SUPPORTING INFORMATION FOR:

Optimizing Formulation and Lyophilization Process for a Fragment Antigen Binding (Fab) Protein Using Solid-state Hydrogen Deuterium Exchange Mass Spectrometry (ssHDX-MS)

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The supporting information contains Figure S1 – S11.

Figure S1: (a) % loss in monomer peak (SEC; 50°C for 3 months) and (b) % increase in acidic peak (SEC; 50°C for 3 months) for formulations F1 UCN to F5 UCN.

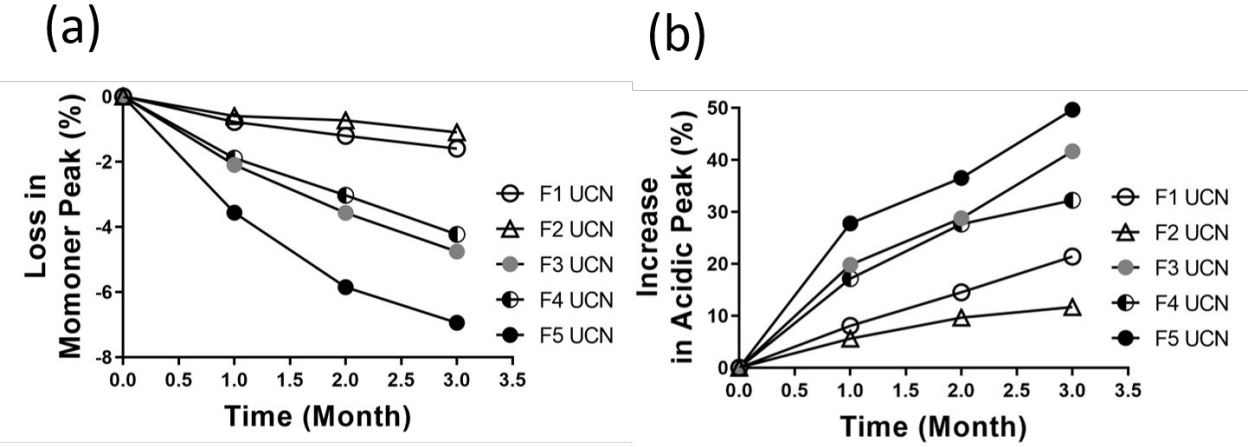

Figure S2: Correlation of % increase in acidic peak (3 months) for formulations F1 UCN to F5 UCN, with residual moisture (a), FT-IR band intensity (b), % moisture gain (c) and number of deuterium taken up after 10 days of incubation in ssHDX-MS (d)

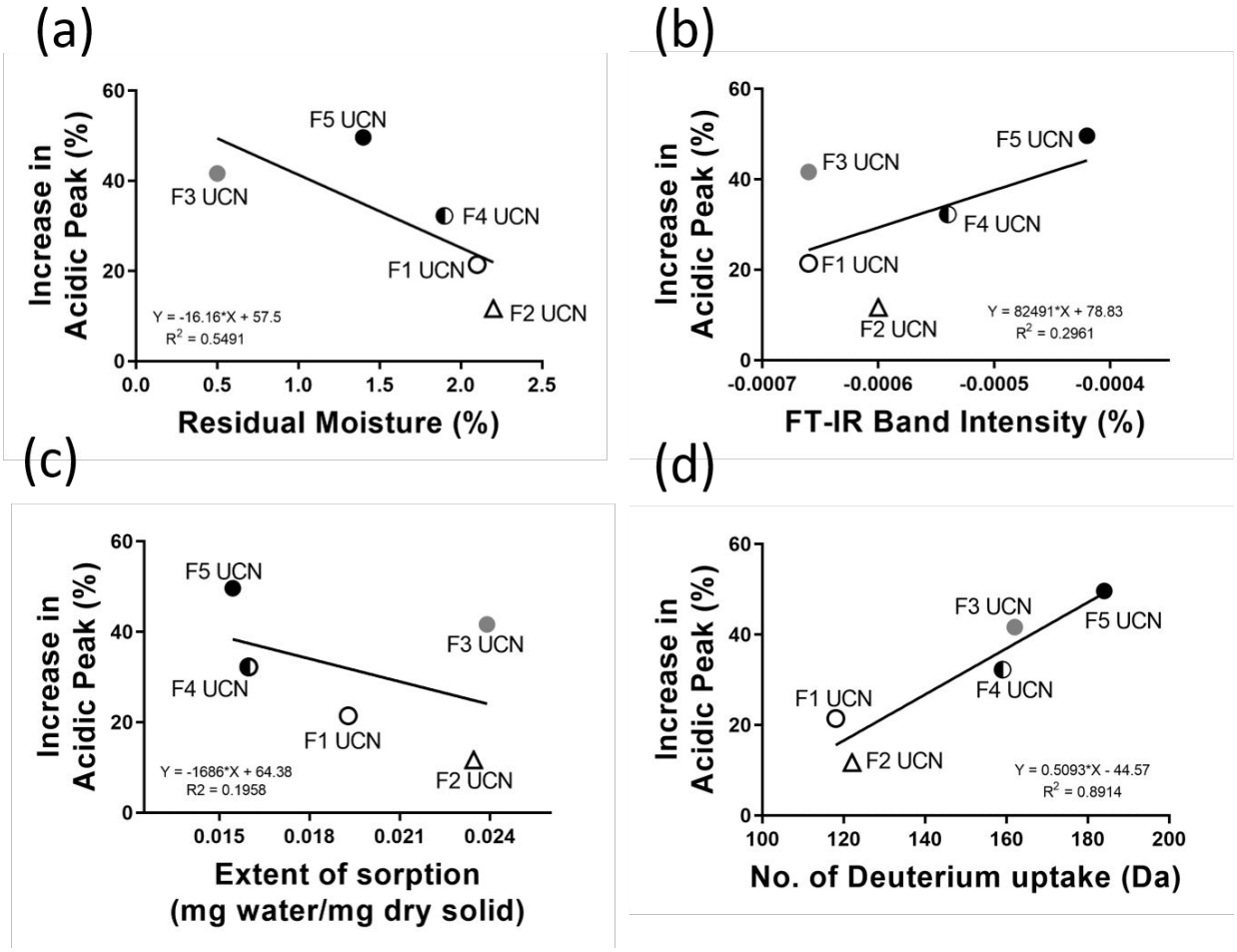

Figure S3: Biexponential kinetic parameters of ssHDX-MS (Eqn. 2) for study 1: N_{fast} (a), N_{slow} (b) K_{fast} (c) and K_{slow} (d). Bars show parameter values for formulations F1 UCN to F5 UCN.

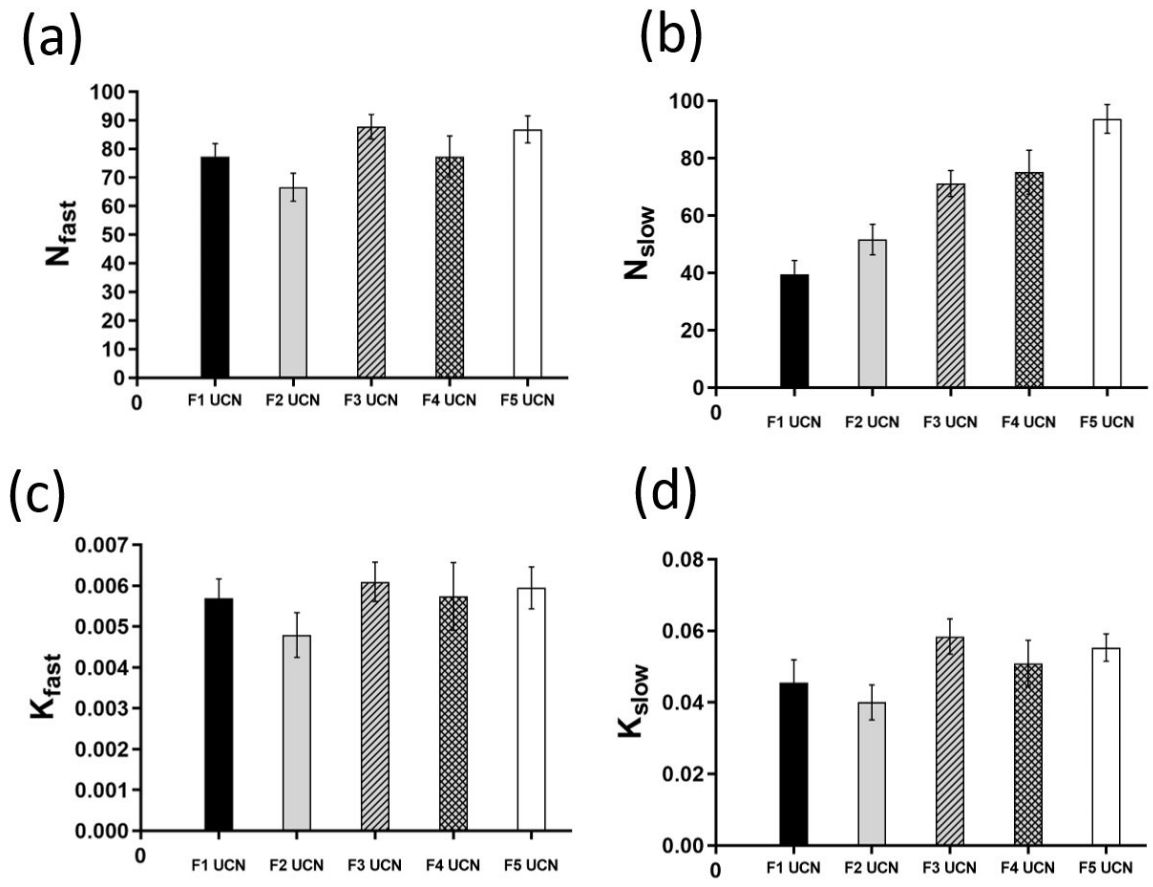

Figure S4: % loss in monomer peak (SEC, (a) and (b)) and % increase in acidic peak (IEC; (c) and (d)) at 50^{o}C as a function of time, and lyophilization processing, for formulations F1 ((a),(c)) and F3 ((b),(d)) produced by CN and UCN.

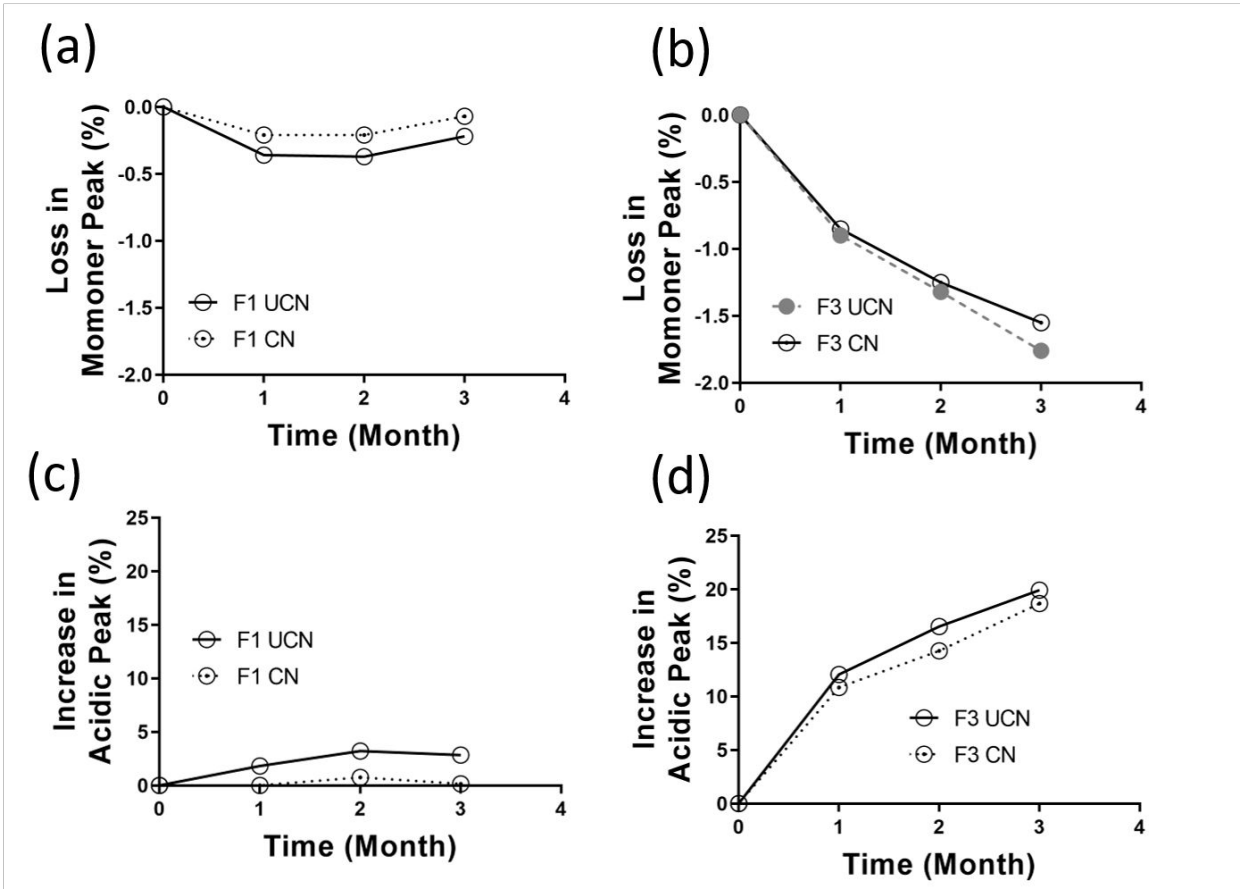

Figure S5: 2nd derivative ssFT-IR of F1 (a) and F3 (b) formulations (CN and UCN)

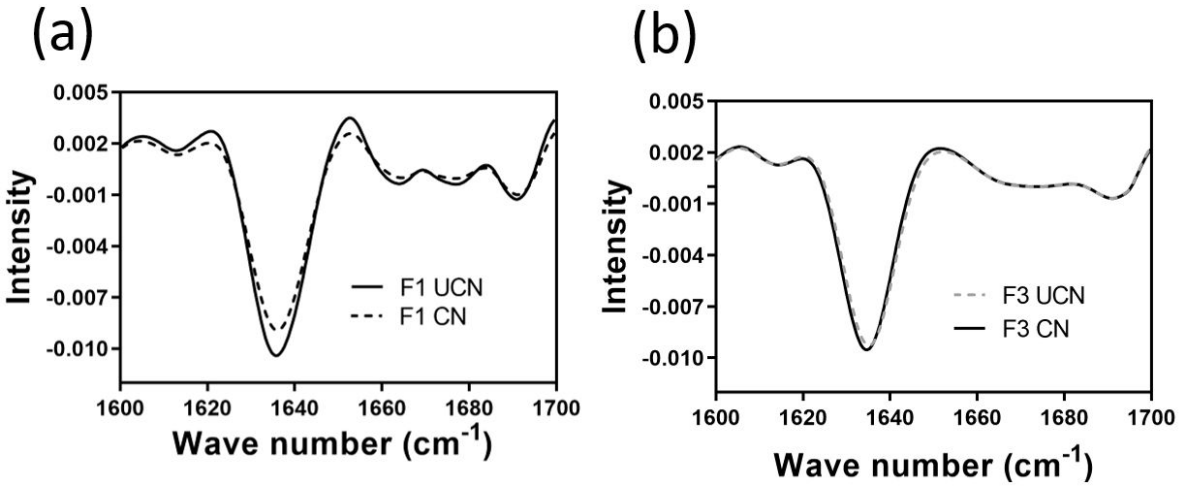

Figure S6: solid state FT-IR of Fab formulation F6 lyophilized using uncontrolled ice nucleation (F6 UCN), controlled ice nucleation (F6 CN) or annealing (F6 AN)

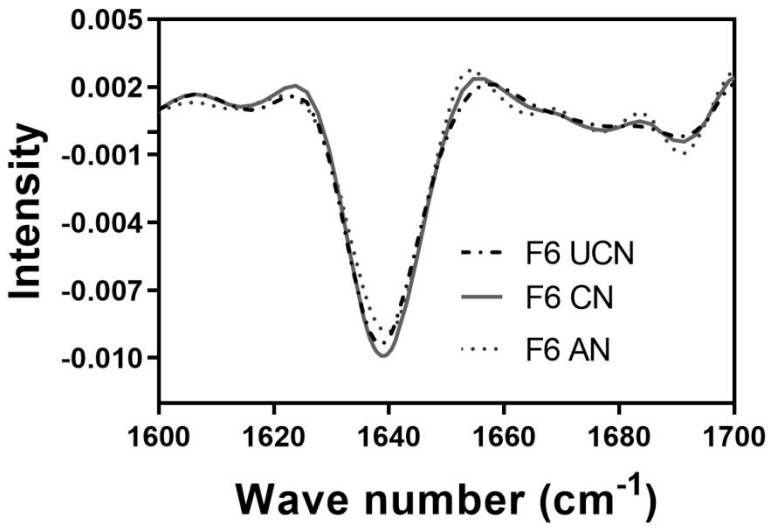

Figure S7: (a) % loss of monomer peak (SEC) and (b) % increase in acidic peak (IEC) vs time (month) for Formulation F6, as a function of different lyophilization processing (UCN, CN, AN)

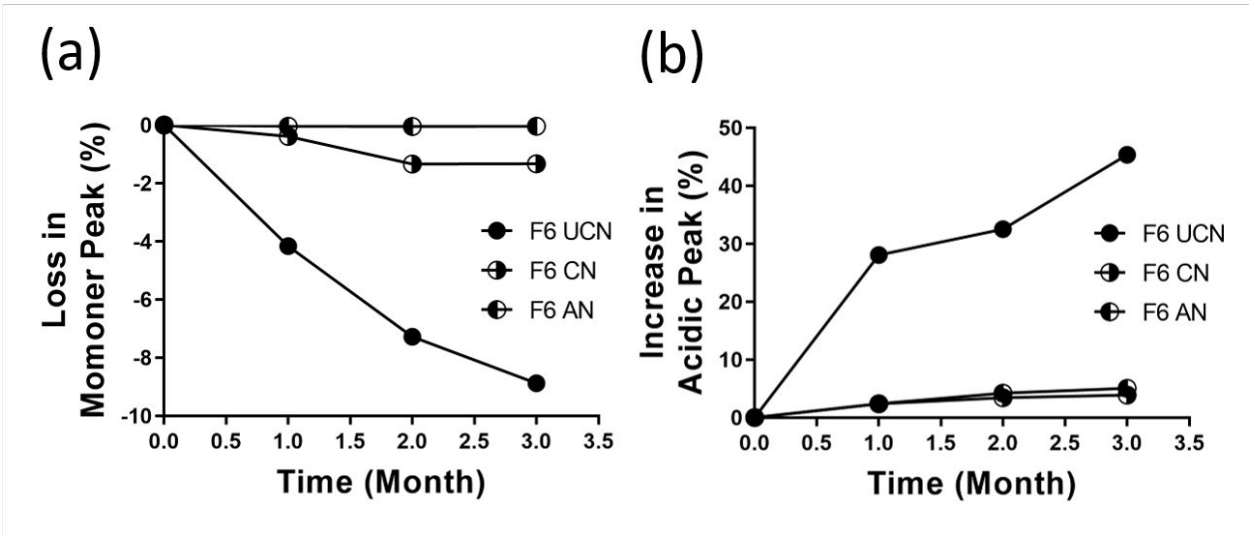

Figure S8: Correlation of % increase in acidic peak by IEC (3 months), for F6 formulations produced using various methods (UCN, CN, AN) with residual moisture (a), ssFT-IR band intensity (b), extent of moisture uptake (c) and number of deuterium taken up after 10 days of incubation (d).

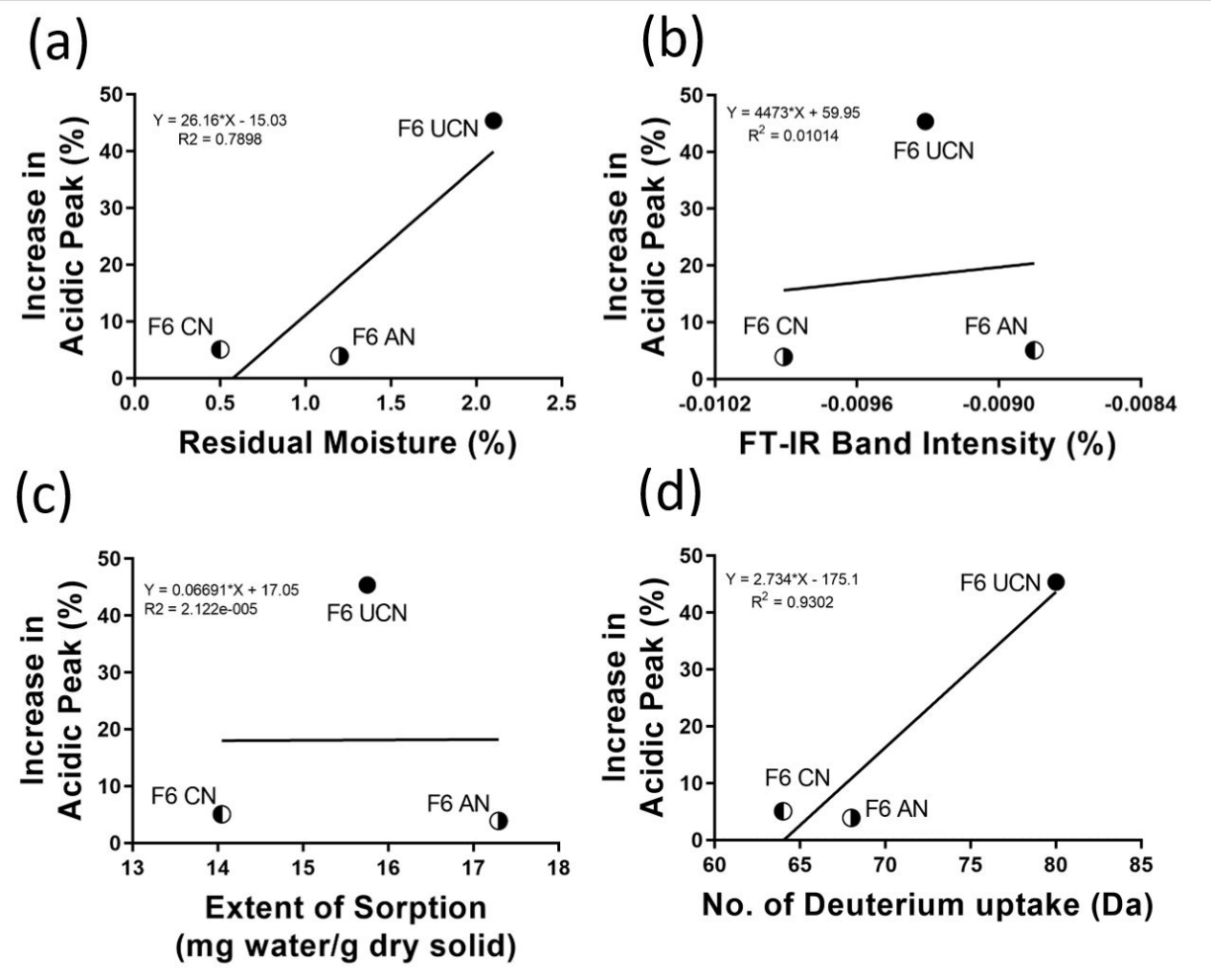

Figure S9: DVS sorption curves of F6 formulations (Uncontrolled ice nucleation, CN and Annealing) at 11% RH and 23°C

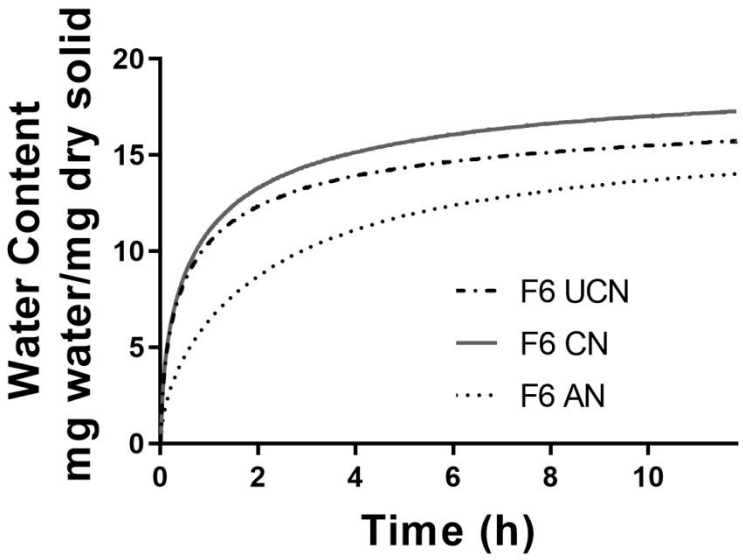

Figure S10: Representative SEC chromatogram, for F1-F5 formulations at 3 month stability time point

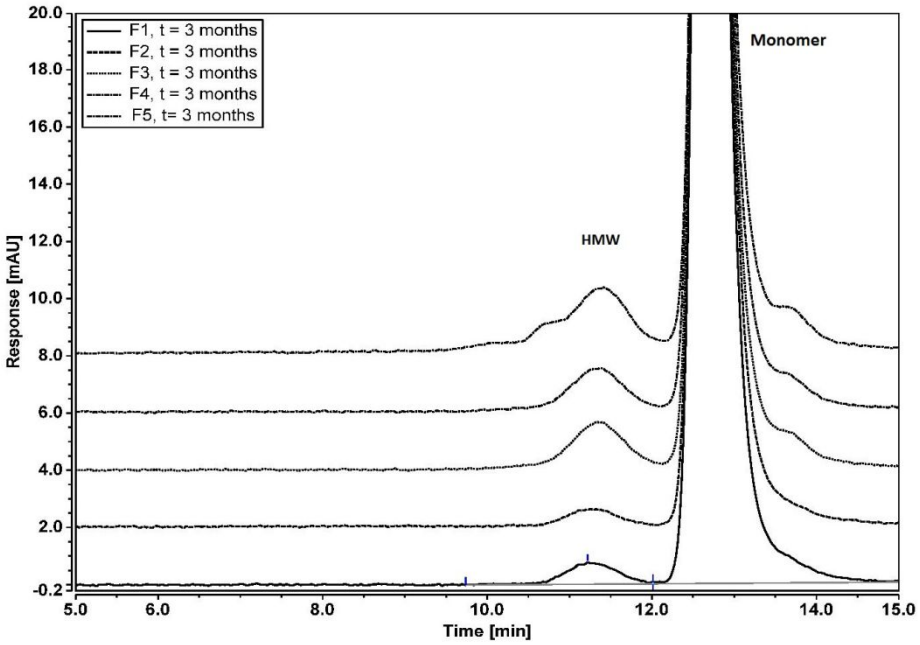

Figure S11: Representative DSC chromatogram for F2 formulation