

# Novel PEPPSI-Type NHC Pd(II) Metallosurfactants on the Base of 1H-Imidazole-4,5-Dicarboxylic Acid: Synthesis and Catalysis in Water–Organic Media

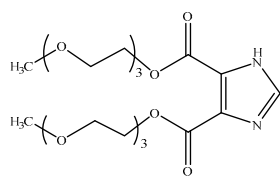
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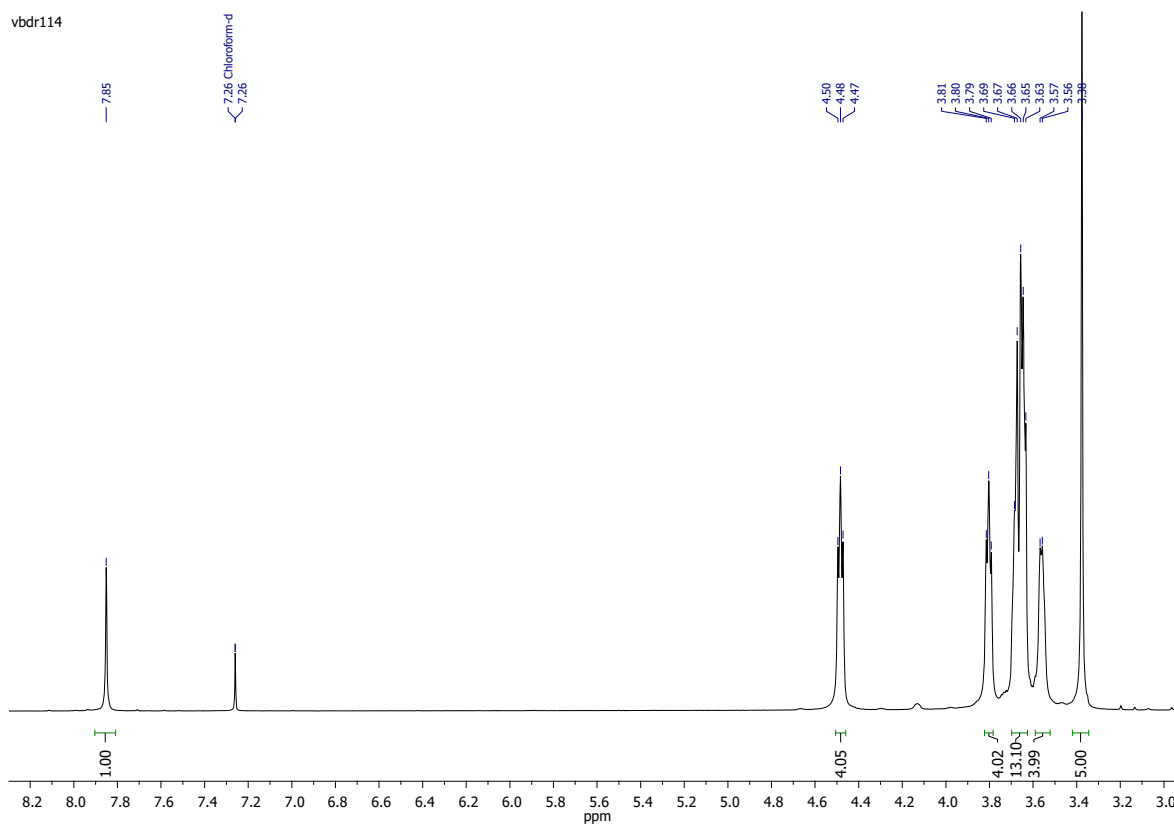
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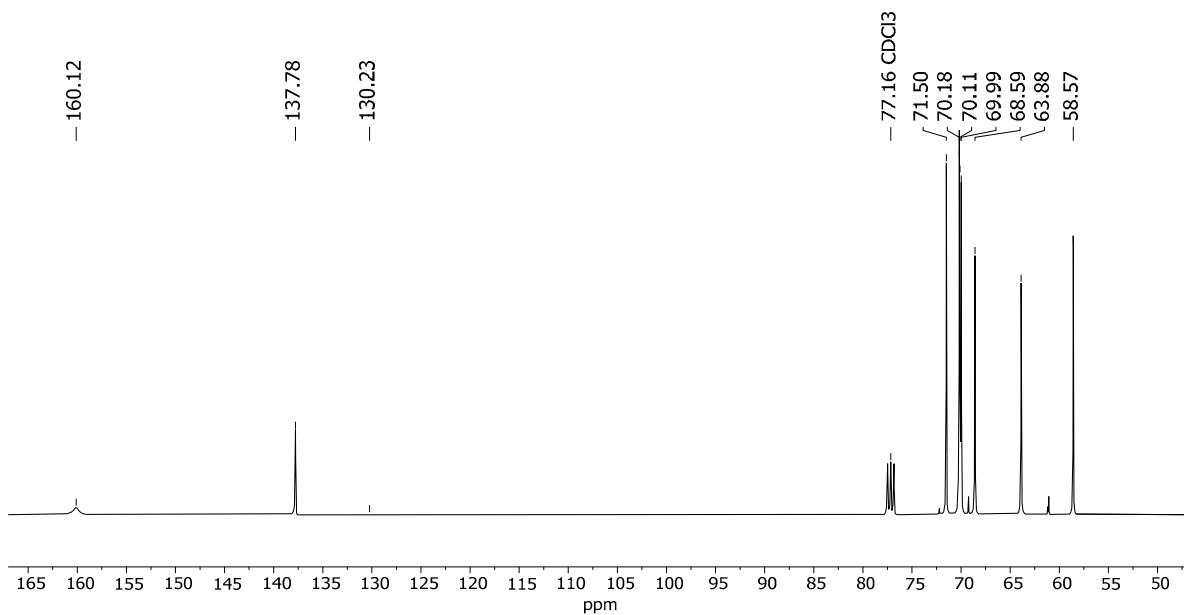
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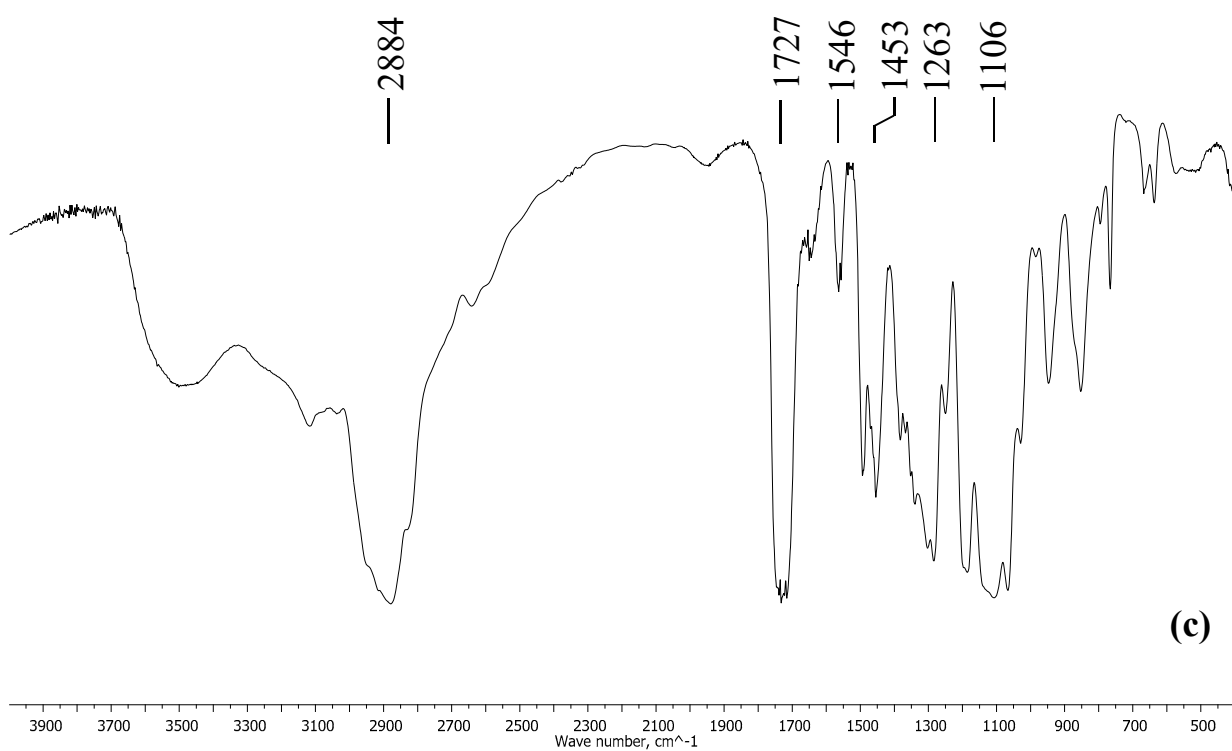
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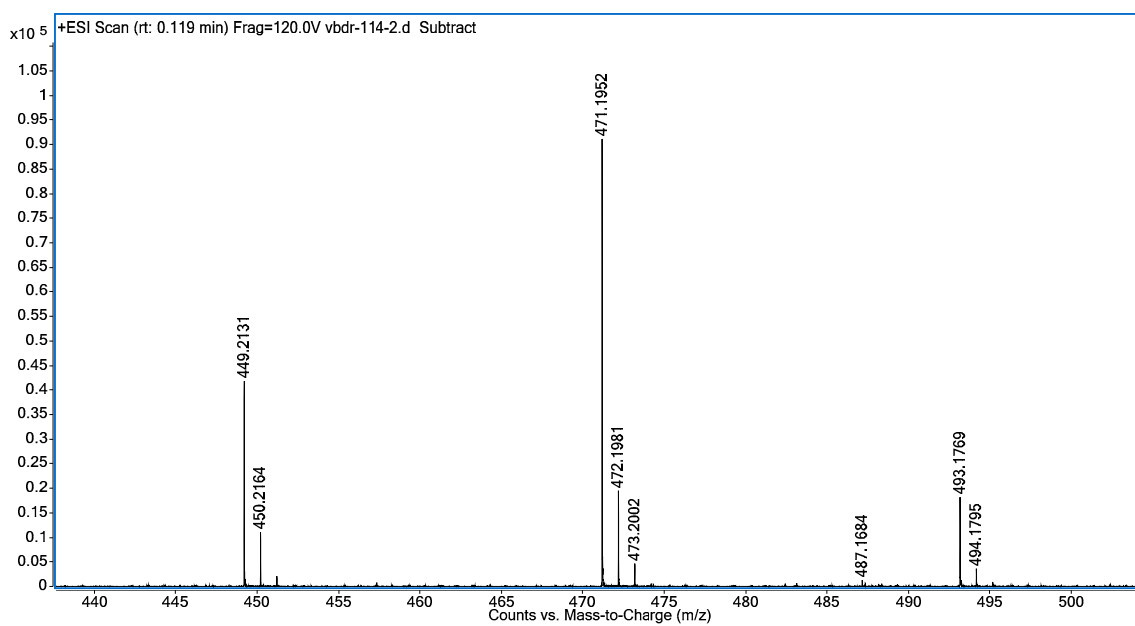
(a)



(b)

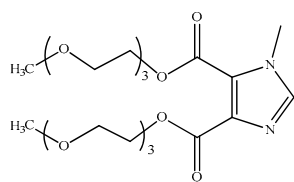


(c)



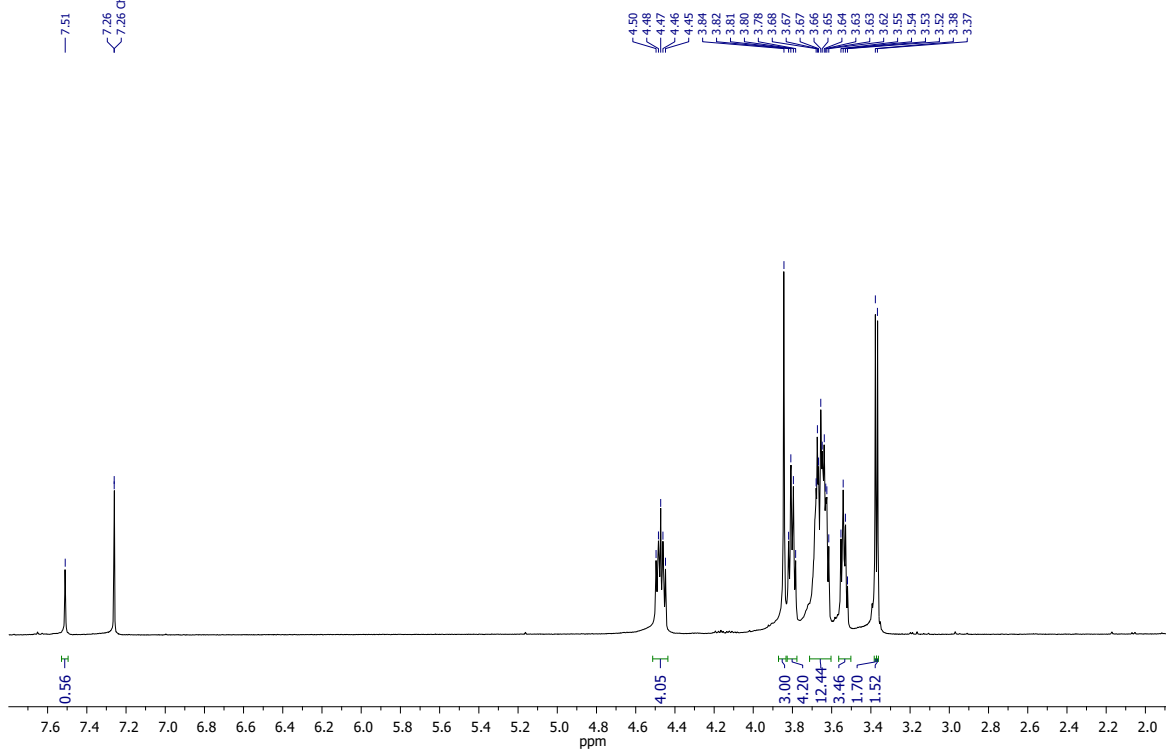
(d)

**Figure S1.** NMR <sup>1</sup>H (a), <sup>13</sup>C (b), FT IR (c) and HRESI MS (d) spectra of 4,5-bis-[2-(2-(2-methoxyethoxy)ethoxy)ethoxycarbonyl]imidazole (**1**).

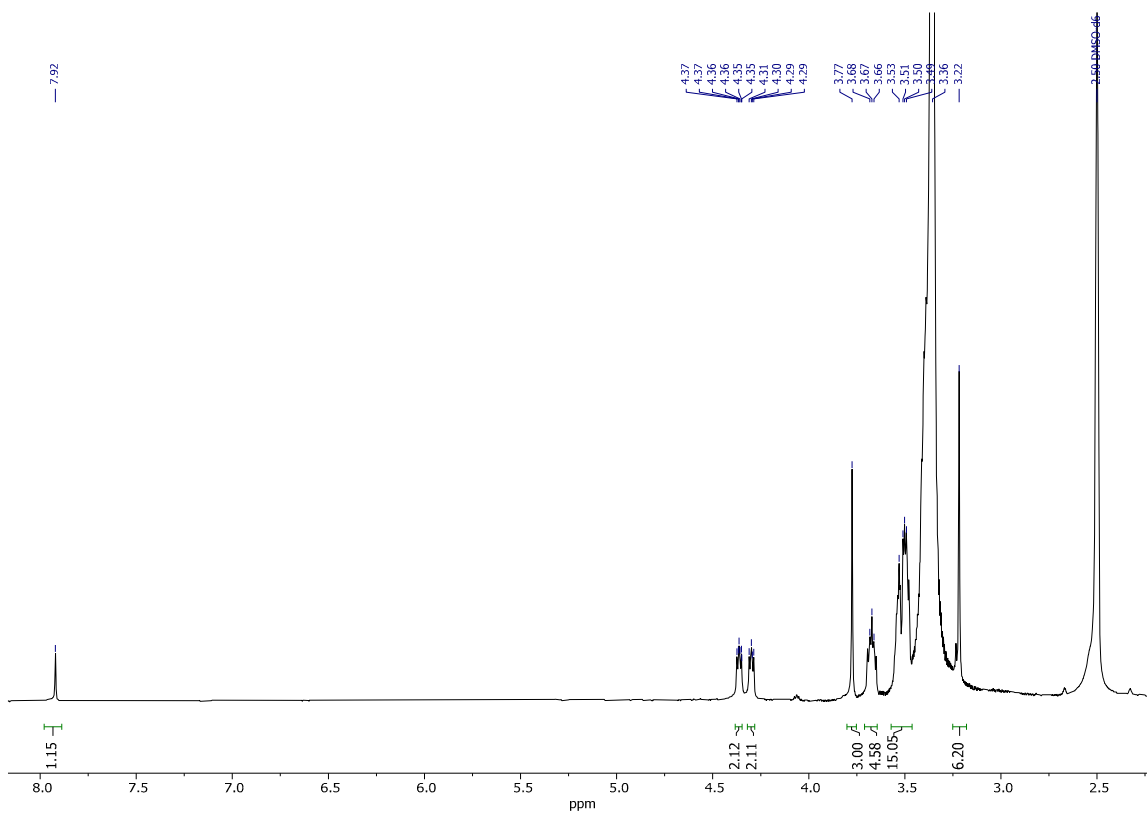


vbdp-24-e

7.26 Chloroform-d

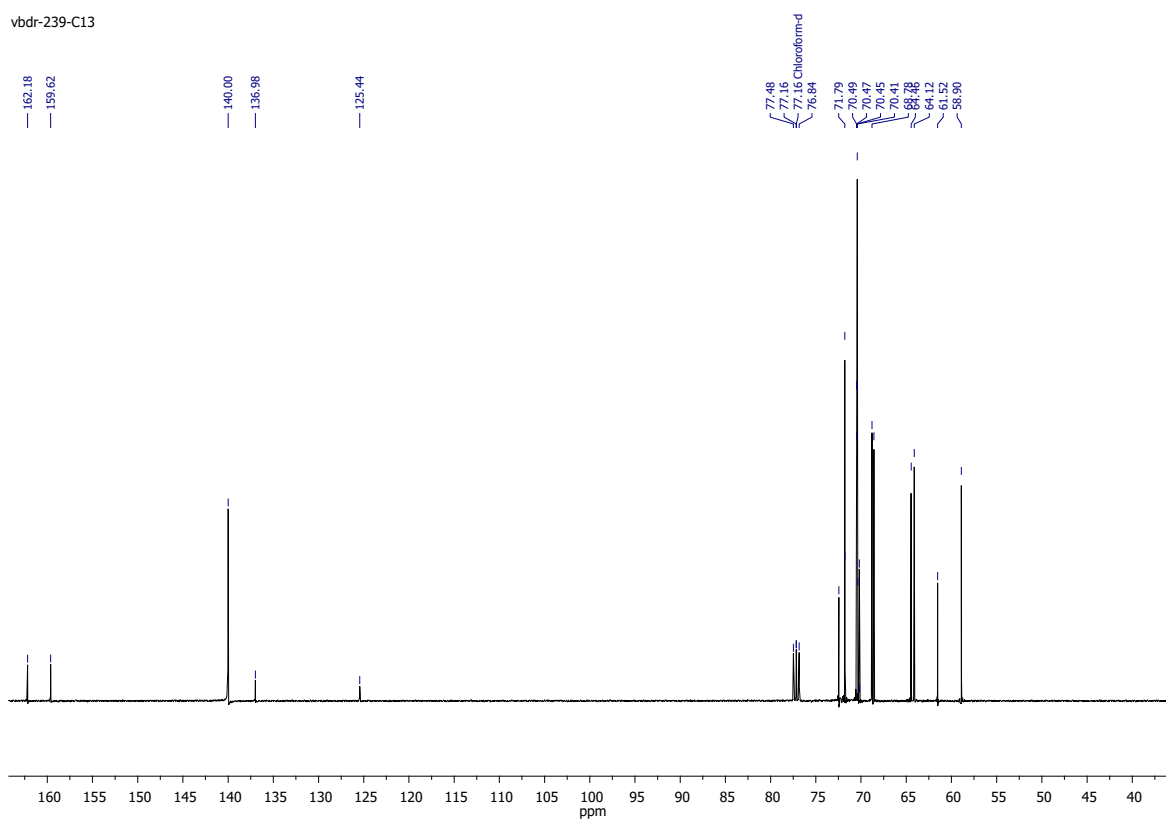


(a)

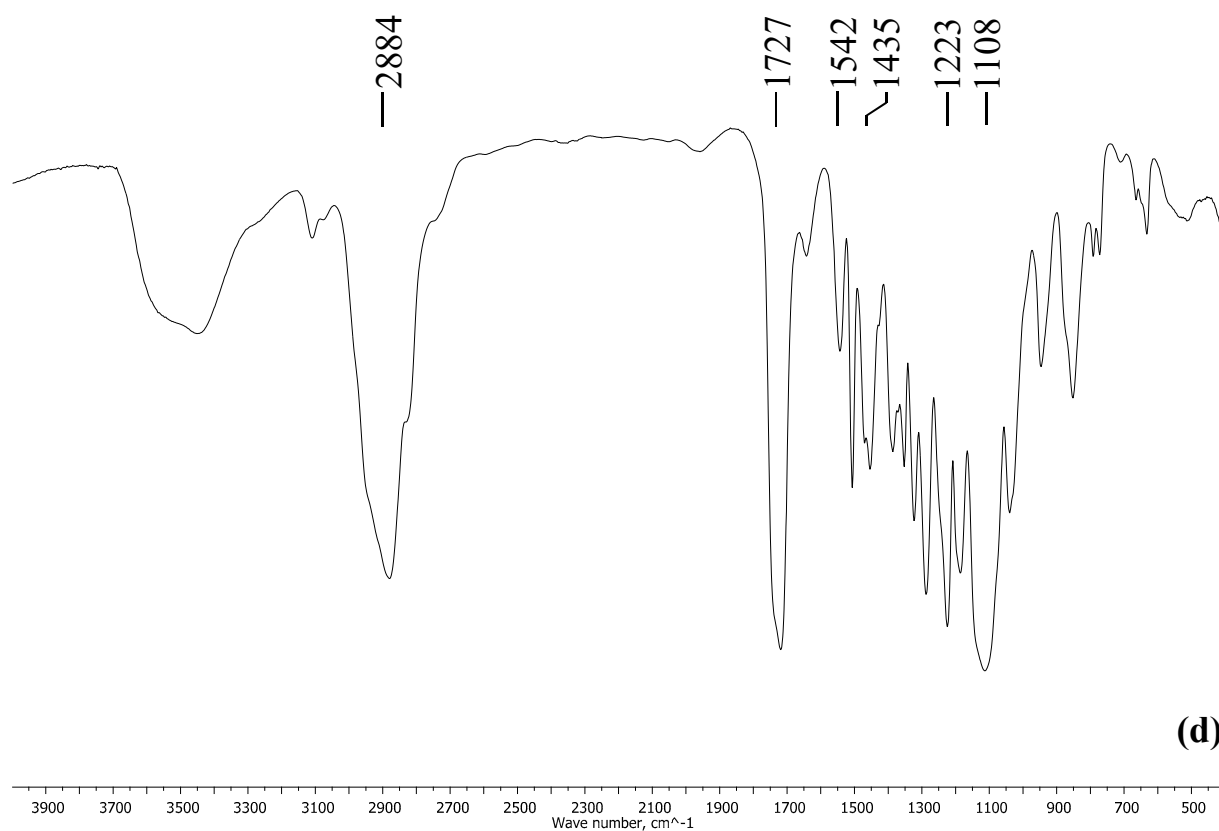


(b)

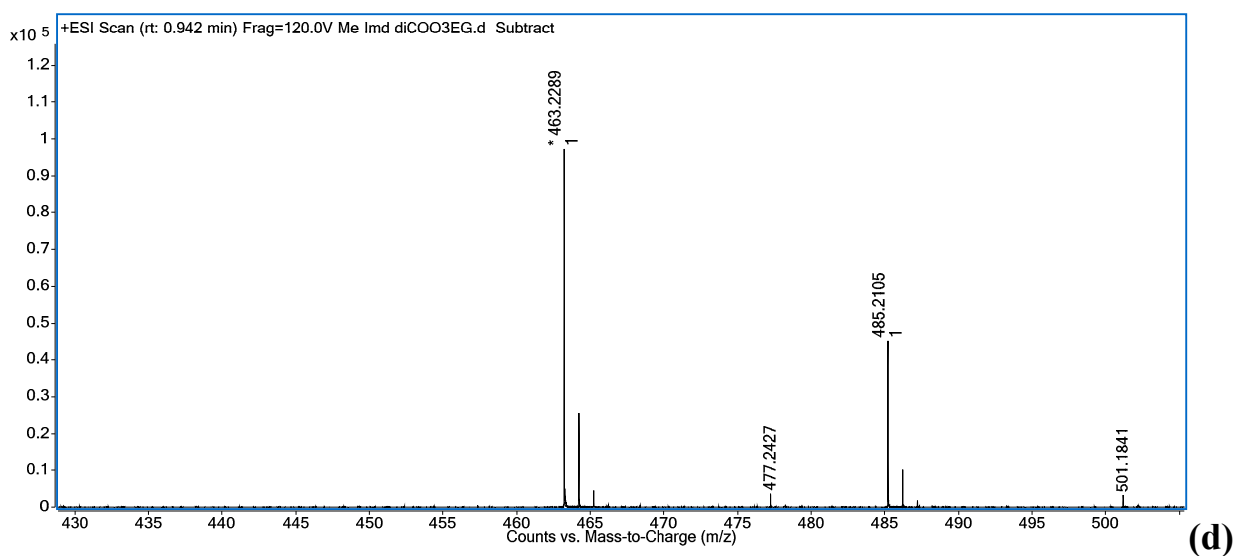
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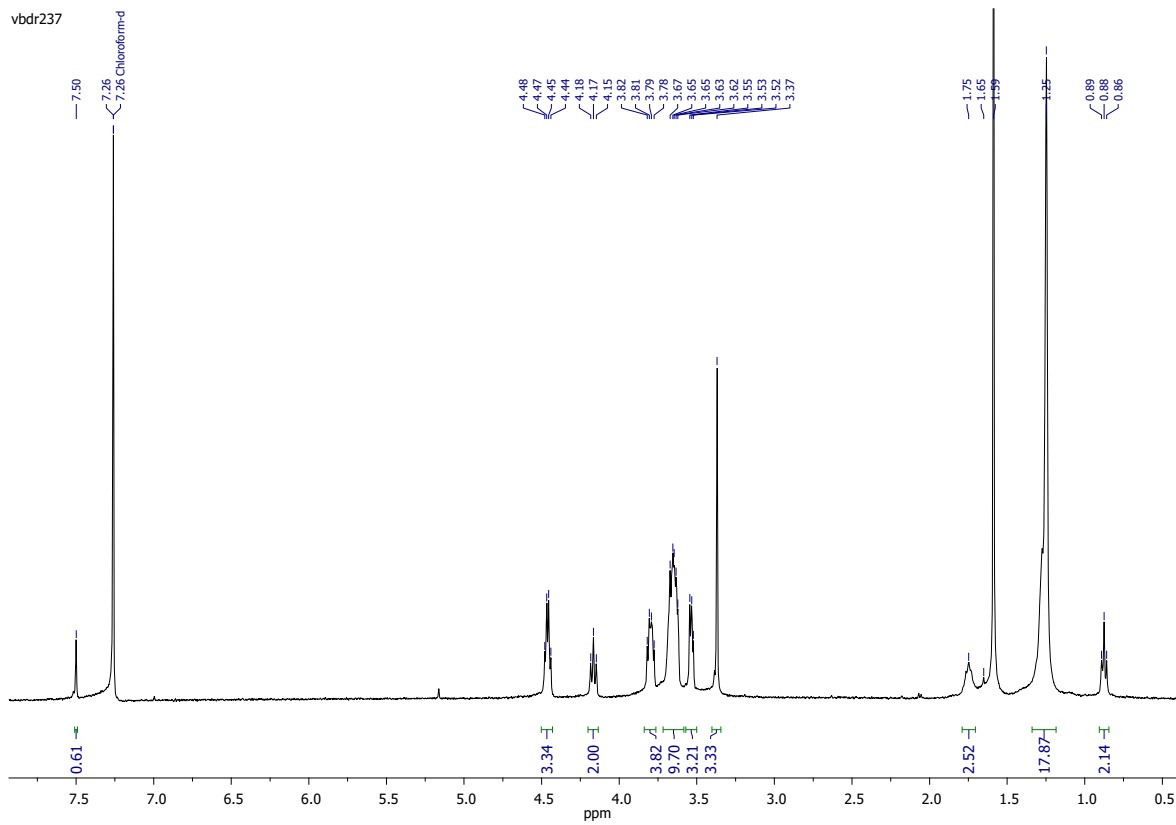
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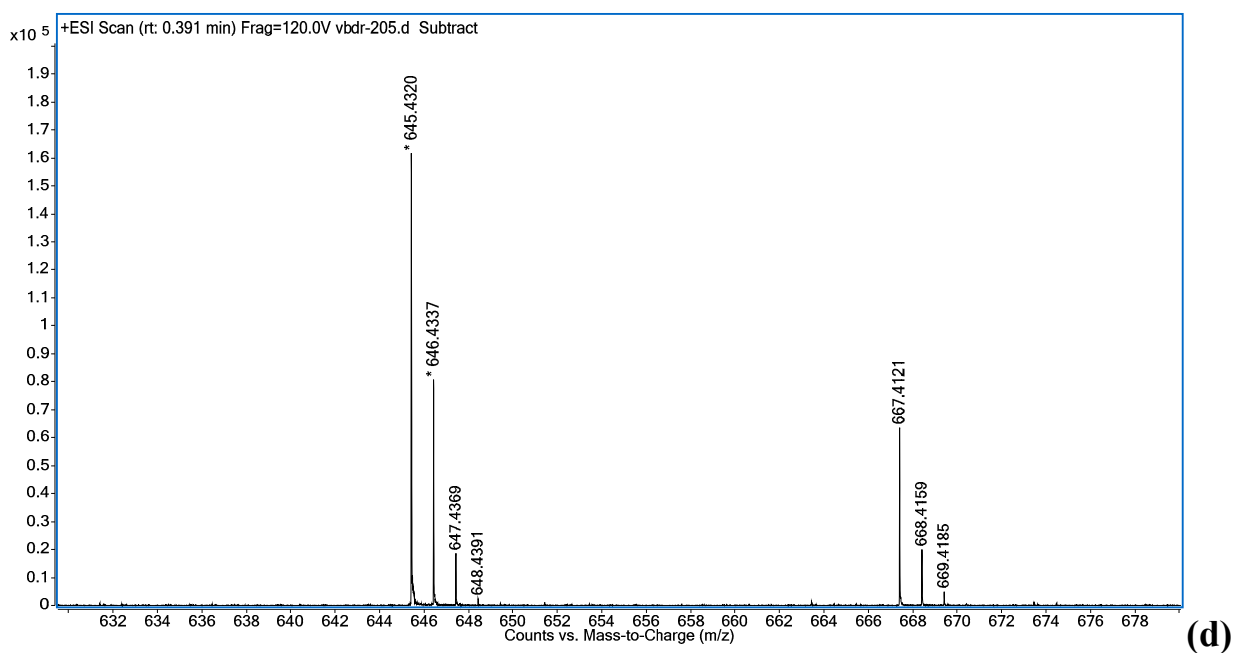
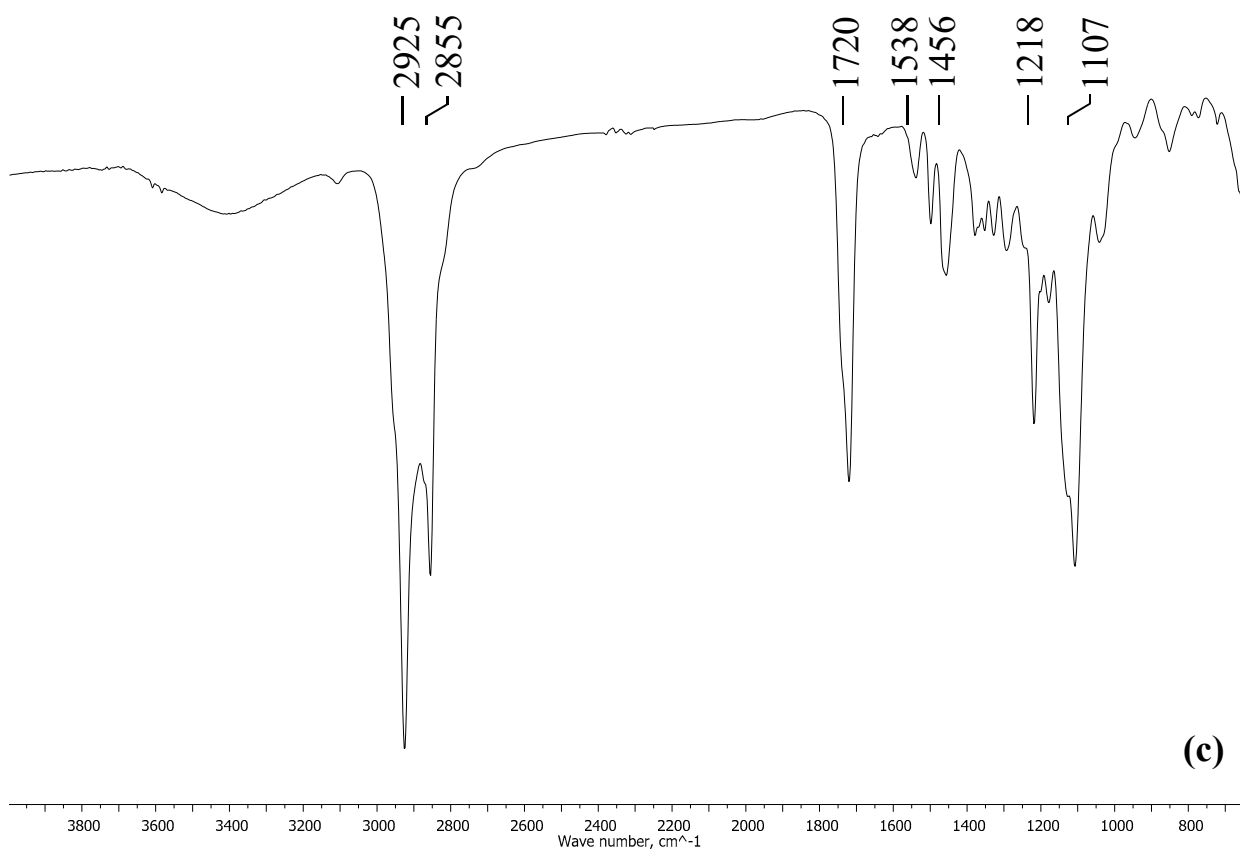


(d)



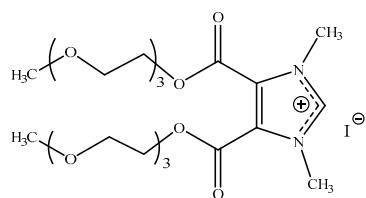
**Figure S2.** NMR  $^1\text{H}$  in  $\text{CDCl}_3$ (a), NMR  $^1\text{H}$  in  $\text{DMSO}-d_6$  (b),  $^{13}\text{C}$  (c), FT IR (d) and HRESI MS (e) spectra of 4,5-bis-[2-(2-(2-methoxyethoxy)ethoxy)ethoxycarbonyl]-1-methylimidazole (**2a**)



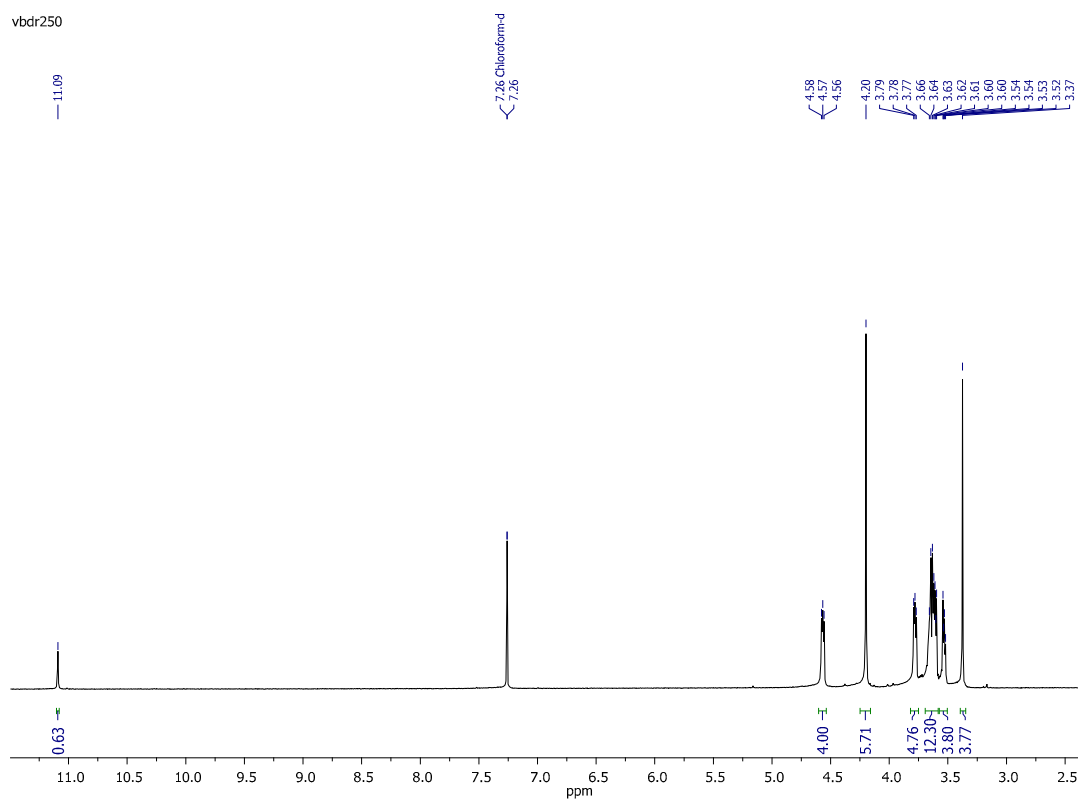


**Figure S3.** NMR  $^1\text{H}$  (a),  $^{13}\text{C}$  (b), FT IR (c) and HRESI MS (d) spectra of 4,5-bis-[2-(2-(2-methoxyethoxy)ethoxy)ethoxycarbonyl]-1-tetradecylimidazole (**2b**)

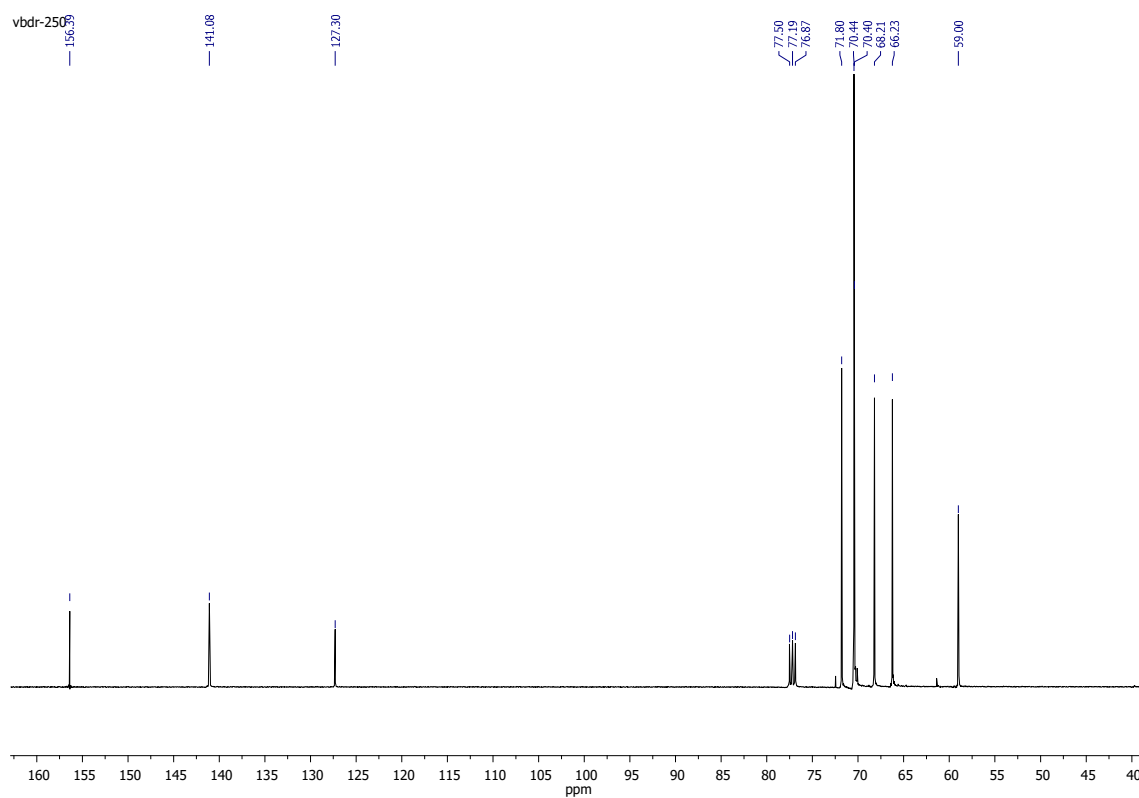




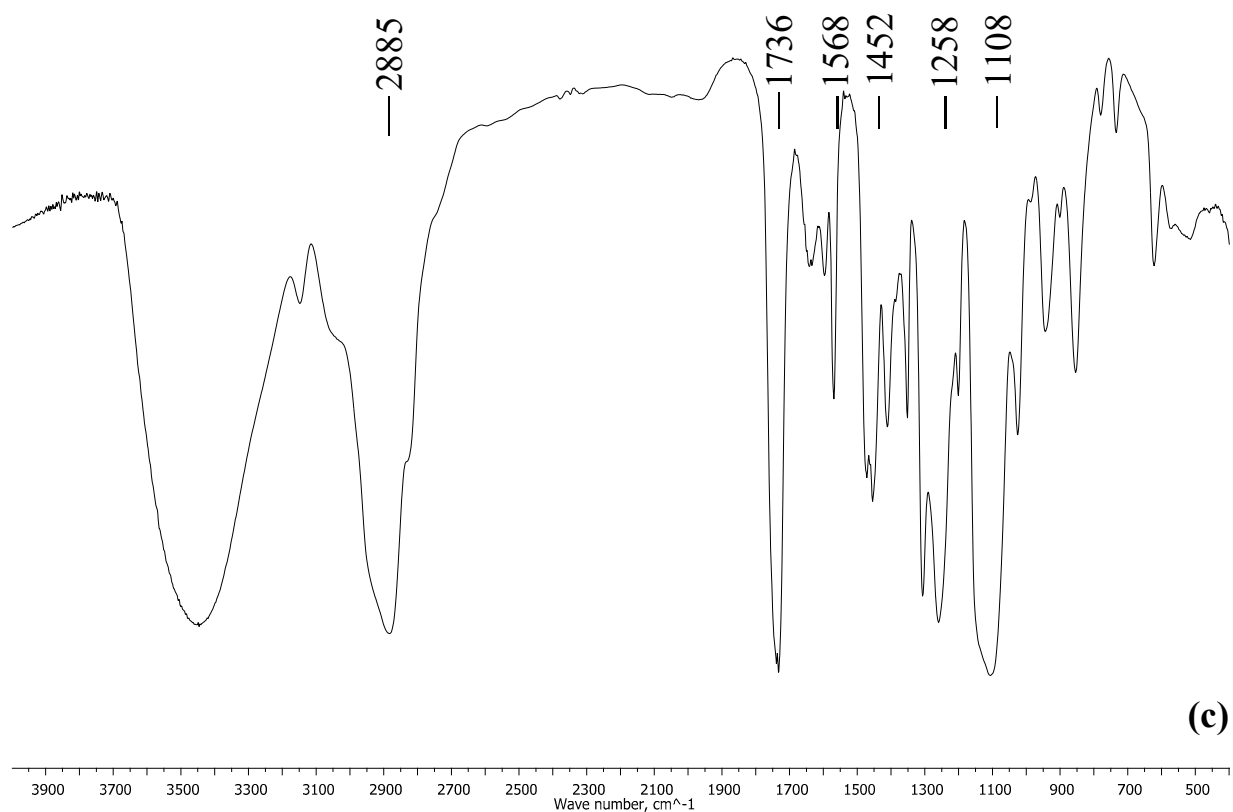
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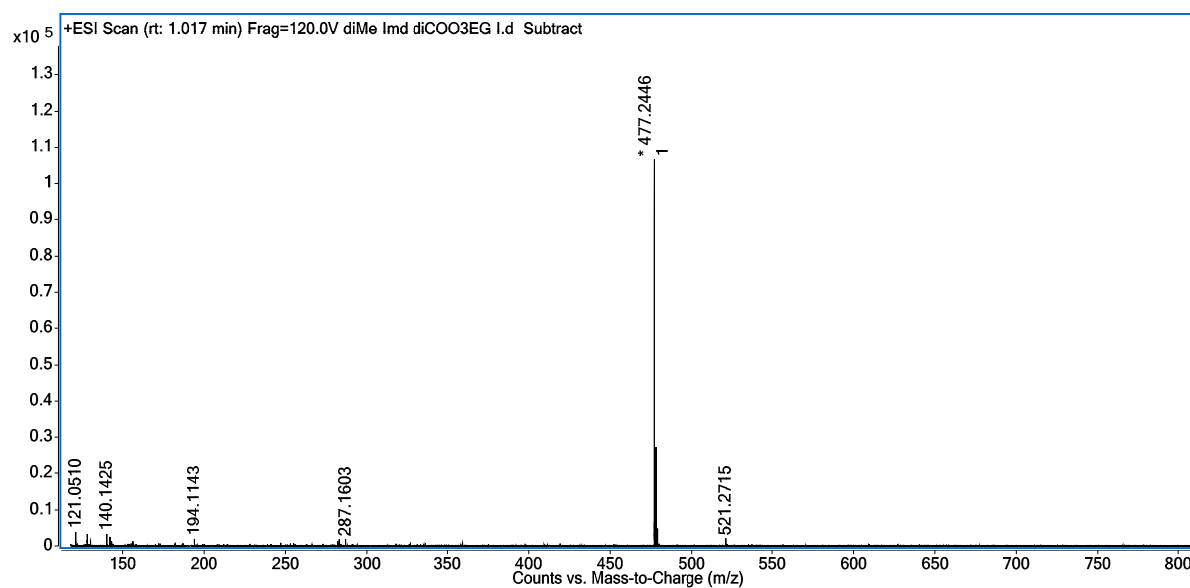
(a)



(b)

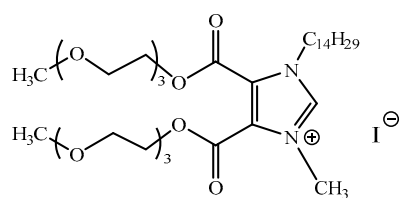


(c)

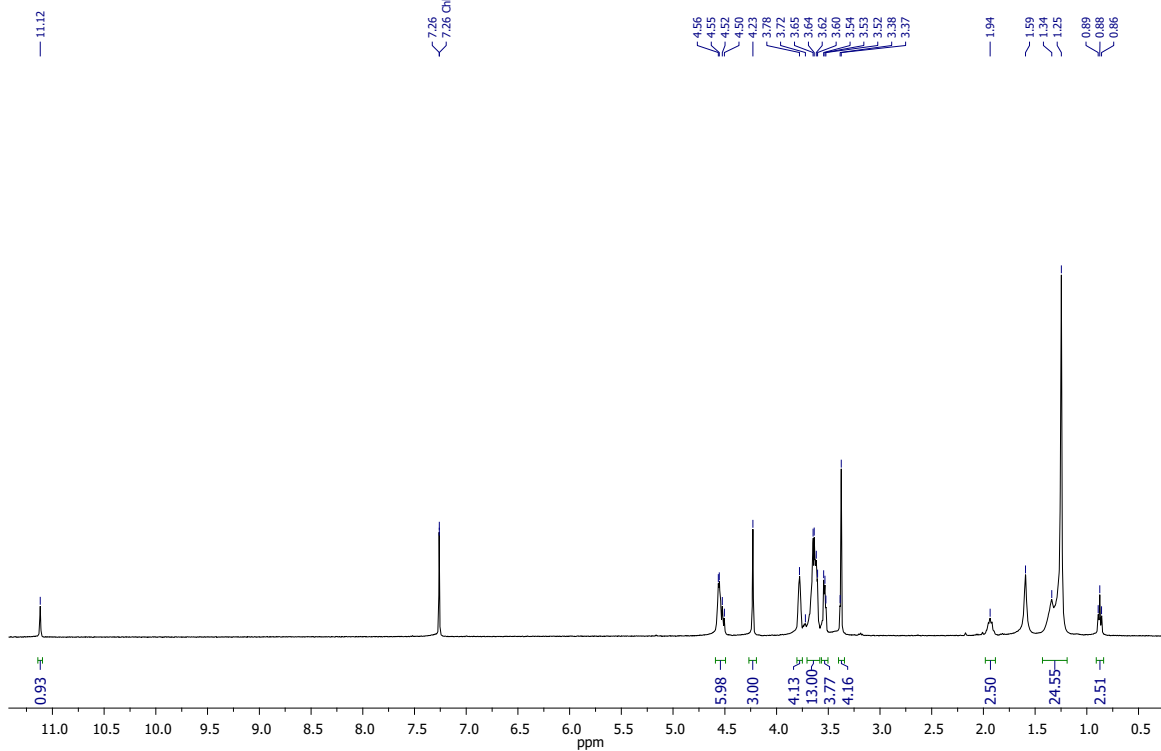


(d)

**Figure S4.** NMR <sup>1</sup>H (a), <sup>13</sup>C (b), FT IR (c) and HRESI MS (d) spectra of 4,5-bis[2-(2-methoxyethoxy)ethoxy)ethoxycarbonyl]-1,3-dimethyl-imidazolium iodide (**3a**)

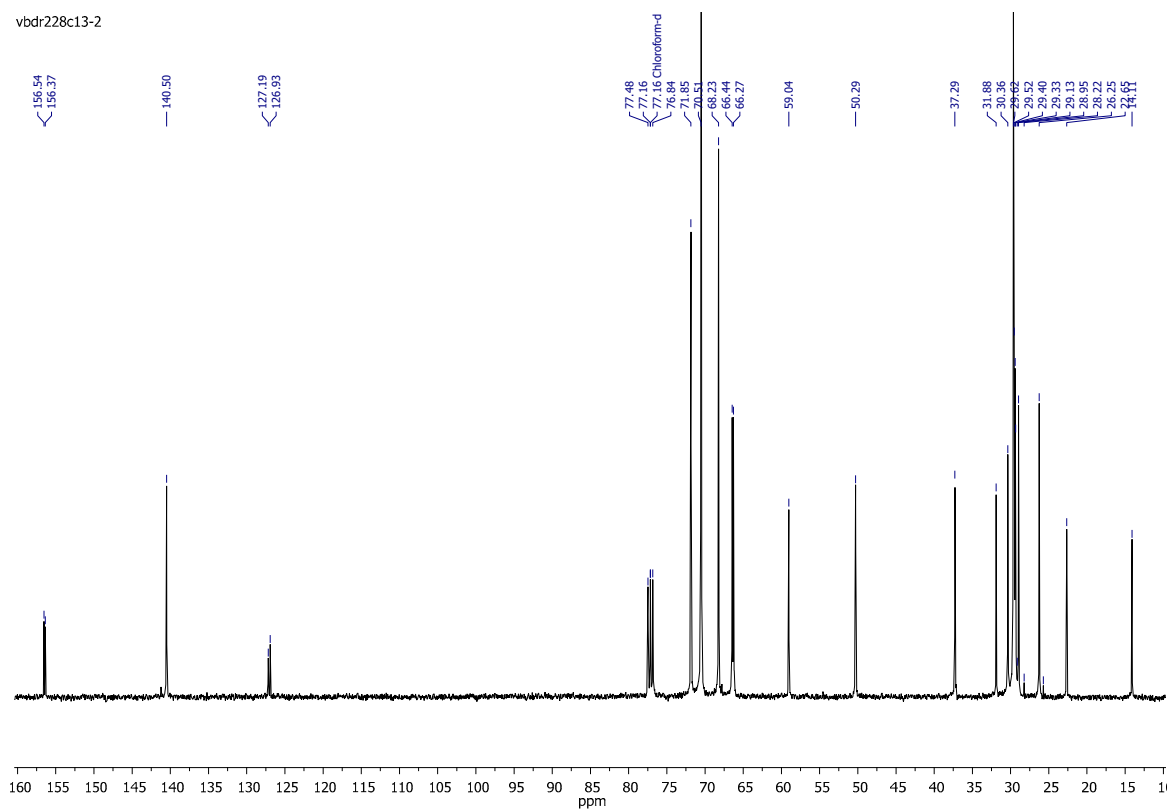


vbdp-11

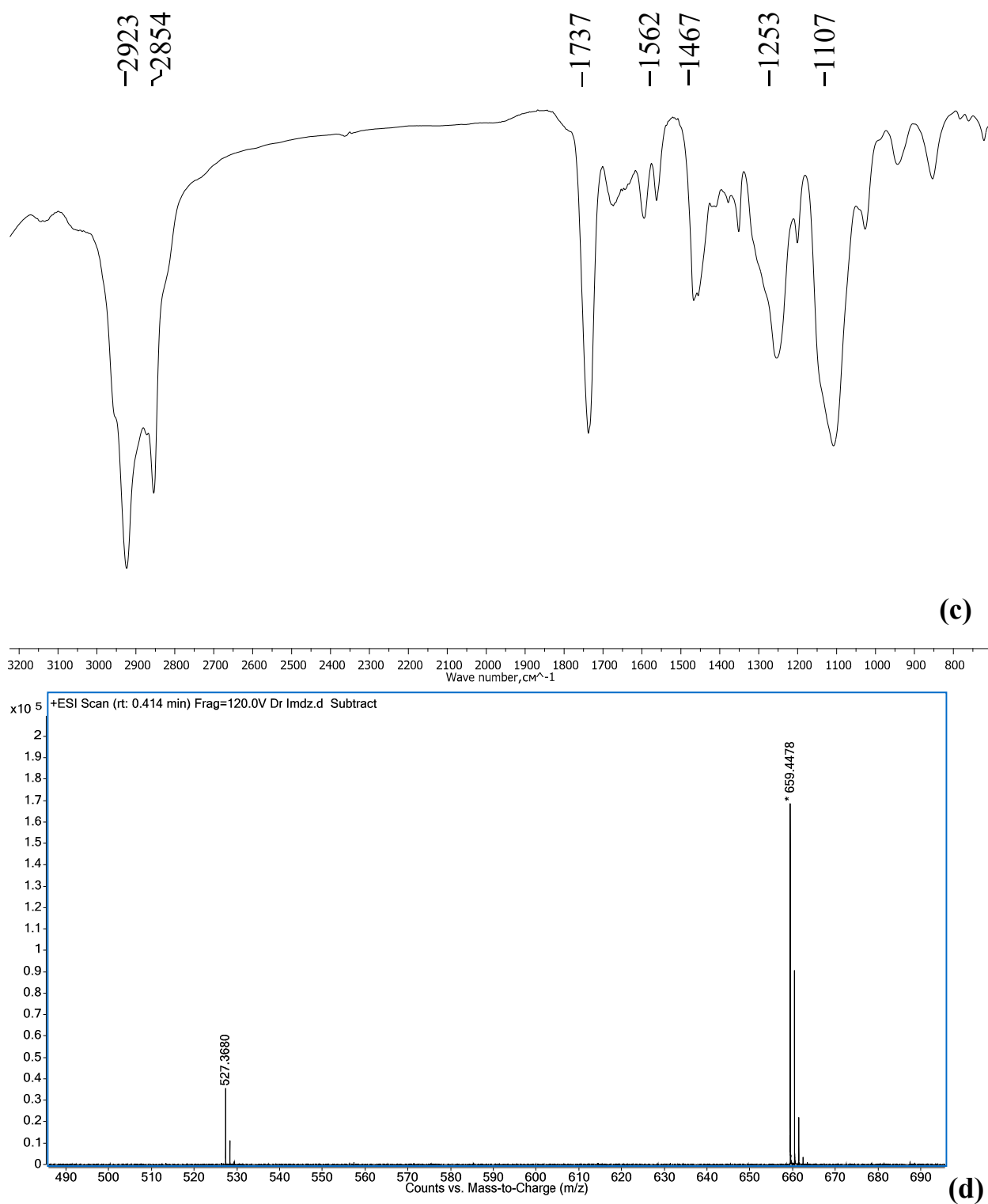


(a)

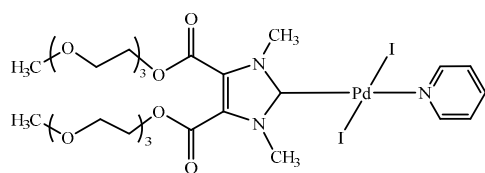
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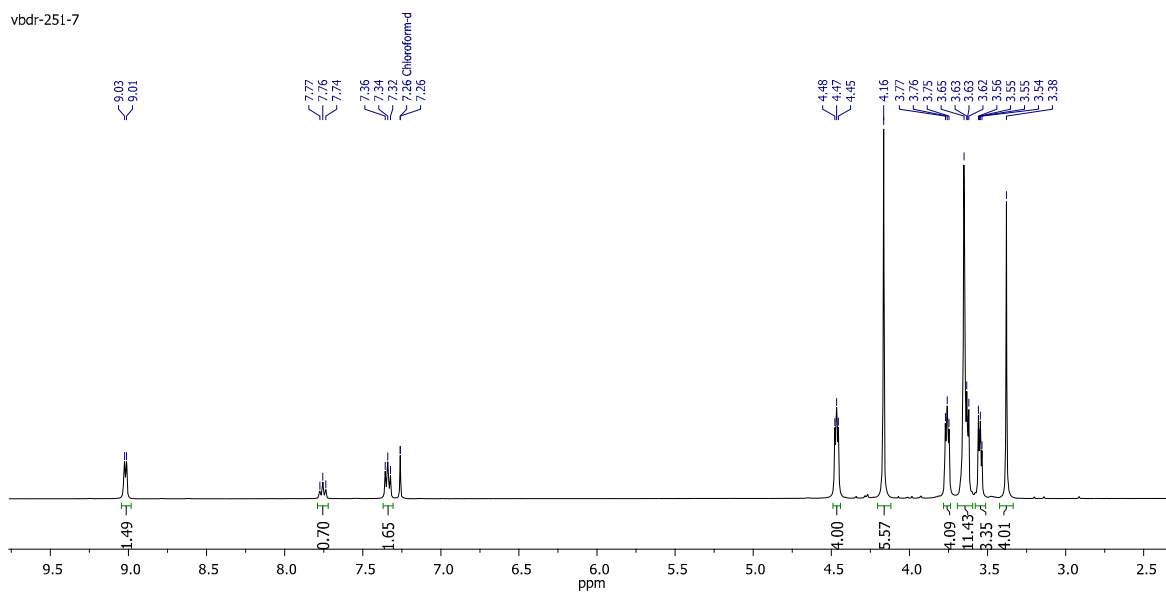
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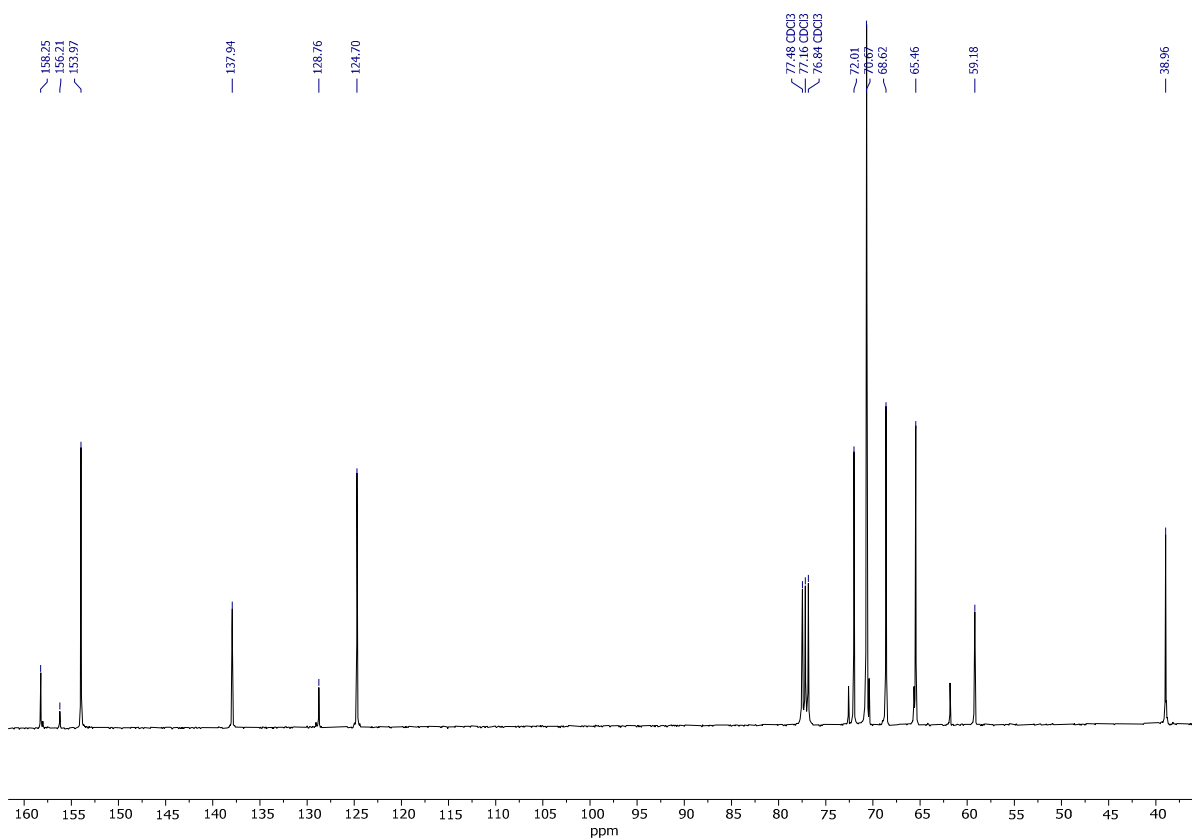
**Figure S5.** NMR <sup>1</sup>H (a), <sup>13</sup>C (b), FT IR (c) and HRESI MS (d) spectra of 4,5-bis[2-(2-methoxyethoxy)ethoxycarbonyl]-1-methyl-3-tetradecylimidazolium iodide (**3b**)



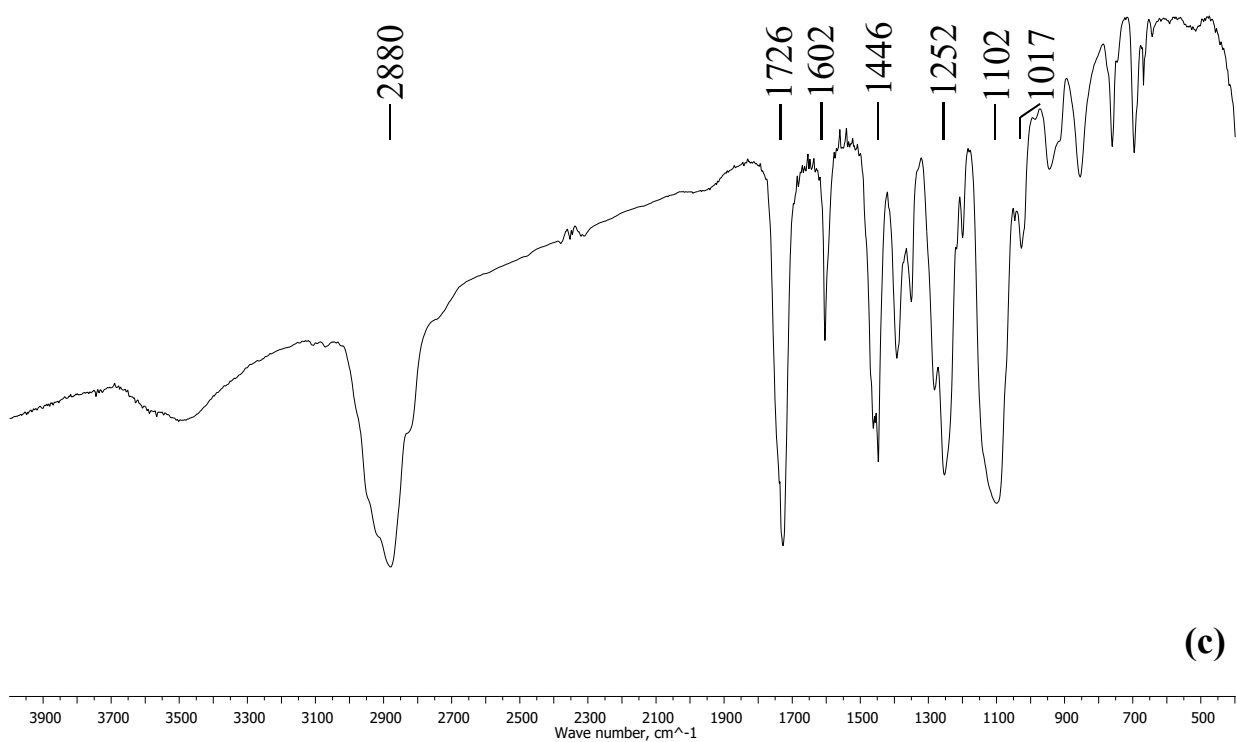
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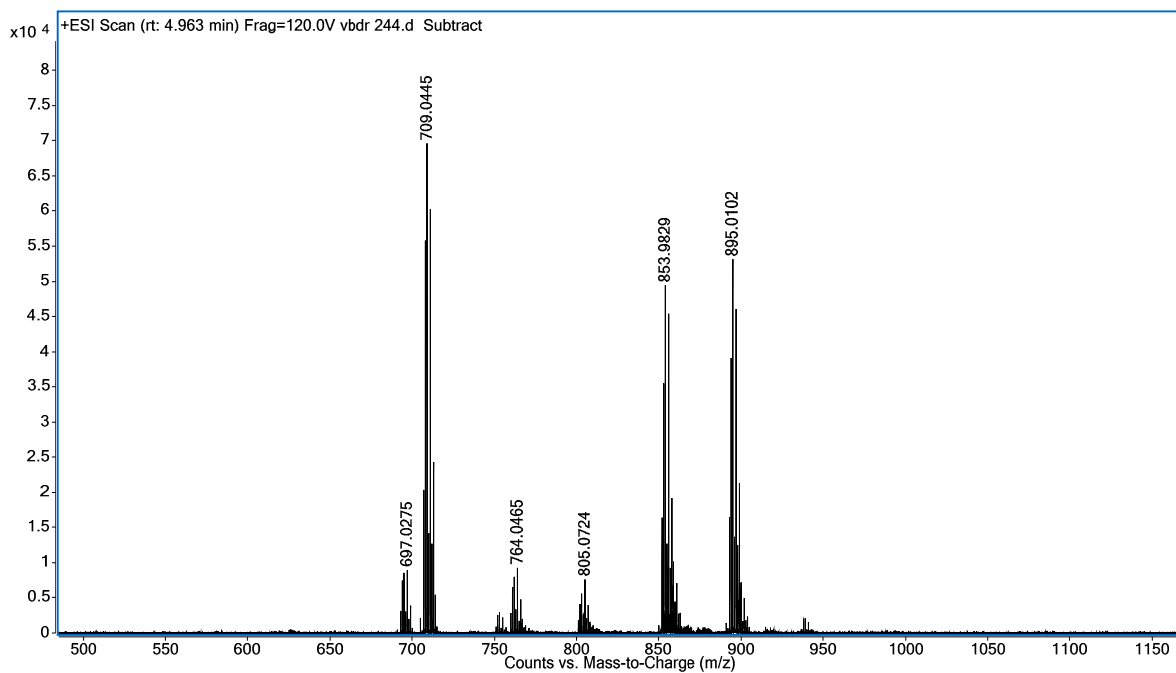
(a)



(b)

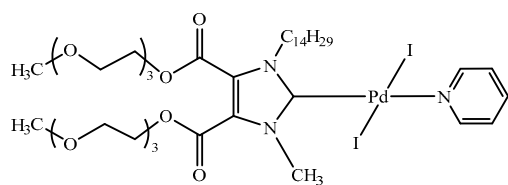


(c)

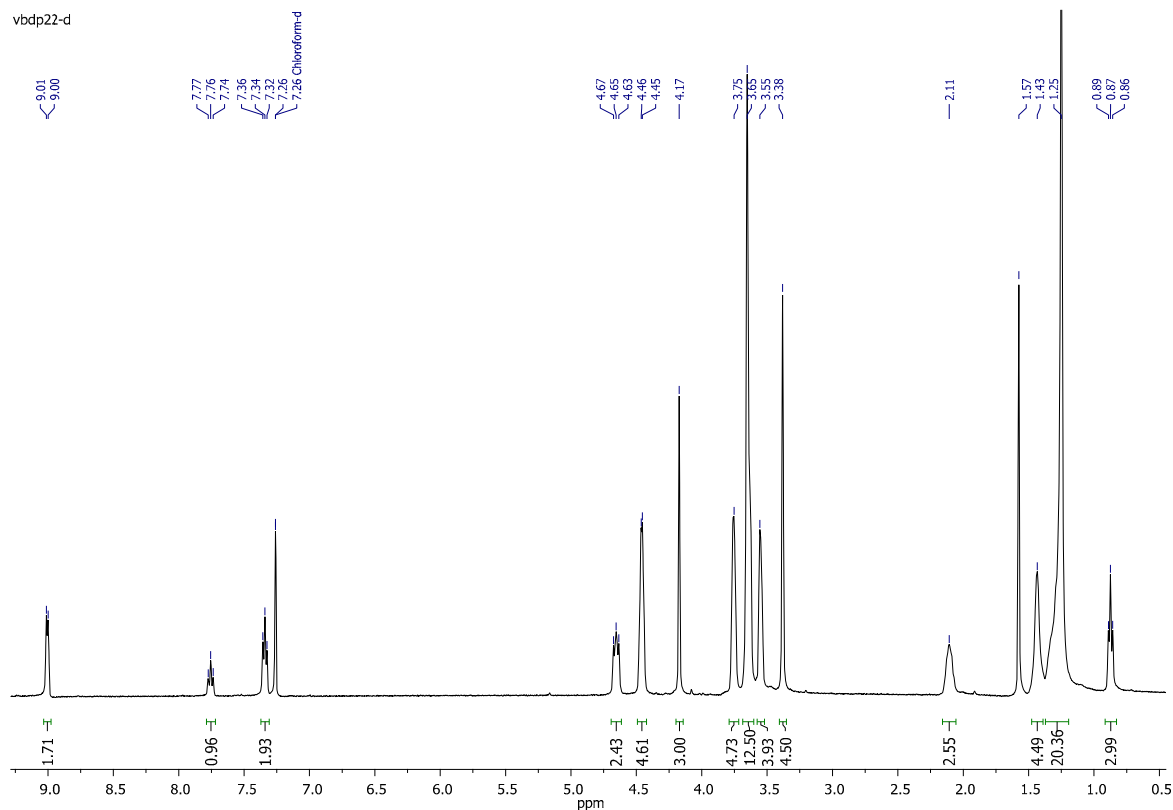


(d)

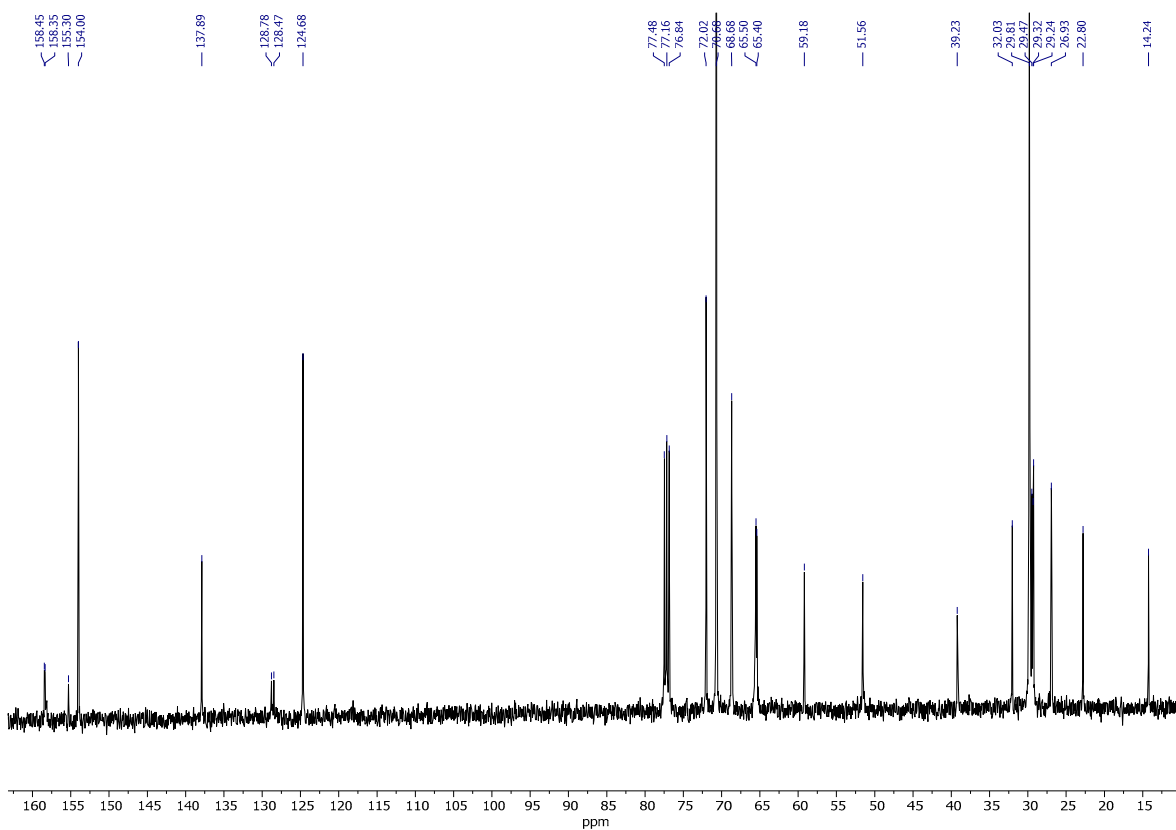
**Figure S6.** NMR <sup>1</sup>H (a), <sup>13</sup>C (b), FT IR (c) and HRESI MS (d) spectra of *trans*-{4,5-bis[2-(2-(2-methoxyethoxy)ethoxy)ethoxycarbonyl]-1,3-dimethylimidazolin-2-ylidene} {pyridine} palladium(II) diiodide (**4a**).



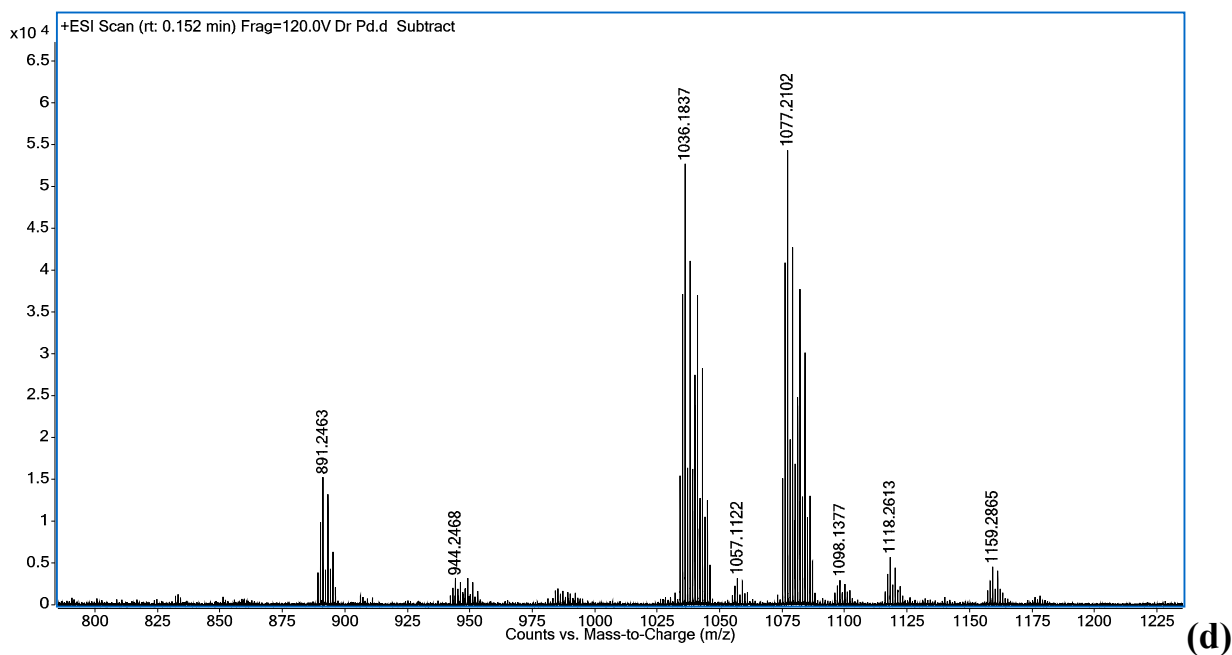
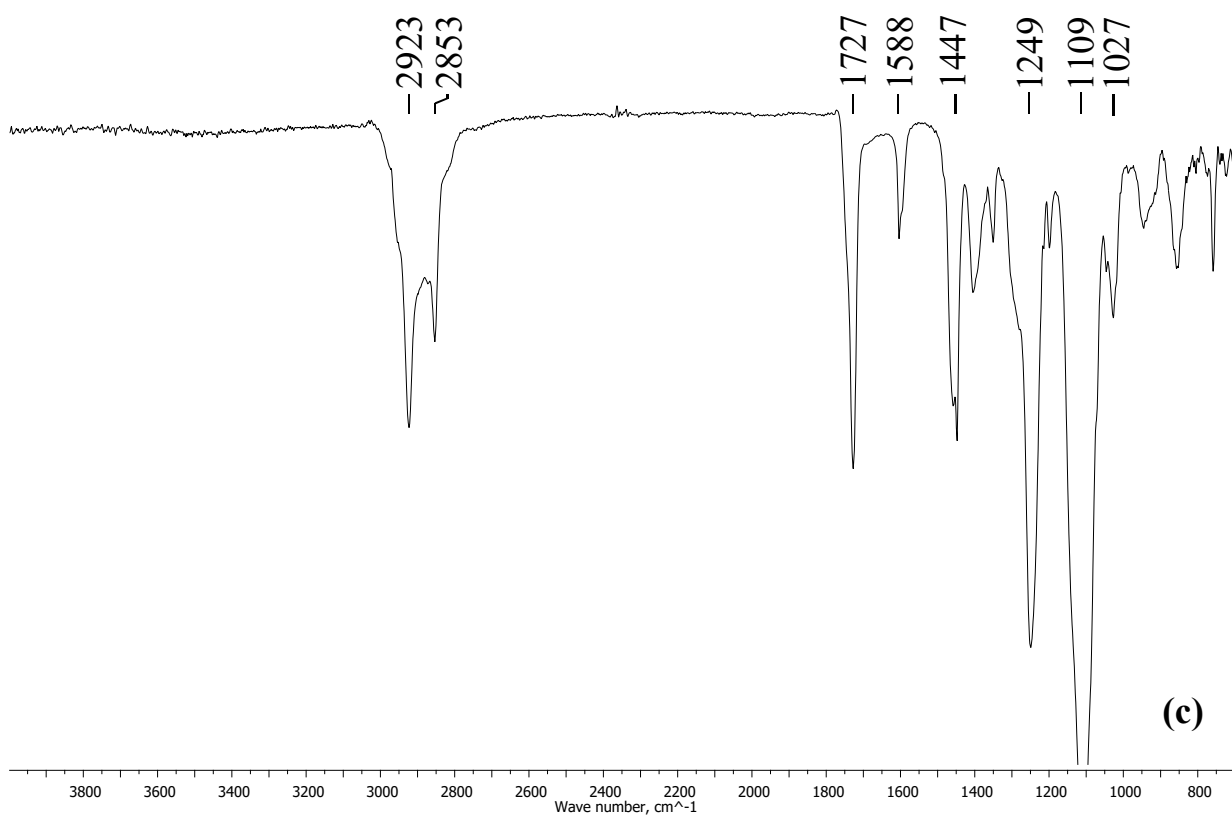
vbdp22-d



(a)

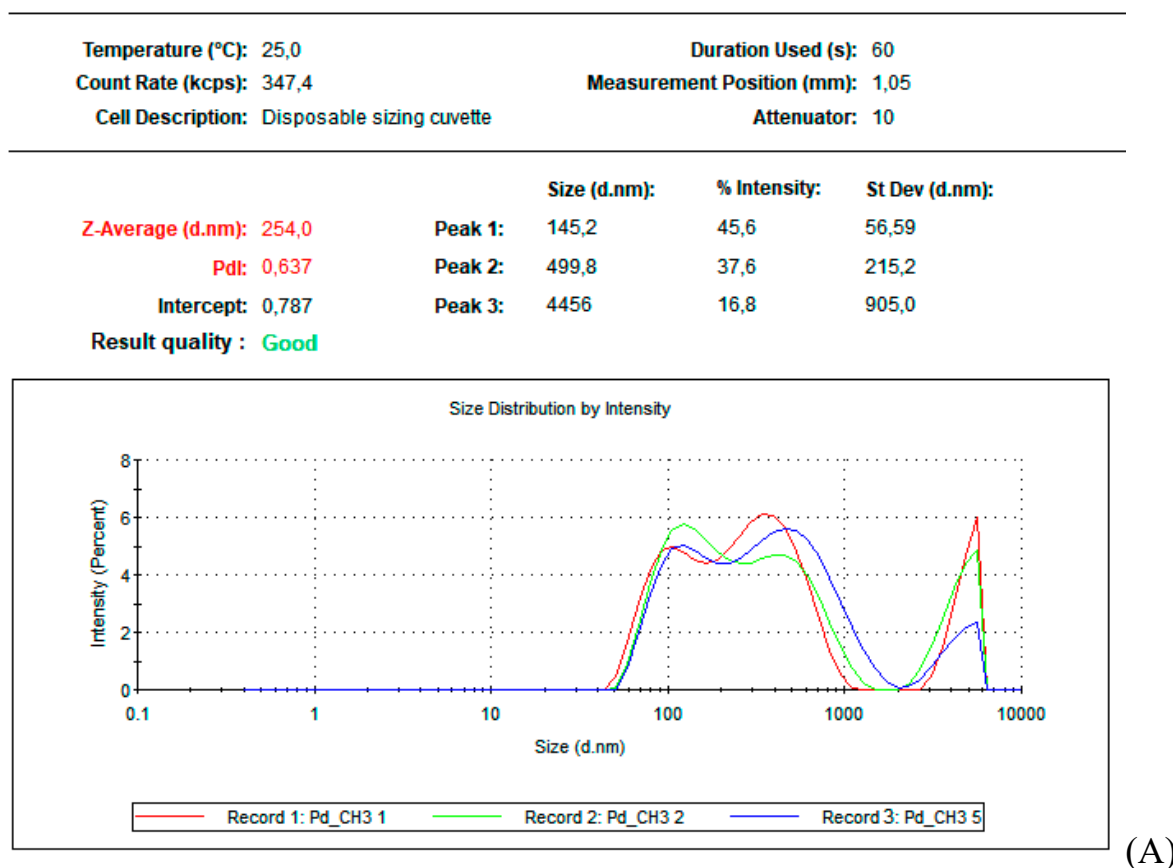


(b)

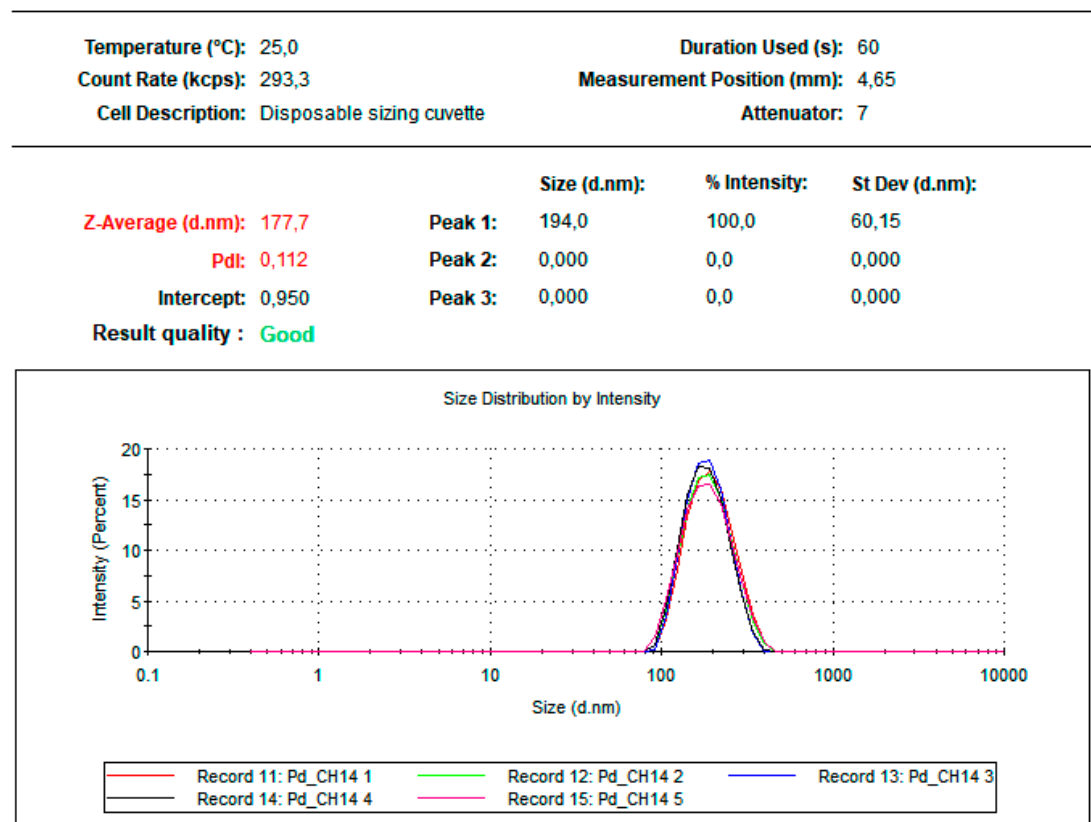


**Figure S7.** NMR <sup>1</sup>H (a), <sup>13</sup>C (b), FT IR (c), HRESI MS (d) spectra of *trans*-{4,5-bis[2-(2-(2-methoxyethoxy)ethoxy)ethoxycarbonyl]-1-methyl-3-tetradecylimidazolin-2-ylidene} {pyridine} palladium(II) diiodide (**4b**).





(A)



(B)

**Figure S8.** DLS intensity vs size graphs for solutions of **4a** (A) and **4b** (B) in water, C [4a,b]= 0.02 mM.