—— **Supplementary Information** ——

Hydrogen Bonded Chiral Sheet Self-assembled from a C_3-Symmetric Tri-carbamate

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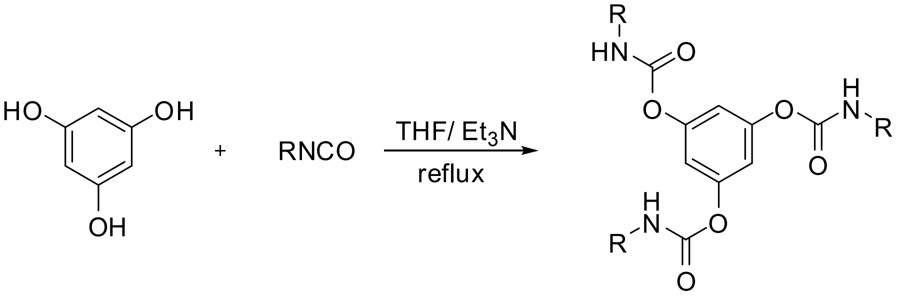
Material and Method

All starting materials were obtained commercially and used as received. Analytical TLC was performed on silica G TLC plates w/UV254 (Sorbent Technologies). ^{1}H NMR and ^{13}C NMR data were collected on a Brüker Advance 500 spectrometer, and processed with its self-bond software. The chemical shifts in spectra were measured in parts per million (ppm) on the delta (δ) scale relative to the resonance of the solvent peak (DMSO-d_6 signal as reference, ^{1}H = 2.50 ppm, ^{13}C = 40.5 ppm). Electrospray Ionization Mass Spectra (ESI-MS) were obtained using 10 mM ammonium acetate as the matrix on a Time-of-Flight MS G1969A Series 6200 spectrometer (Agilent Technologies Co. Ltd.) with Fragmentor 250 V and ESI 5000 V. IR spectra were acquired on a Perkin Elmer Spectrum 400 FT-IR/FT-FIR spectrometer. The X-ray data were collected by a Brüker D8 single crystal X-ray diffractometer (Apex II). X-ray powder diffraction spectra were recorded on a X'PERT-PRO X-ray diffractometer (PANalytical, Netherlands) equipped with a 3 kW copper tube X-ray generator of $\lambda = 0.1541$ nm under 40 mA and 45 kV. Spectra were collected at room temperature in a 2θ range of 3°~35° at a scanning rate of 3° /min. TEM measurements were performed with a Hitachi 7500 TEM with accelerate voltage 80 kV. TEM samples from quick injection were prepared as following: 100 μL of a certain clear solution of tri-carbamate **1** was quickly injected into a 20 mL of vial with 10 mL of water in with vigorous stirring. Afterwards, the solution was agitated using an ultrasonic instrument for about 10 min and aged overnight. Then, the solution was placed on a 200 mesh copper grid with formvar carbon as a support film and completely air dried prior to being observed by TEM.

Synthesis of Benzene-1,3,5-triyl tris(propylcarbamate)



R = -C_3H_7, tri-carbamate **1**

Scheme 1S. Synthesis of benzene-1,3,5-triyl tris(propylcarbamate) **1**.

A flame dried 50 mL round bottom flask equipped with a magnetic stir bar was charged with 1-isocyanatopropane (2.12 g, 25 mmol) and a catalytic amount of triethylamine (5 drops) in 10 mL of tetrahydrofuran (THF). The mixture was stirred at room temperature for 5 minutes. Phloroglucinol (0.94 g, 7.5 mmol) in 5 mL of THF was added drop wise for 10 minutes. Then, the mixture was refluxed for 17 hours. The mixture was concentrated by evaporating two thirds of the solvent with a rotavapor, and then precipitated in 250 mL of ice cold water. The solid product was filtered on a Buchner funnel and washed several times with deionized water. The tri-carbamate **1** (m.p 143-145°) was obtained as a white solid (2.64 g, 94%) by filtration. Crystals of compound **1** for powder and single crystal X-ray diffraction analysis were obtained by slow evaporation of ethyl acetate, which can also be grown by slow evaporation of acetonitrile or THF/H_2O (20:1). ^{1}H NMR (DMSO-d_6, 500 MHz) δ 0.87 (t, J = 7.0 Hz 9H), 1.46 (m, 6H), 3.00 (m, 6H), 6.72 (s, J = 5.0 3H), 7.81 (t, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 12.2, 23.3, 43.2, 112.8, 152.4, 154.6; IR (Nujol) cm^{-1} 3308, 2923, 1711, 1534, 1456, 1250, 1143, 1035; HRMS calculated for $C_{18}H_{27}N_3O_6$ (M+H$^+$), 382.1978, (M+NH$_4^+$) 399.2243; found 382.1972, 399.2238.

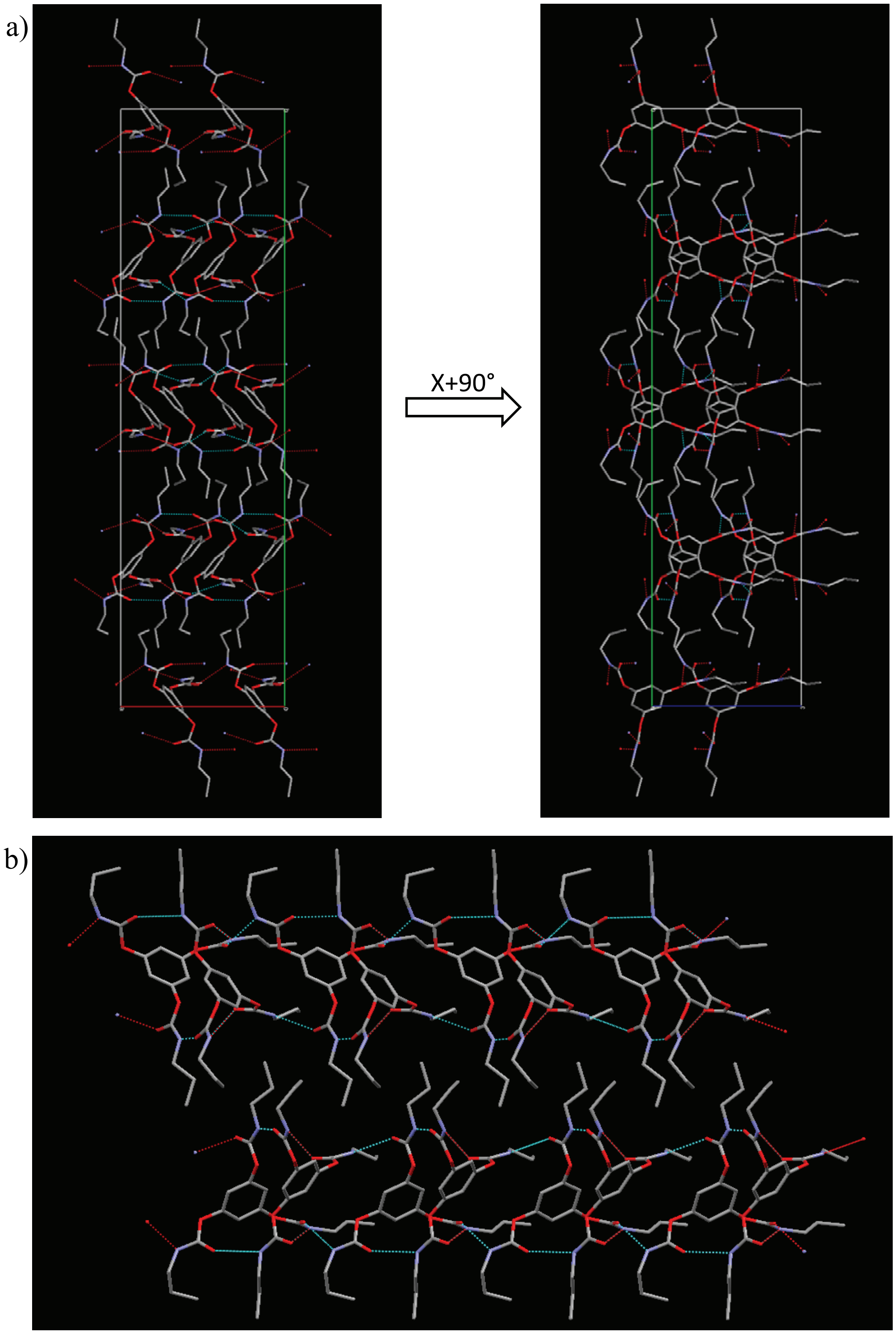
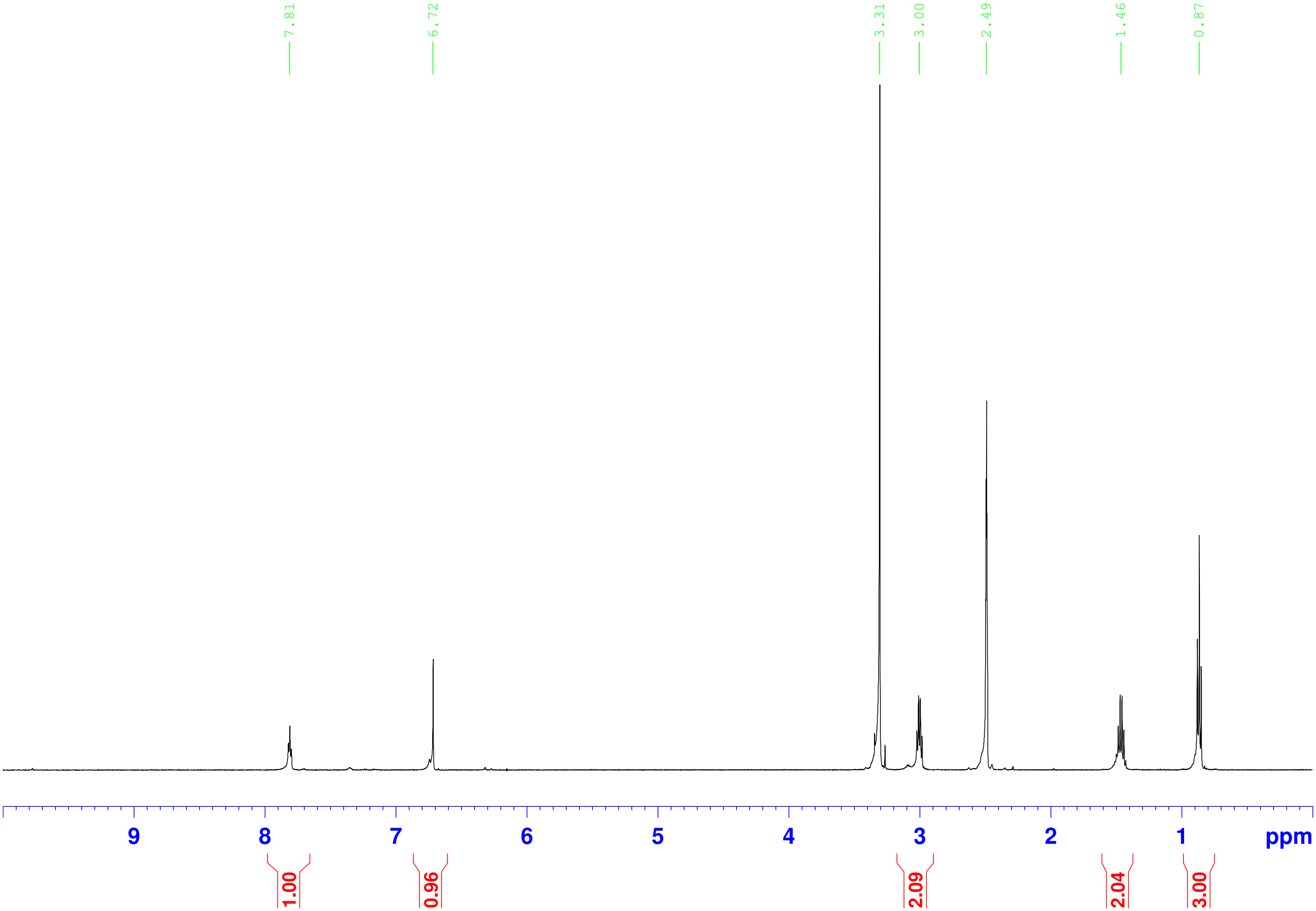


Fig. 1S Crystal packing of benzene-1,3,5-triyl tris(propylcarbamate) **1**: (a) Unit Cell; (b) Side view of the two layered sheet.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6
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ppm
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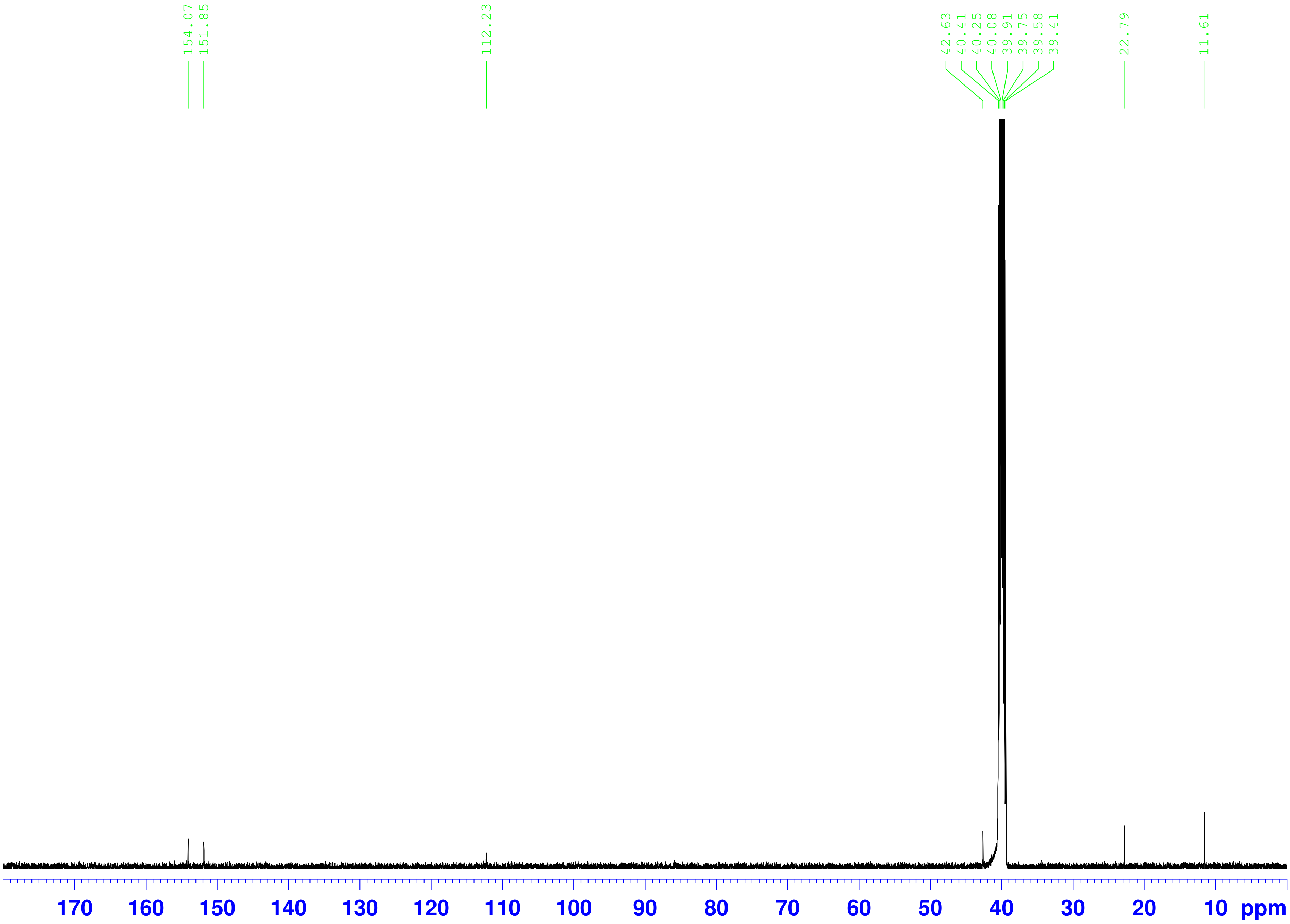
2.04
3.00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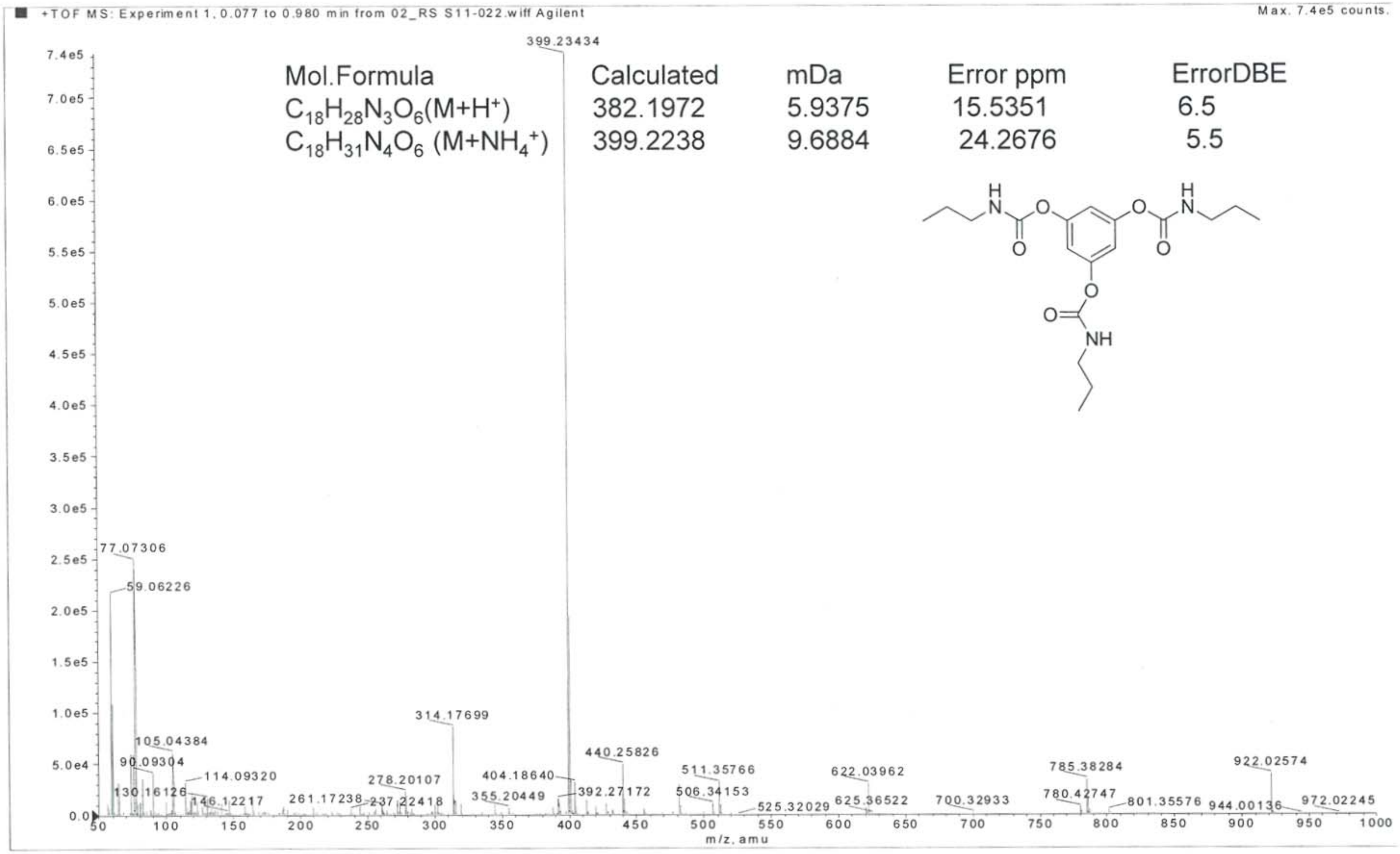
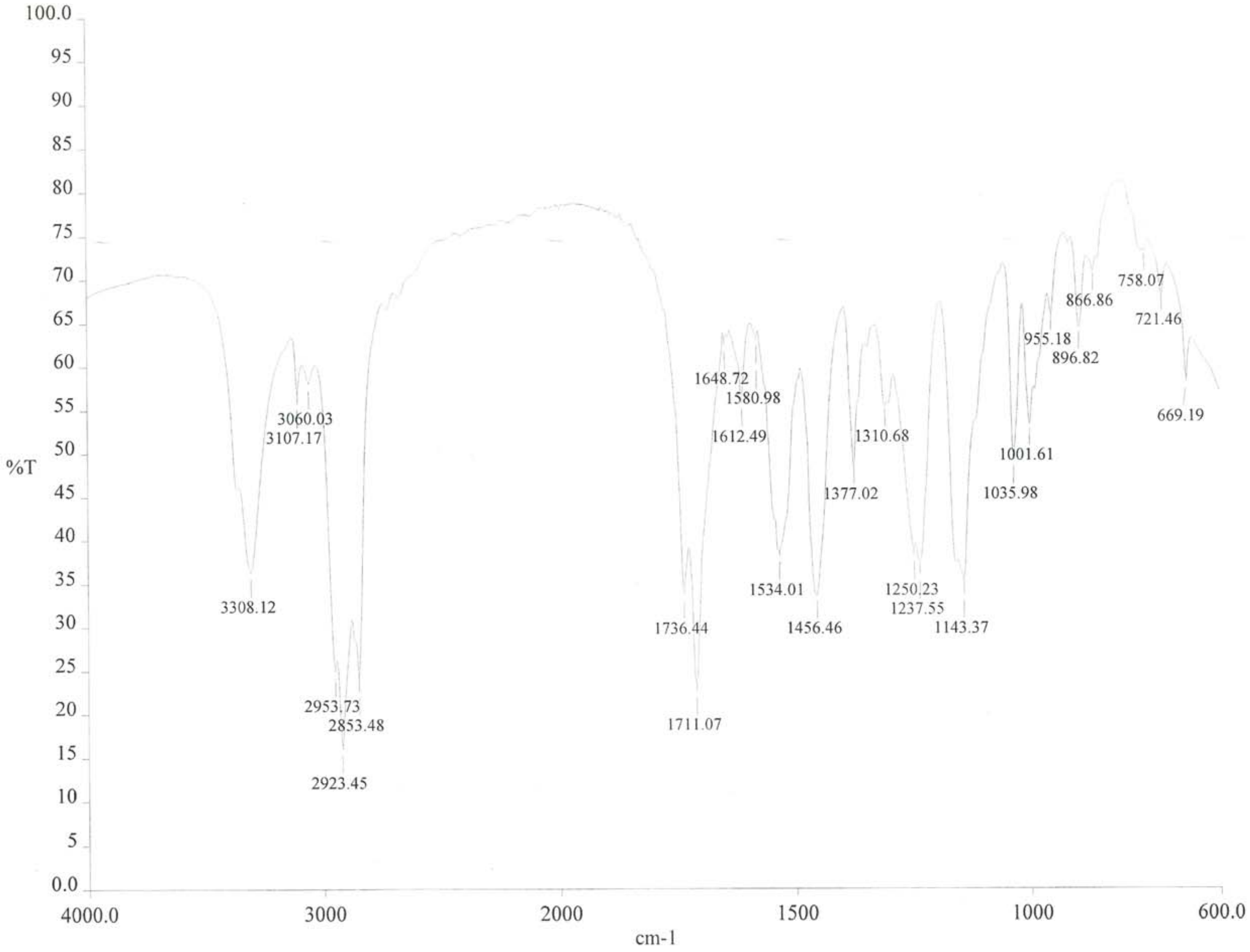


Mol.Formula	Calculated	mDa	Error ppm	ErrorDBE
$C_{18}H_{28}N_3O_6(M+H^+)$	382.1972	5.9375	15.5351	6.5
$C_{18}H_{31}N_4O_6$ $(M+NH_4^+)$	399.2238	9.6884	24.2676	5.5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2000
1500
1000
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