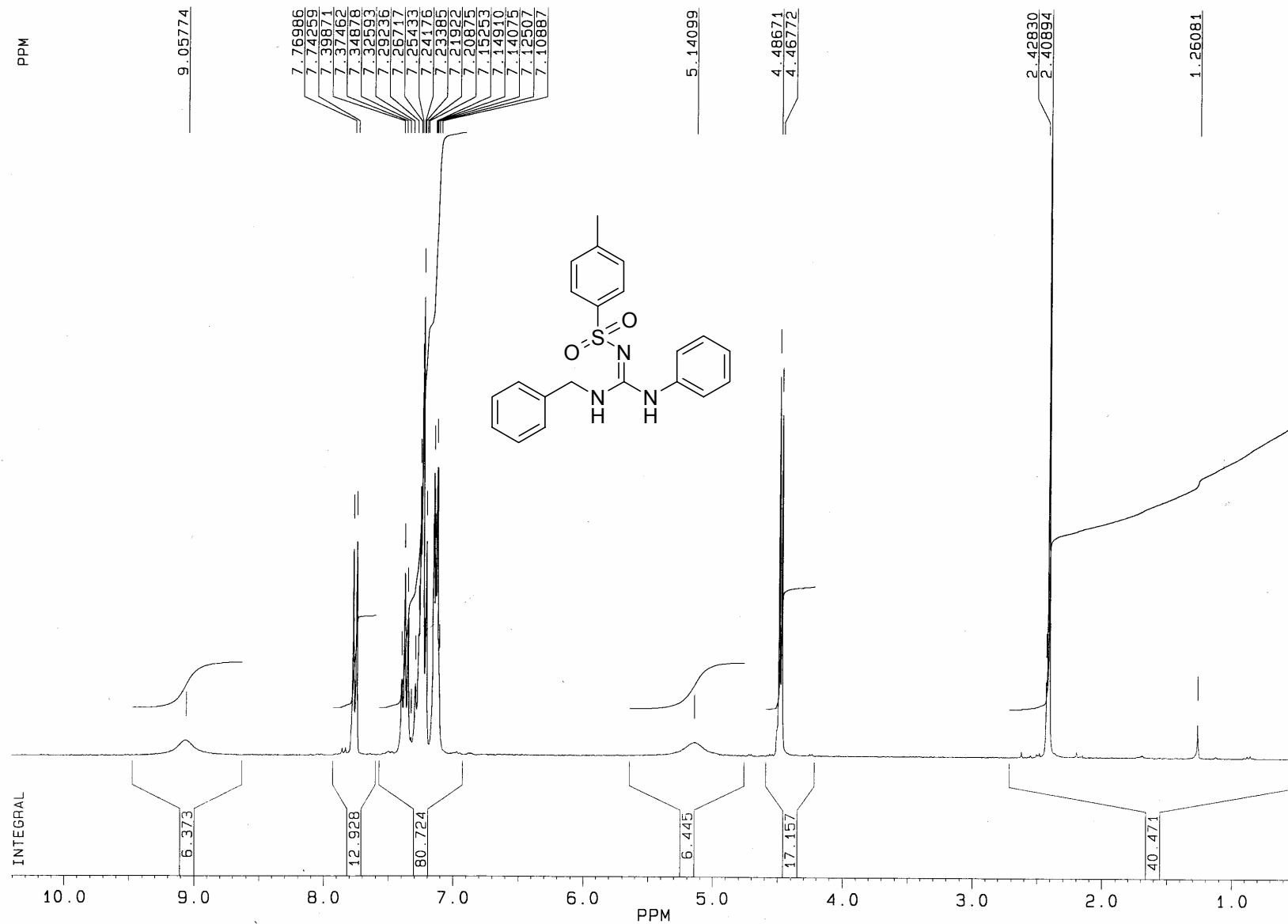


SUPPORTING INFORMATION

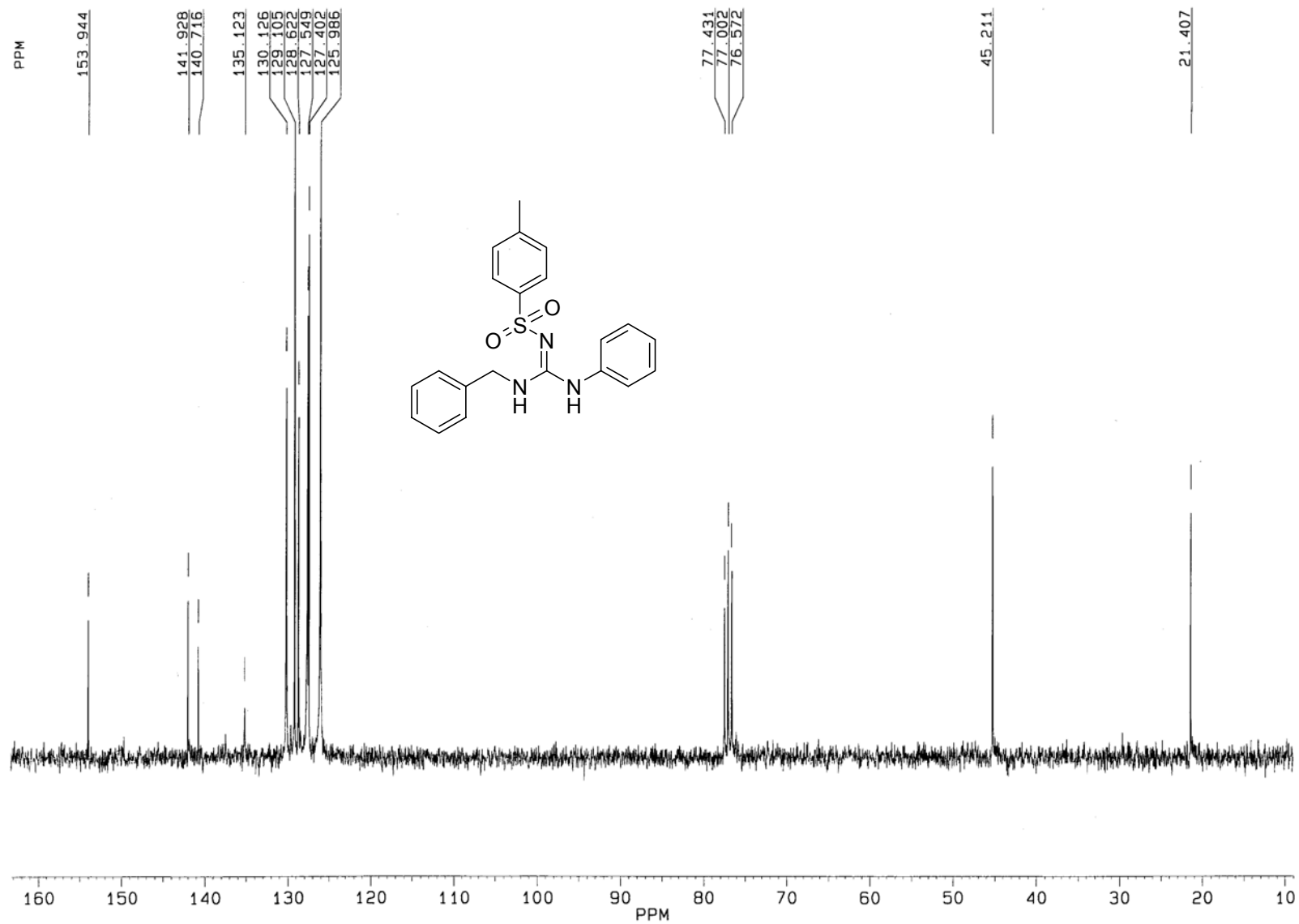
Title: Design, Synthesis and Recognition Properties of Urea-Type Anion Receptors in Low Polar Media

Author(s): Luca Pescatori, Arturo Arduini, Andrea Pochini, Franco Ugozzoli, Andrea Secchi*

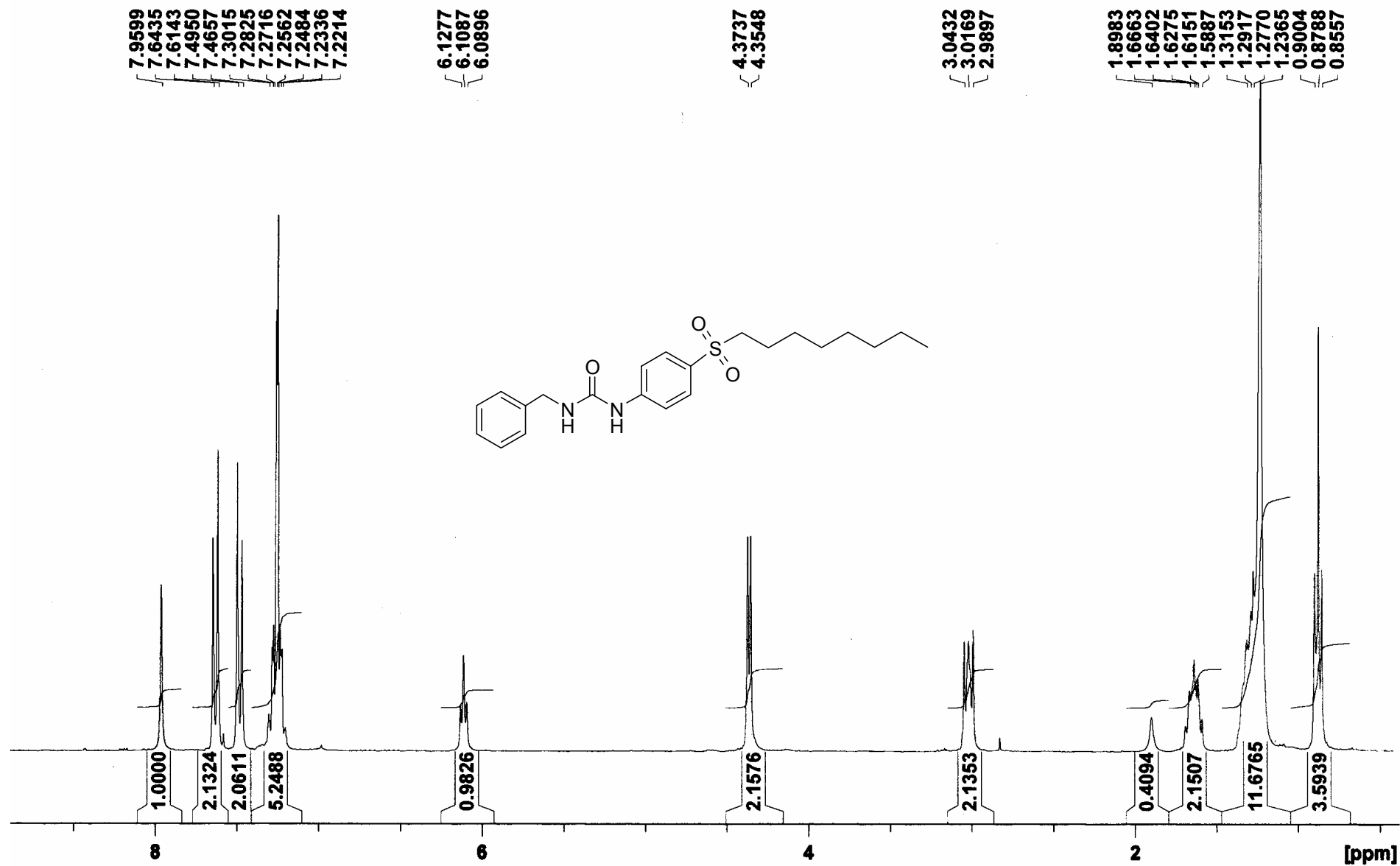
Ref. No.: O200700740



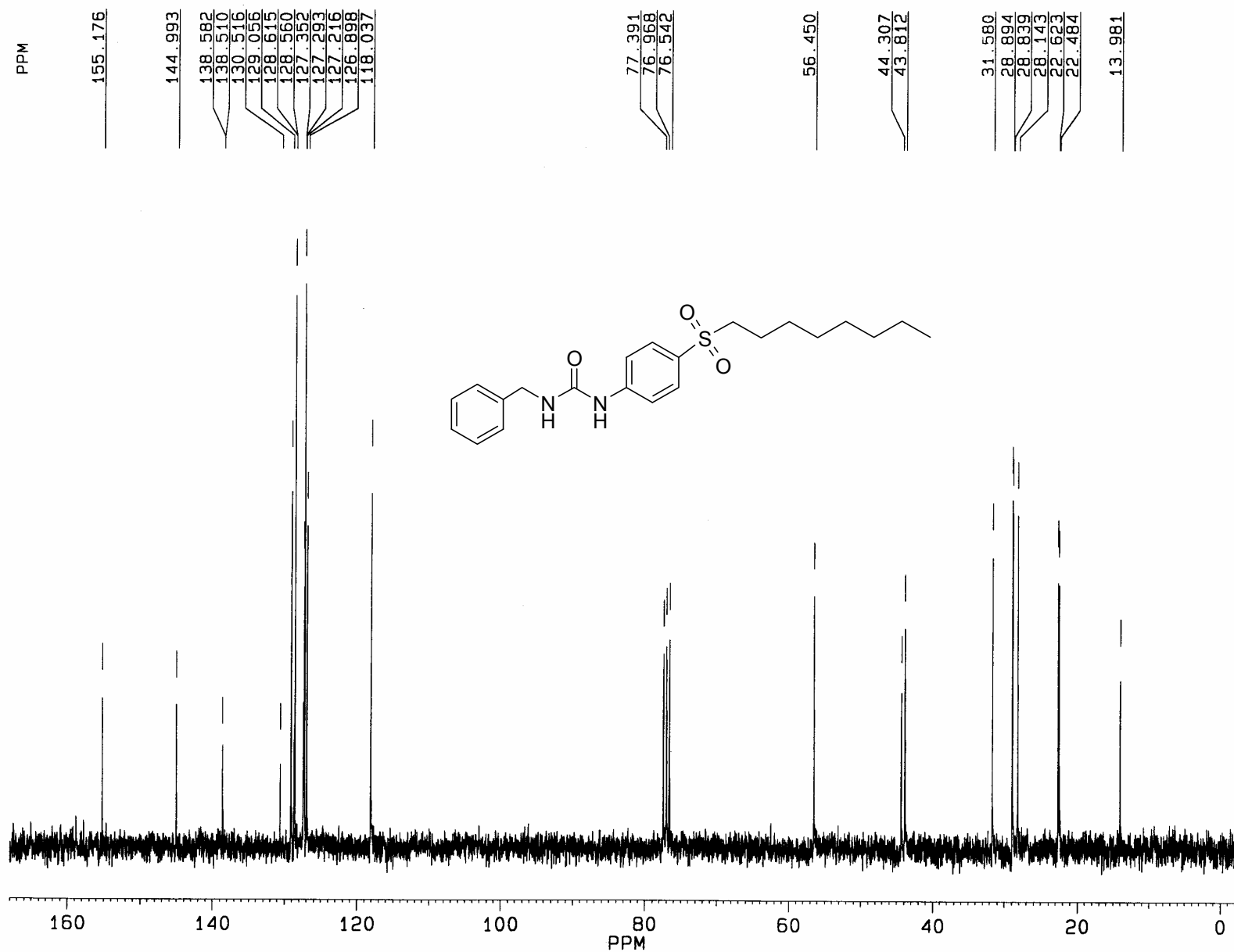
¹H NMR (300 MHz, CDCl₃) of *N*-[1-Benzylamino-1-phenylaminomethylidene]-4-methylbenzenesulfonamide **1**.

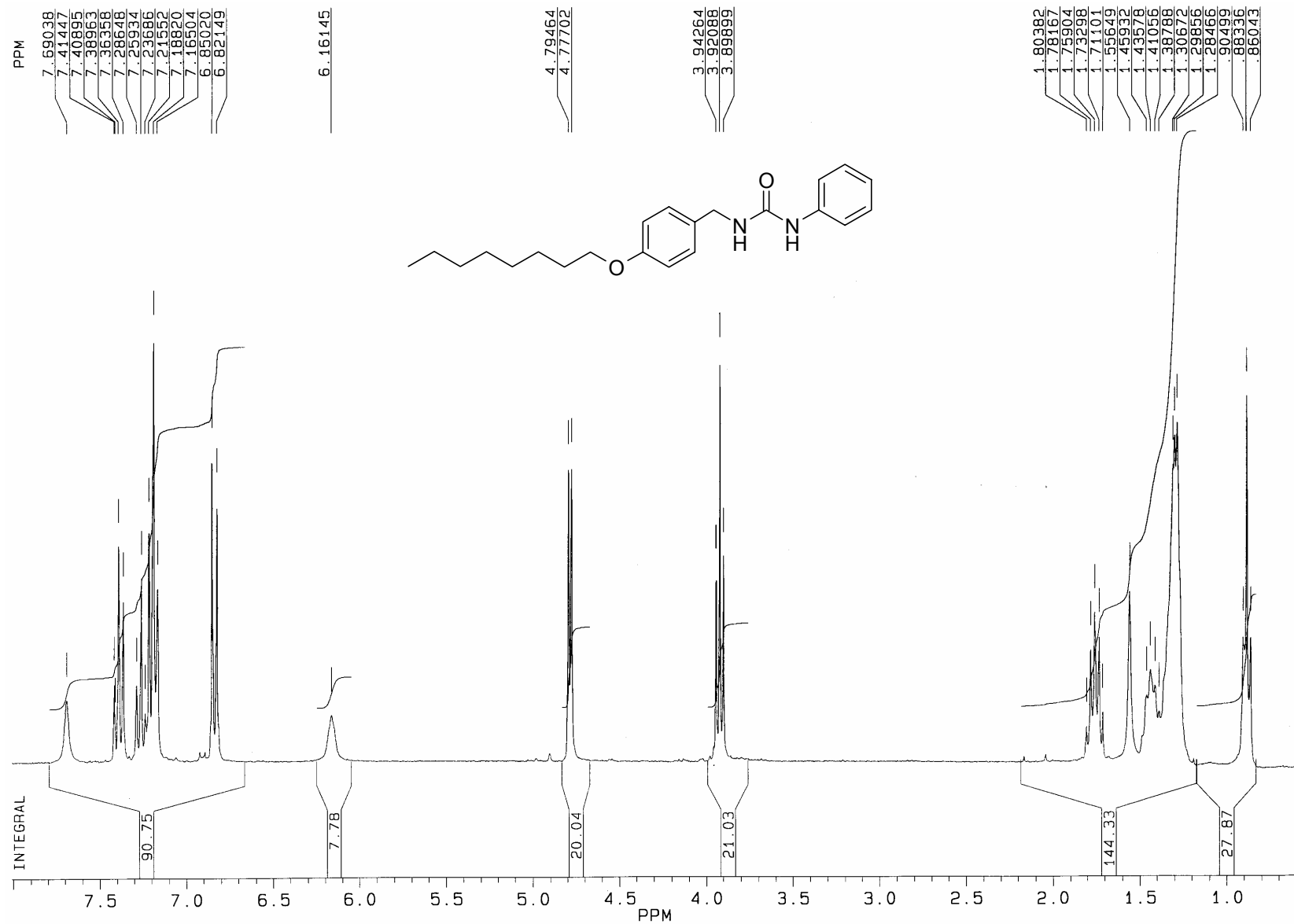


^{13}C NMR (75 MHz, CDCl_3) of *N*-[1-Benzylamino-1-phenylaminomethylidene]-4-methylbenzenesulfonamide **1**.

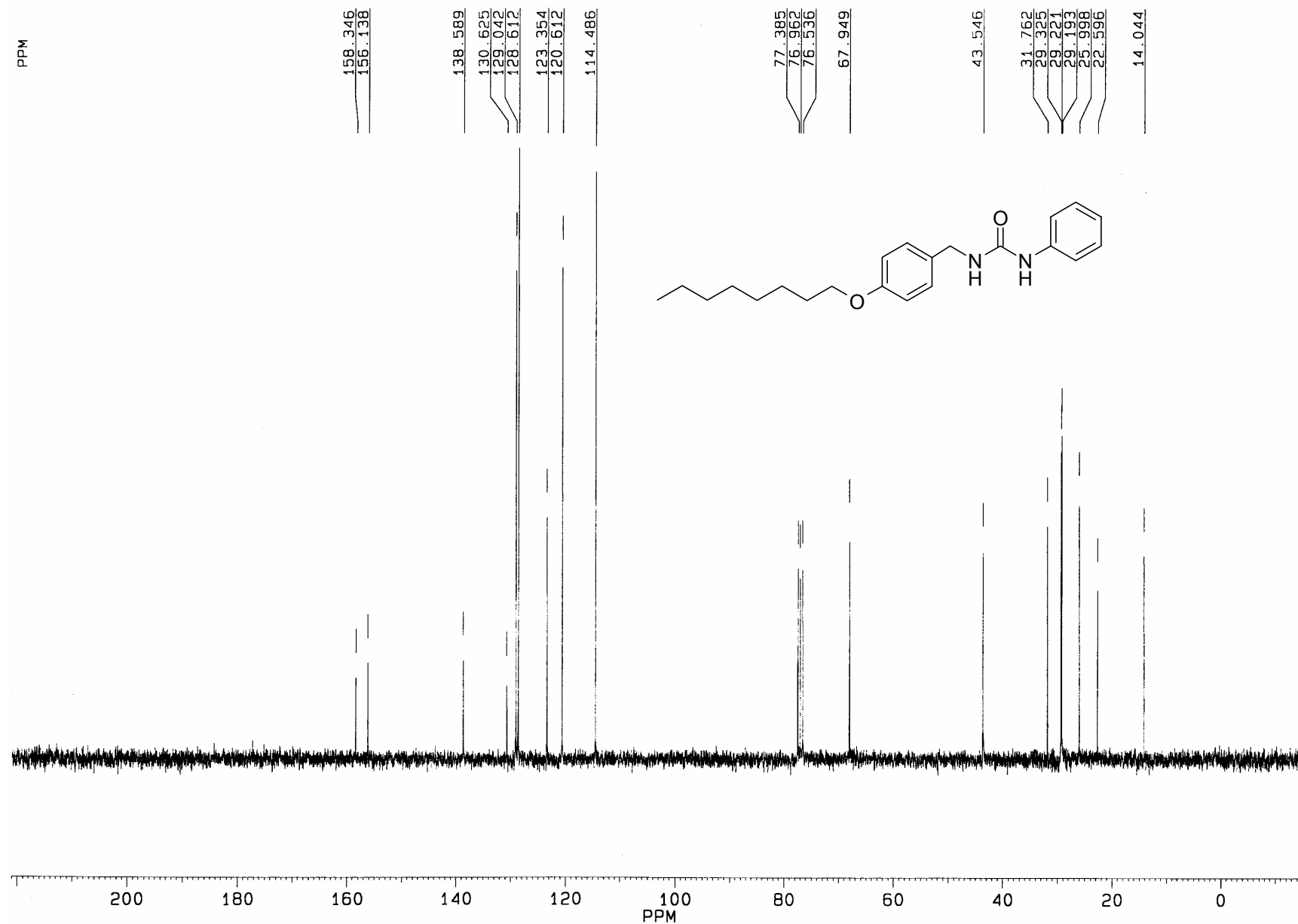


¹H NMR (300 MHz, CDCl₃) of 1-benzyl-3-[4-(octylsulfonyl)phenyl]urea 11.

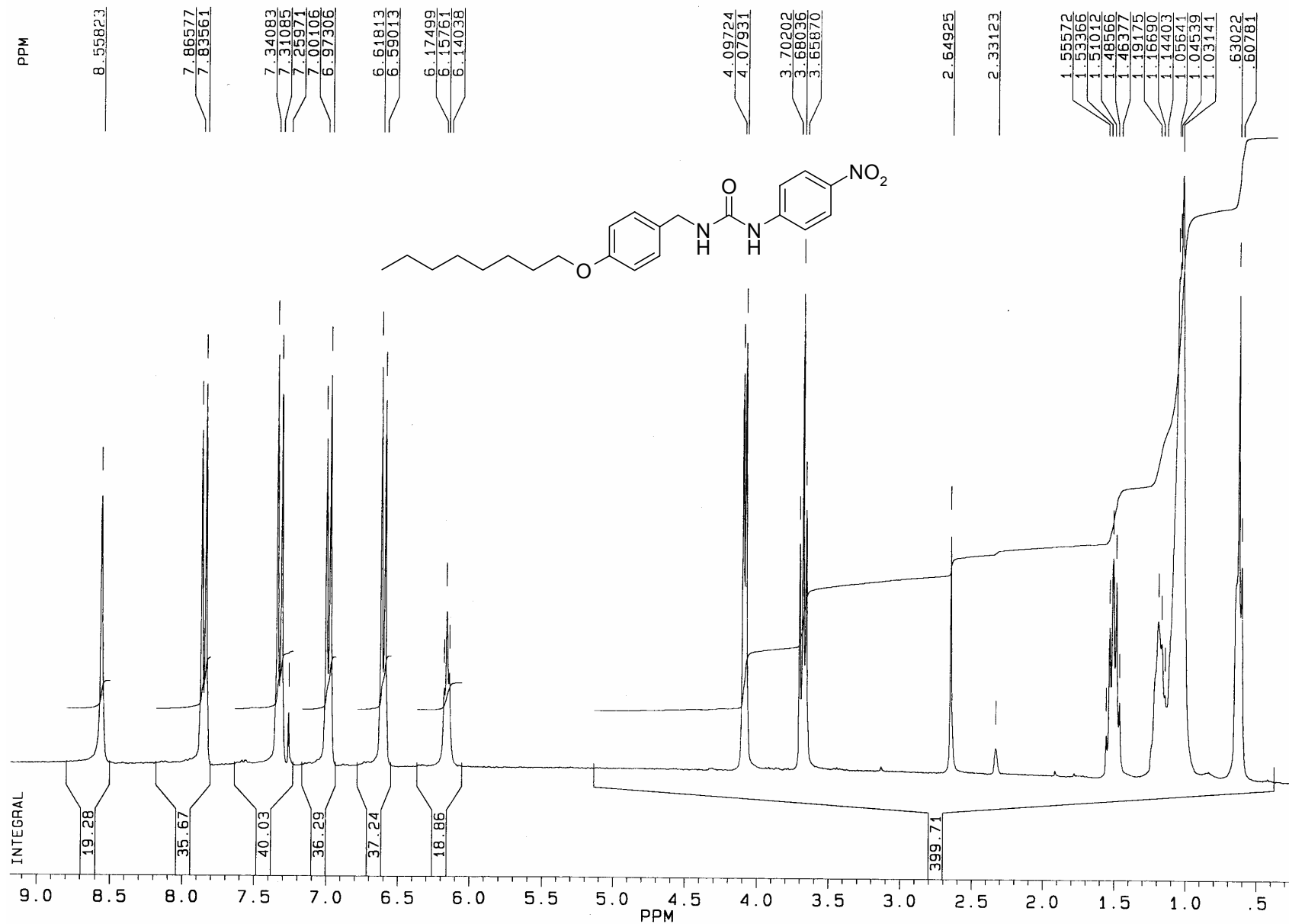


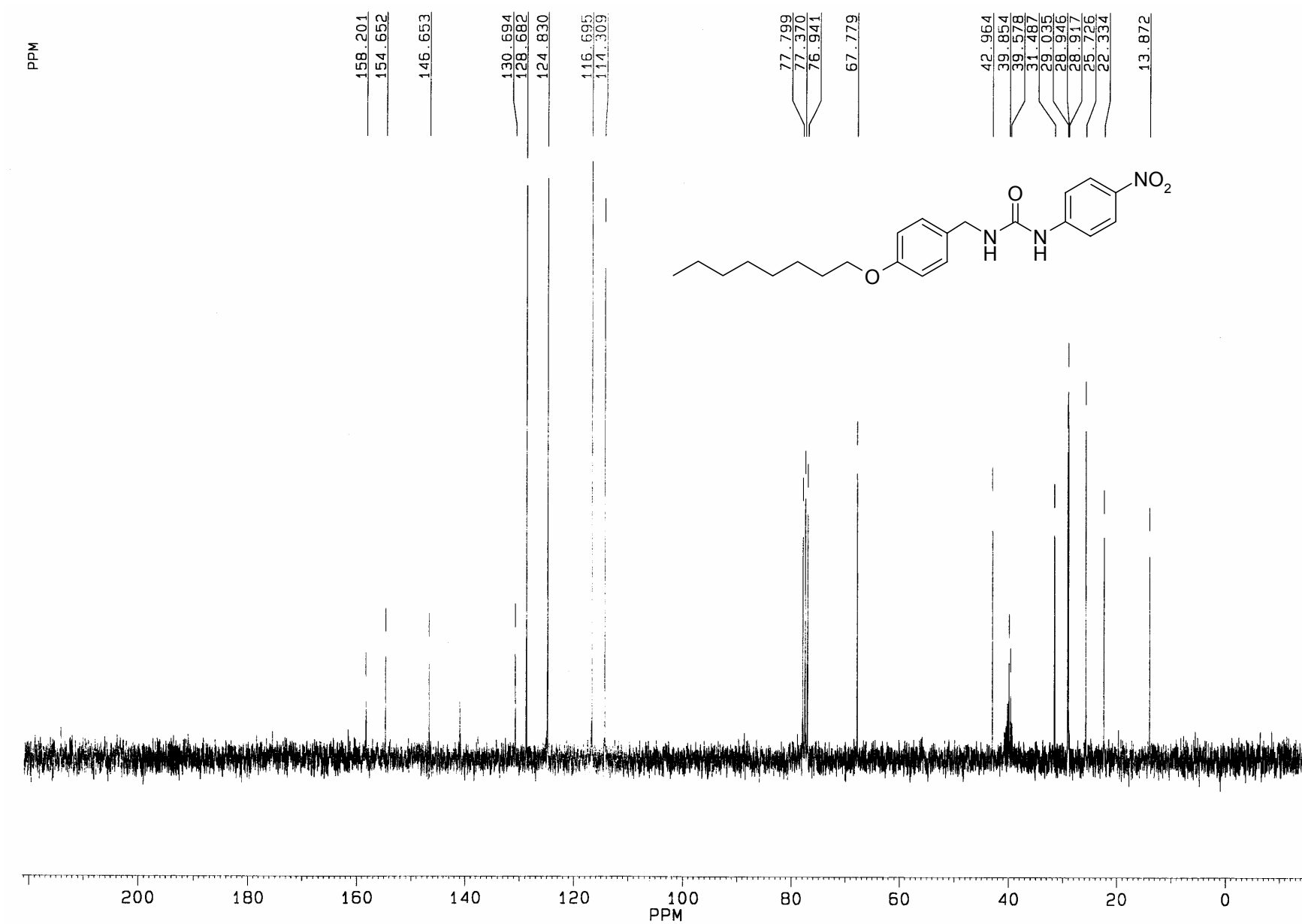


¹H NMR (300 MHz, CDCl₃) of 1-[4-(octyloxy)benzyl]-3-phenylurea **12**.

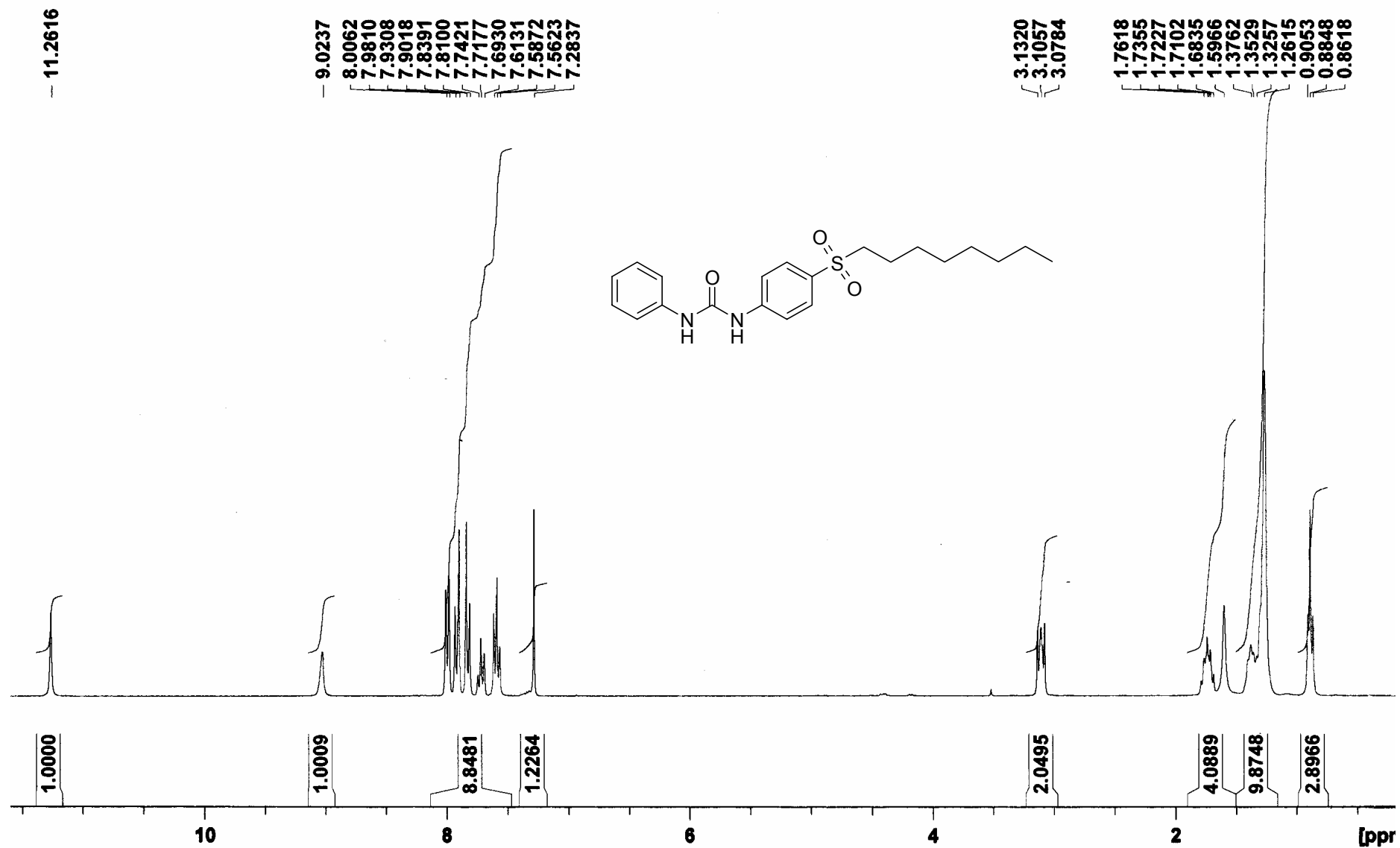


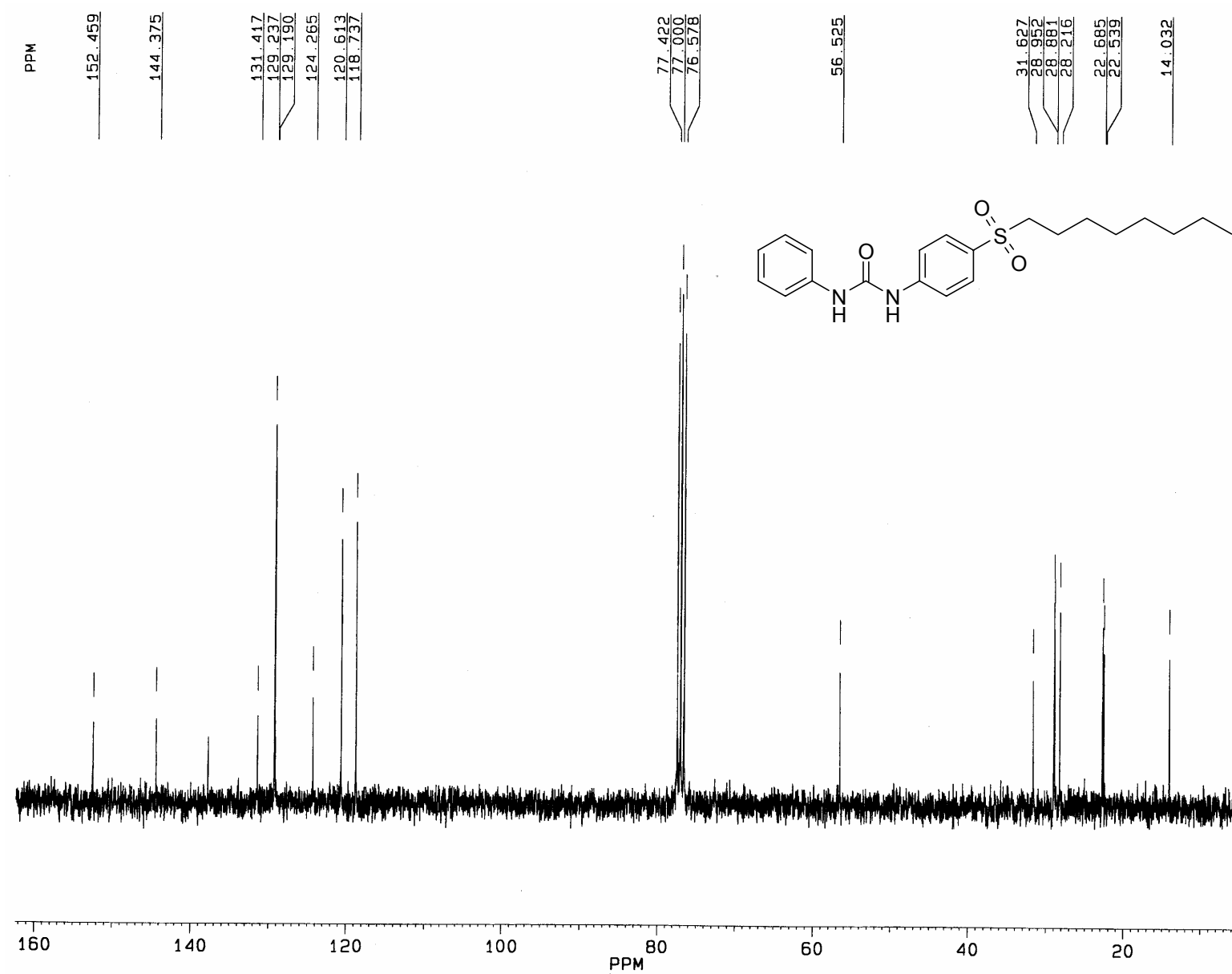
¹³C NMR (75 MHz, CDCl₃) of 1-[4-(octyloxy)benzyl]-3-phenylurea **12**.



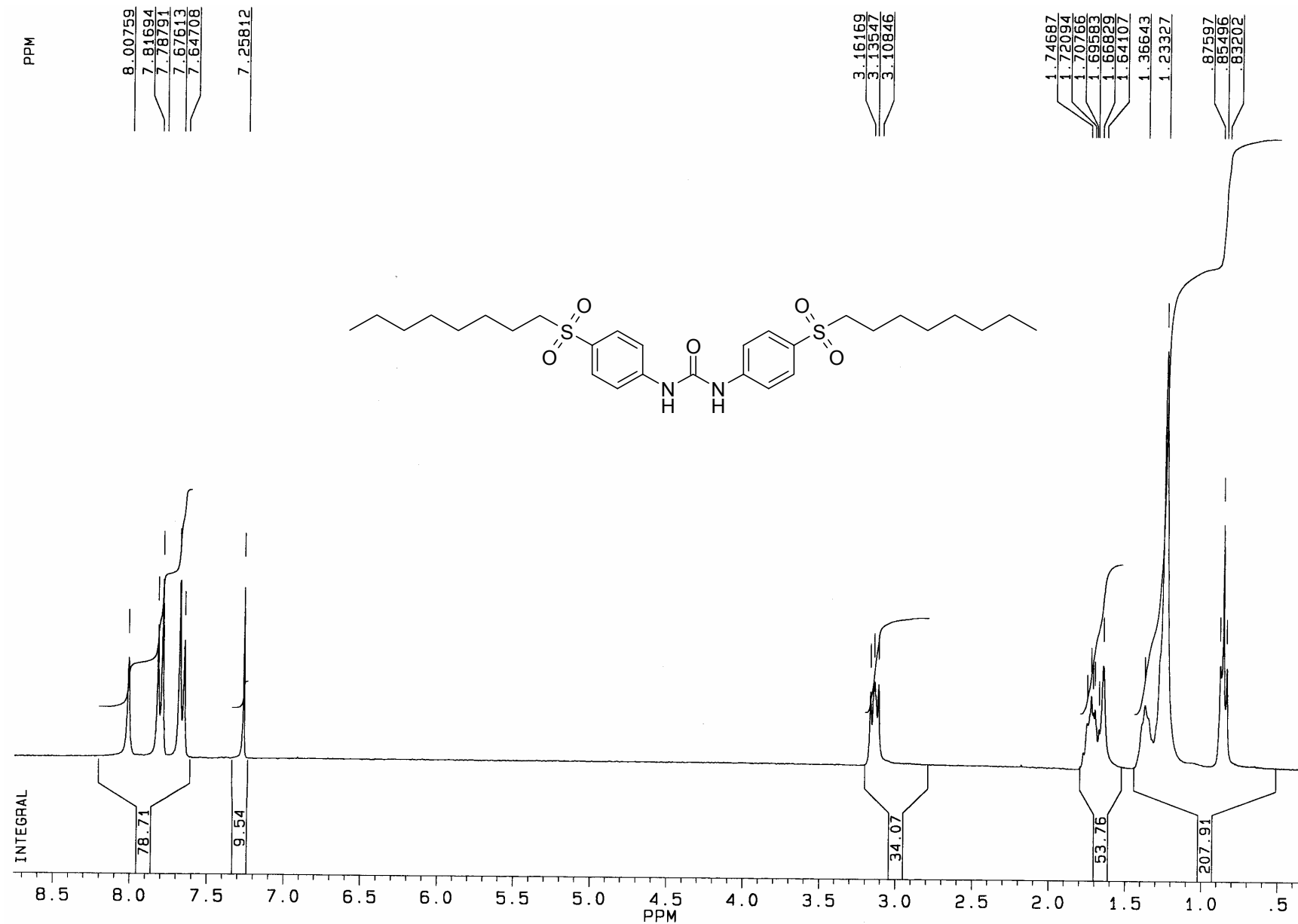


¹³C NMR (75 MHz, CDCl₃/DMSO-*d*₆) of 1-(4-nitrophenyl)-3-[4-(octyloxy)benzyl]urea **13**.

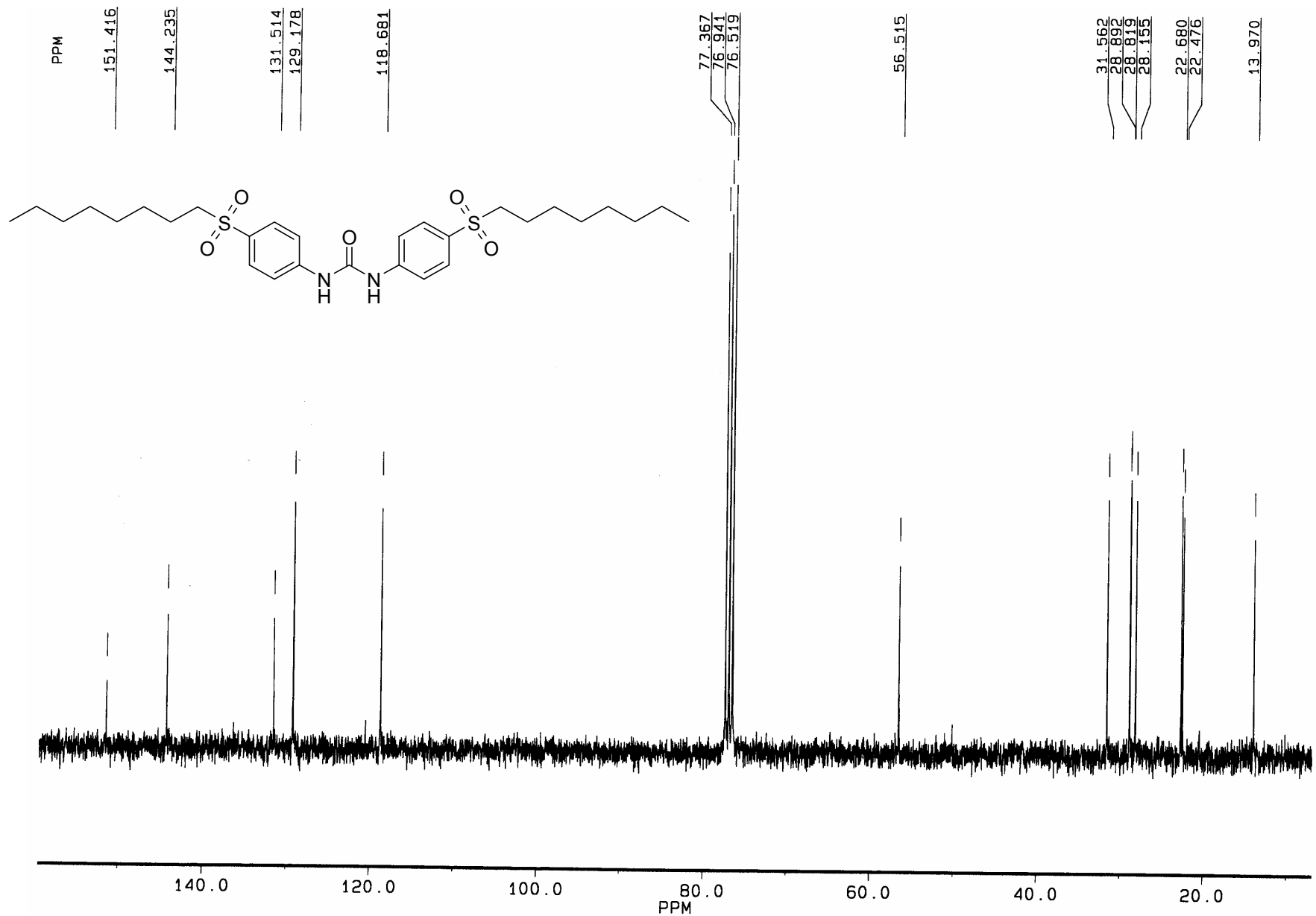




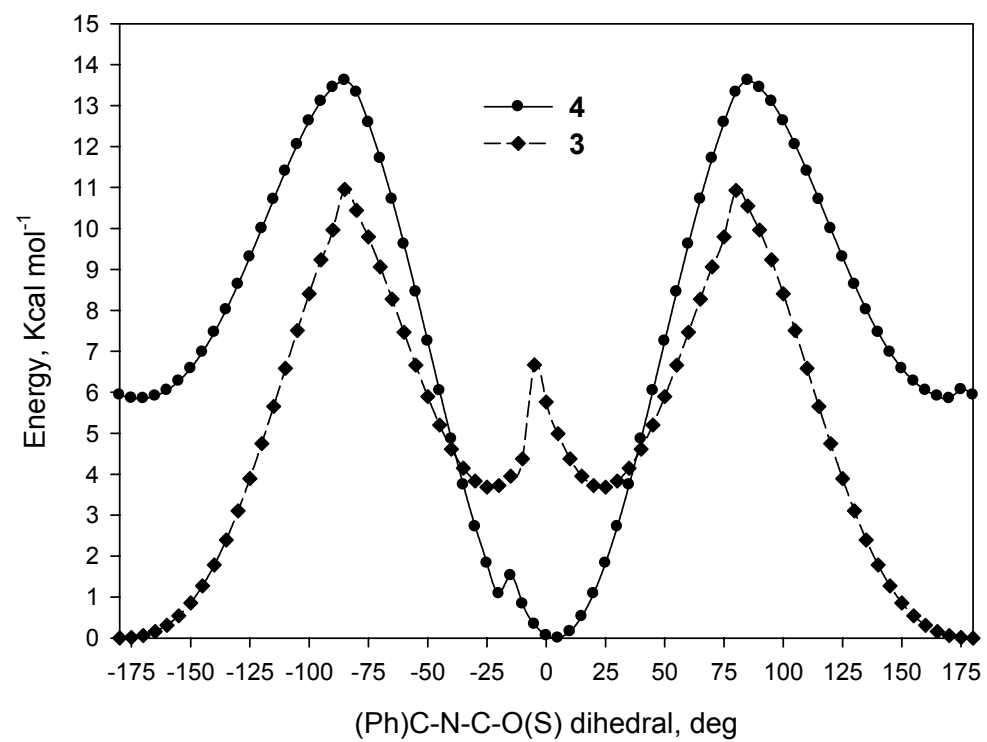
¹³C NMR (75 MHz, CDCl₃) of 1-[4-(octylsulfonyl)phenyl]-3-phenylurea **14**.



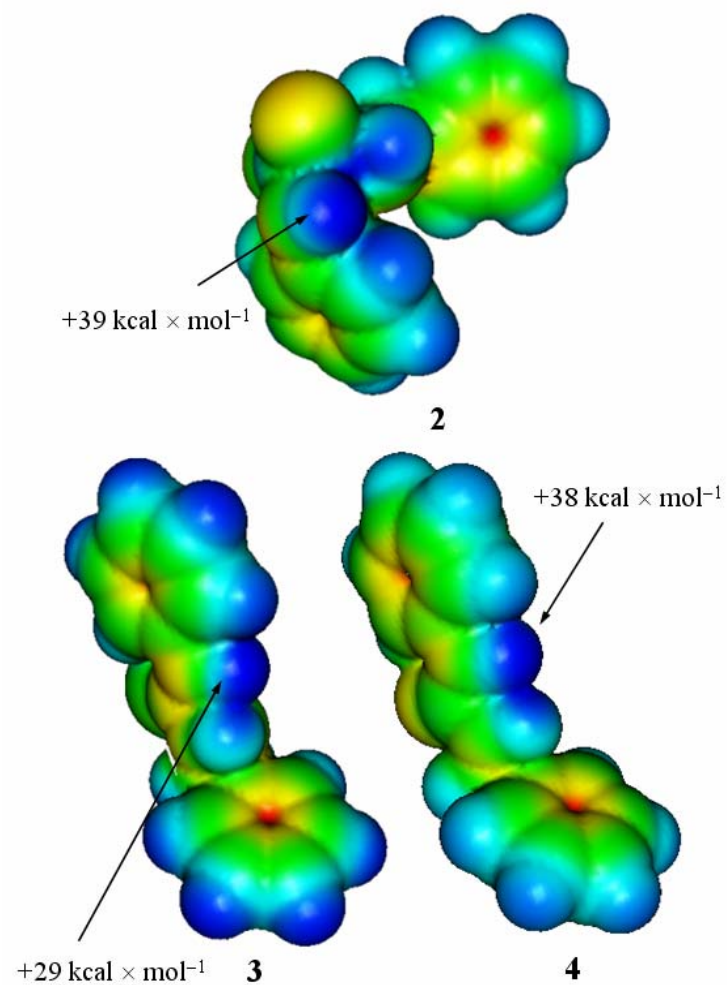
¹H NMR (300 MHz, CDCl₃) of 1,3-bis[4-(octylsulfonyl)phenyl]urea **15**.



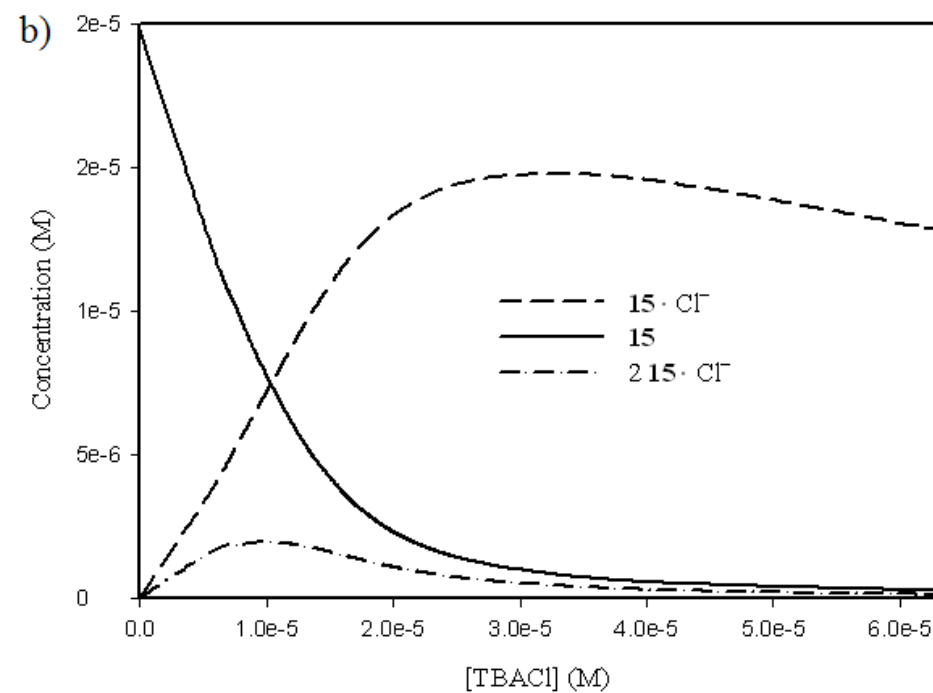
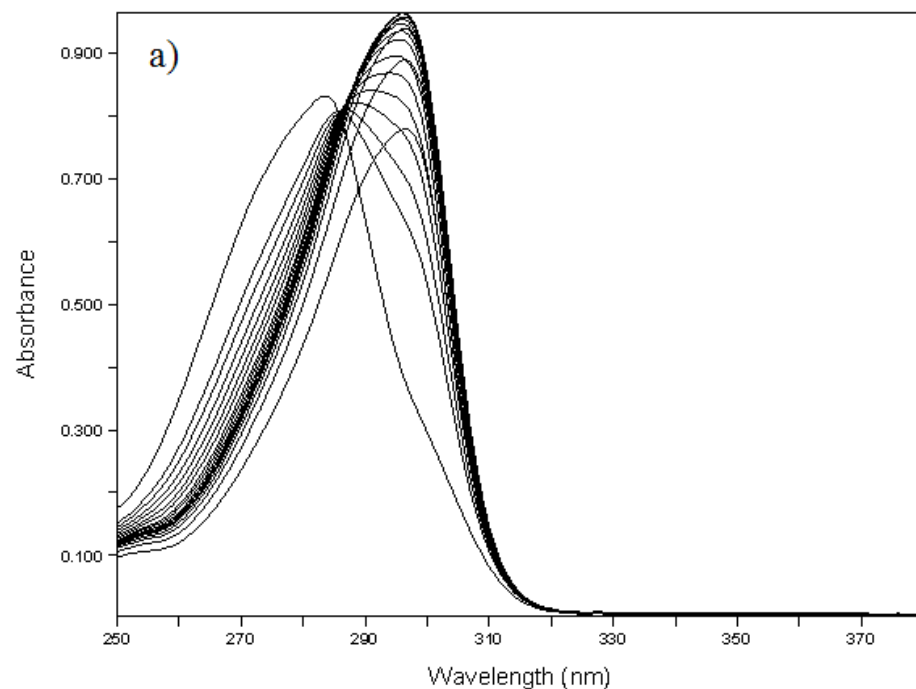
¹³C NMR (75 MHz, CDCl₃) of 1,3-bis[4-(octylsulfonyl)phenyl]urea **15**.



Rotational barriers obtained varying (Ph)C–N–C–O(S) dihedral from –180 to 180 for **3** and **4**



Molecular Electrostatic Potential (MEP) plotted onto the van der Waals surfaces. Mapping colours from red (negative) to blue (positive): **2** (-74 to $+39 \text{ kcal} \times \text{mol}^{-1}$), **3** (-70 to $+29 \text{ kcal} \times \text{mol}^{-1}$), and **4** (-72 to $+38 \text{ kcal} \times \text{mol}^{-1}$).



a) Family of spectra for the titration of a solution of **15** [2.0×10^{-5} M] with a solution of TBACl [2.0×10^{-4} M] in CHCl_3 ; b) distribution diagram relative to the chromophoric species present in solution during the titration.