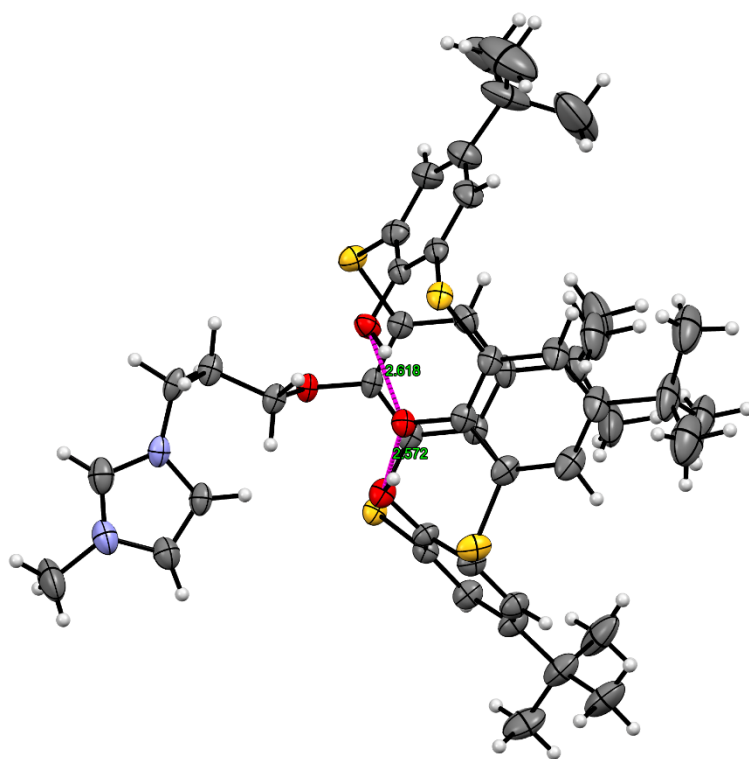


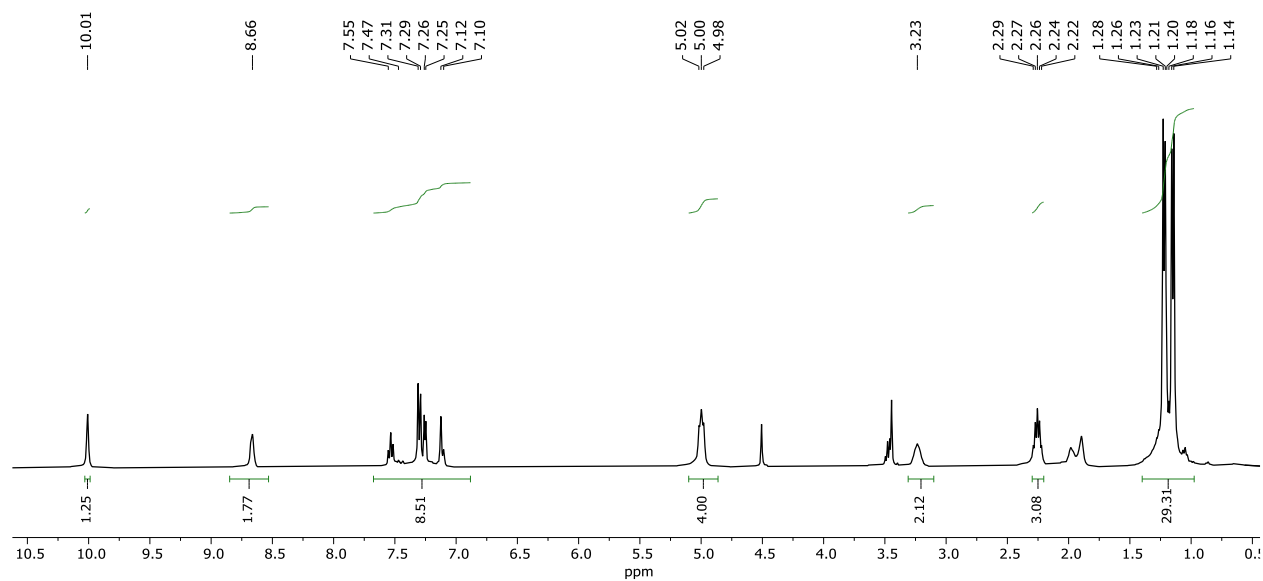
# PEPPSI-Type Pd(II) – NHC Complexes on the Base of p-tert-Butylthiacalix[4]arene: Synthesis and Catalytic Activities

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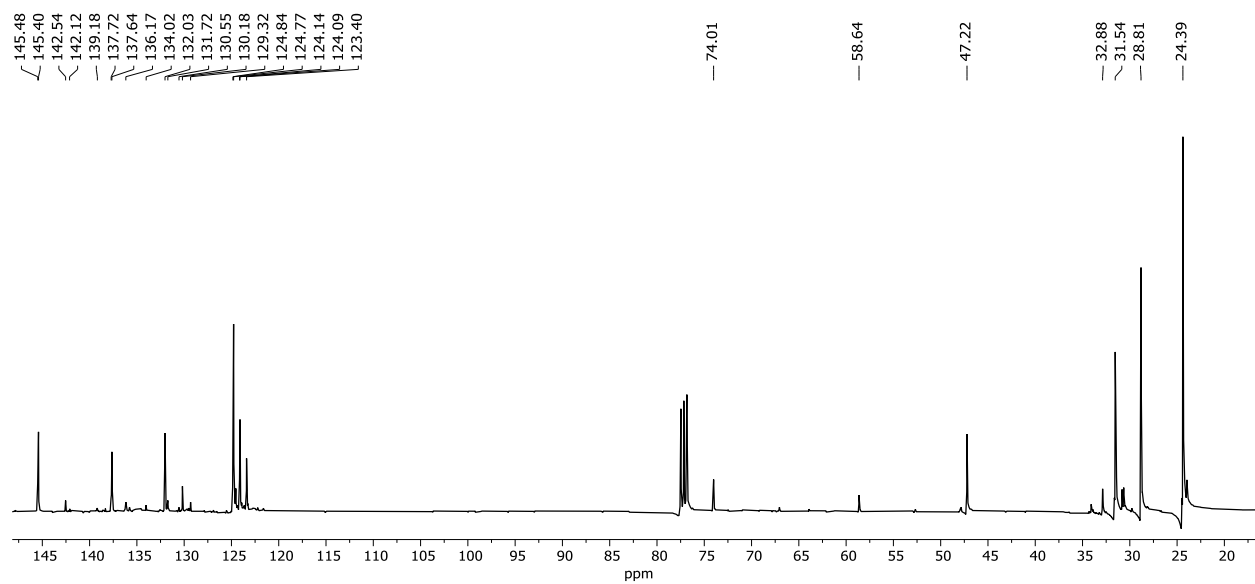
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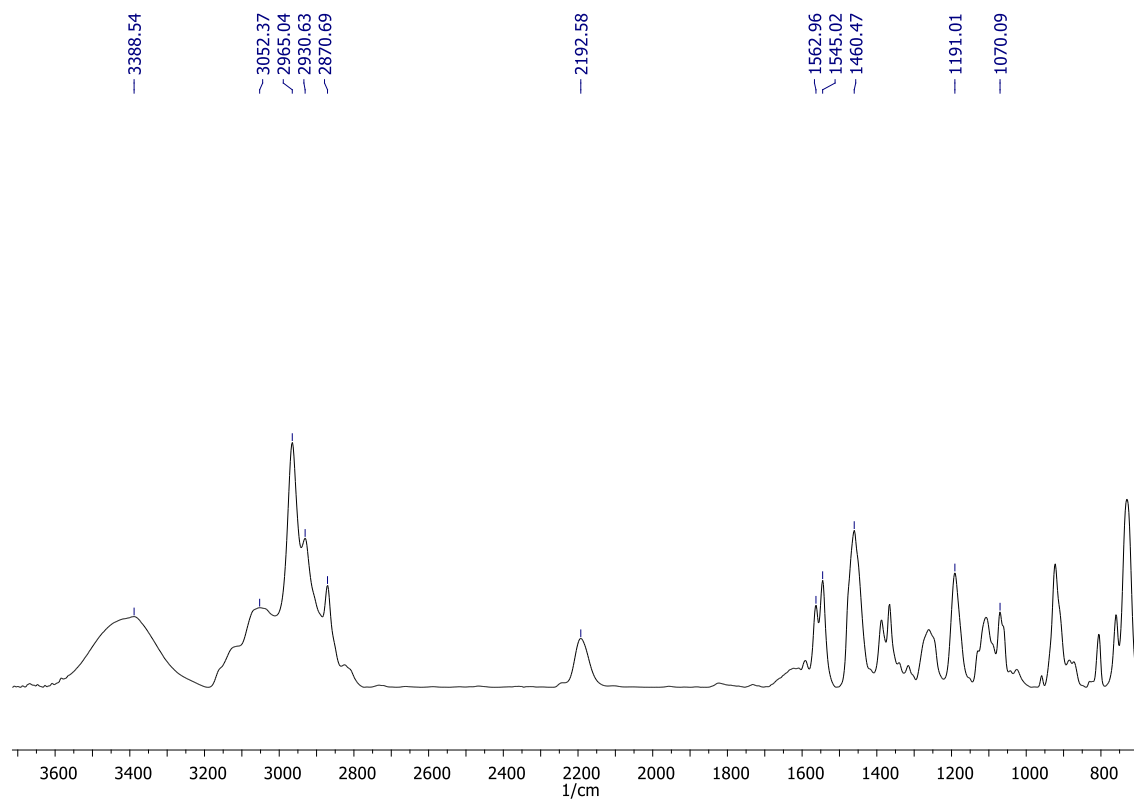
**Figure S1.** ORTEP representation of **2** showing 50% probability thermal ellipsoids. C atoms – grey, N atoms – blue, O atoms – red, S atoms – yellow.



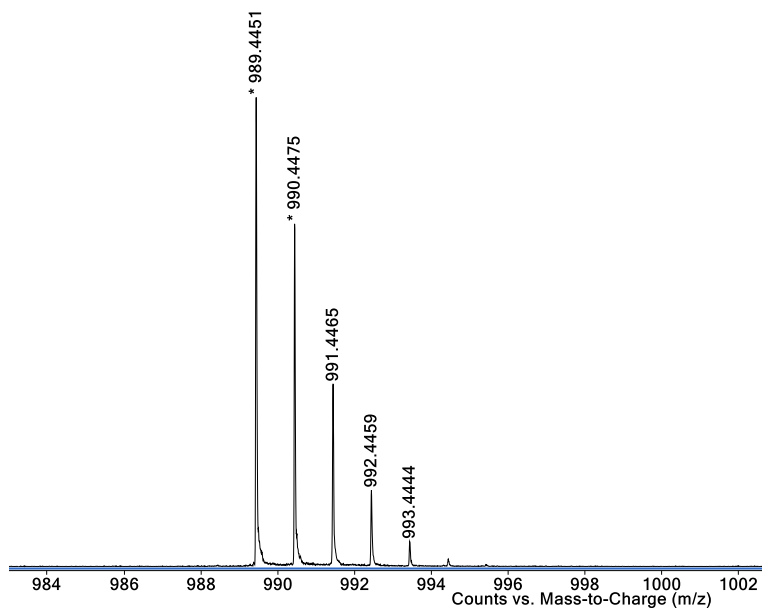
**(a)**



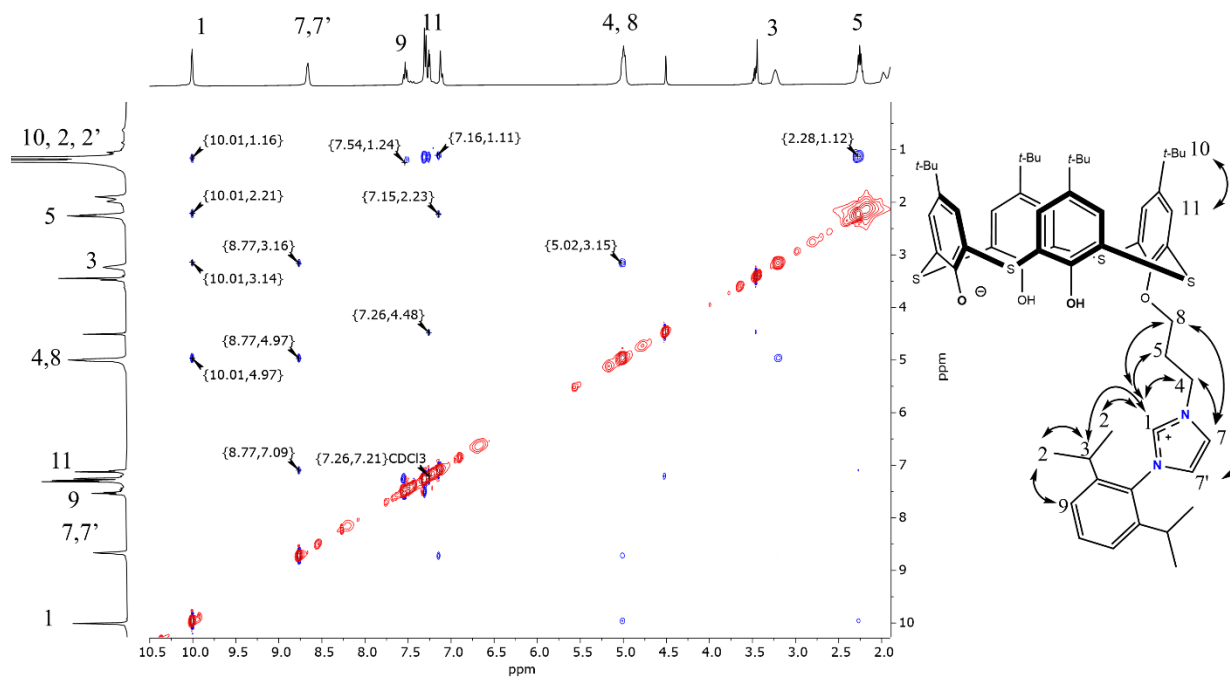
(b)



(c)

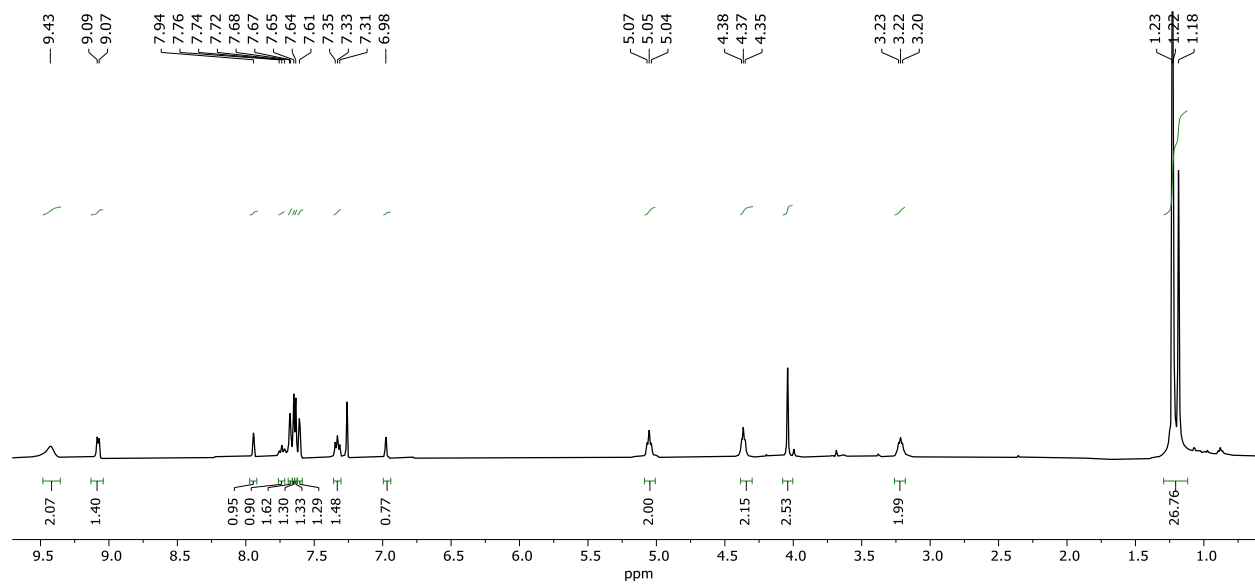


(d)

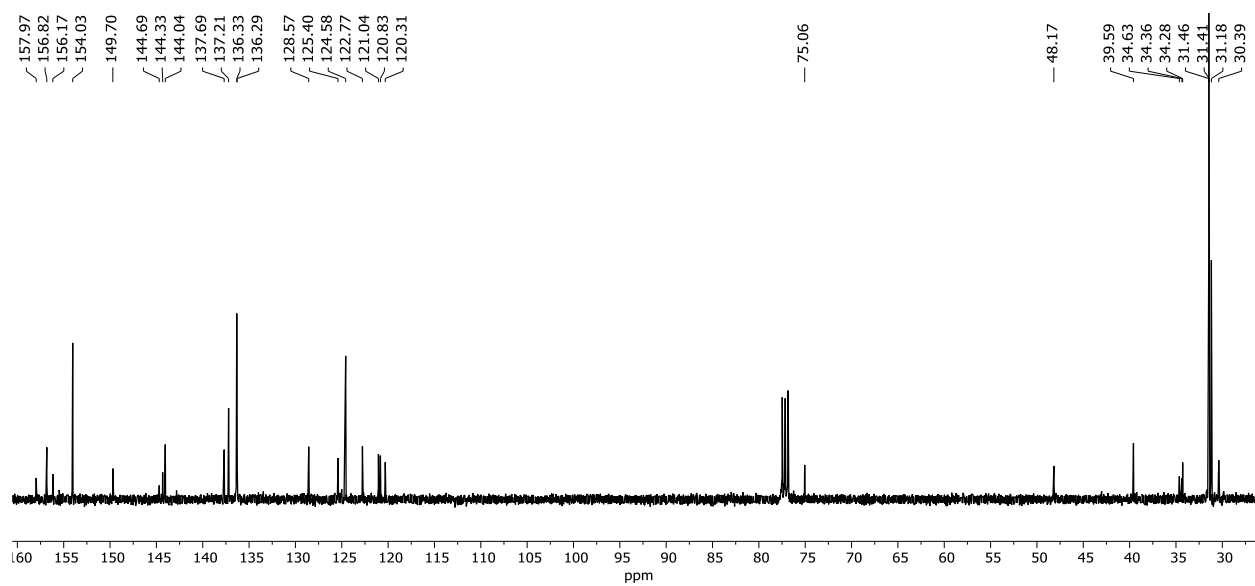


(e)

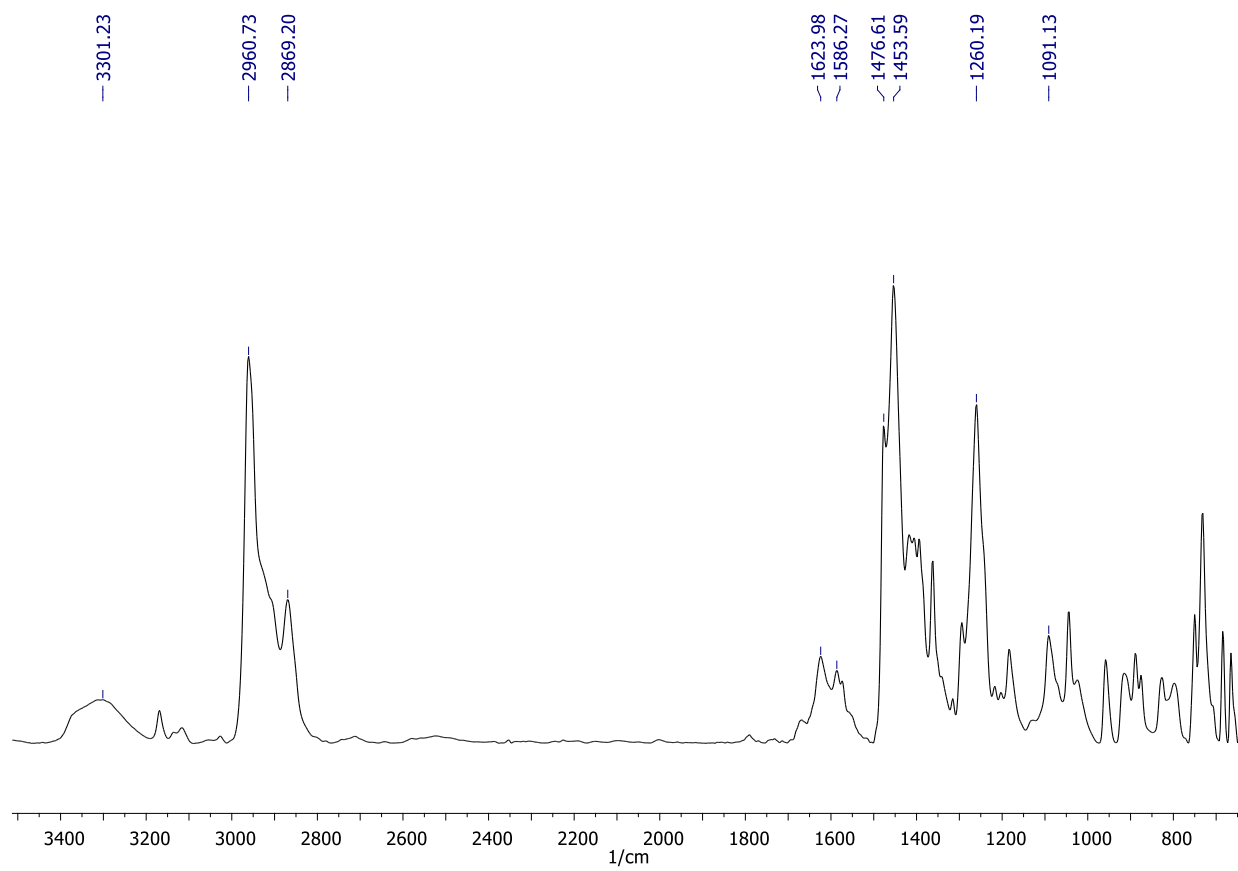
**Figure S2.** NMR  $^1\text{H}$  (a),  $^{13}\text{C}$  (b), FT IR (c), HR ESIMS (d) and NOESY ( $^1\text{H}$ - $^1\text{H}$ ) NMR spectra (e) of 5,11,17,23-tetra-*tert*-butyl-25, 27-dihydroxy-26-oxido-28-(3-(3-*N*-(2',6' di-*isopropylphenyl*)limidazolium)propoxy) -2,8,14,20-tetrathiacalix[4]arene (**3**)



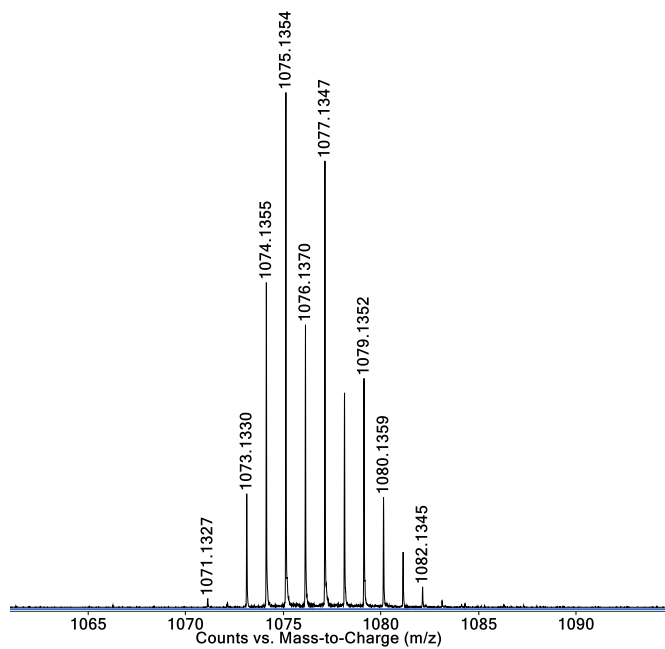
**(a)**



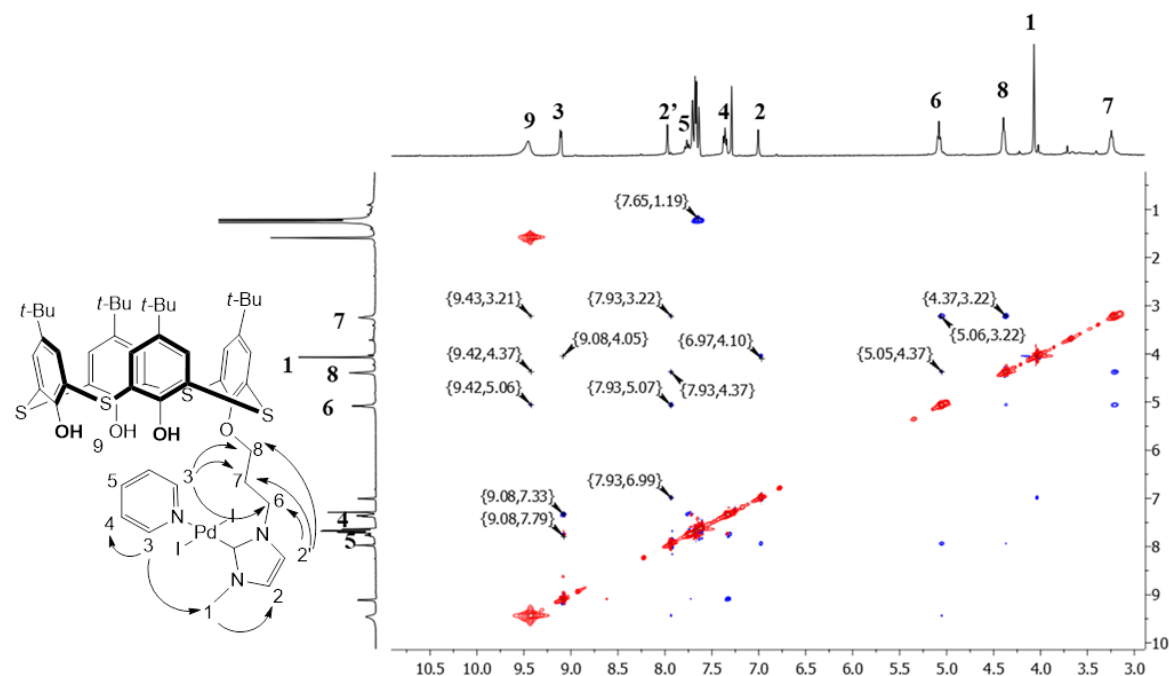
**(b)**



(c)

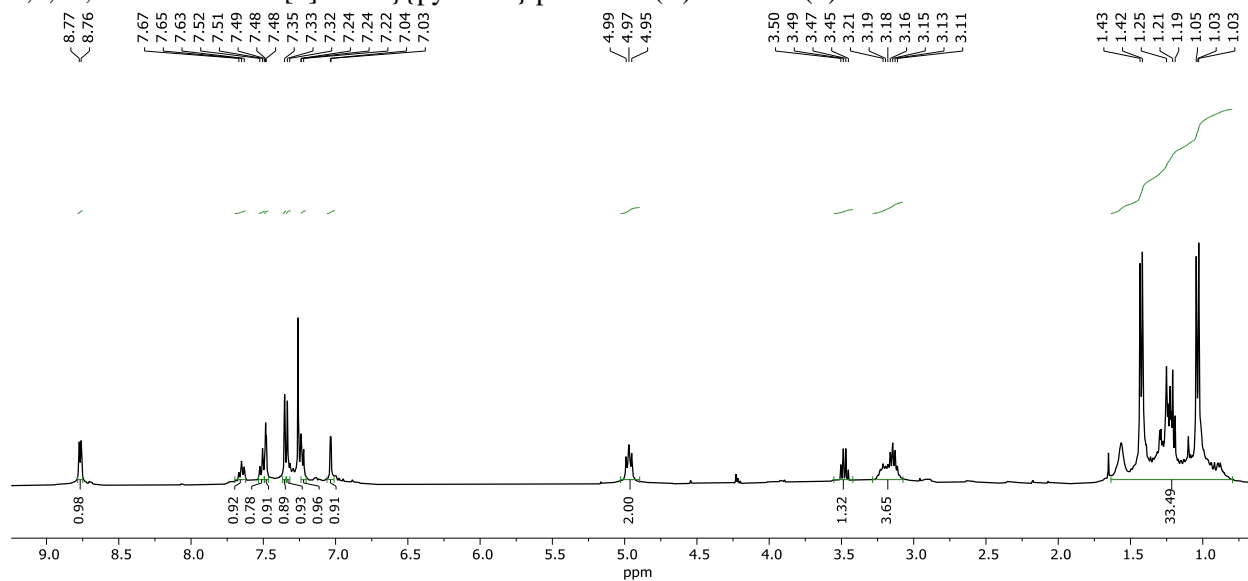


(d)

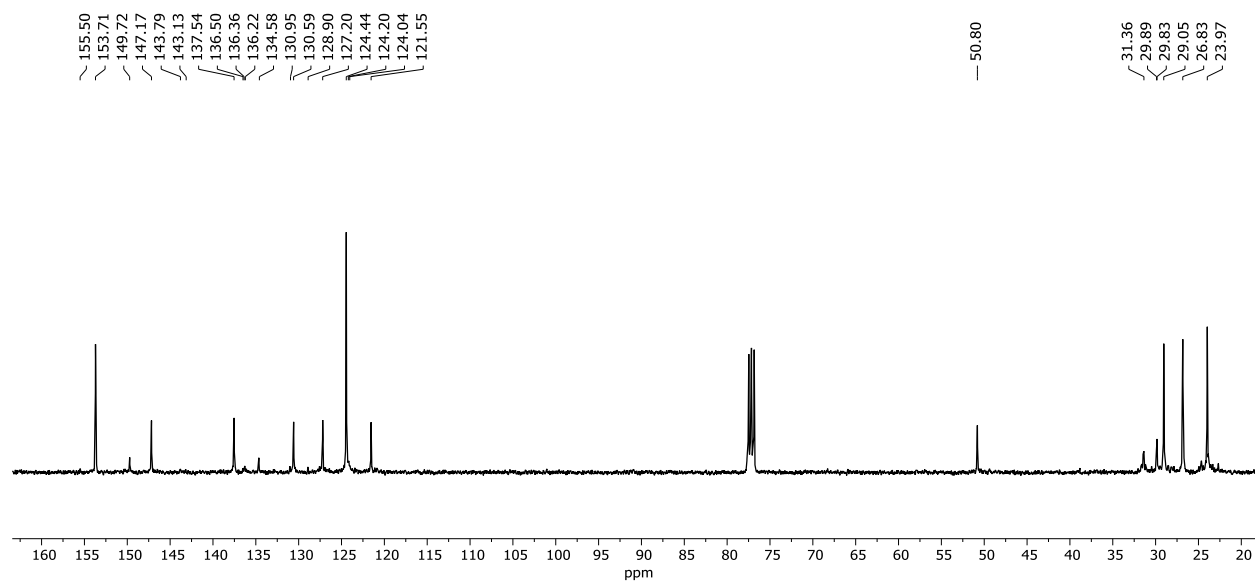


(e)

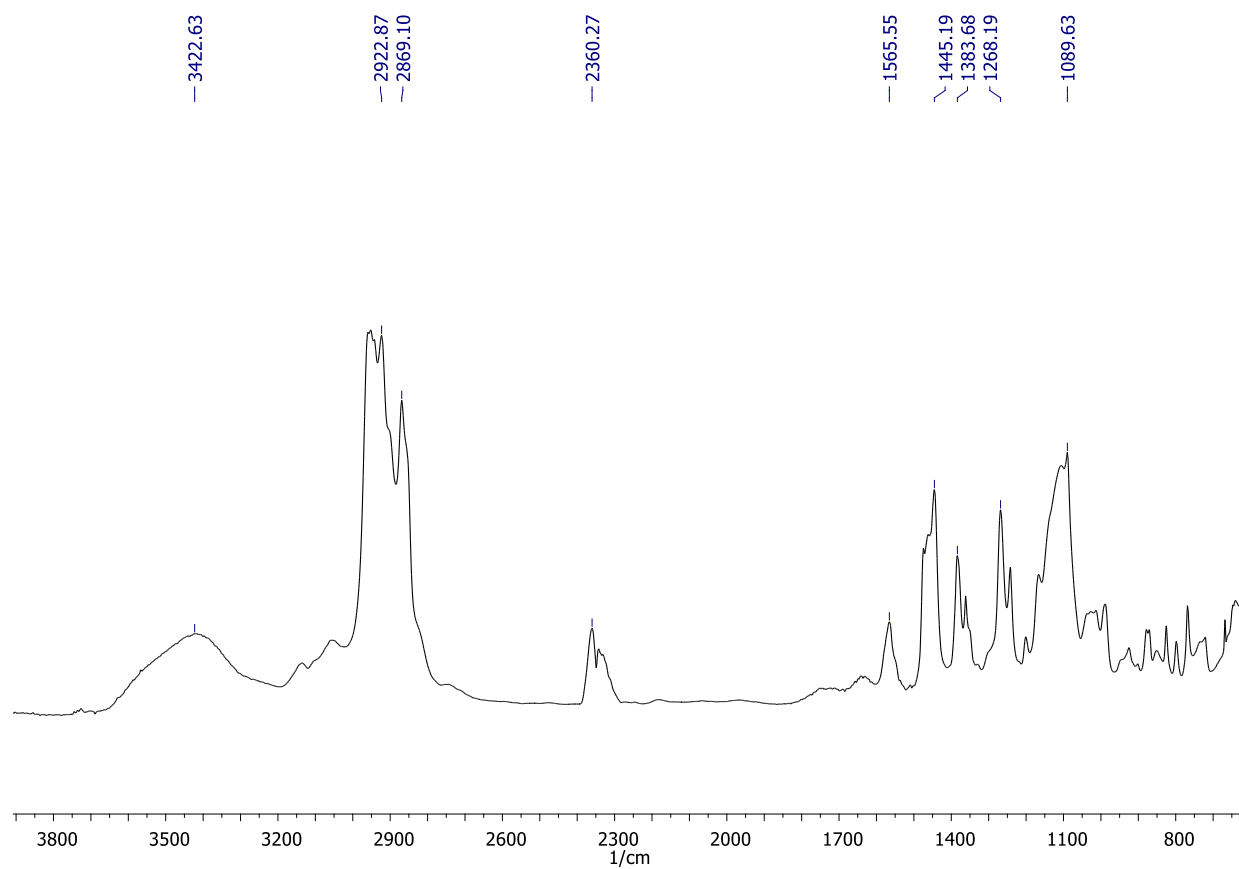
**Figure S3.** NMR  $^1\text{H}$  (a),  $^{13}\text{C}$  (b), FT IR (c), HR ESIMS (d) and NOESY ( $^1\text{H}$ - $^1\text{H}$ ) NMR spectra (e) of trans - {5,11,17,23-tetra-*tert*-butyl-25, 26, 27-trihydroxy-28-(3-(3-*N*-methylimidazolin-2-ylidene)propoxy) - 2,8,14,20-tetrathiocalix[4]arene }{pyridine} palladium(II) diiodide (**4**).



(a)

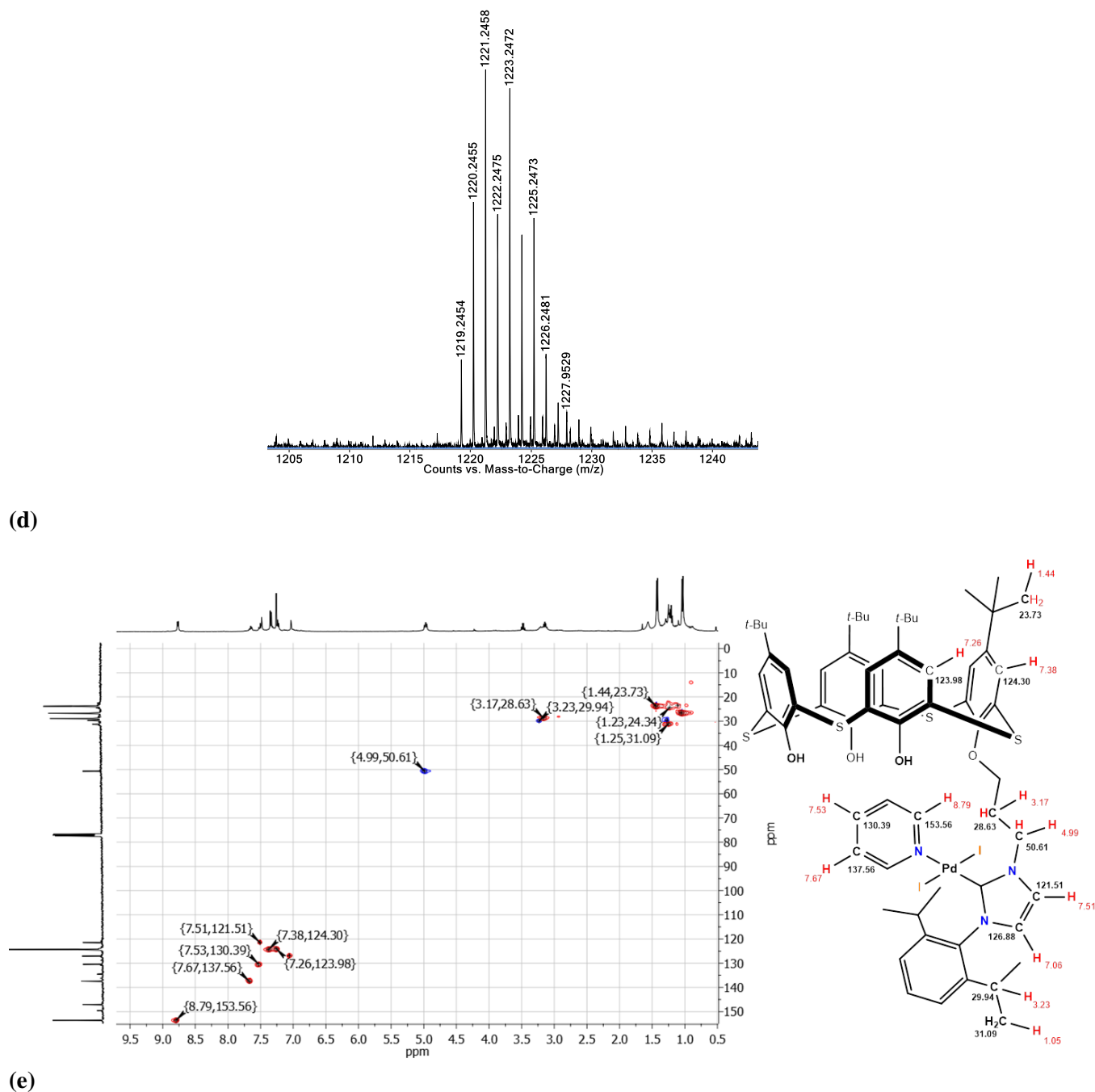


(b)



(c)





**Figure S4.** NMR  $^1\text{H}$  (a),  $^{13}\text{C}$  (b), FT IR (c), HR ESIMS (d) and HSQC ( $^1\text{H}$ - $^{13}\text{C}$ ) spectra (e) of trans - {5,11,17,23-tetra-*tert*-butyl-25, 26, 27-trihydroxy-28-(3-(3-N-(2',6' di-isopropylphenyl)imidazolin-2-ylidene)propoxy) -2,8,14,20-tetrathiacalix[4]arene } {pyri-dine} palladium(II) diiodide (**5**).