



**Fig. 7. 2D-NMR study on LPMO binding to substrates.** His83, one of the copper ligands together with His155 and His1 side-chain and terminal amine (N) (A), participates in cellulose binding on LPMO (C) as shown by strong signal displacement in the  $^1\text{H}$ - $^{15}\text{N}$  heteronuclear single quantum (HSQC) spectra acquired in the absence (black contour) and the presence (cyan contour) of a cellulose hexasaccharide (Glc6) (the unaffected signal of Val42 is shown as reference) (B). More interestingly, a smaller but significant displacement of the above NMR signal in the presence of CDH suggests that the same site, near the catalytic copper, is also involved in binding of CDH, or other copper-reducing molecules, for LPMO activation. The strongest interactions (NMR displacements) correspond to red surface in A, followed by blue surface. Adapted from Courtade et al. (2016).