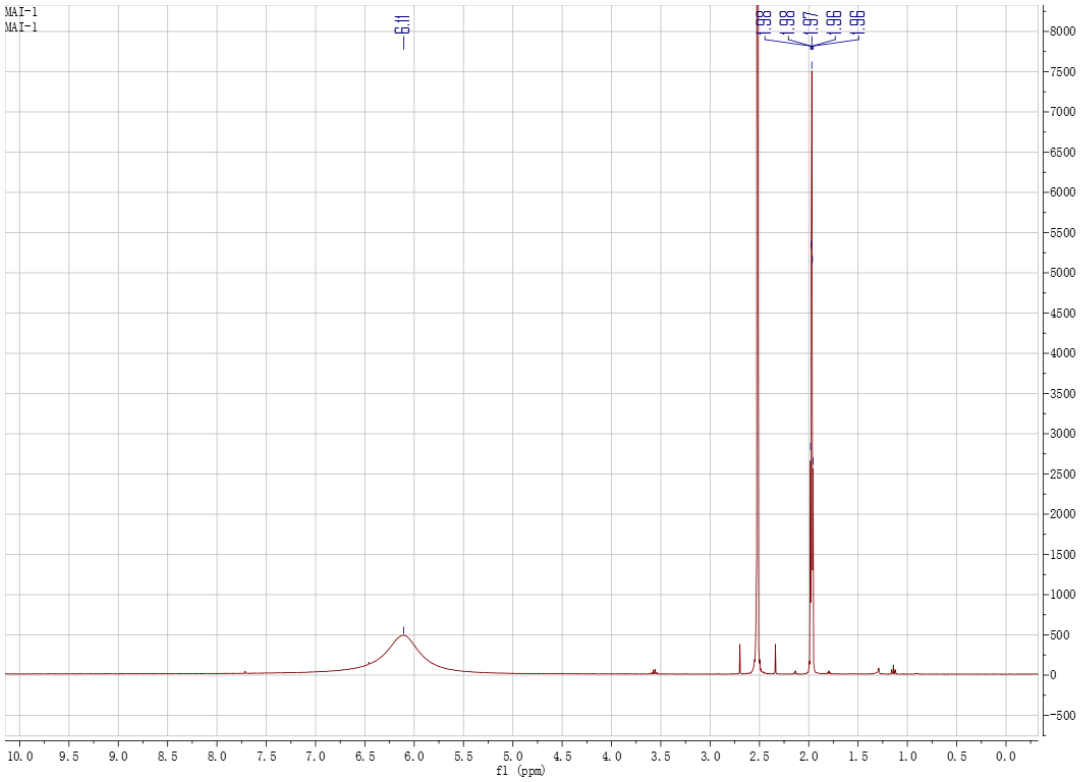



Figure S21 The $^{1}$H NMR of pure MAI in acetonitrile-$D_3$.

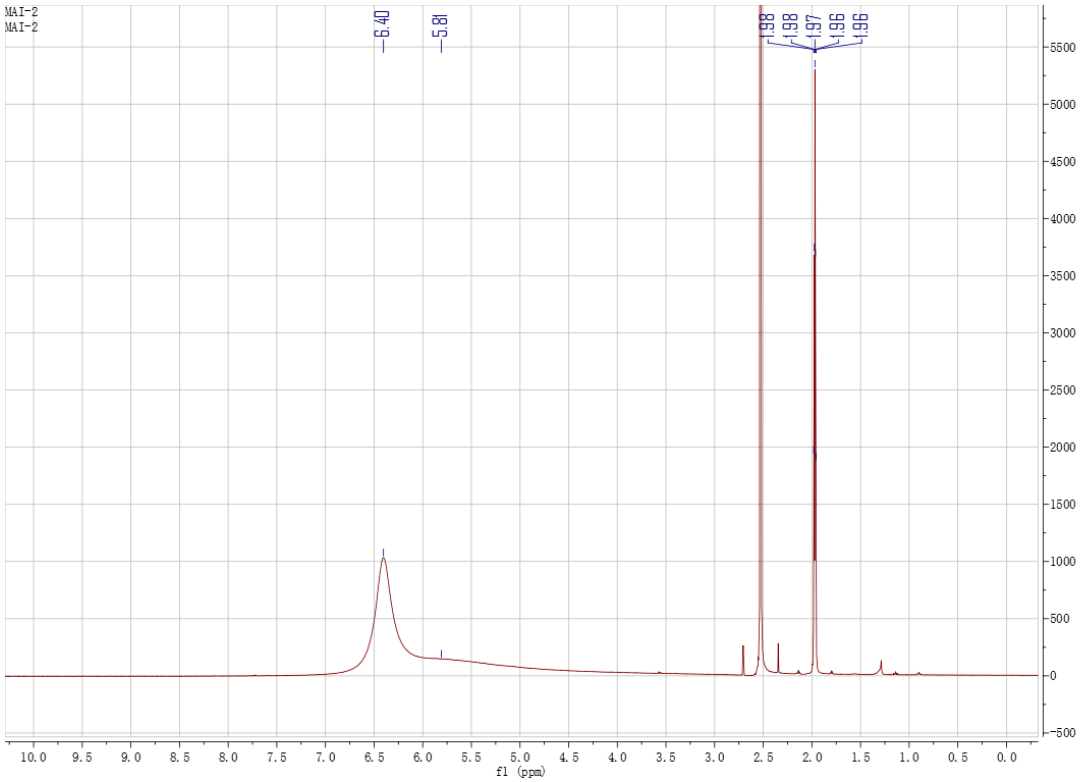



Figure S22 The $^{1}$H NMR of MAI with equivalent thiourea in acetonitrile-$D_3$.

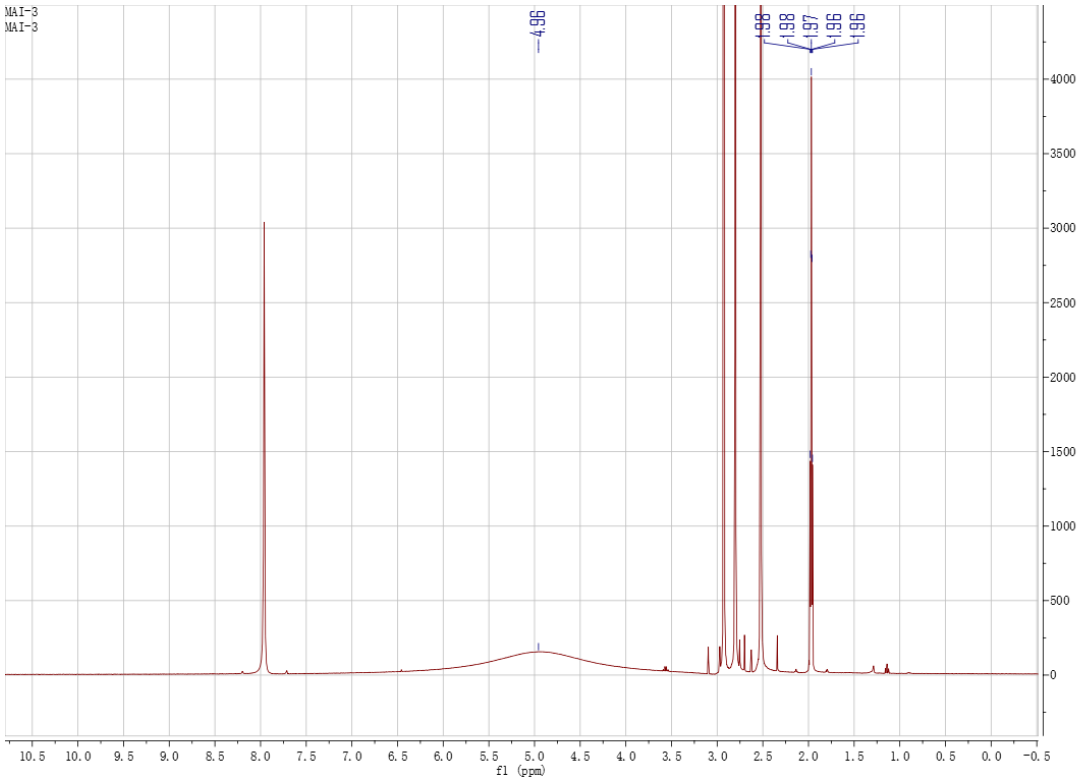



Figure S23 The $^{1}$H NMR of MAI with equivalent DMF in acetonitrile-$D_3$.

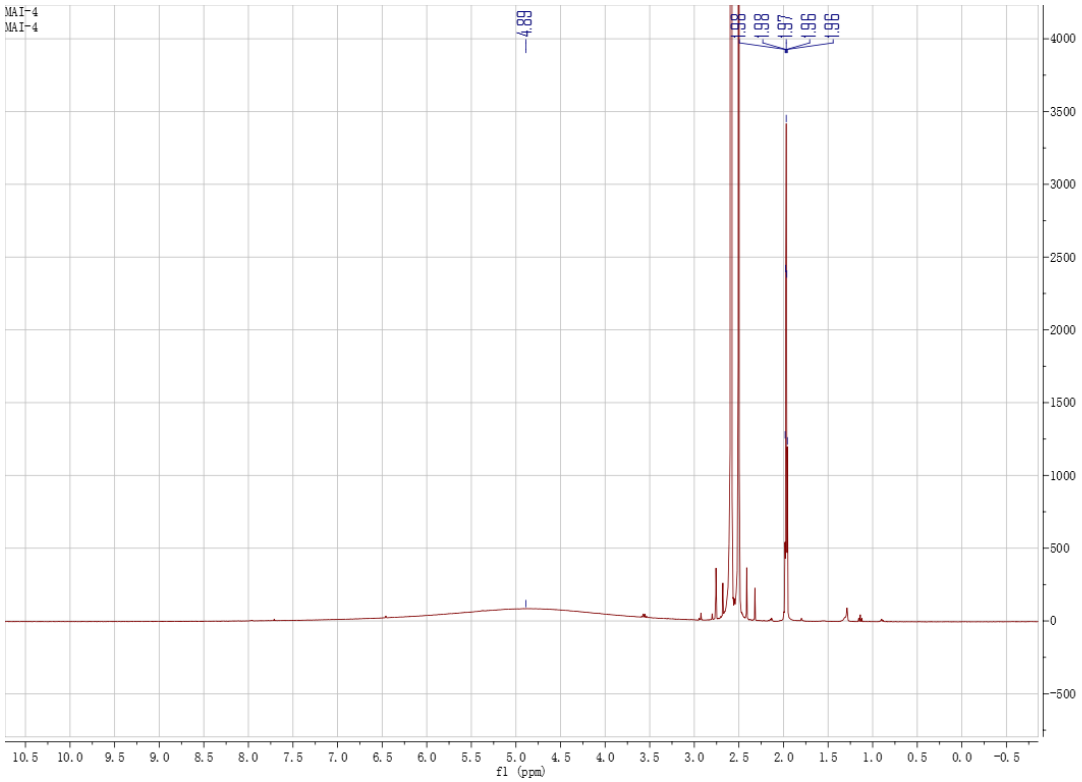



Figure S24 The $^{1}H$ NMR of MAI with equivalent DMSO in acetonitrile-$D_3$.

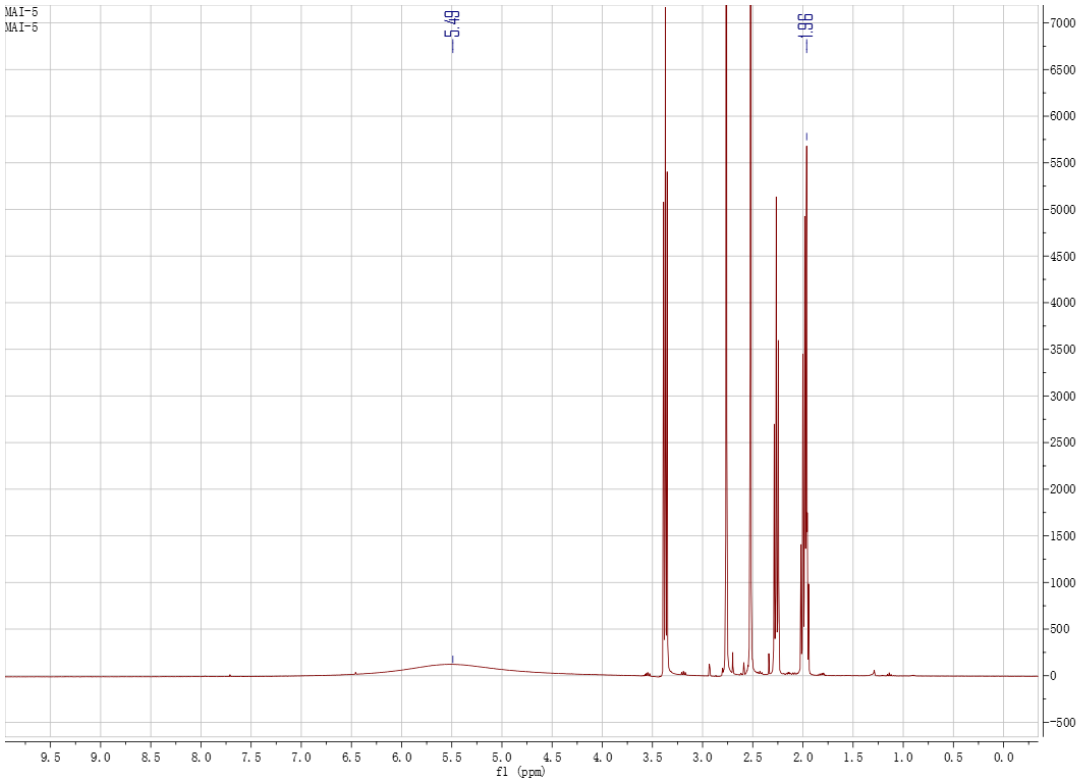



Figure S25 The $^{1}H$ NMR of MAI with equivalent NMP in acetonitrile-$D_3$.

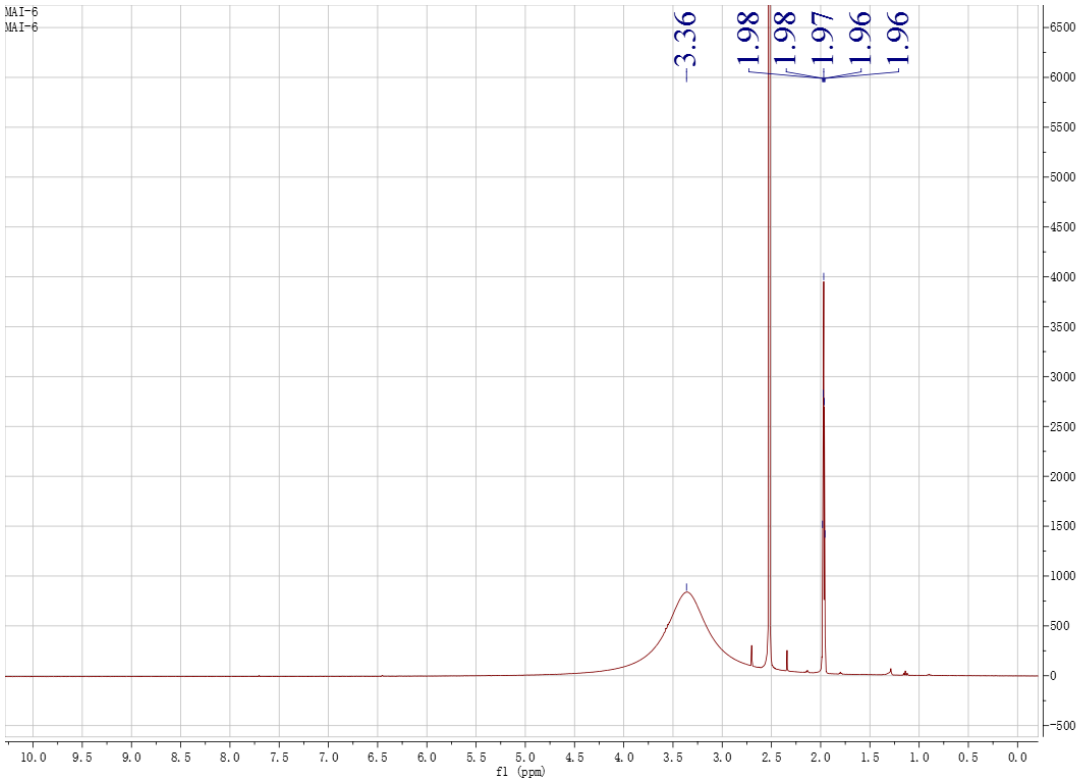



Figure S26 The $^{1}H$ NMR of MAI with equivalent $H_2O$ in acetonitrile-$D_3$.