Fe(II) spin crossover (SCO) materials based on N1-substituted ligands are very sensitive towards subtle modifications in the ligand design. Recently developed synthetic approaches towards systematically N1-functionalized tetrazoles gave access to a broad library of homologous ligands for a systematic study on the steric impact of the ligands’ substitution pattern. In a series of 3-halogen substituted 1-propyl-1H-tetrazoles SCO-active Fe(II)-complexes were obtained, featuring a higher spin transition temperature than the parent compound (figure 1a). Various analytical methods confirmed, that the halogen substitution had only an impact on the steric demand of the ligand but does not affect the electronic properties. A similar effect was observed for the methyl-substituted 1-[(1,1'-biphenyl)-4-ylmethyl]-1H-tetrazoles (figure 1b), were the variation of the methyl-position had a notable impact on the crystal packing, affecting therethrough the SCO behaviour. In the contribution is highlighted, how valuable information towards tuneable SCO materials is achieved based on such structure-property correlations.

Figure 1 SCO in a series of a) 1-propyl-1H-tetrazoles b) 1-[(1,1'-biphenyl)-4-ylmethyl]-1H-tetrazoles