

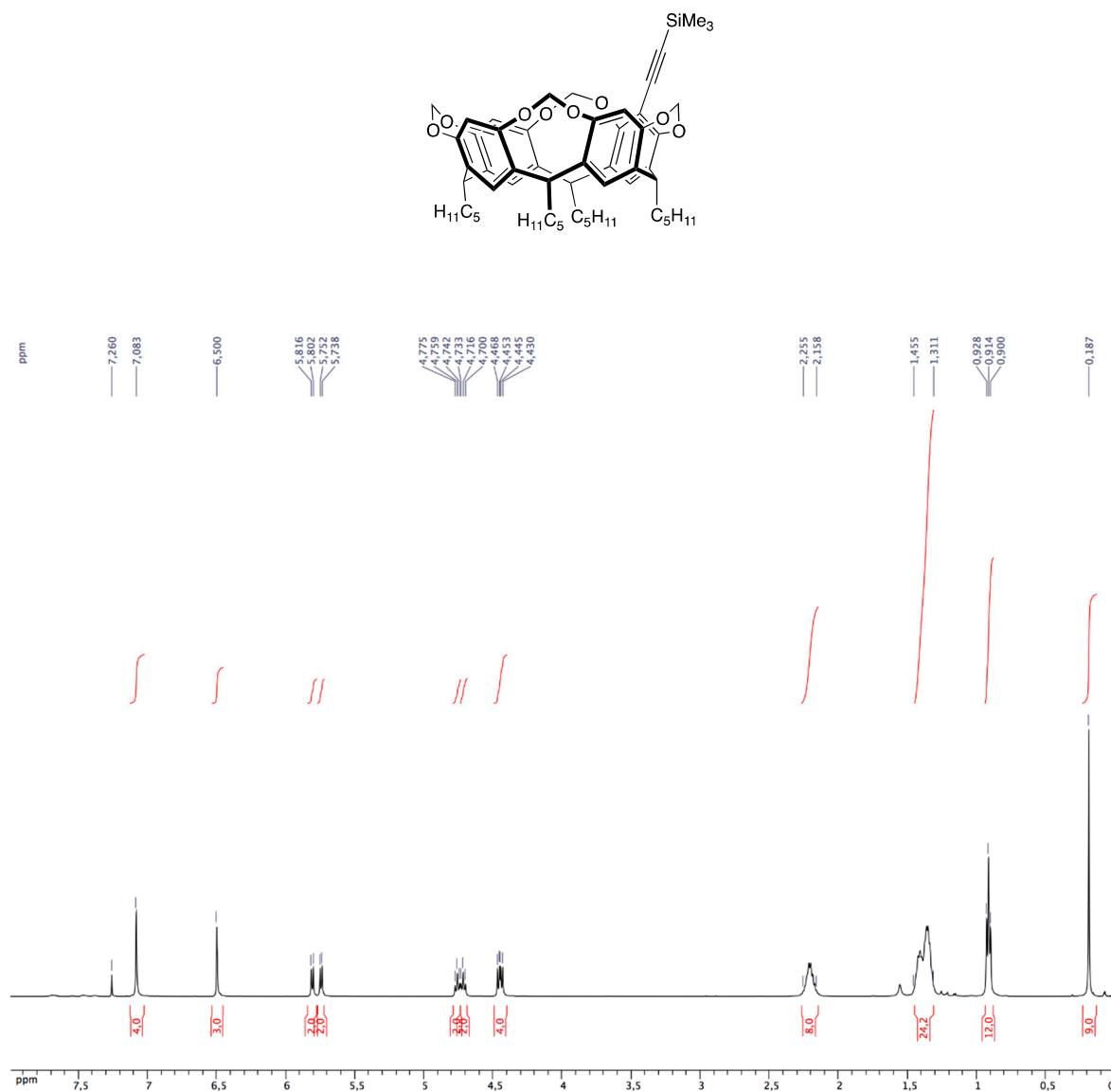
Synthesis of the first resorcin[4]arene-functionalised triazolium salts and their use in Suzuki-Miyaura cross-coupling reactions

David Sémeril, Dominique Matt, and Rengan Ramesh

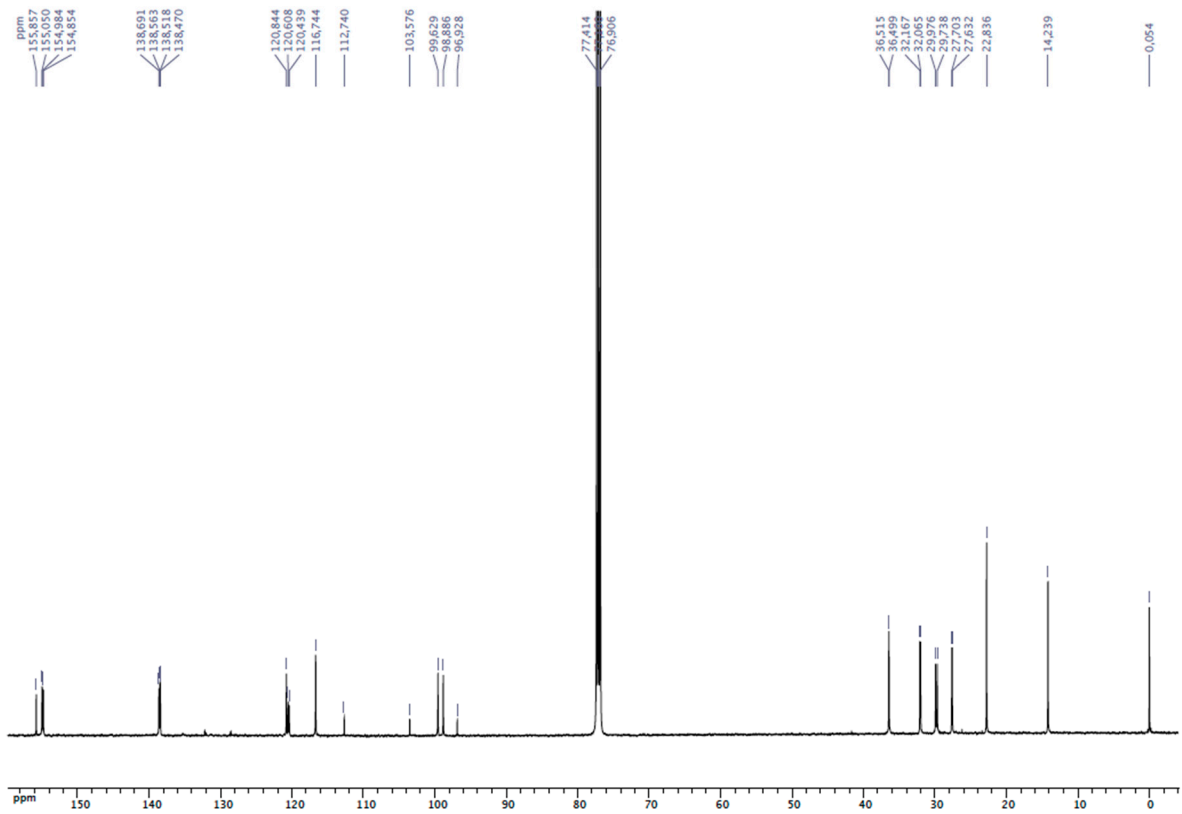
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Characterising data of 5-(trimethylsilyl)ethynyl-4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentylresorcin[4]arene (4)

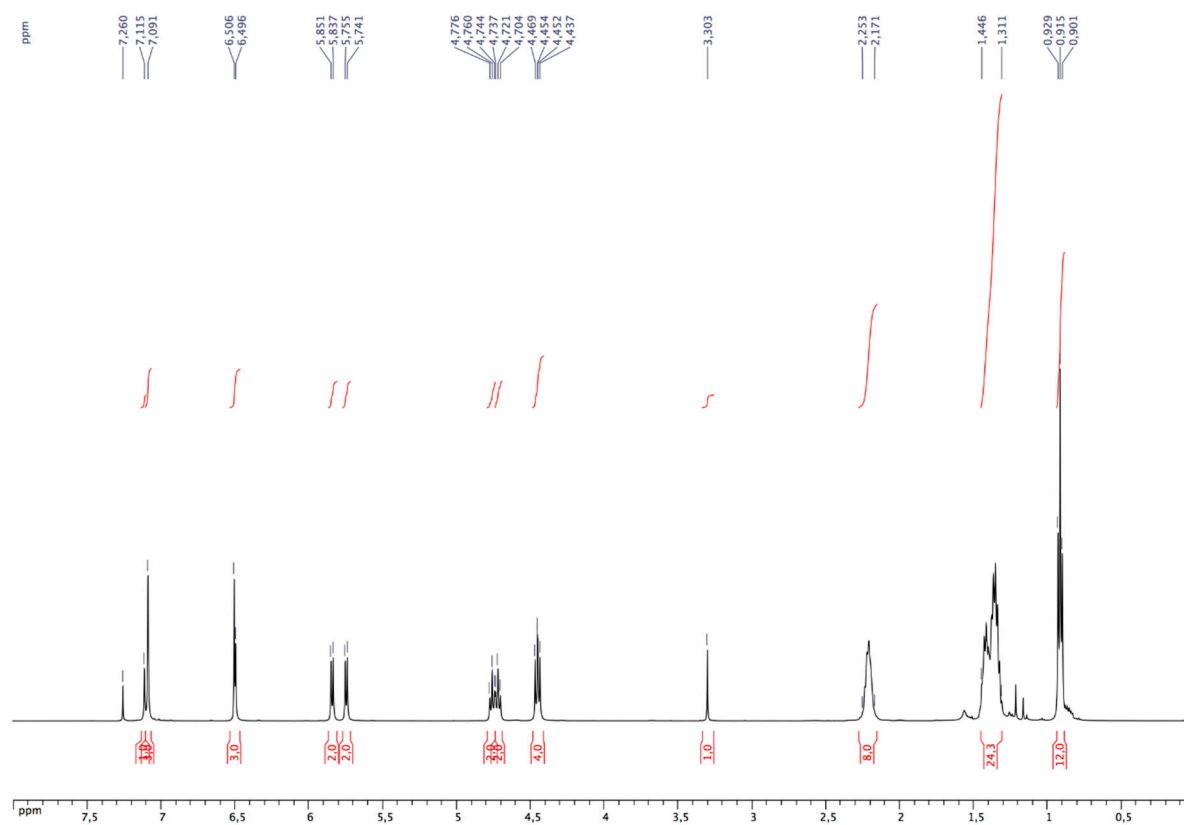
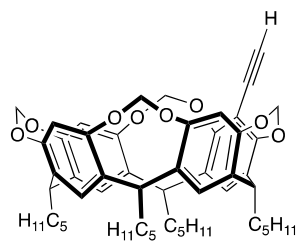


^1H NMR spectrum of 4 (CDCl_3)

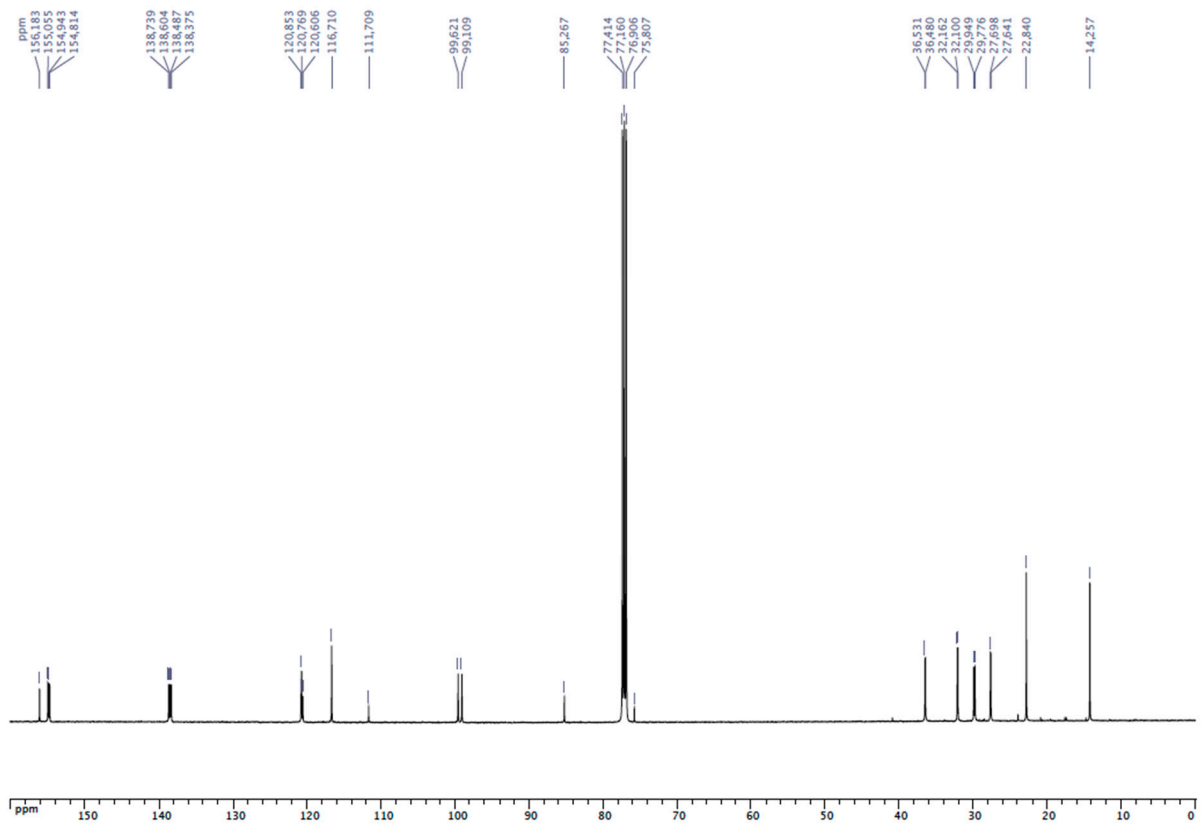


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** (CDCl_3)

Characterising data of 5-ethynyl-4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentylresorcin [4]arene (5)

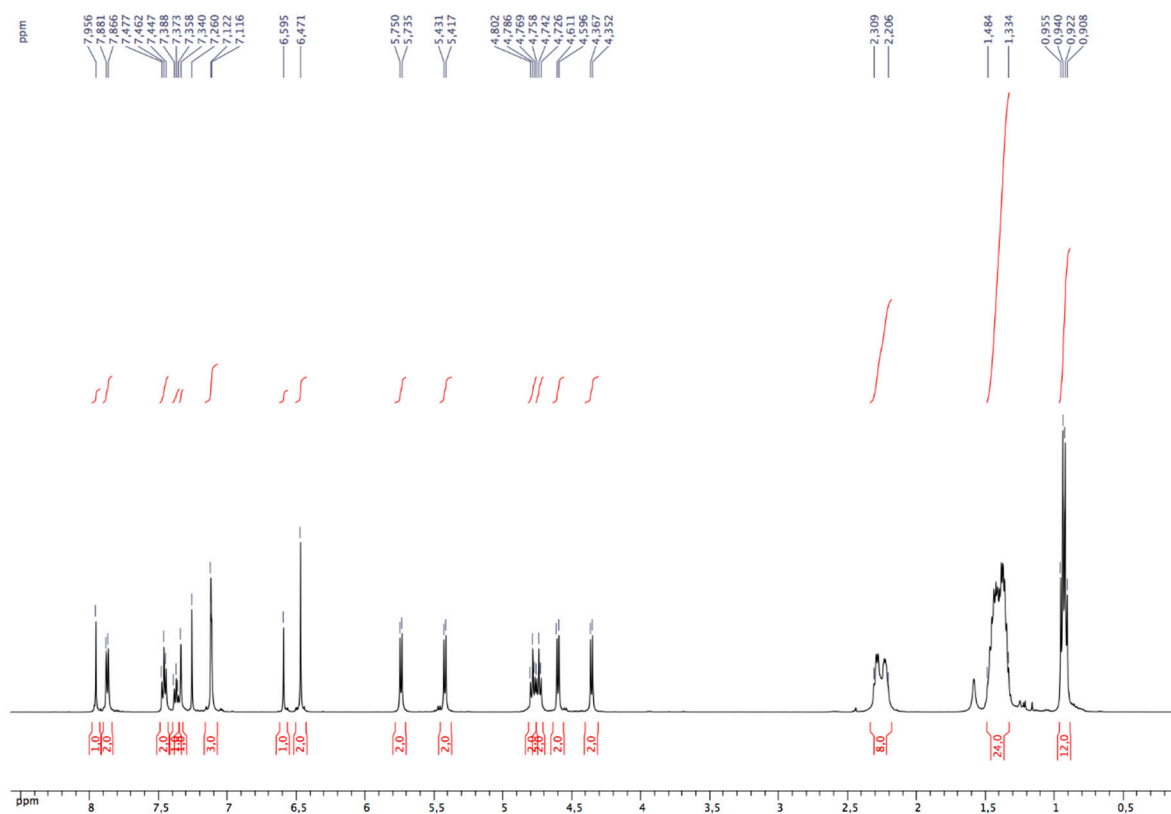
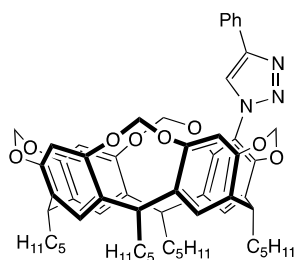


¹H NMR spectrum of 5 (CDCl₃)

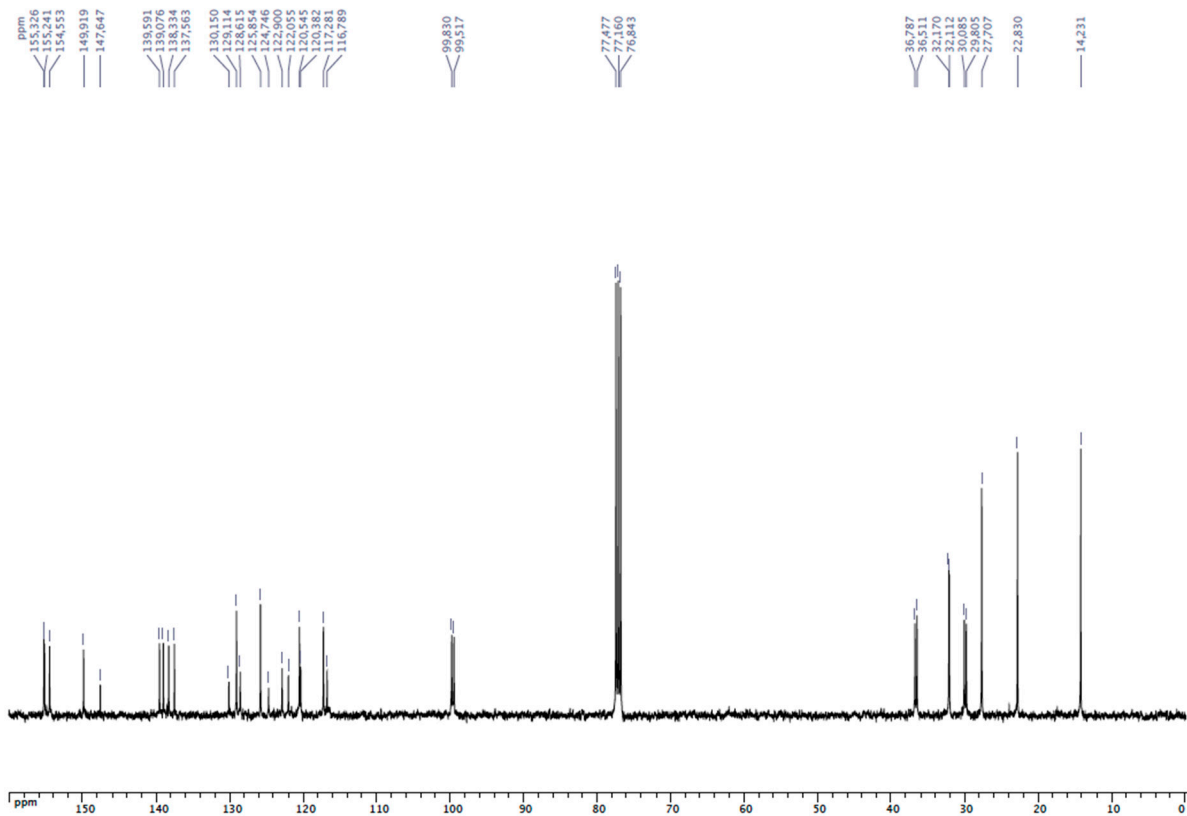


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5** (CDCl_3)

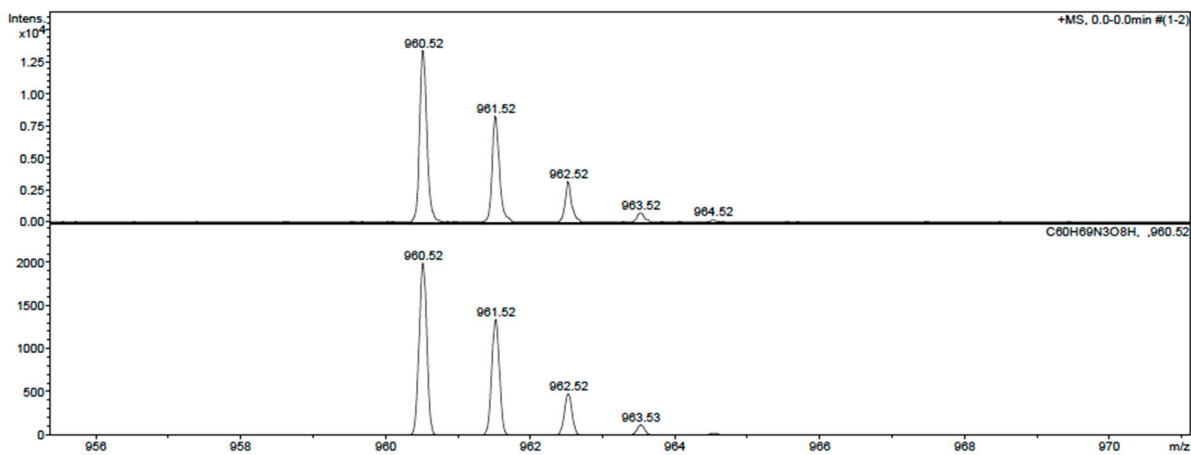
Characterising data of 1*H*-1,2,3-triazole,1-{4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentyl resorcin[4]arene-5-yl}-4-phenyl (7)



¹H NMR spectrum of 7 (CDCl₃)

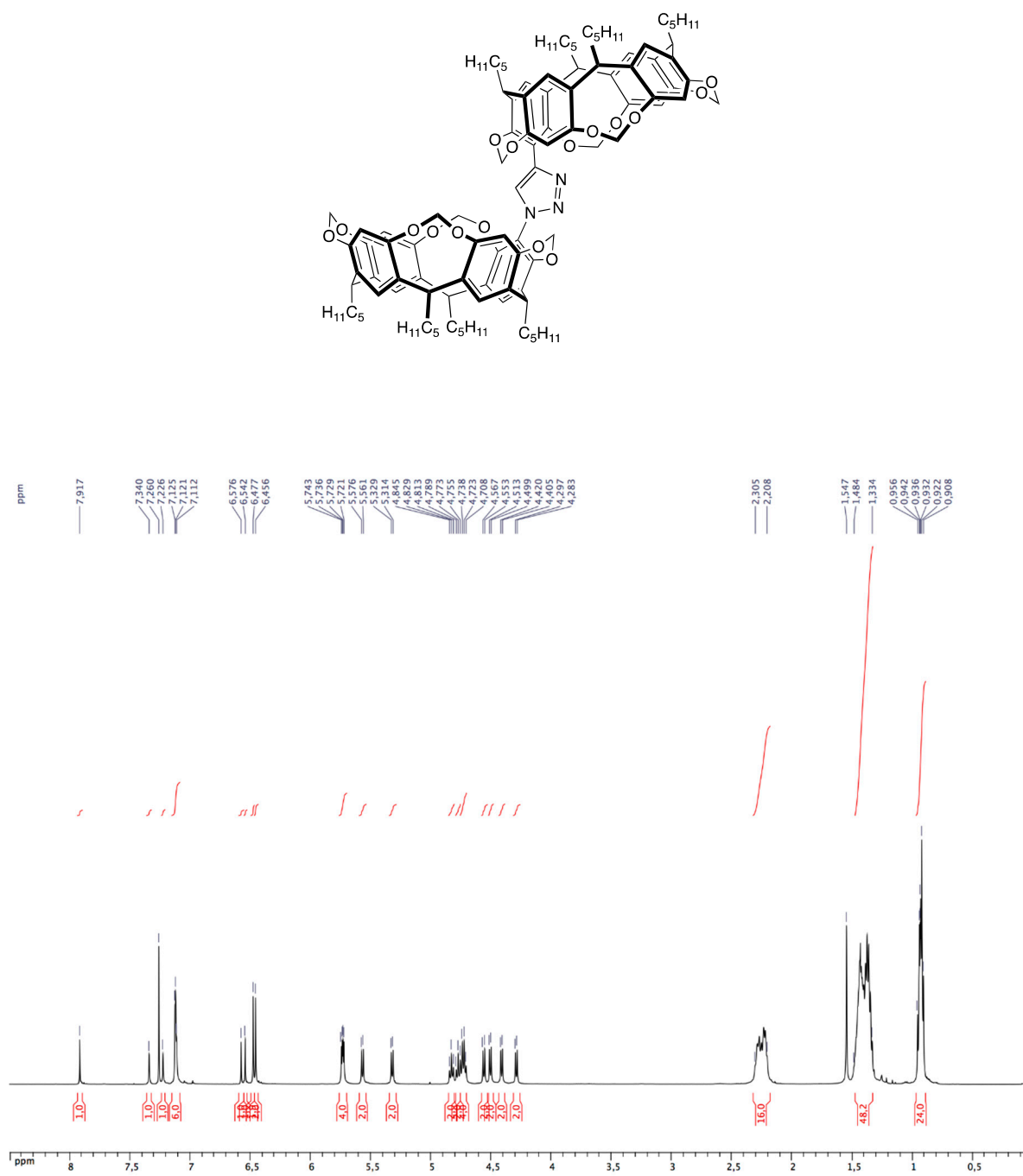


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7** (CDCl_3)

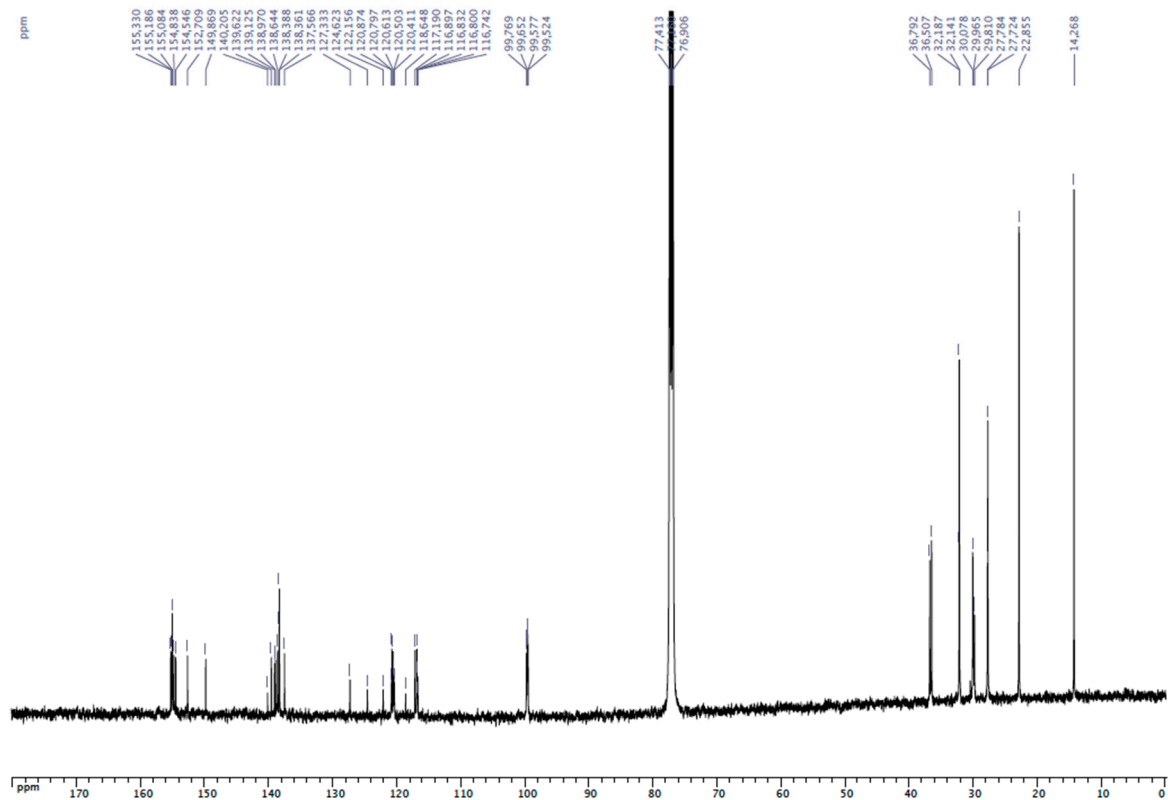


ESI-TOF spectrum of **7** (measured top and calculated for $\text{C}_{60}\text{H}_{70}\text{N}_3\text{O}_8$ bottom)

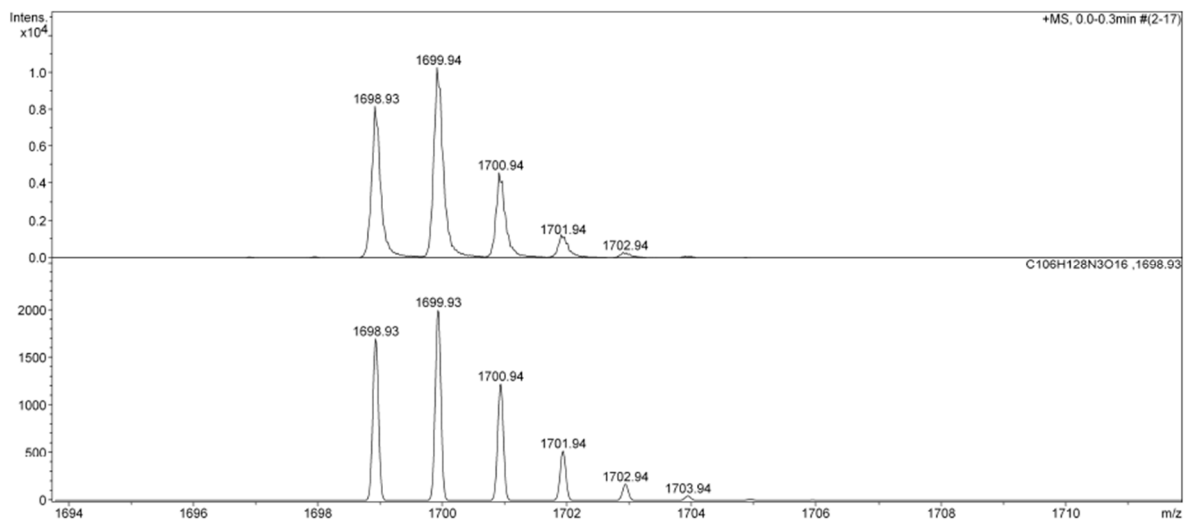
Characterising data of 1*H*-1,2,3-triazole,1,4-bis{4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentylresorcin[4]arene-5-yl} (8)



¹H NMR spectrum of **8** (CDCl₃)

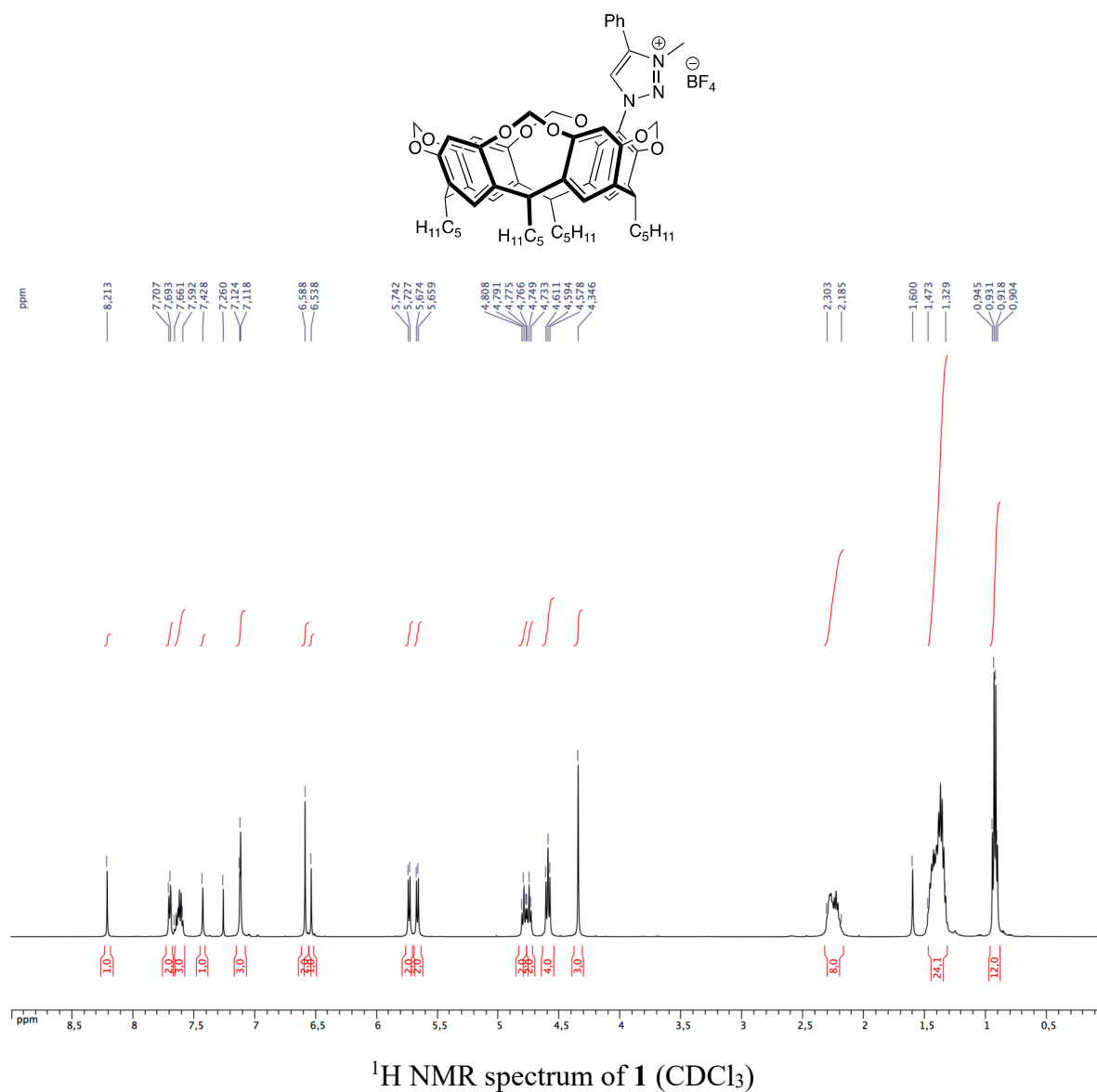


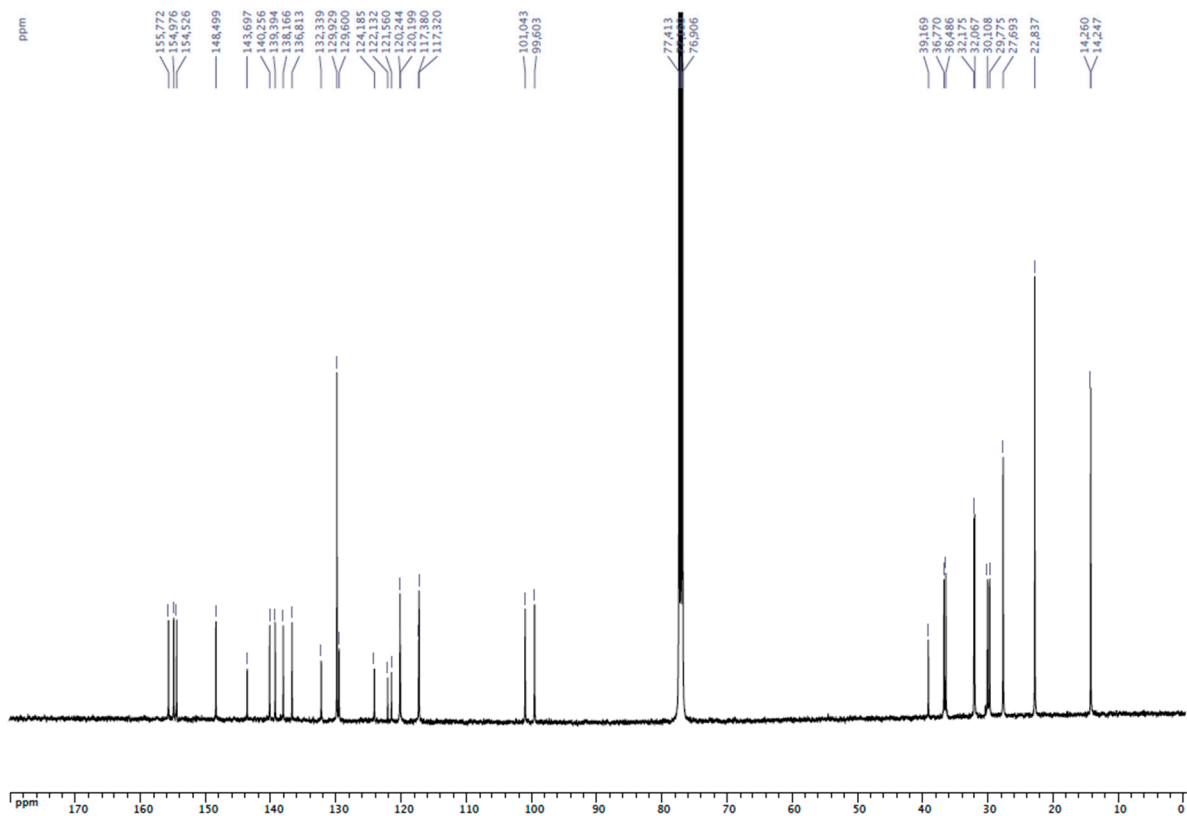
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8** (CDCl_3)



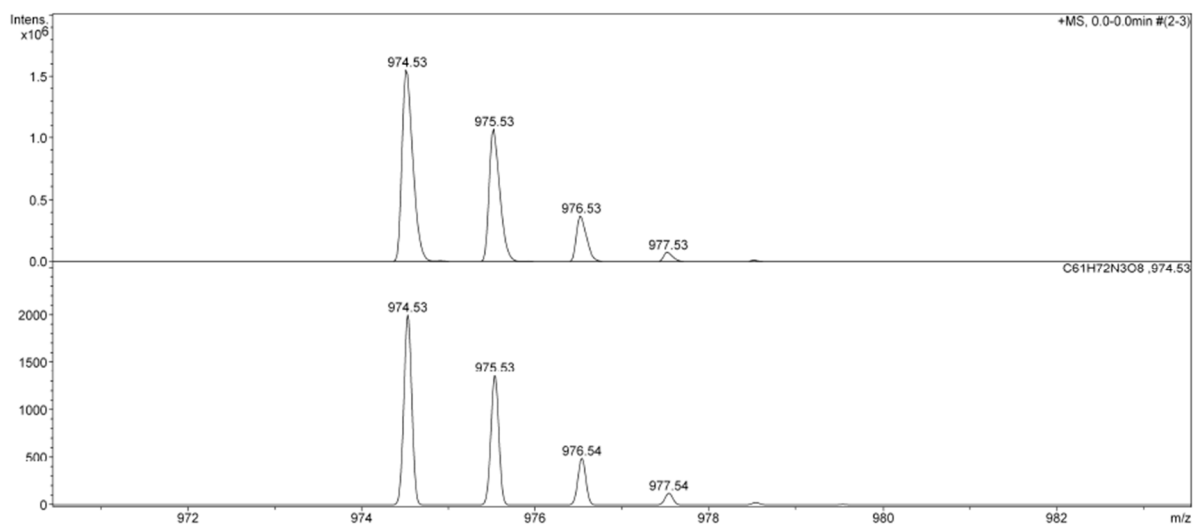
ESI-TOF spectrum of **8** (measured top and calculated for $\text{C}_{106}\text{H}_{128}\text{N}_3\text{O}_{16}$ bottom)

Characterising data of 1-{4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentylresorcin[4]arene-5-yl}-4-phenyl-3-methyl-1*H*-1,2,3-triazolium tetrafluoroborate (1)



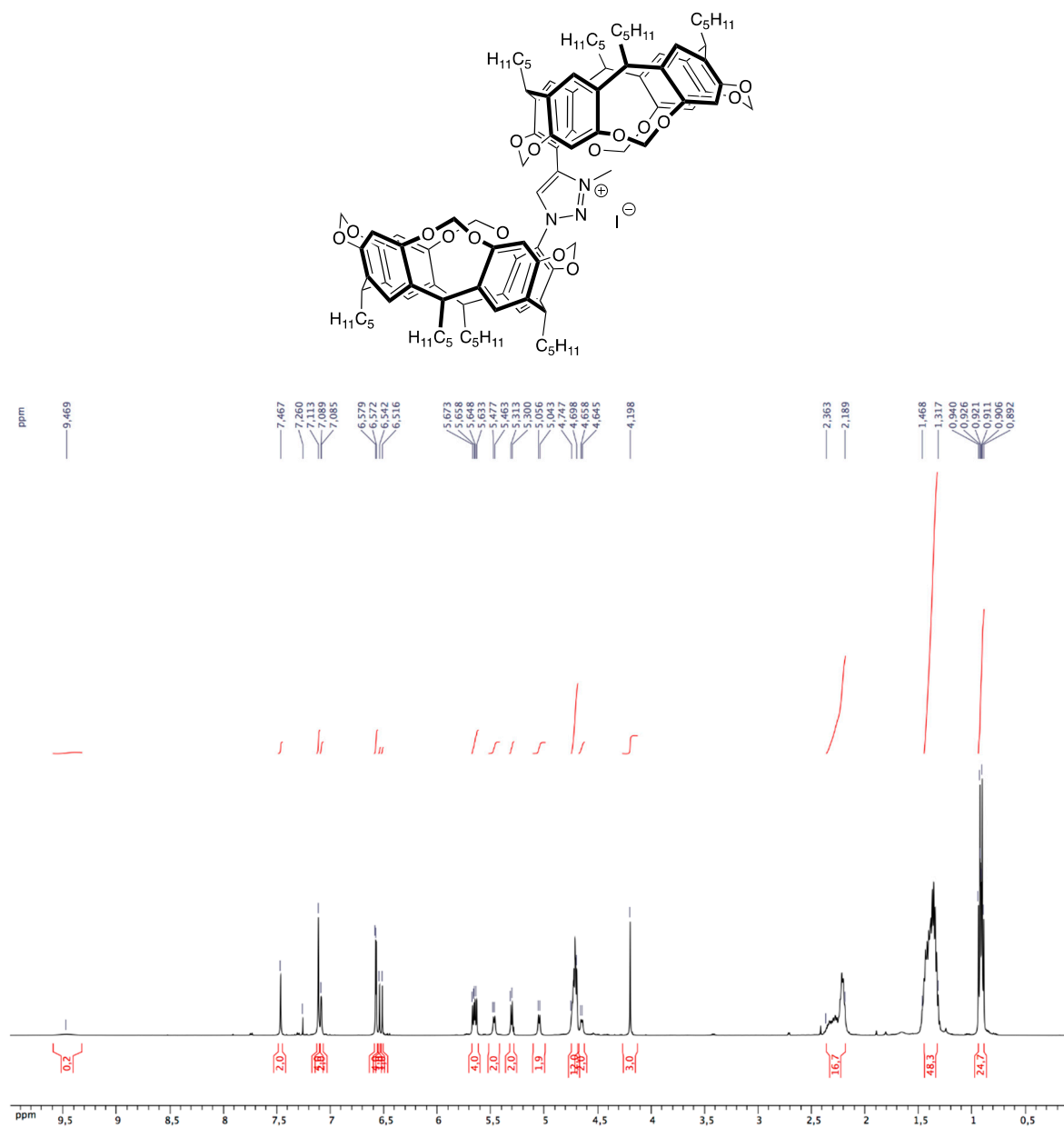


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** (CDCl_3)

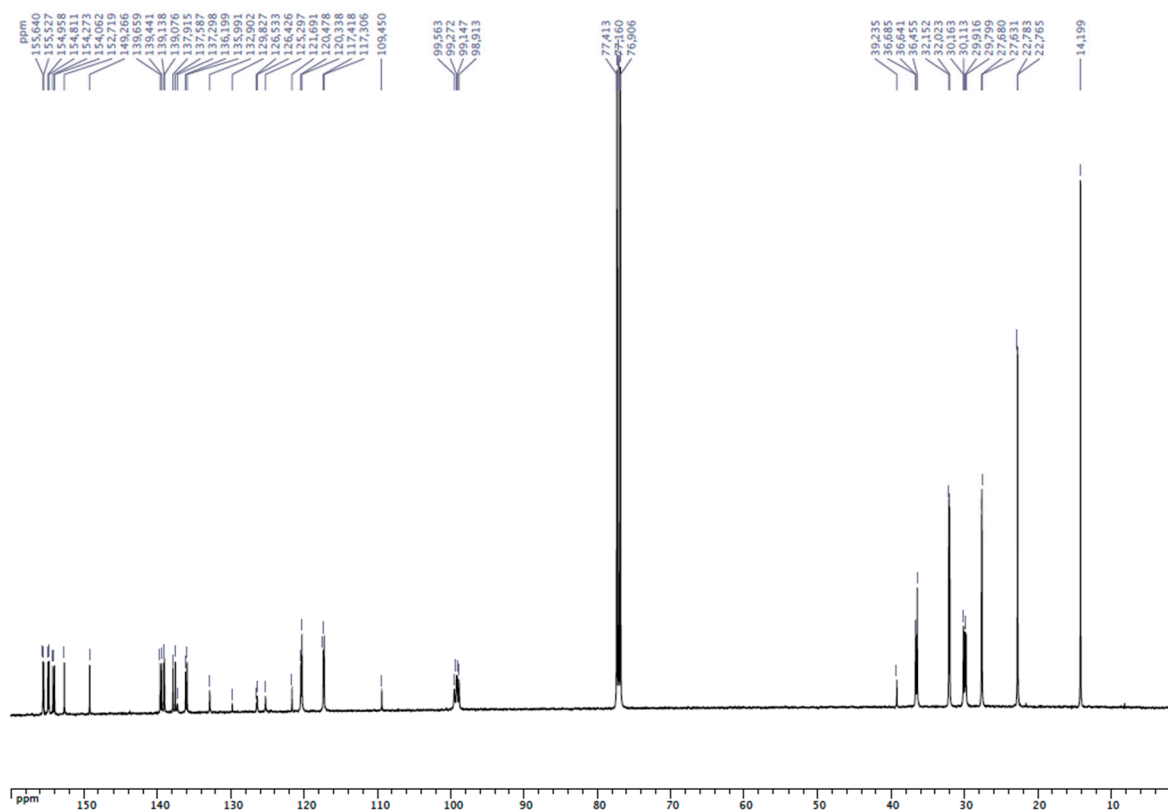


ESI-TOF spectrum of **1** (measured top and calculated for $\text{C}_{61}\text{H}_{72}\text{N}_3\text{O}_8$ bottom)

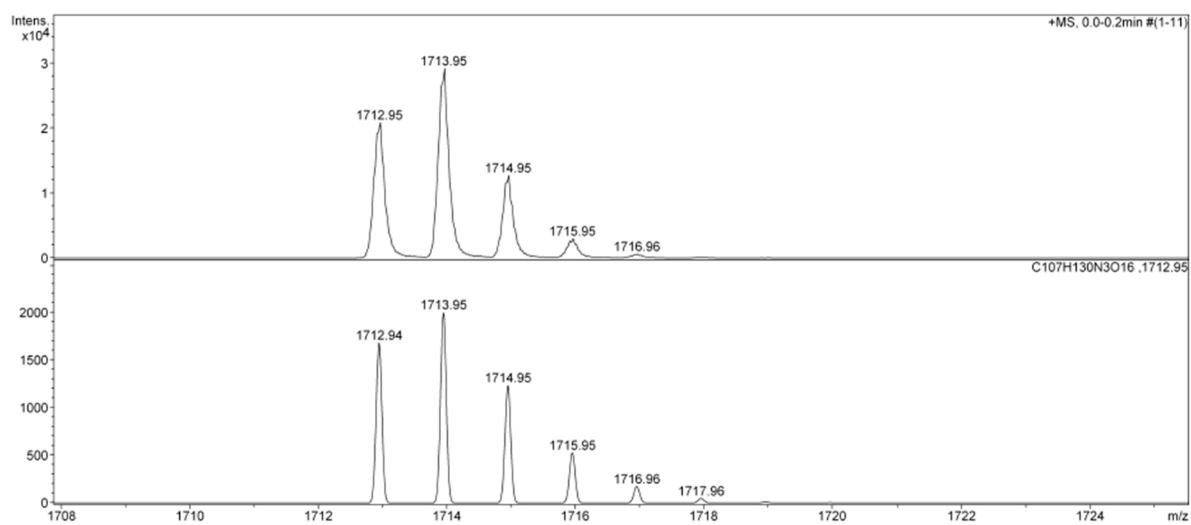
Characterising data of 1,4-bis{4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentylresorcin[4] arene-5-yl}-3-methyl-1*H*-1,2,3-triazolium iodide (**2**)



1H NMR spectrum of **2** ($CDCl_3$)

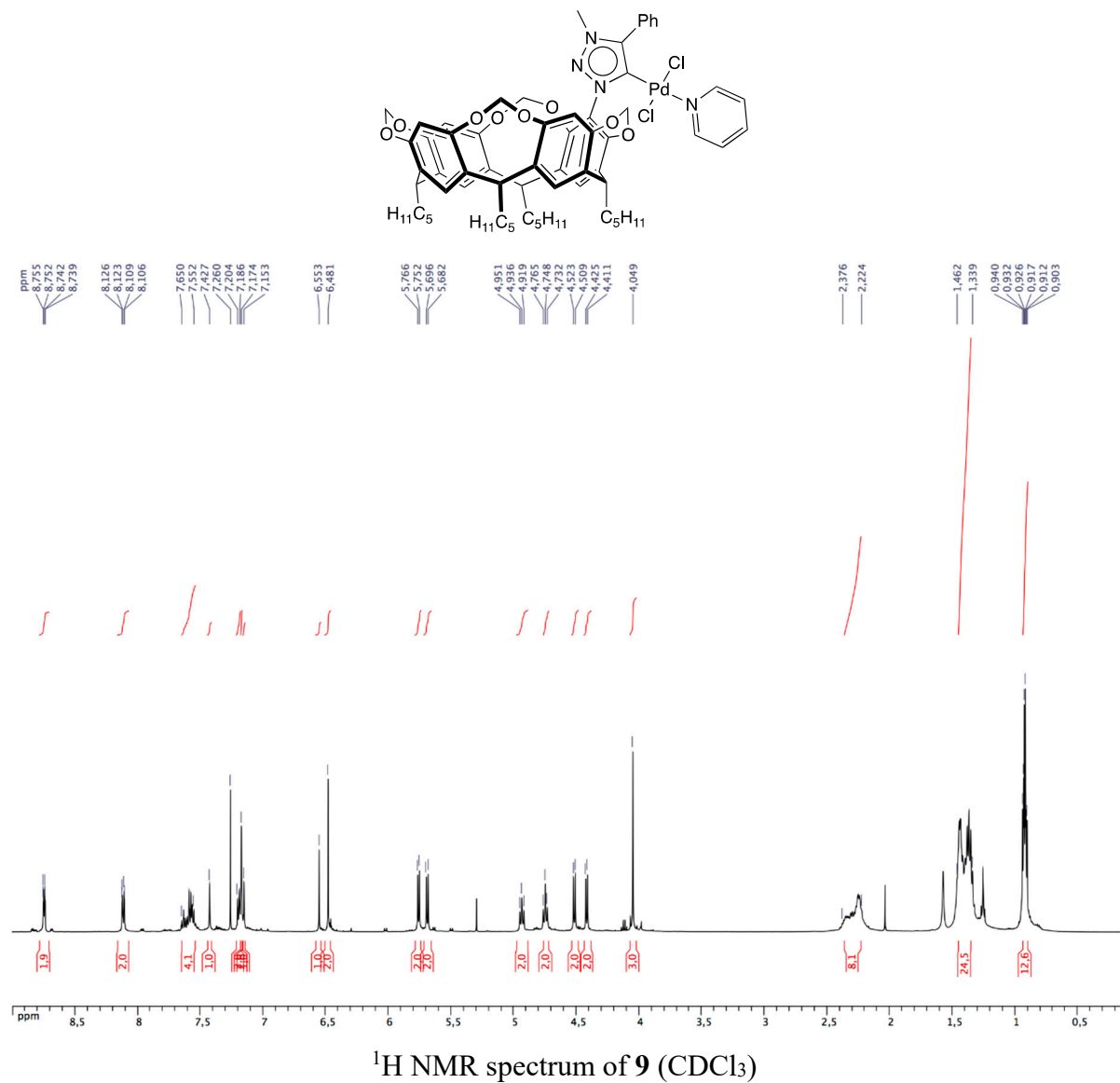


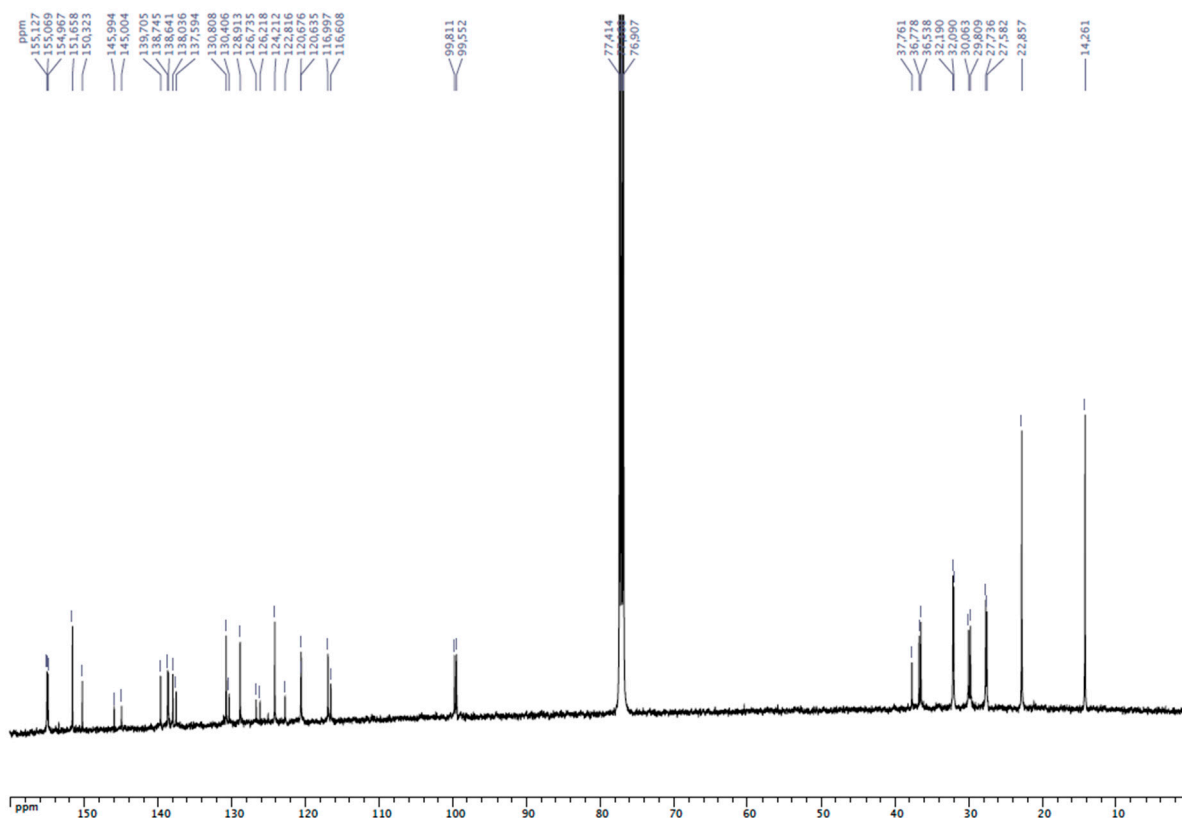
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** (CDCl_3)



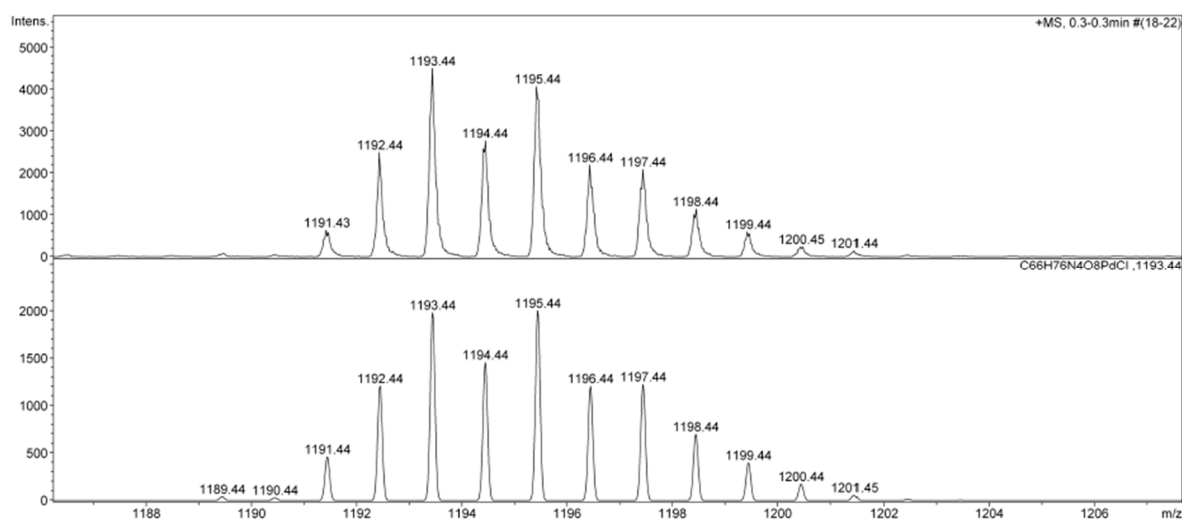
ESI-TOF spectrum of **2** (measured top and calculated for $\text{C}_{107}\text{H}_{130}\text{N}_3\text{O}_{16}$ bottom)

Characterising data of *trans*-dichloro-[1-[4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentylresorcin[4]arene-5-yl]-4-phenyl-3-methyl-1*H*-1,2,3-triazol-5-ylidene}pyridine palladium(II) (**9**)



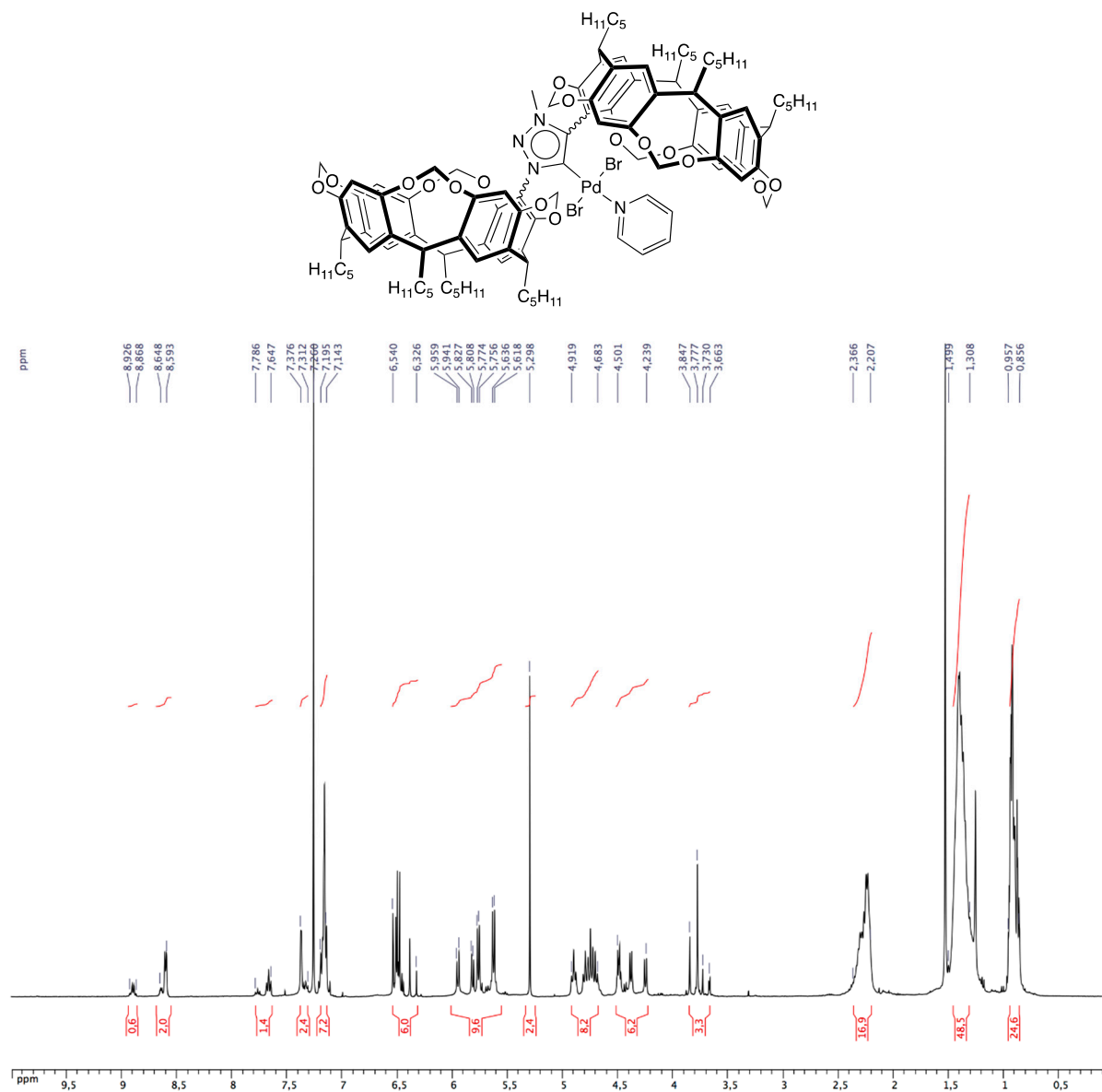


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** (CDCl_3)

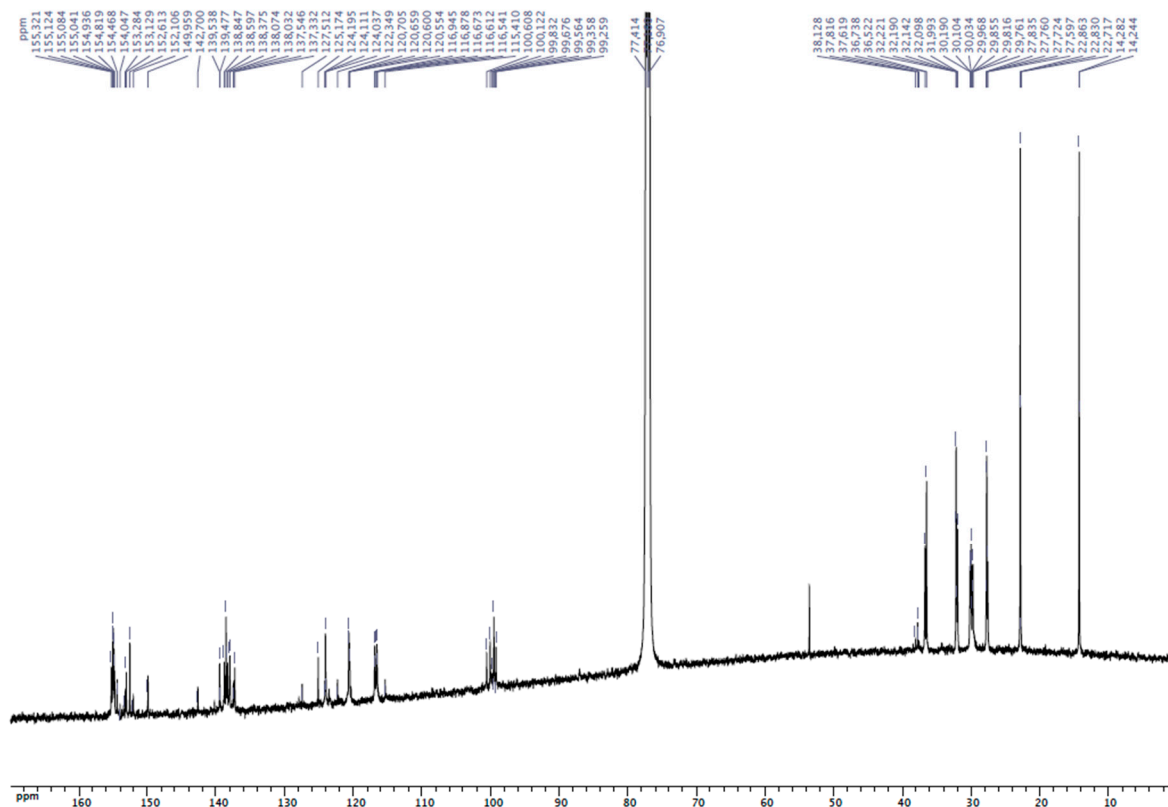


ESI-TOF spectrum of the **9** (measured top and calculated for $\text{C}_{66}\text{H}_{76}\text{N}_4\text{O}_8\text{PdCl}$ bottom)

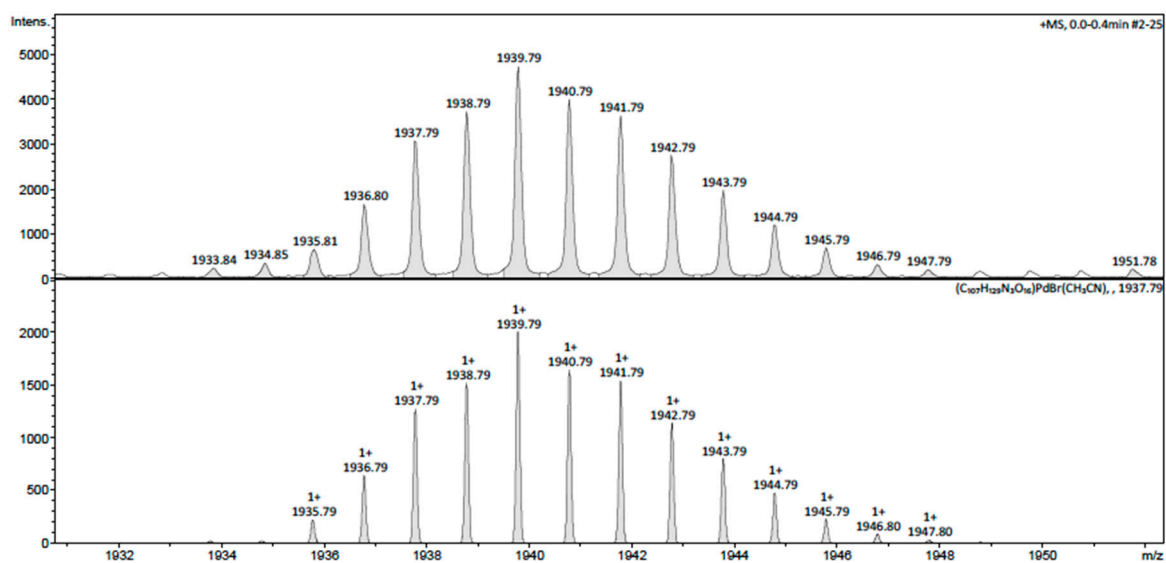
Characterising data of *trans*-dibromo-[1,4-bis[4(24),6(10),12(16),18(22)-tetramethylenedioxy-2,8,14,20-tetrapentylresorcin[4]arene-5-yl]-3-methyl-1*H*-1,2,3-triazol-5-ylidene]pyridine palladium(II) (10)



¹H NMR spectrum of 10 (CDCl₃)

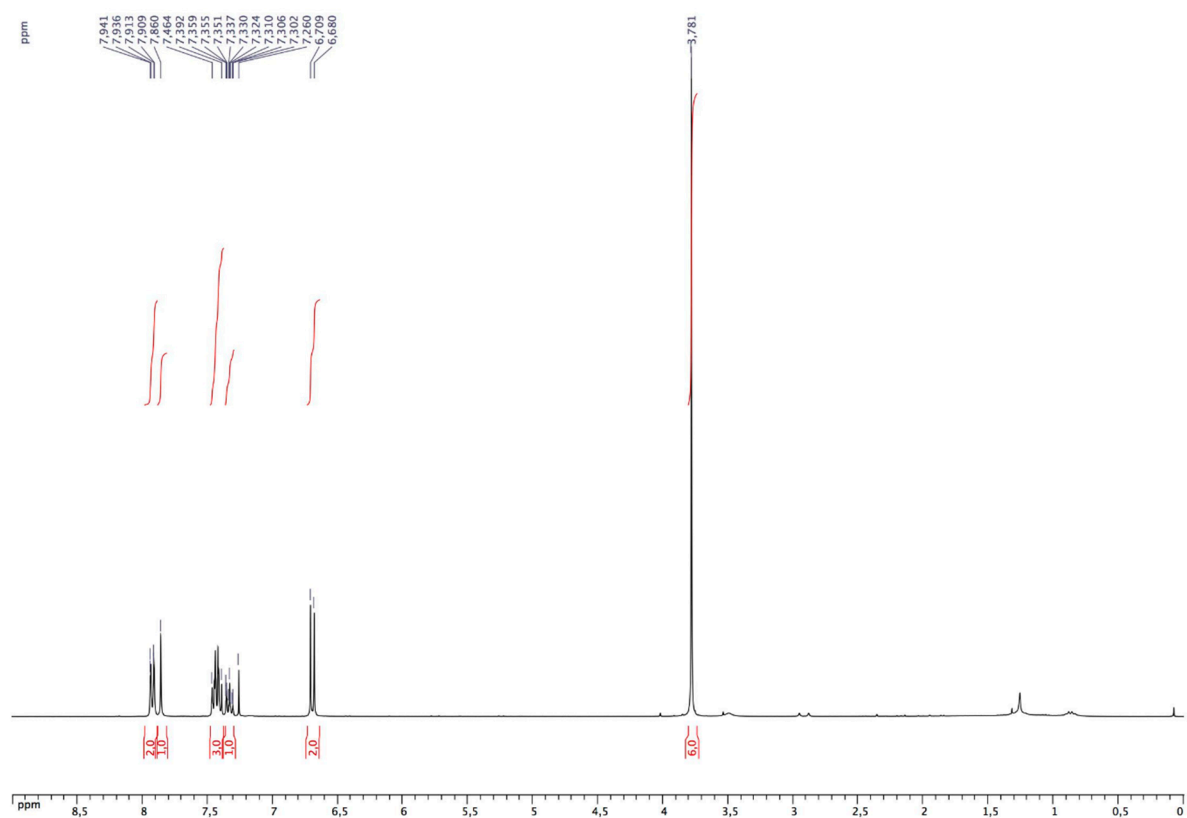
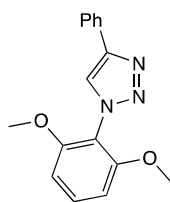


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10** (CDCl_3)

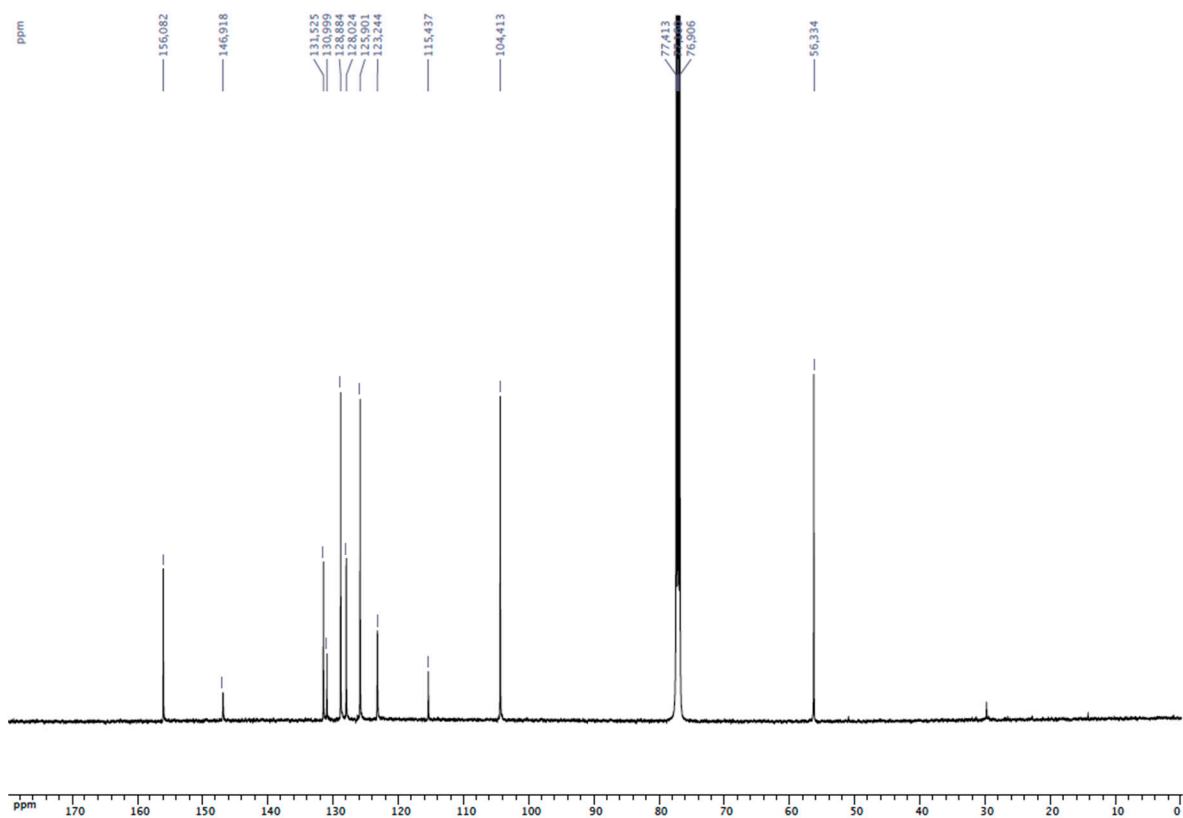


ESI-TOF spectrum of **10** (measured top and calculated for $\text{C}_{111}\text{H}_{132}\text{N}_4\text{O}_{16}\text{PdBr}$ bottom)

Characterising data of 1-(2,6-dimethoxyphenyl)-4-phenyl-1H-1,2,3-triazole

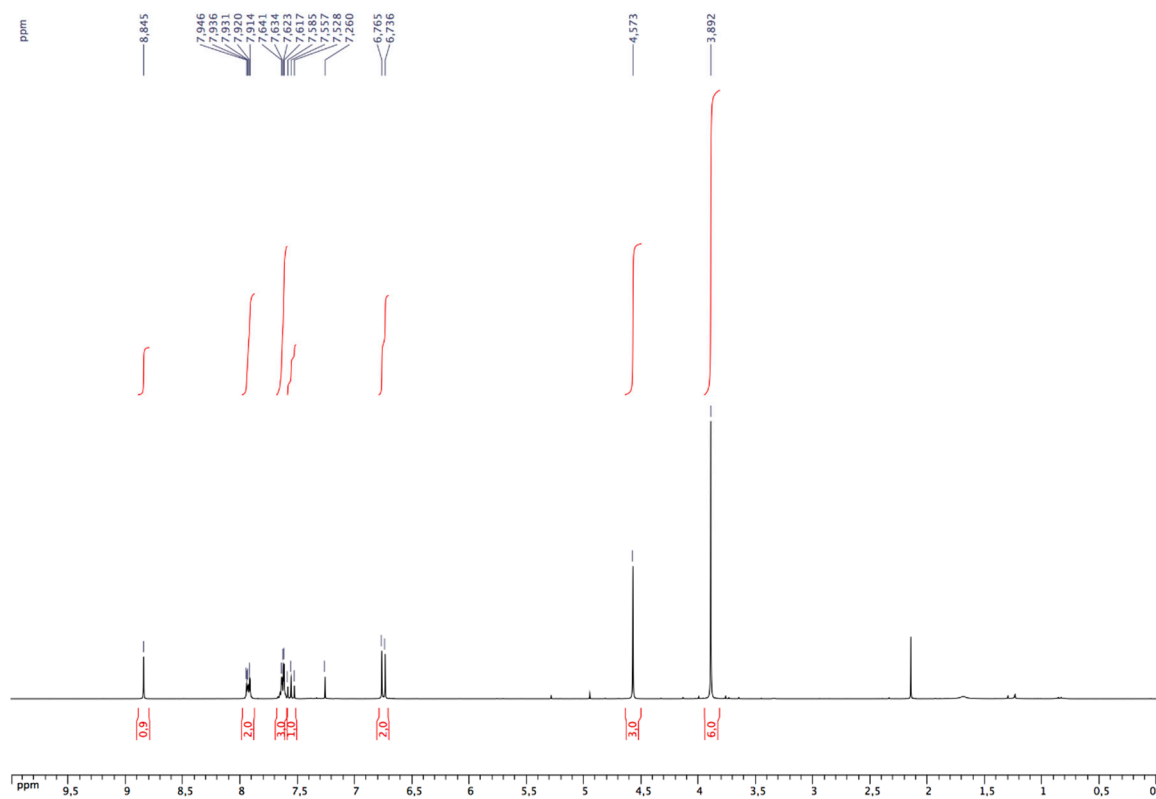
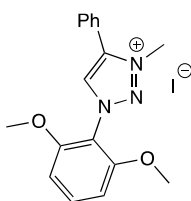


¹H NMR spectrum of 1-(2,6-dimethoxyphenyl)-4-phenyl-1H-1,2,3-triazole (CDCl₃)

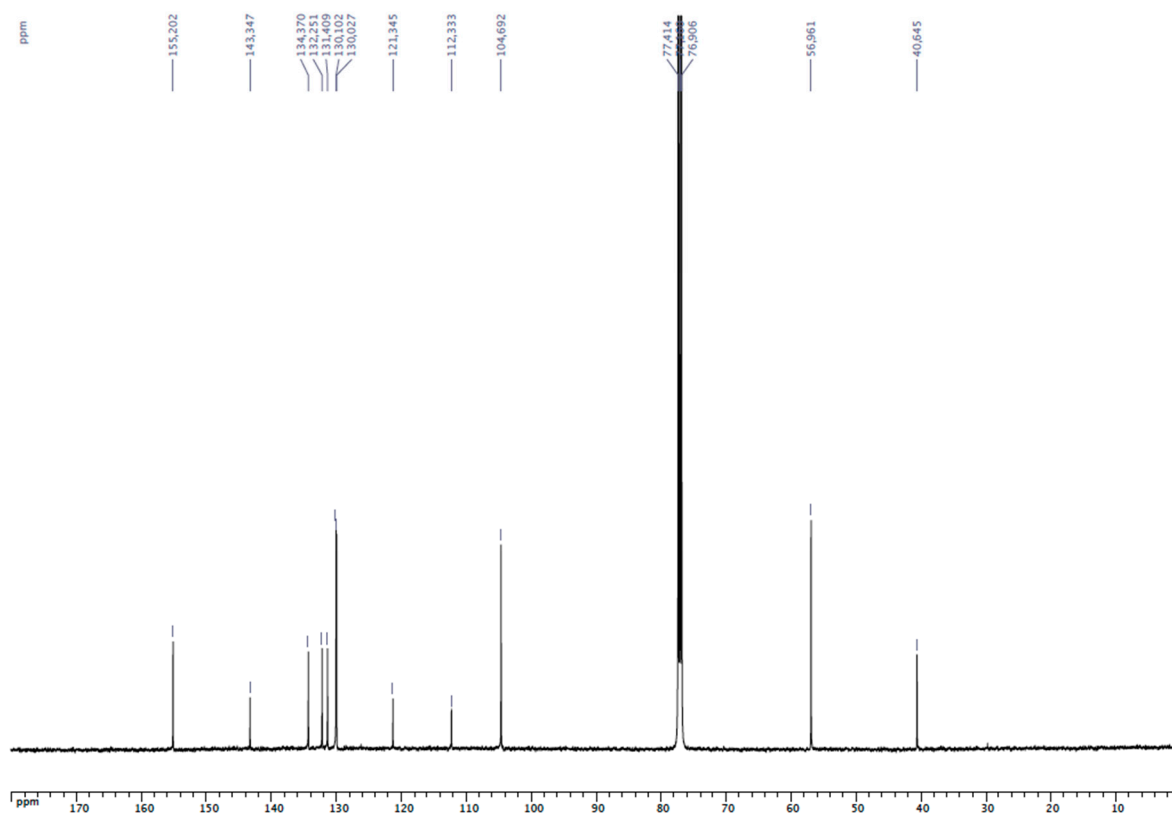
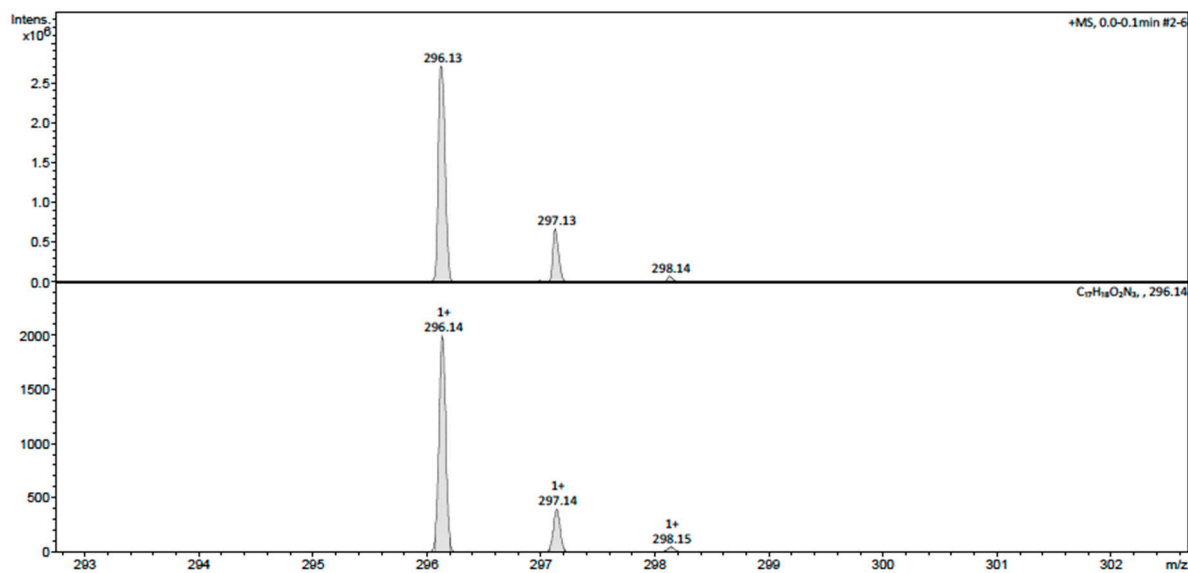


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 1-(2,6-dimethoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (CDCl_3)

Characterising data of 1-(2,6-dimethoxyphenyl)-3-methyl-4-phenyl-1*H*-1,2,3-triazolium iodide (11)



¹H NMR spectrum of **11** (CDCl₃)

 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **11** (CDCl_3)ESI-TOF spectrum of **11** (measured top and calculated for $\text{C}_{17}\text{H}_{18}\text{O}_2\text{N}_3$ bottom)