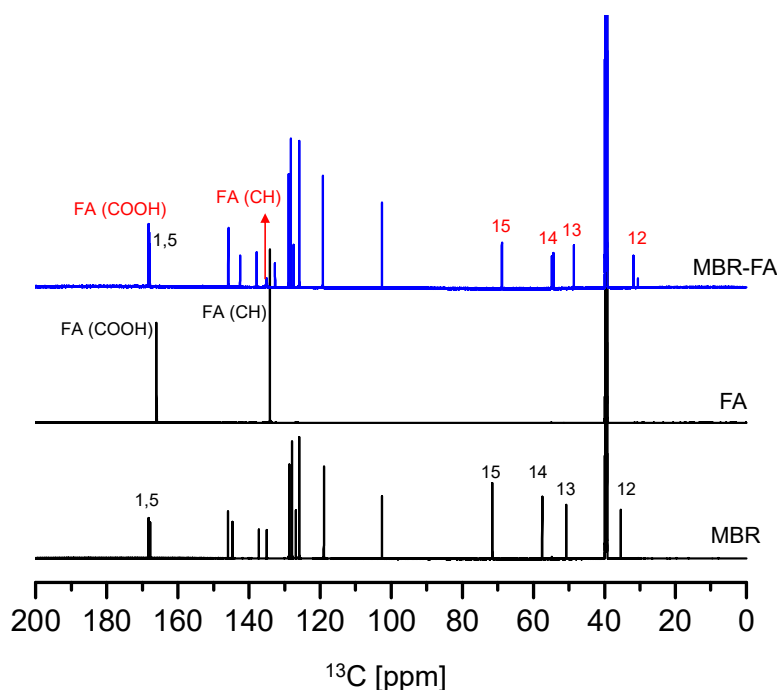
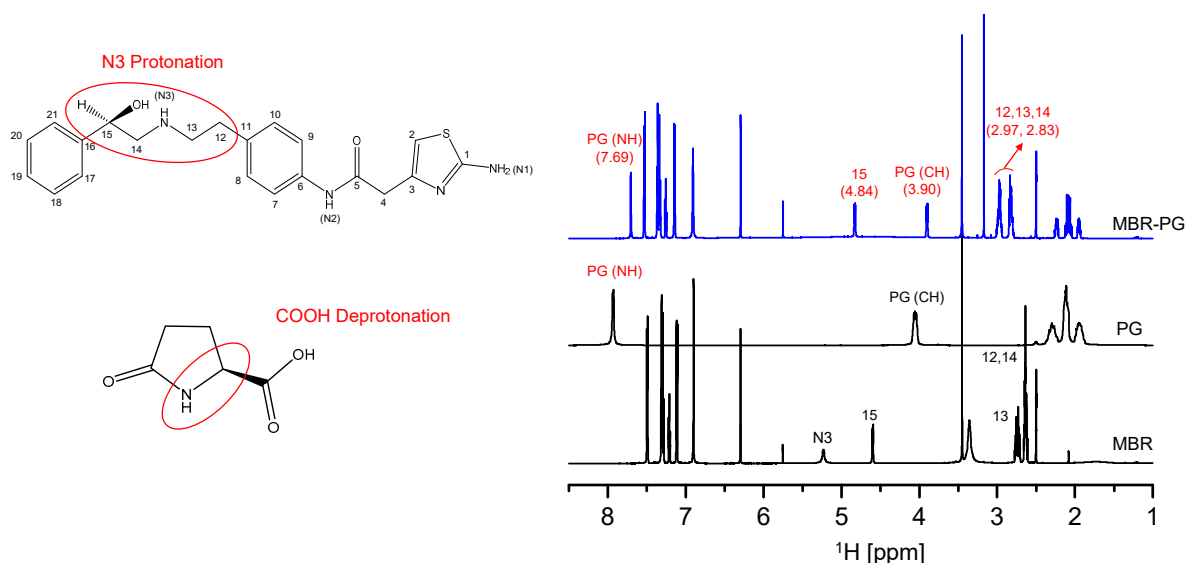


# Supplementary Materials: Co-Amorphous Screening for the Solubility Enhancement of Poorly Water-Soluble Mirabegron and Investigation of Their Intermolecular Interactions and Dissolution Behaviors

Ji-Hun An, Changjin Lim, Alice Nguvoko Kiyonga, In Hwa Chung, In Kyu Lee, Kilwoong Mo, Minho Park, Wonno Youn, Won Rak Choi, Young-Ger Suh and Kiwon Jung



**Figure S1.** Solution-state  $^{13}\text{C}$ -NMR spectra for MBR-FA co-amorphous, MBR and FA ( $\text{DMSO-}d_6$ ).



**Figure S2.** Solution-state  $^1\text{H}$ -NMR spectra for MBR-PG co-amorphous, MBR and PG ( $\text{DMSO-}d_6$ ).

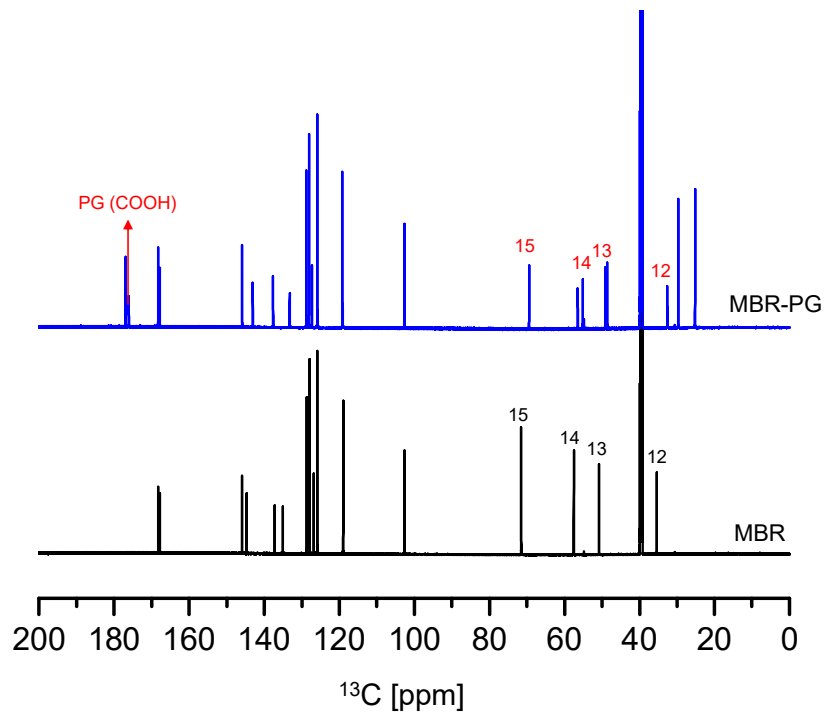


Figure S3. Solution-state  $^{13}\text{C}$ -NMR spectra for MBR-PG co-amorphous and MBR ( $\text{DMSO-}d_6$ ).

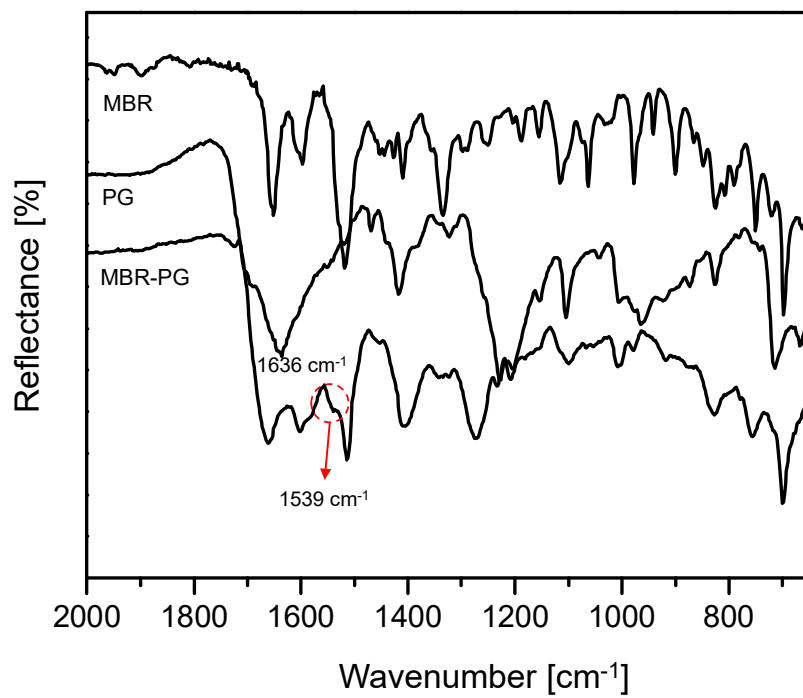
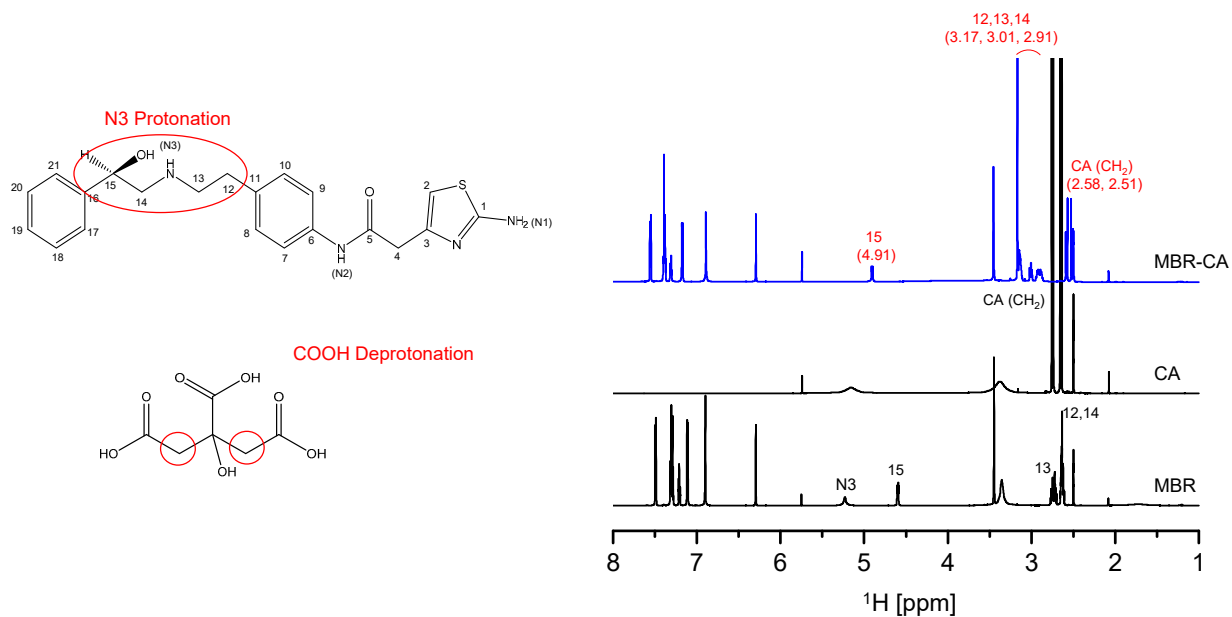
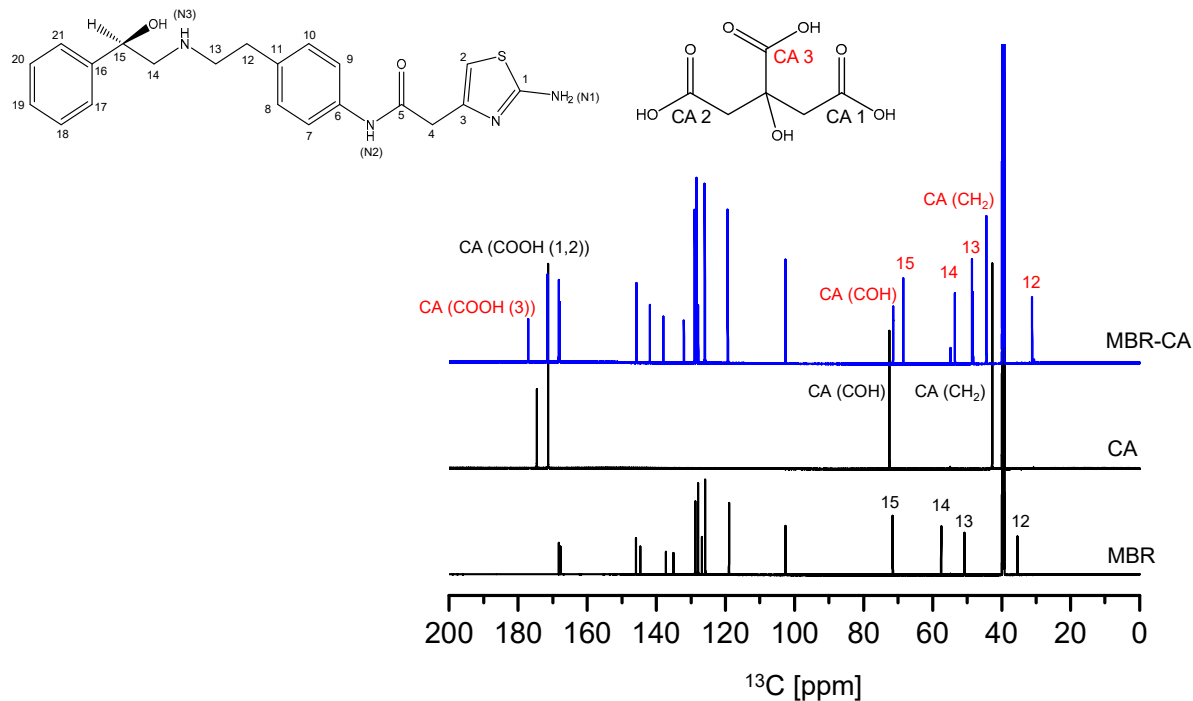


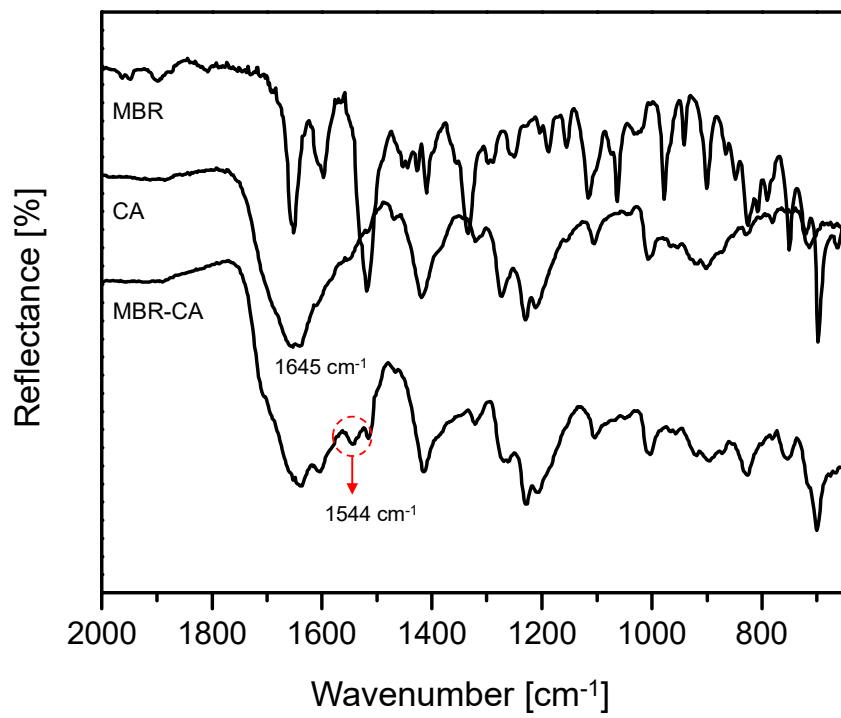
Figure S4. ATR-FTIR spectra for MBR-PG co-amorphous, MBR and PG.



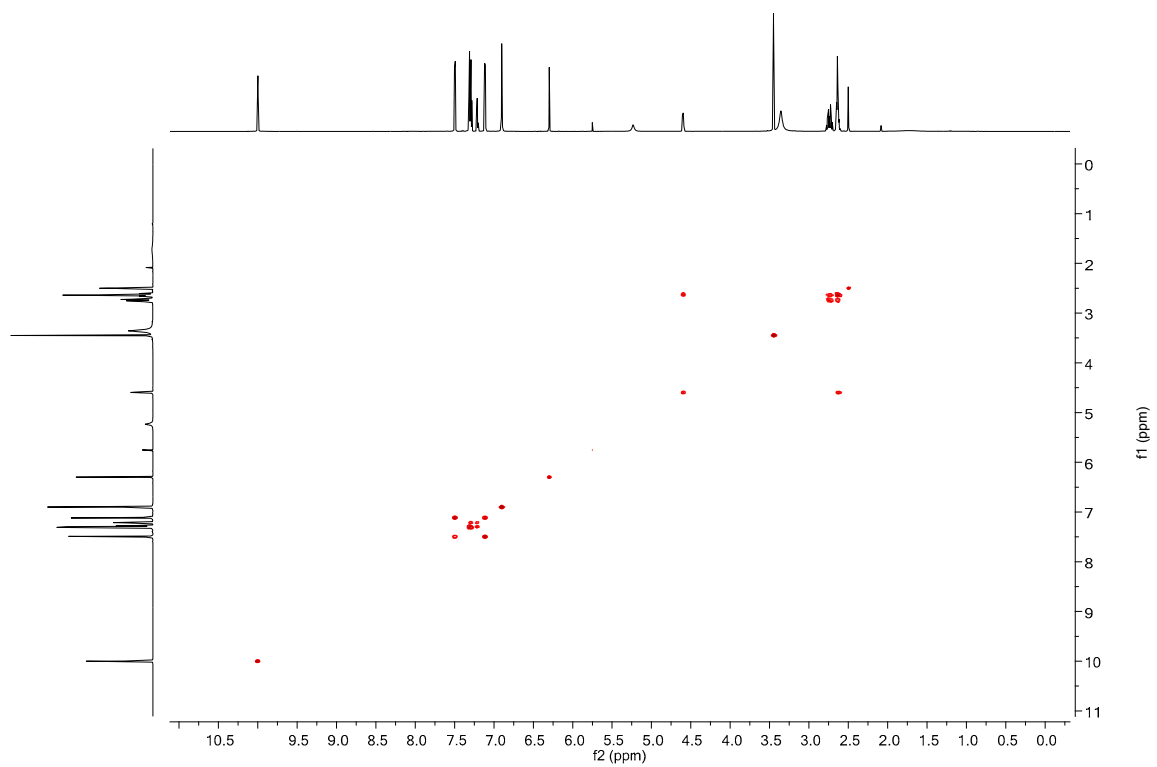
**Figure S5.** Solution-state  $^1\text{H}$ -NMR spectra for MBR-CA co-amorphous, MBR and CA (DMSO- $d_6$ ).



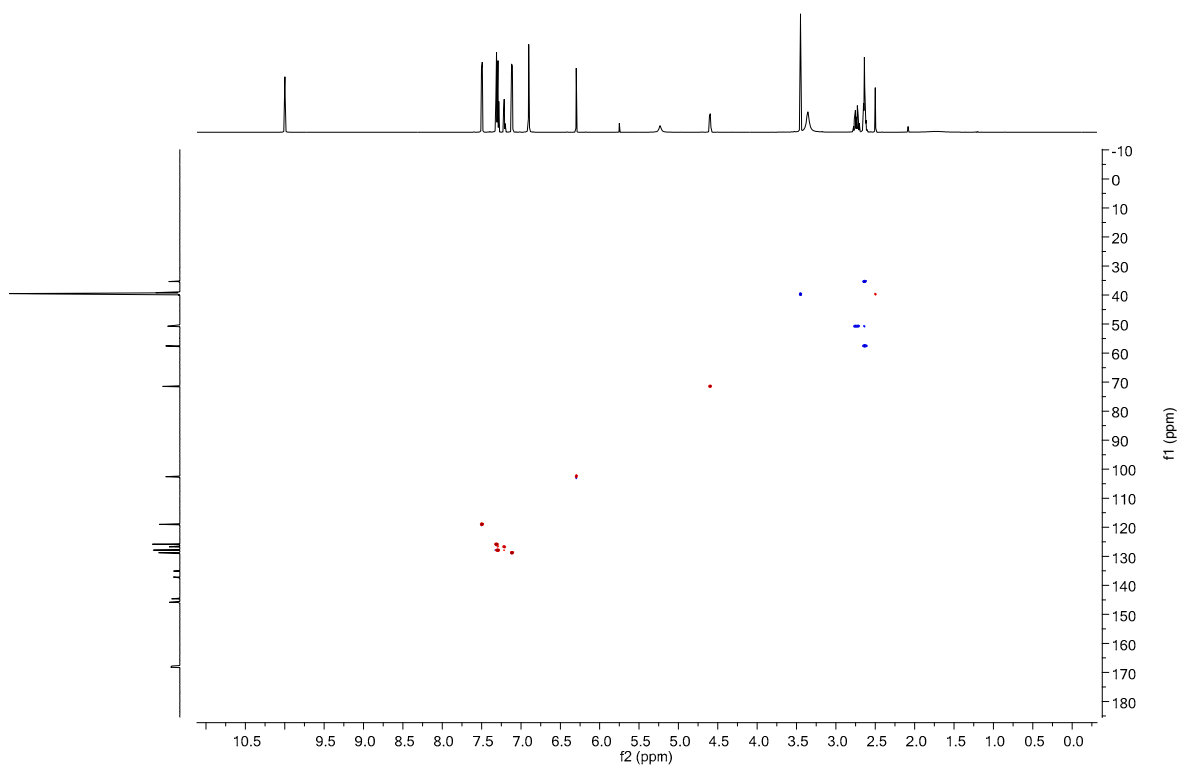
**Figure S6.** Solution-state  $^{13}\text{C}$ -NMR spectra for MBR-CA co-amorphous, MBR and CA (DMSO- $d_6$ ).



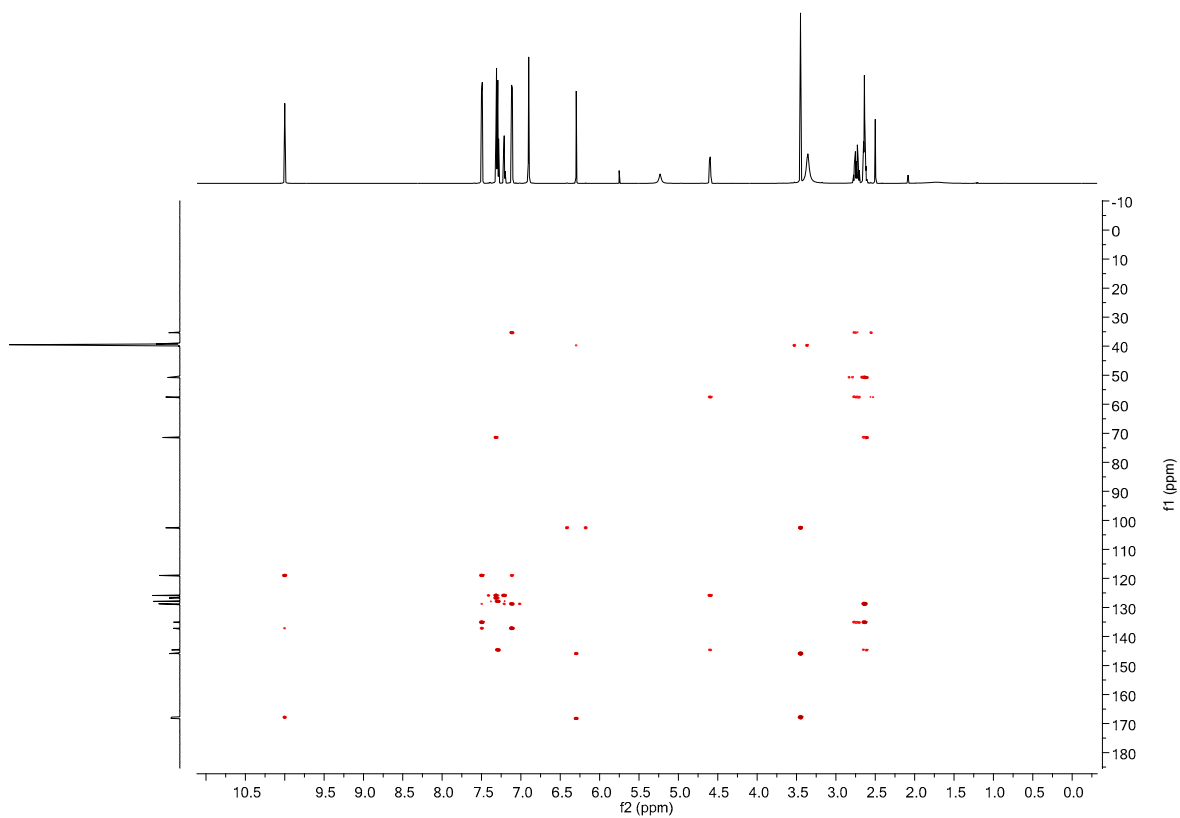
**Figure S7.** ATR-FTIR spectra for MBR-CA co-amorphous, MBR and CA.



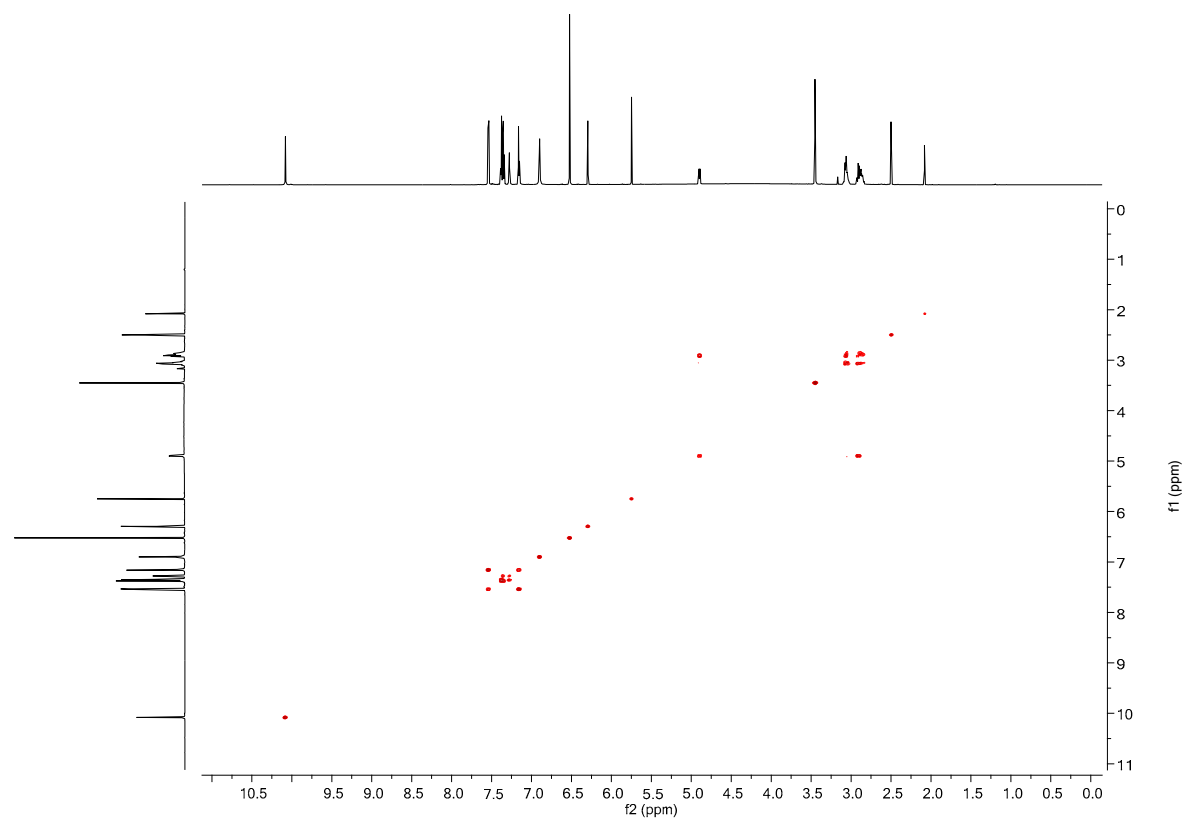
**Figure S8.** Solution-state 2D ( $^1\text{H}$ - $^1\text{H}$  COSY) NMR spectrum of MBR ( $\text{DMSO-}d_6$ ).



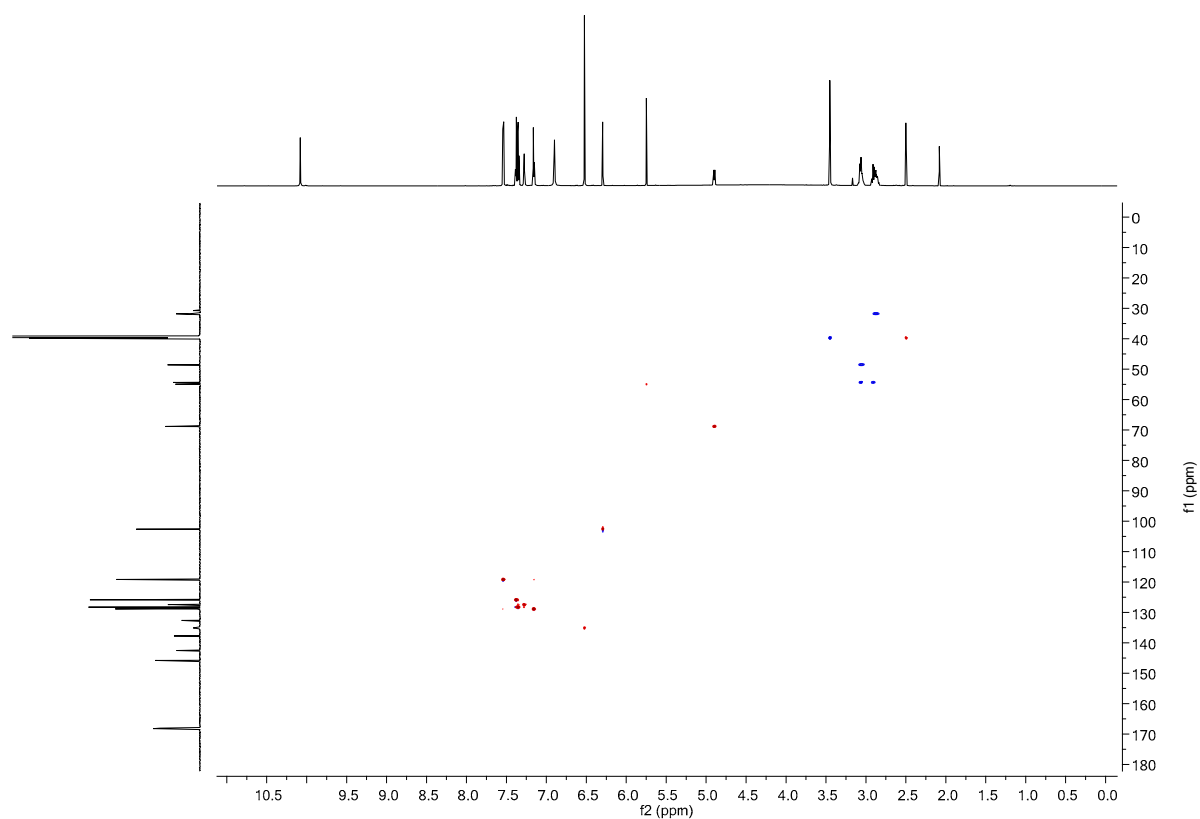
**Figure S9.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{H}$  HSQC) NMR spectrum of MBR ( $\text{DMSO}-d_6$ ).



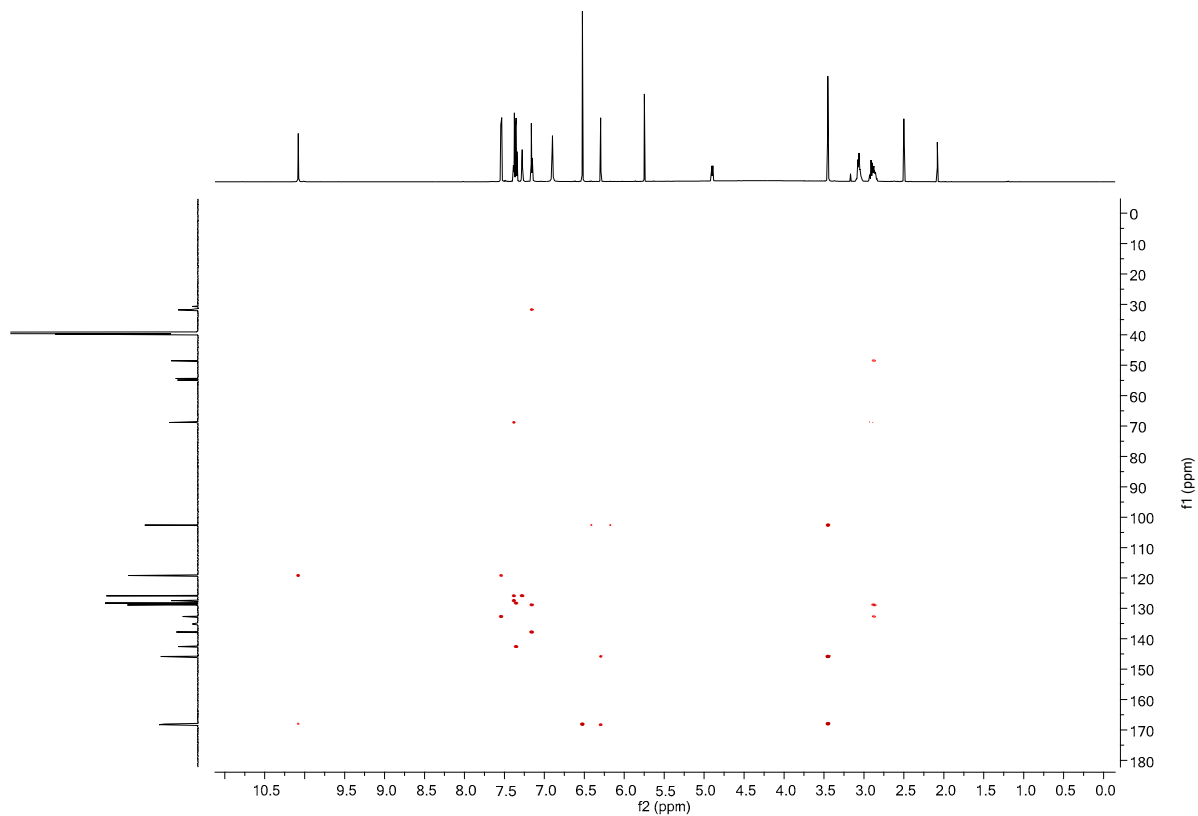
**Figure S10.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{H}$  HMBC) NMR spectrum of MBR ( $\text{DMSO}-d_6$ ).



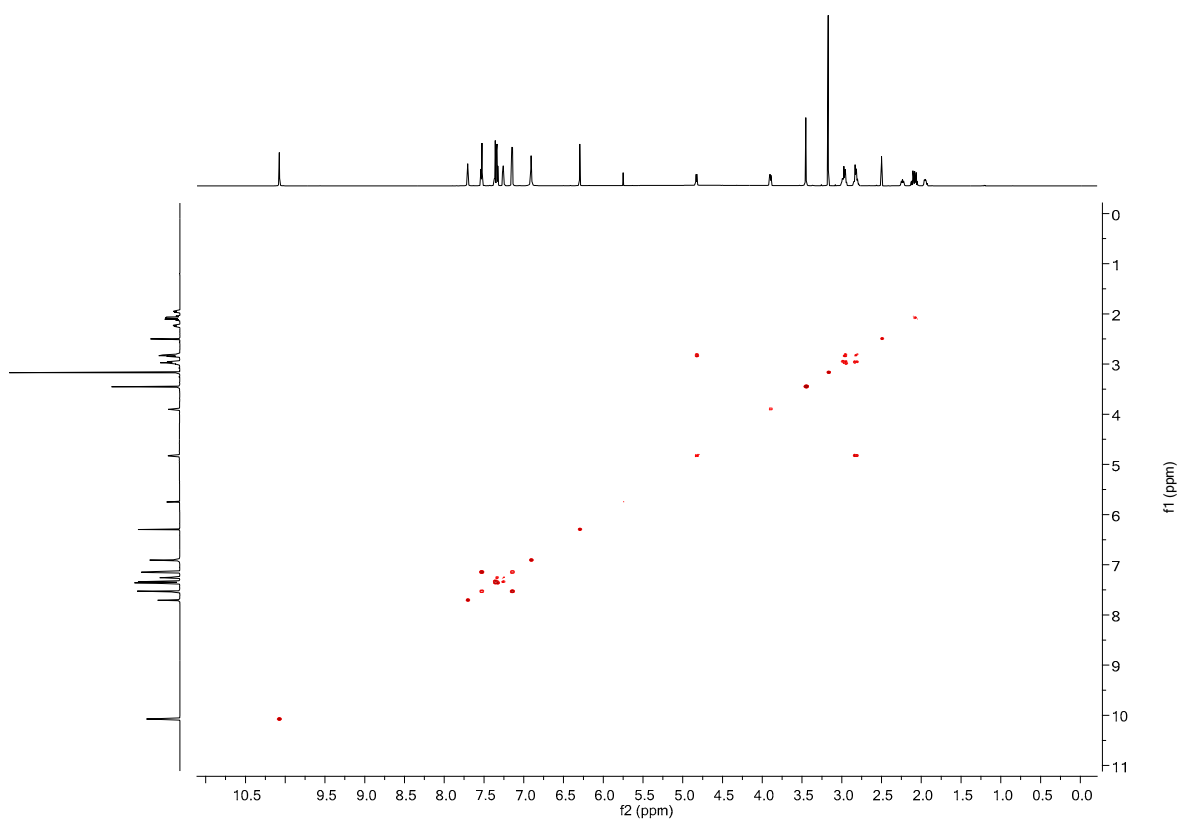
**Figure S11.** Solution-state 2D ( $^1\text{H}$ - $^1\text{H}$  COSY) NMR spectrum of MBR-FA co-amorphous ( $\text{DMSO-}d_6$ ).



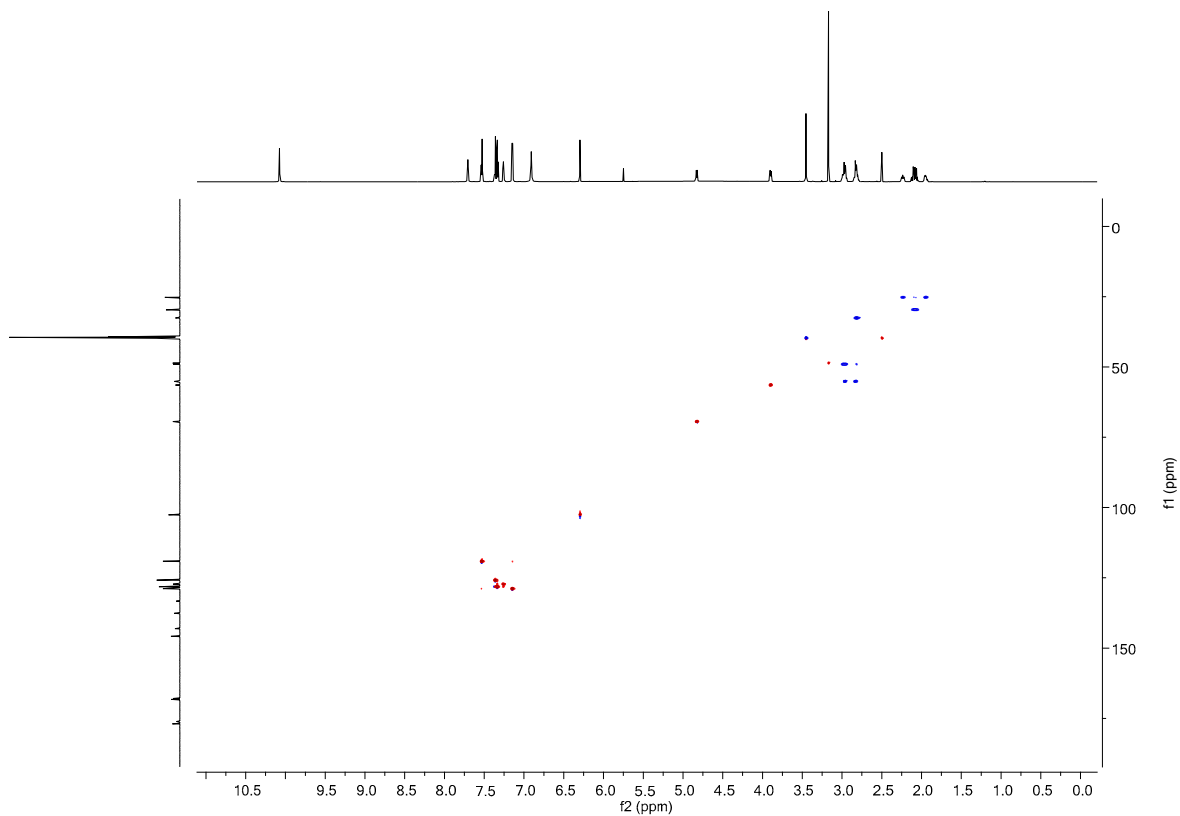
**Figure S12.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{C}$  HSQC) NMR spectrum of MBR-FA co-amorphous ( $\text{DMSO-}d_6$ ).



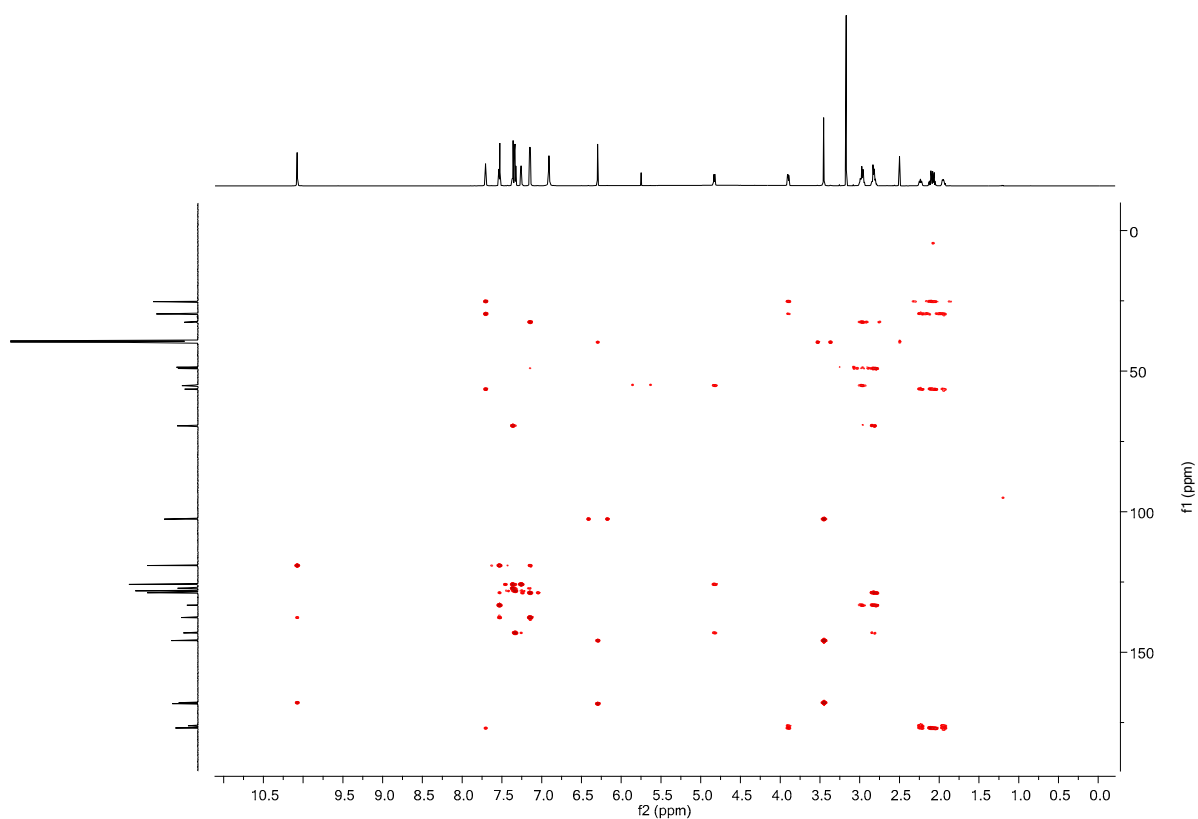
**Figure S13.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{C}$  HMBC) NMR spectrum of MBR-FA co-amorphous ( $\text{DMSO-}d_6$ ).



**Figure S14.** Solution-state 2D ( $^1\text{H}$ - $^1\text{H}$  COSY) NMR spectrum of MBR-PG co-amorphous ( $\text{DMSO-}d_6$ ).

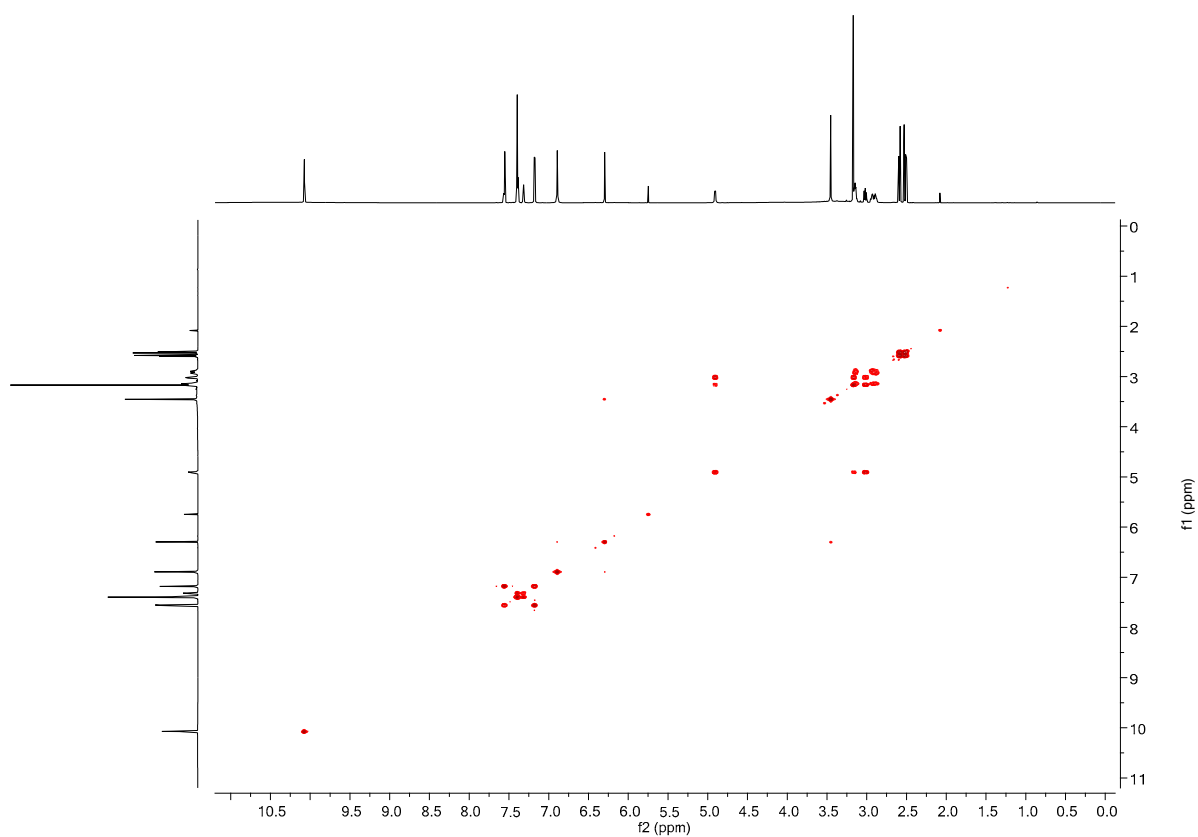


**Figure S15.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{C}$  HSQC) NMR spectrum of MBR-PG co-amorphous ( $\text{DMSO-}d_6$ )

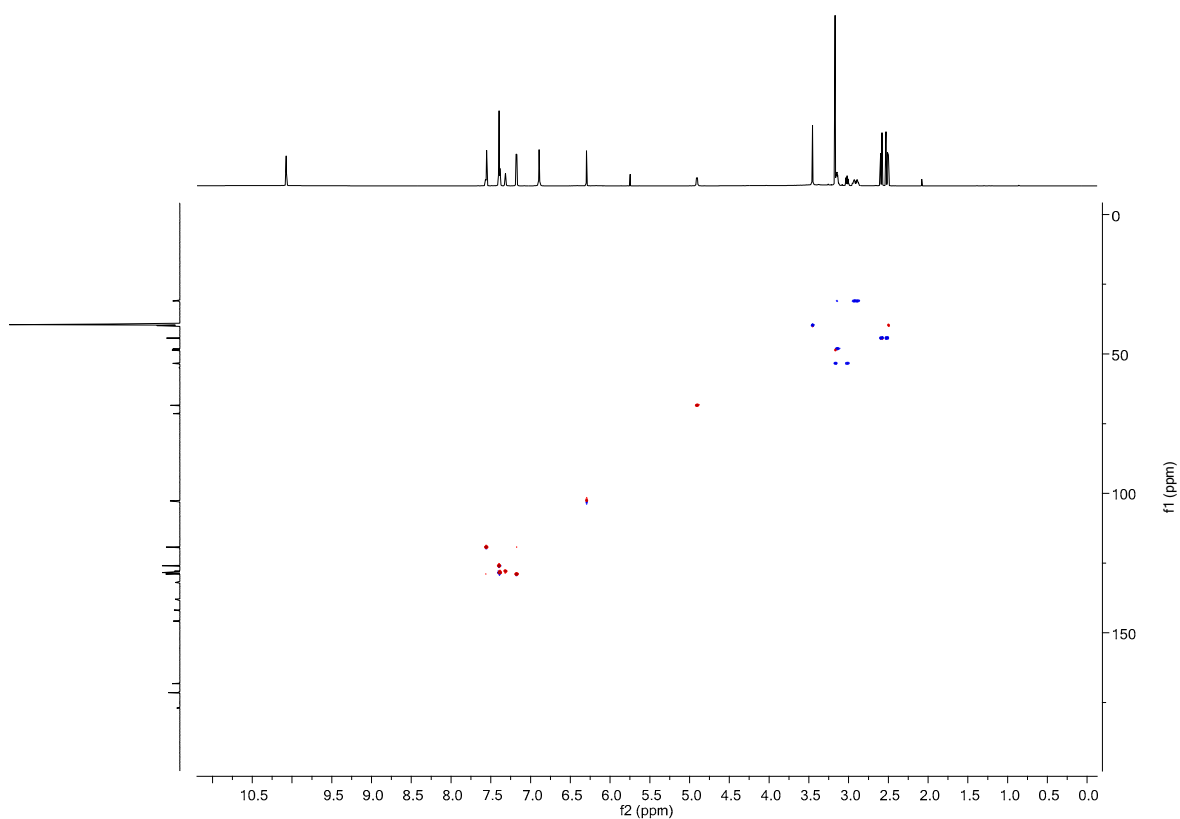


**Figure S16.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{C}$  HMBC) NMR spectrum of MBR-PG co-amorphous ( $\text{DMSO-}d_6$ ).

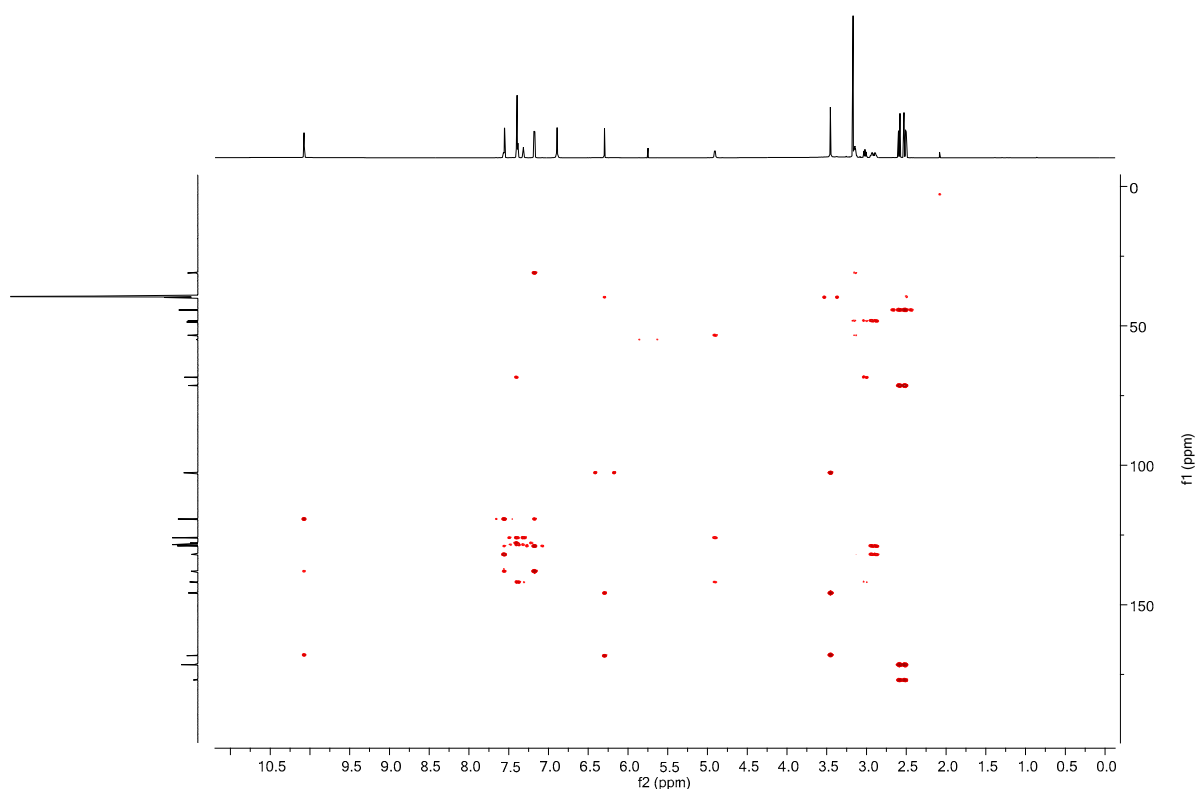




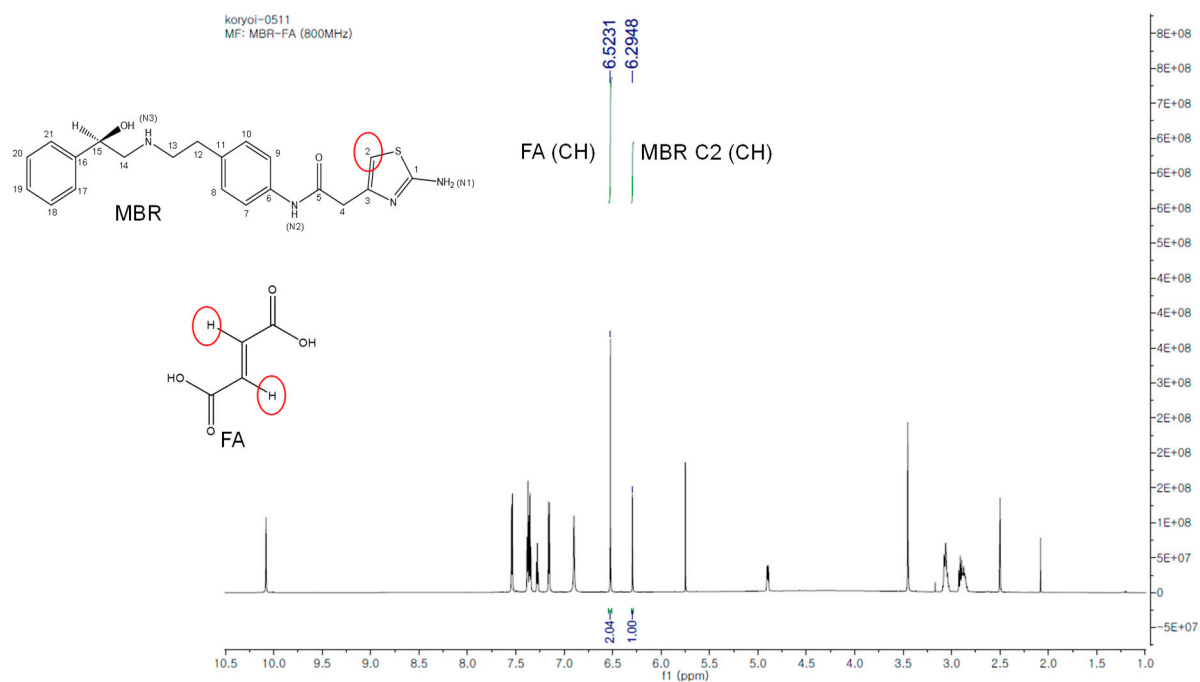
**Figure S17.** Solution-state 2D ( $^1\text{H}$ - $^1\text{H}$  COSY) NMR spectrum of MBR-CA co-amorphous ( $\text{DMSO-}d_6$ ).



**Figure S18.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{C}$  HSQC) NMR spectrum of MBR-CA co-amorphous ( $\text{DMSO-}d_6$ ).



**Figure S19.** Solution-state 2D ( $^1\text{H}$ - $^{13}\text{C}$  HMBC) NMR spectrum of MBR-CA co-amorphous ( $\text{DMSO-}d_6$ ).



**Figure S20.** Solution-state  $^1\text{H}$ -NMR spectrum of MBR-FA co-amorphous.

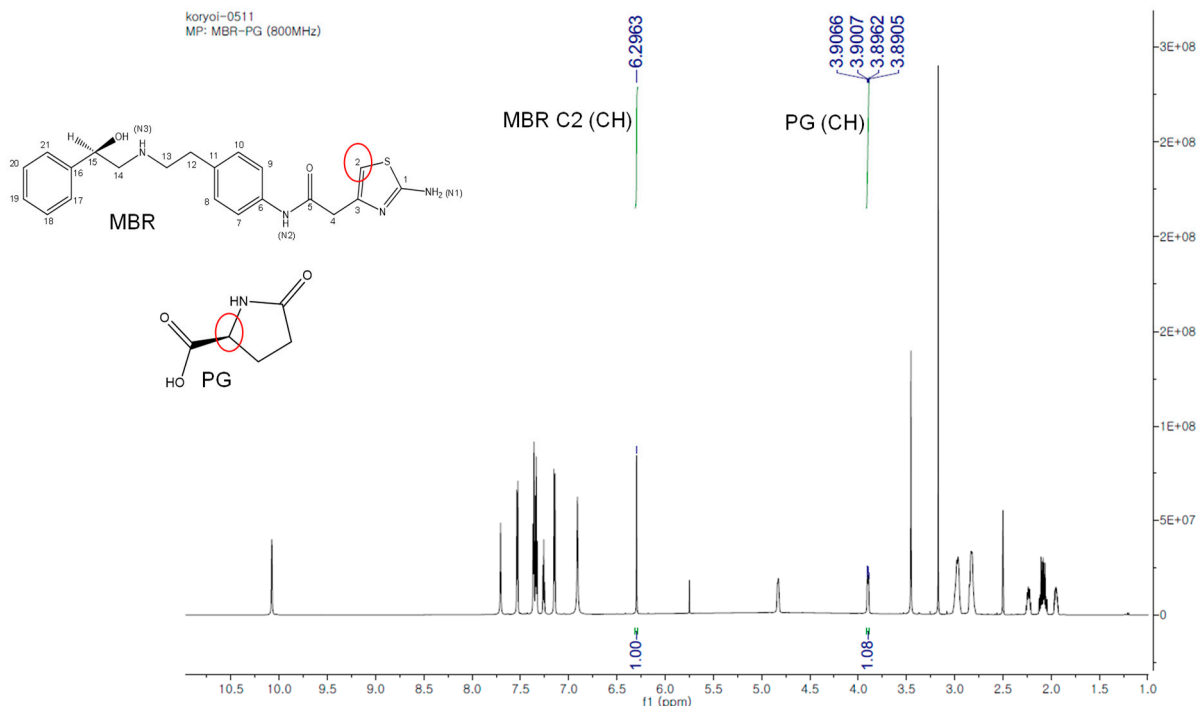


Figure S21. Solution-state  $^1\text{H}$ -NMR spectrum of MBR-PG co-amorphous.

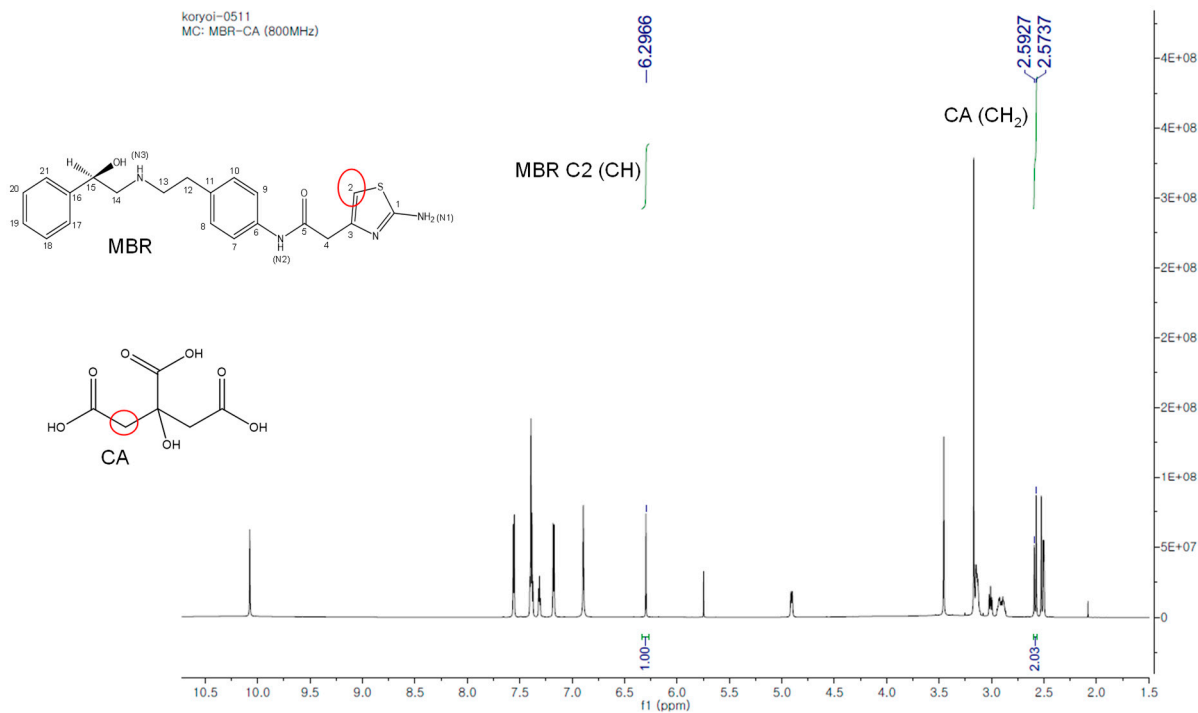


Figure S22. Solution-state  $^1\text{H}$ -NMR spectrum of MBR-CA co-amorphous.

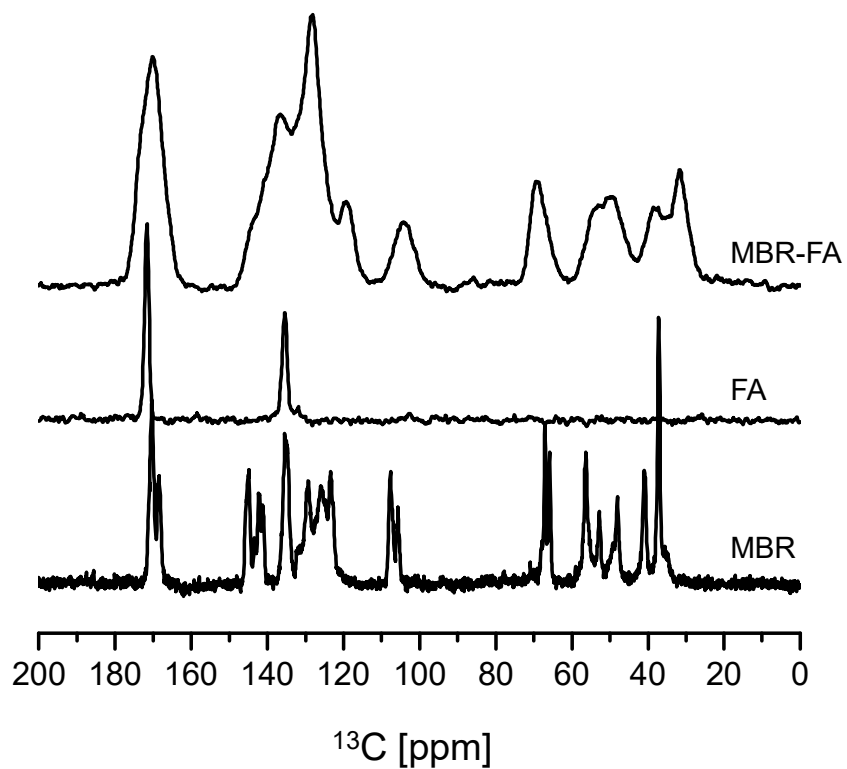


Figure S23. Solid-state CP/MAS  $^{13}\text{C}$ -NMR spectra for MBR-FA co-amorphous, MBR and FA.

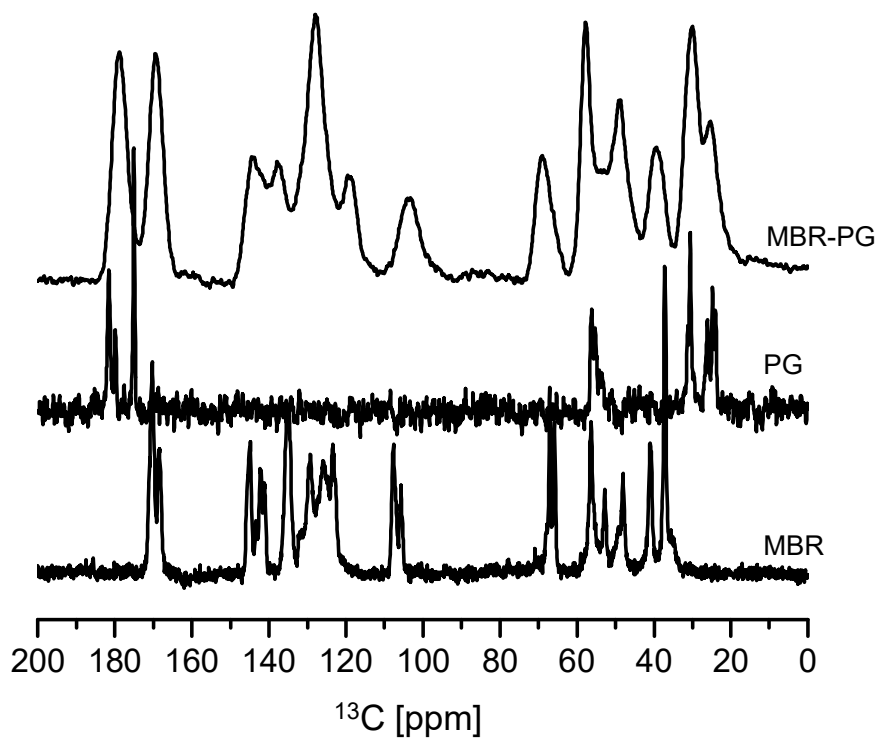


Figure S24. Solid-state CP/MAS  $^{13}\text{C}$ -NMR spectra for MBR-PG co-amorphous, MBR and PG.

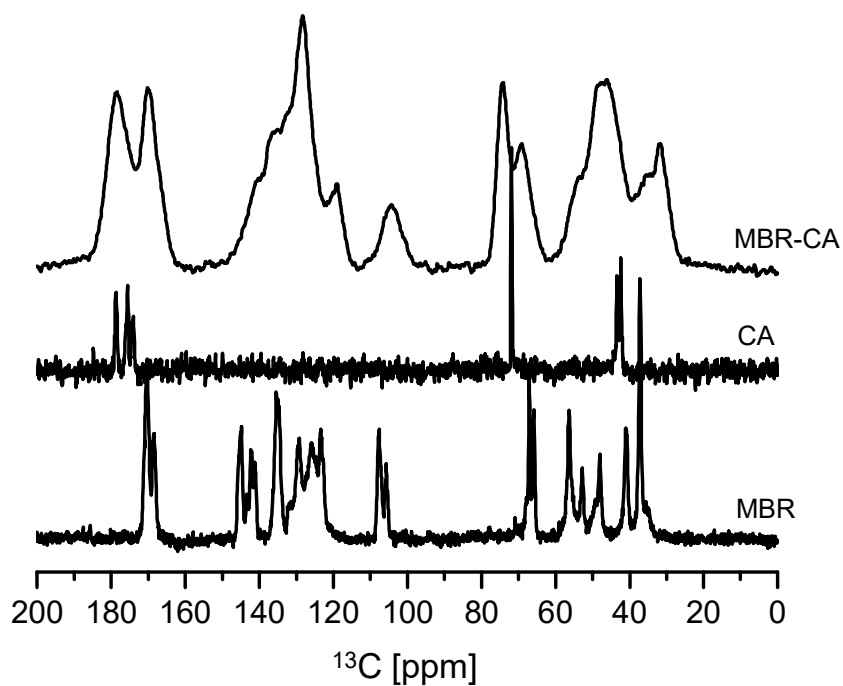


Figure S25. Solid-state CP/MAS  $^{13}\text{C}$ -NMR spectra for MBR-CA co-amorphous, MBR and CA.

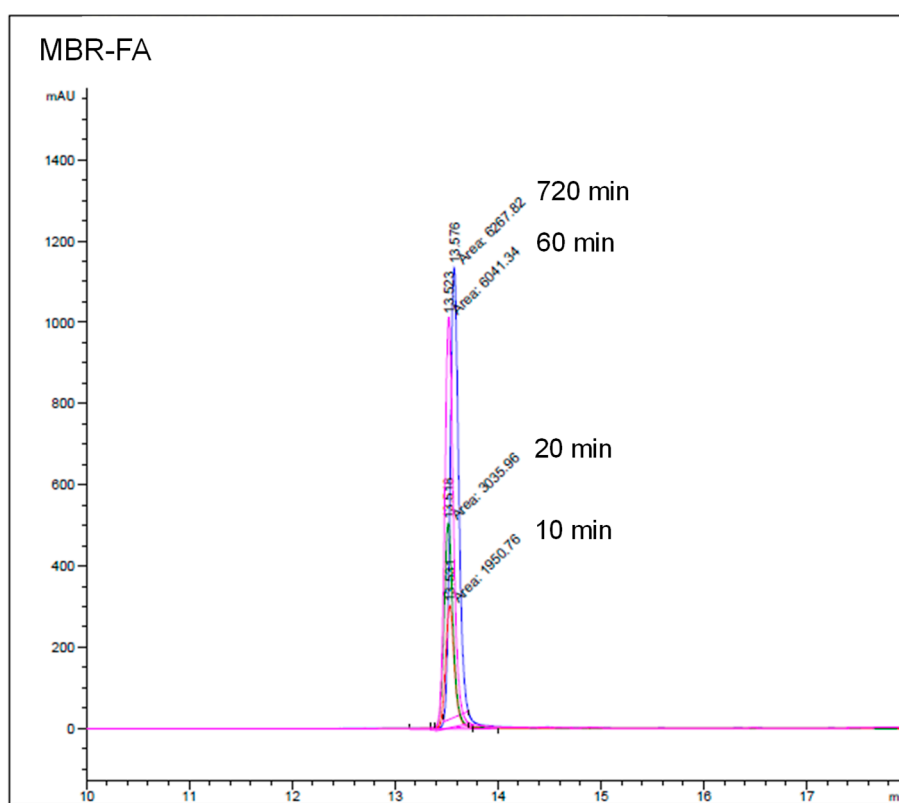
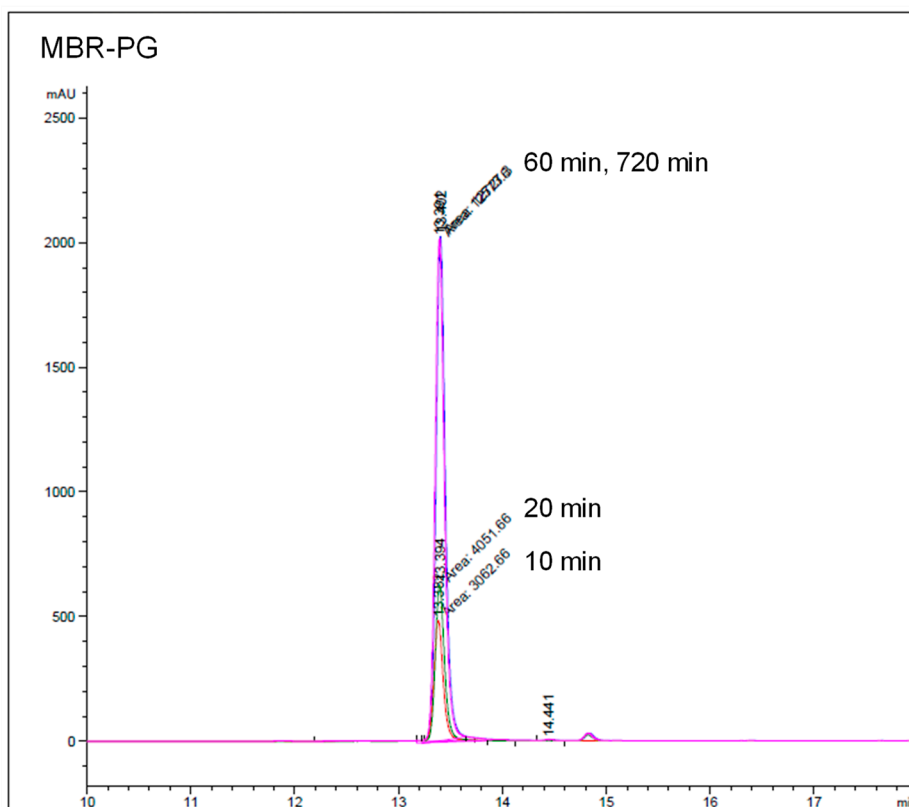
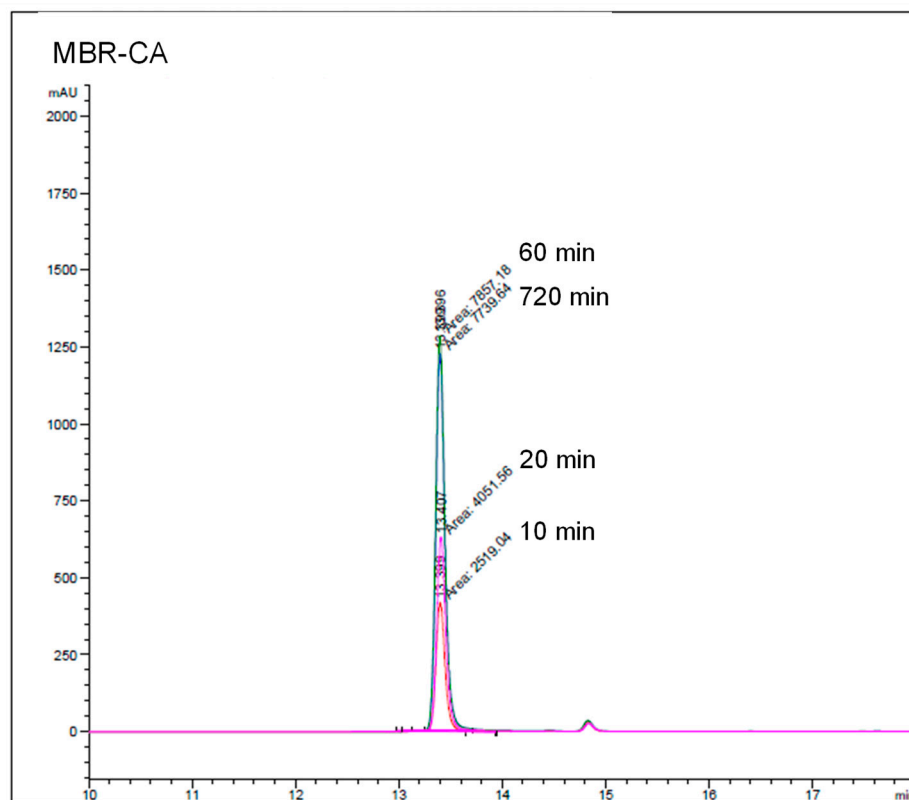


Figure S26. High-performance liquid chromatography (HPLC) chromatograms of the dissolution of MBR-FA at 10 min, 20 min, 60 min and 720 min.



**Figure S27.** HPLC chromatograms of the dissolution of MBR-PG at 10 min, 20 min, 60 min and 720 min.



**Figure S28.** HPLC chromatograms of the dissolution of MBR-CA at 10 min, 20 min, 60 min and 720 min.