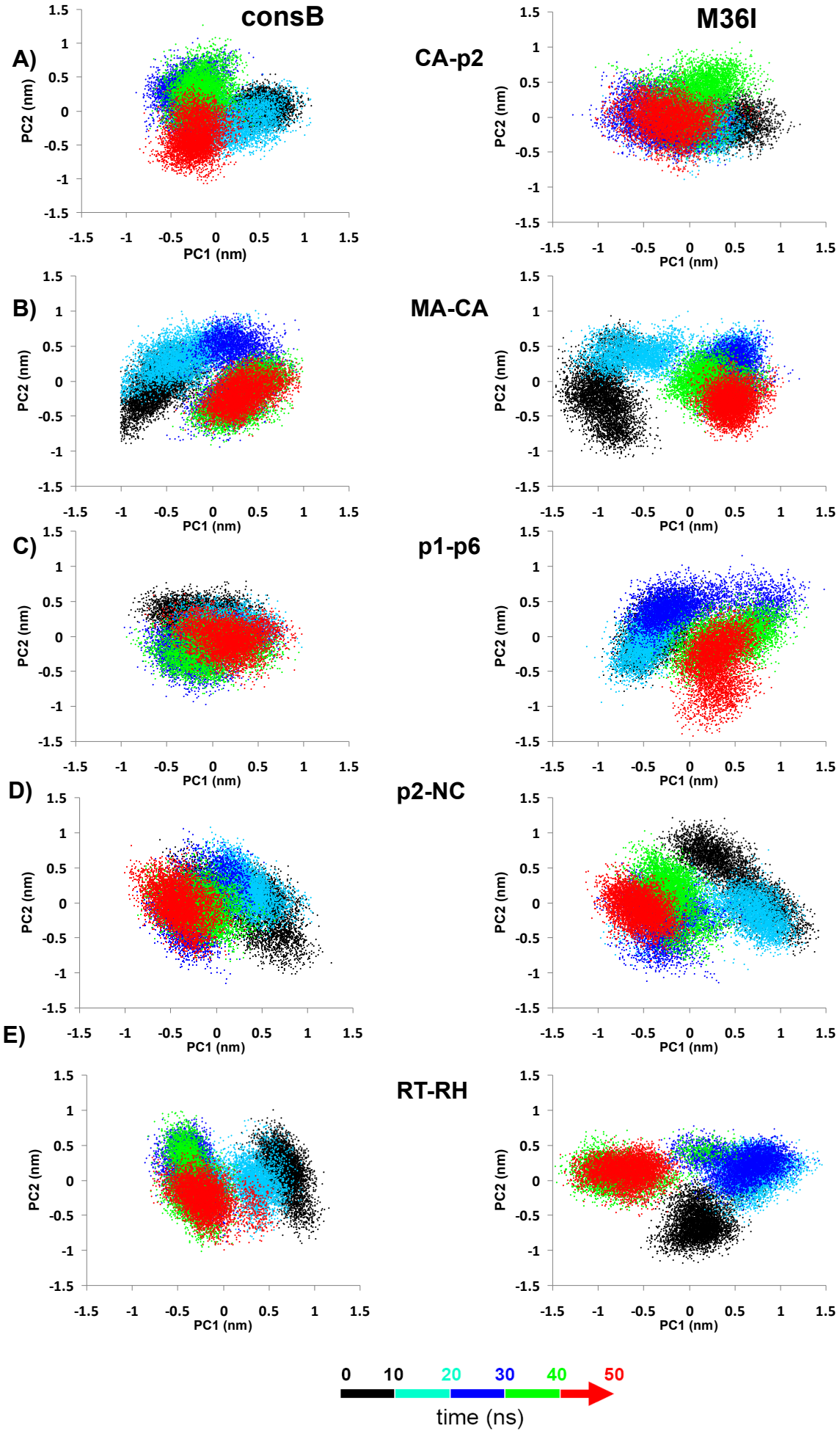Additional file 7 – Conformational sampling along the first two PC space