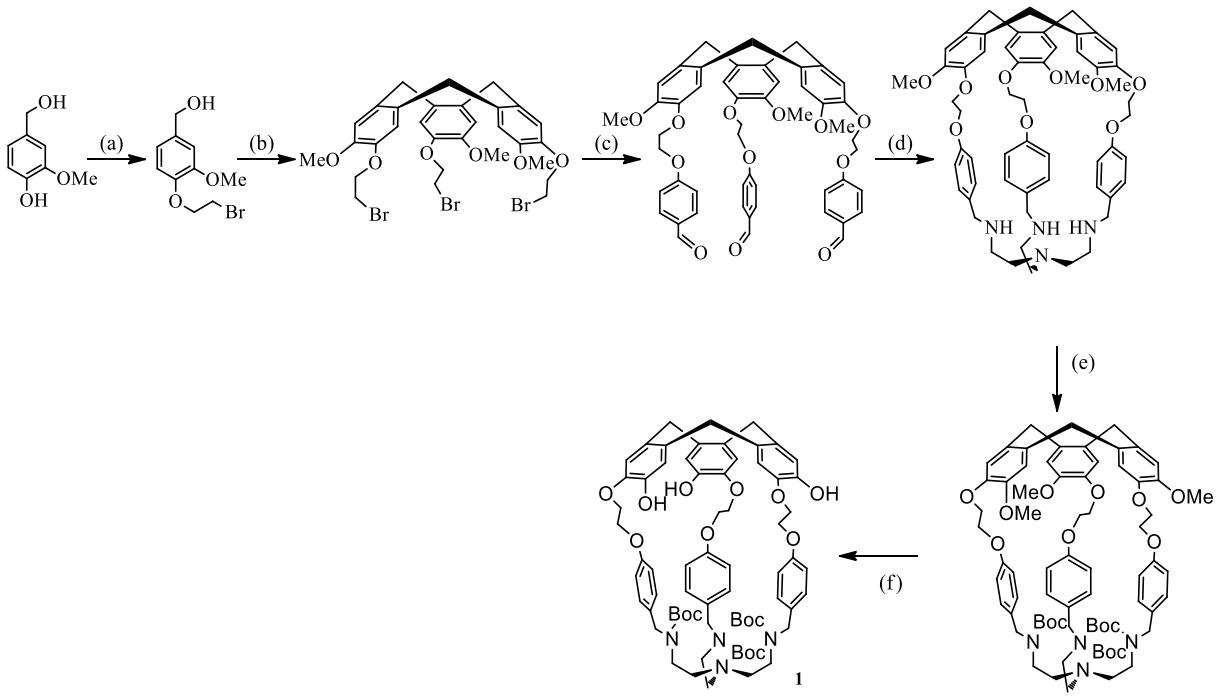
Supporting Information

Synthesis and physico-chemical properties of the first water soluble Cu(II)@hemicryptophane complex

Aline Schmitt,[a] Christophe Bucher,[a] Vincent Maurel,[b] Jean-Pierre Dutasta*[a] and Alexandre Martinez*[a]

[a] Dr. A. Schmitt, Dr. C. Bucher, Dr. J.-P. Dutasta, Dr. A. Martinez Laboratoire de Chimie, École Normale Supérieure de Lyon, CNRS, UCBL, 46, Allée d'Italie, F-69364 Lyon, France
[a] Dr Vincent Maurel, Laboratoire de Résonances Magnétiques, CEA-Grenoble/INAC/SCIB/LRM, UMR-E 3 CEA-UJF, 17, rue des Martyrs 38054 Grenoble CEDEX 09
[c] Pr. A. Martinez, Aix Marseille Universite, Centrale Marseille, CNRS, iSm2 UMR 7313, 13397, Marseille, France



Scheme S-1. Synthesis of hemicryptophane **1**.[1] Reactions conditions: (a) 1,2-dibromoethane, K_2CO_3, EtOH, 50°C, 6 h, 48%; (b) $Sc(OTf)_3$, CH_2Cl_2, reflux, 1 night, 23%; (c) 4-hydroxybenzaldehyde, Cs_2CO_3, DMF, 40°C, 1 night, 95% ; (d) (i) tris(2-aminoethyl)amine, $CHCl_3$/MeOH 50/50, rt, 1 night 2) $NaBH_4$, rt, 3h, 77%. (e) Boc_2O, CH_2Cl_2, 2h, rt, 91%; (f) PPh_2Li, THF, 60°C, 55%;

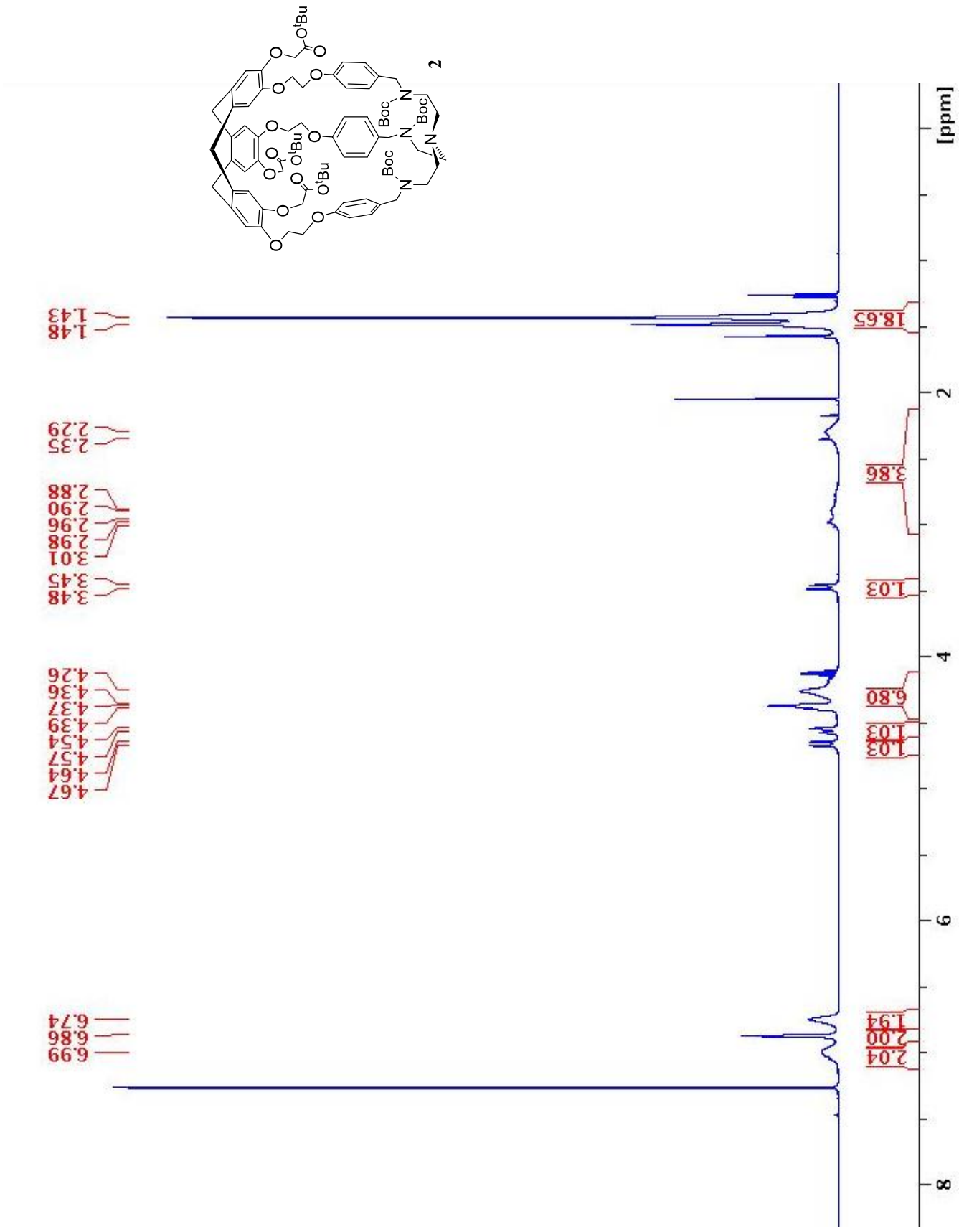


Figure S-1. ^{1}H NMR of hemicryptophane **2** ($CDCl_3$, 298 K, 500.10 MHz)

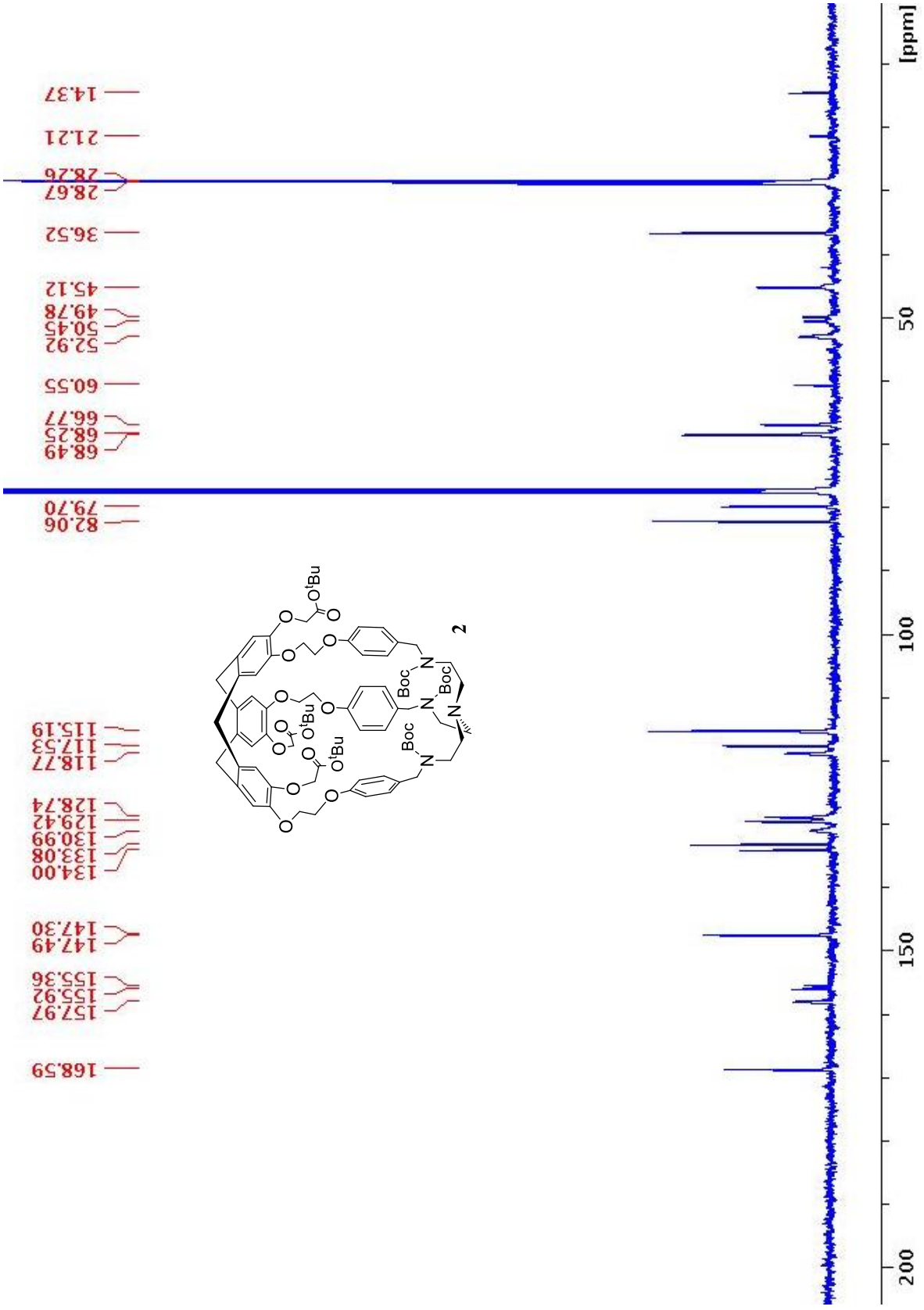


Figure S-2. ^{13}C NMR of hemicryptophane **2** ($CDCl_3$, 298 K, 125.76 MHz)

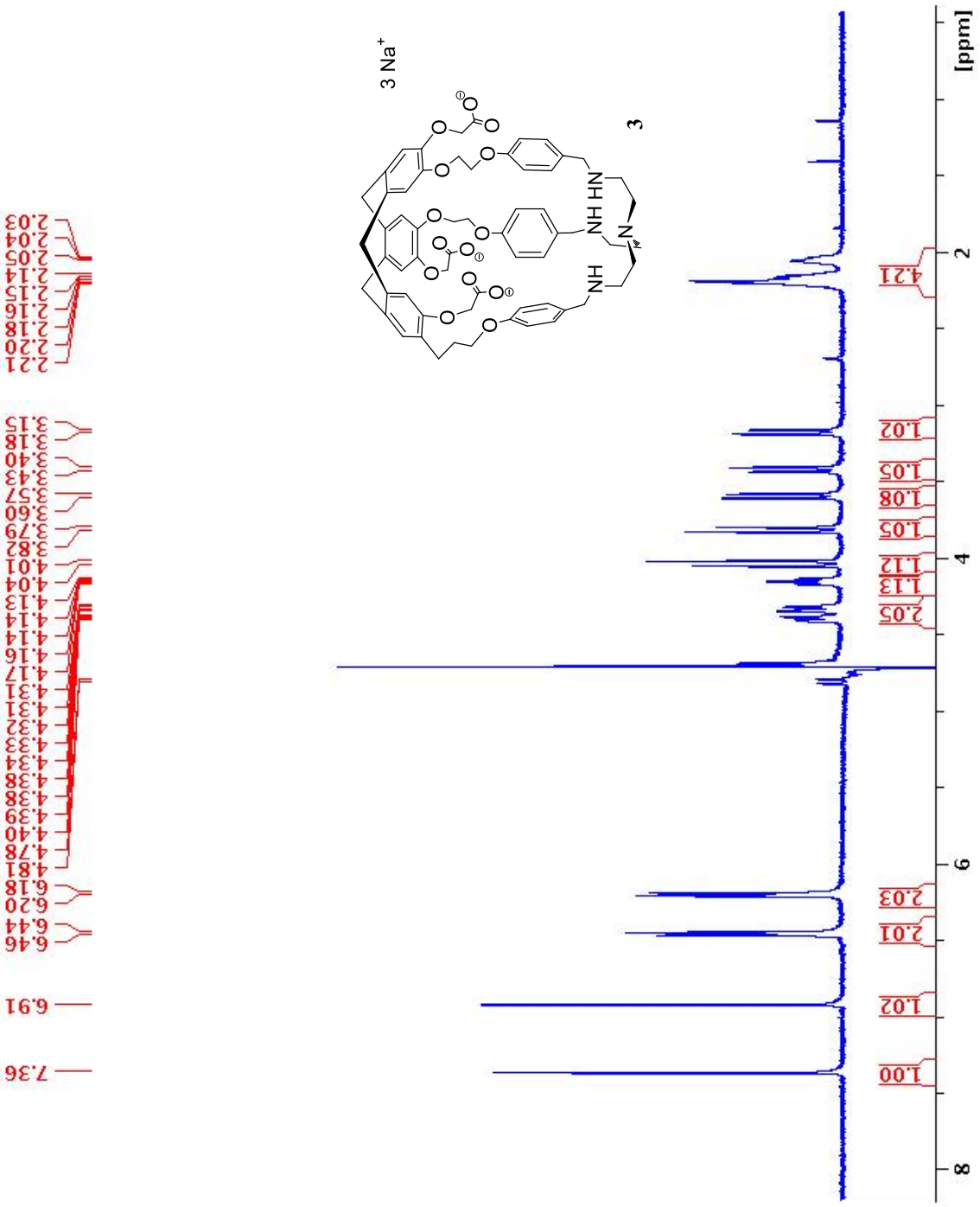


Figure S-3. ^{1}H NMR of hemicryptophane **3** ($CDCl_3$, 298 K, 500.10 MHz)

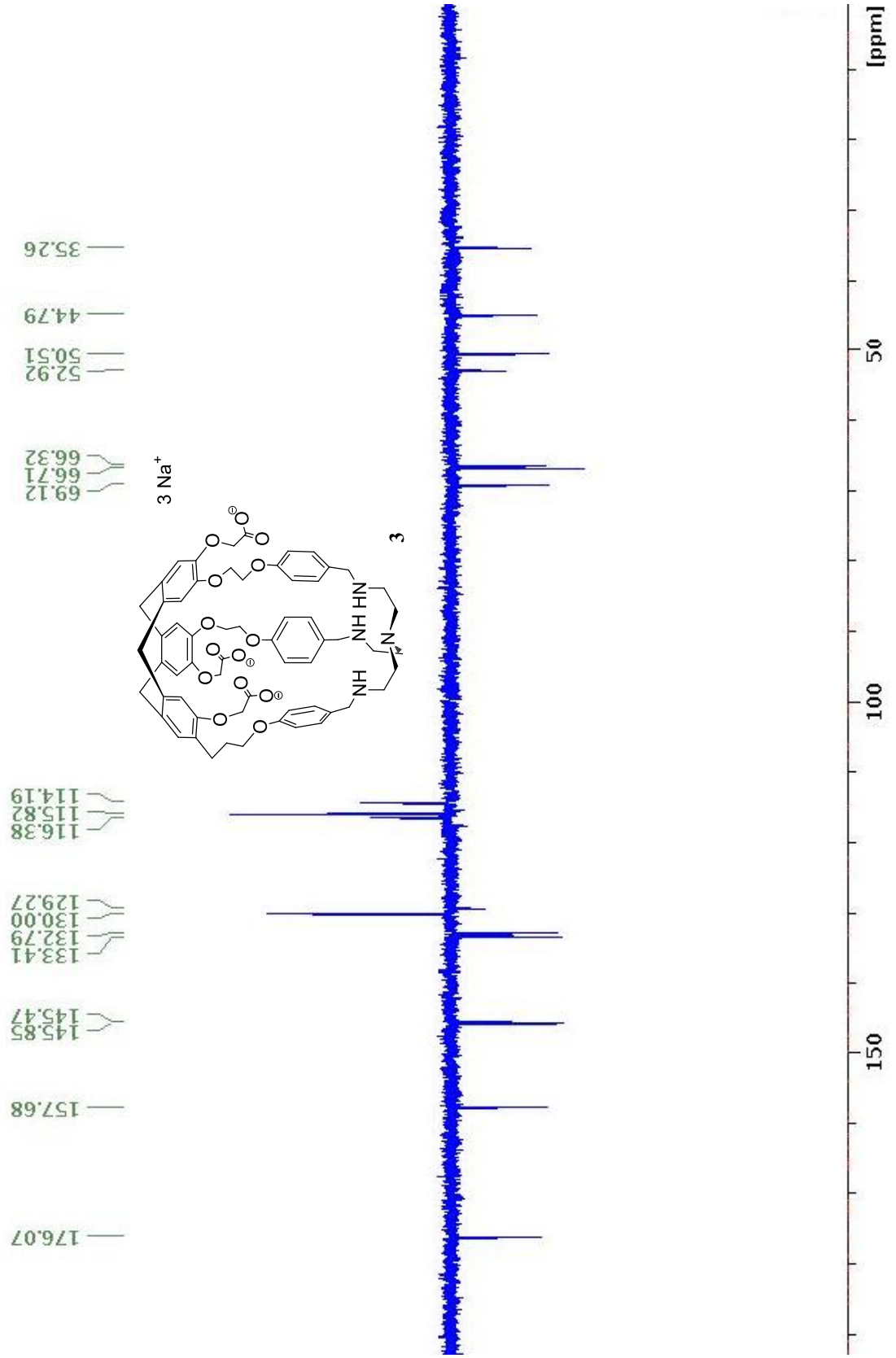


Figure S-4. ^{13}C NMR of hemicryptophane **3** ($CDCl_3$, 298 K, 125.76 MHz)

Reference

1 A. Schmitt, V. Robert, J.-P. Dutasta and A. Martinez, *Org. Lett*., 2014, **16**, 2374–2377.