

Supporting Information

Template-Directed Synthesis of Kinetically and Thermodynamically Stable Molecular Necklace Using Ring Closing Metathesis

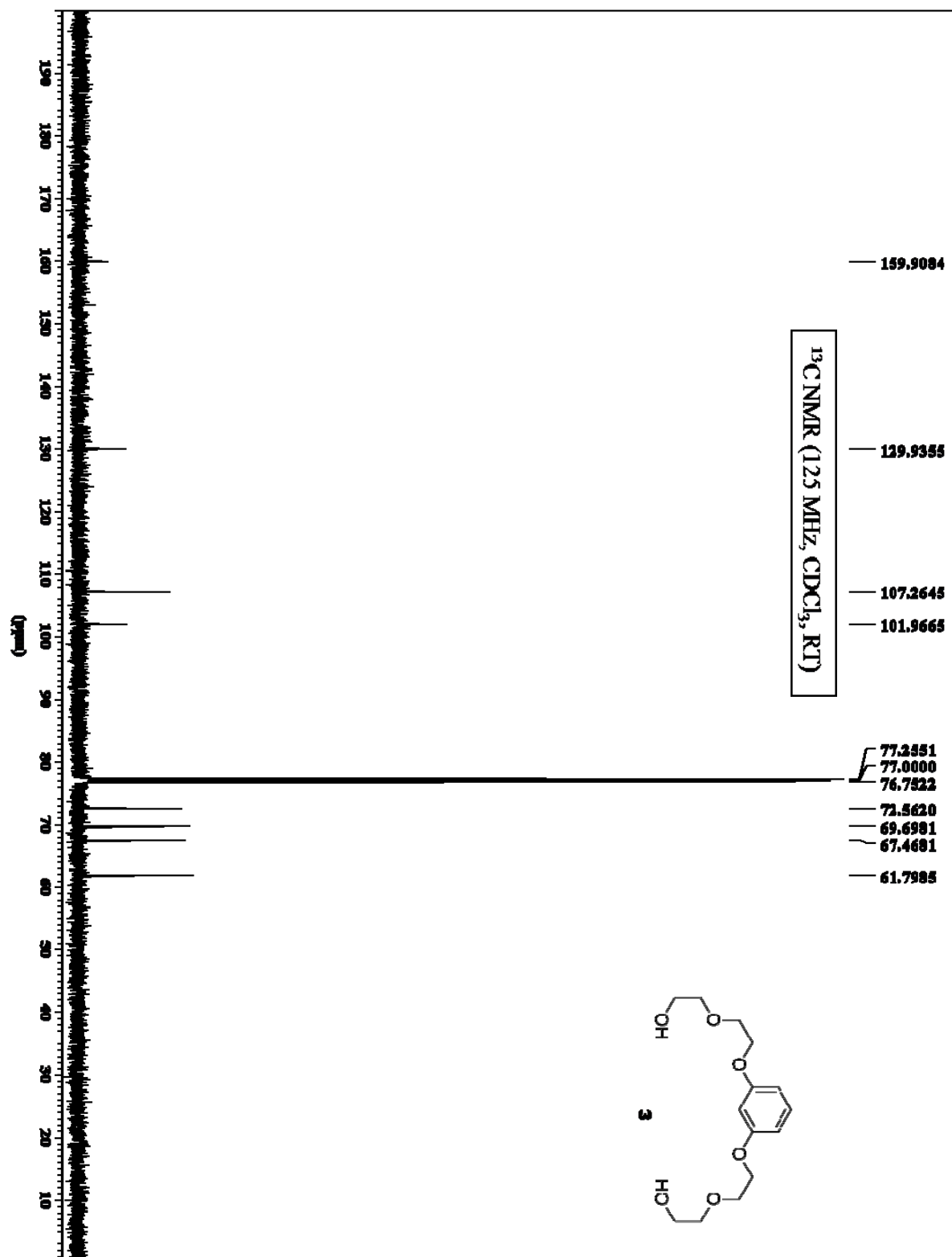
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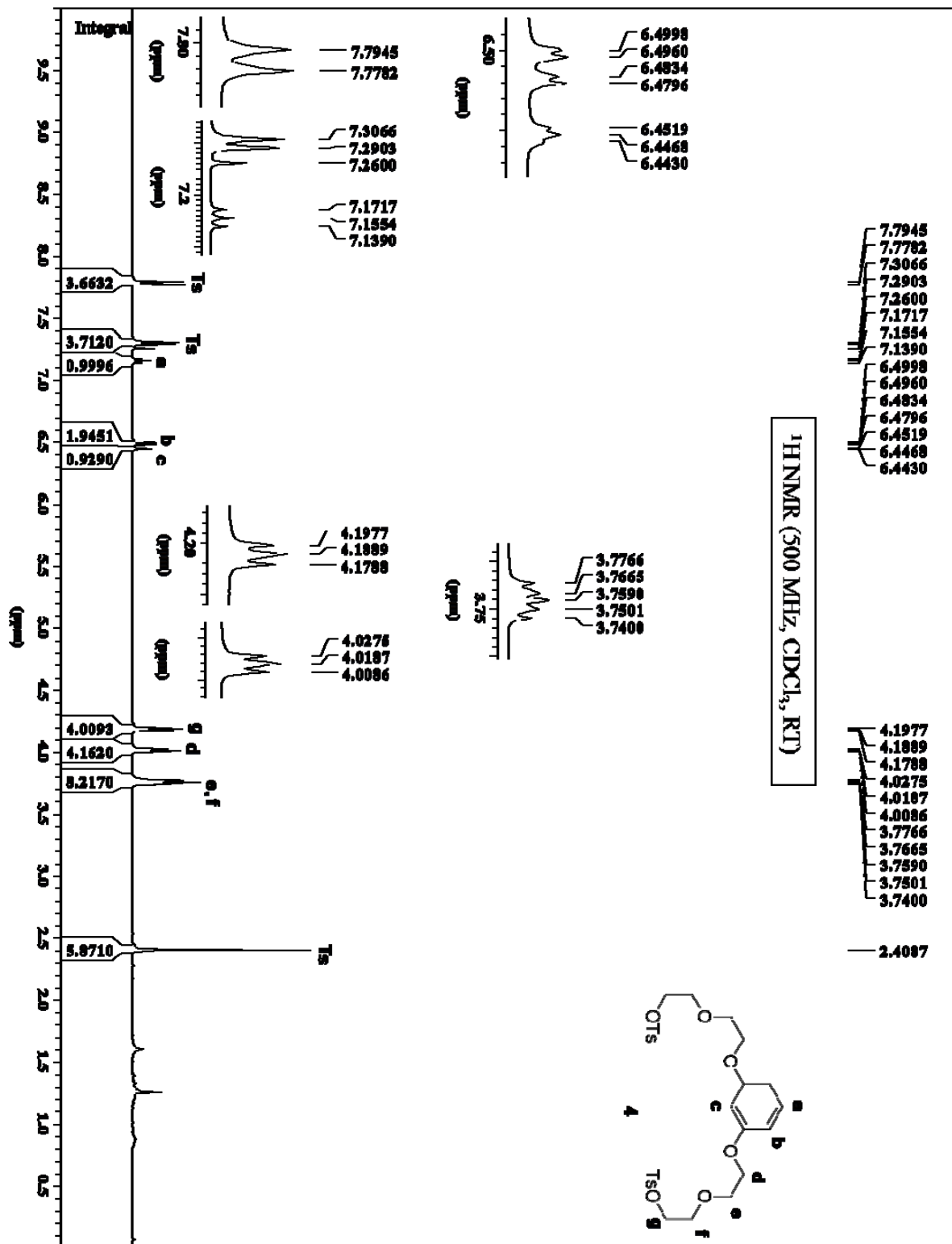
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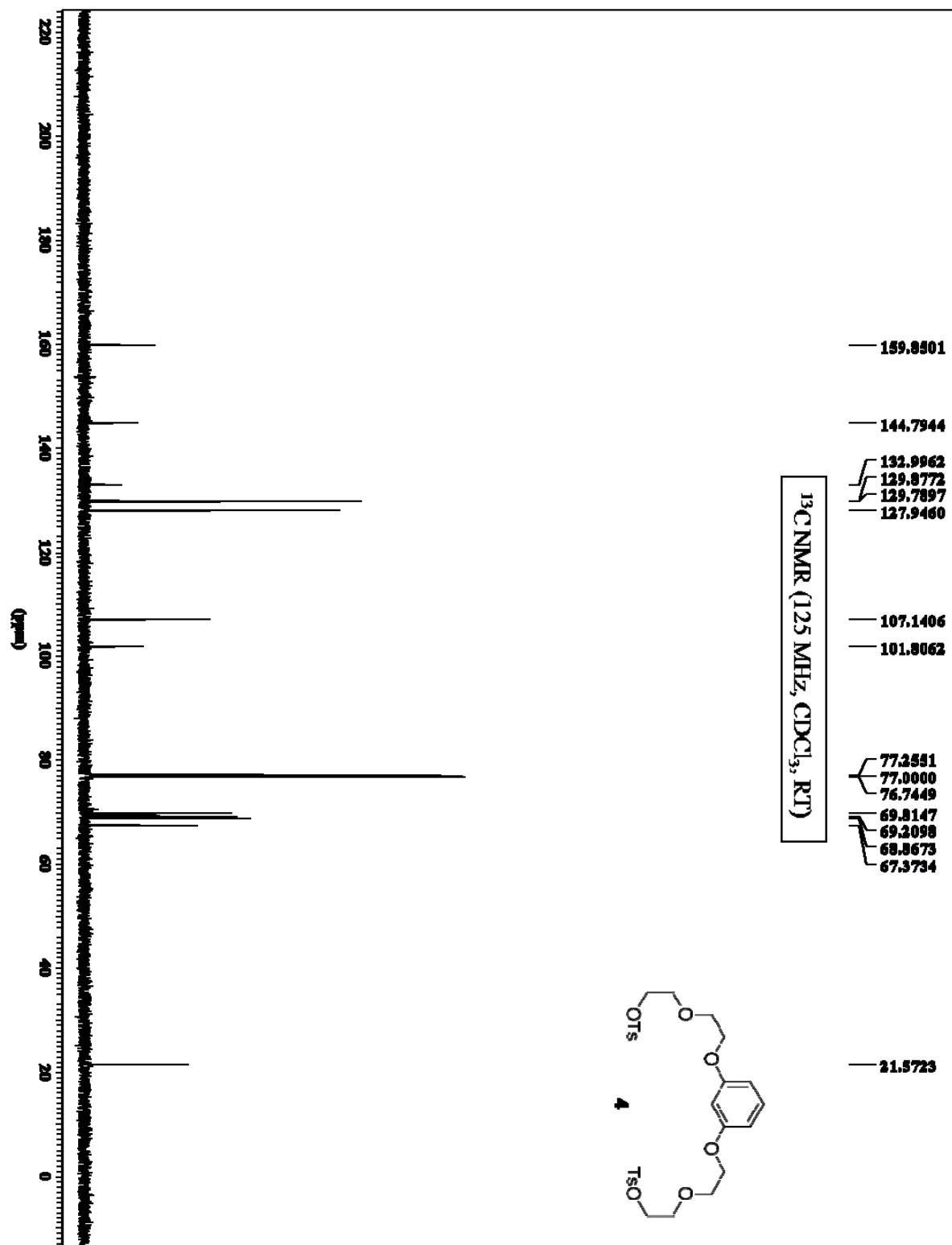
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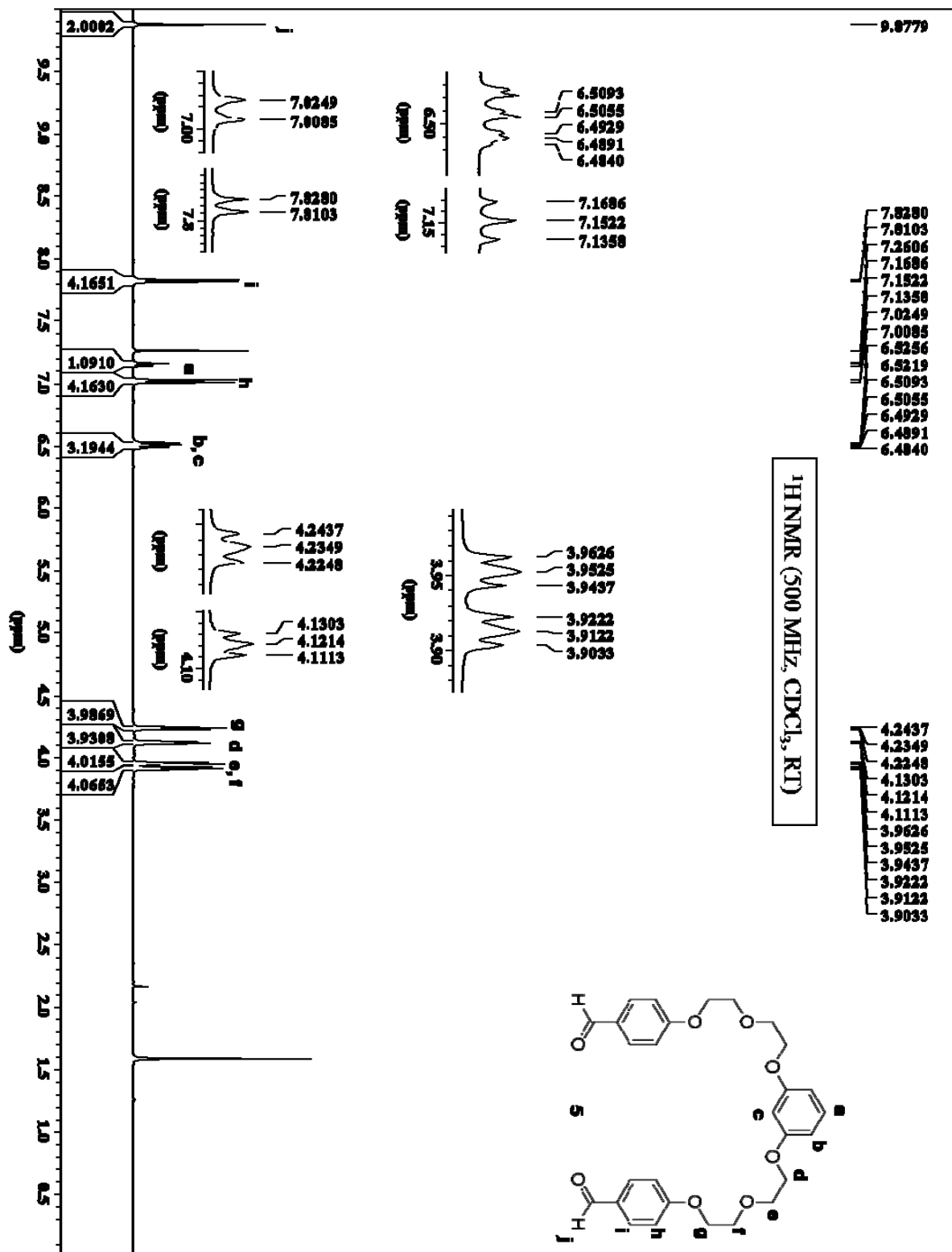
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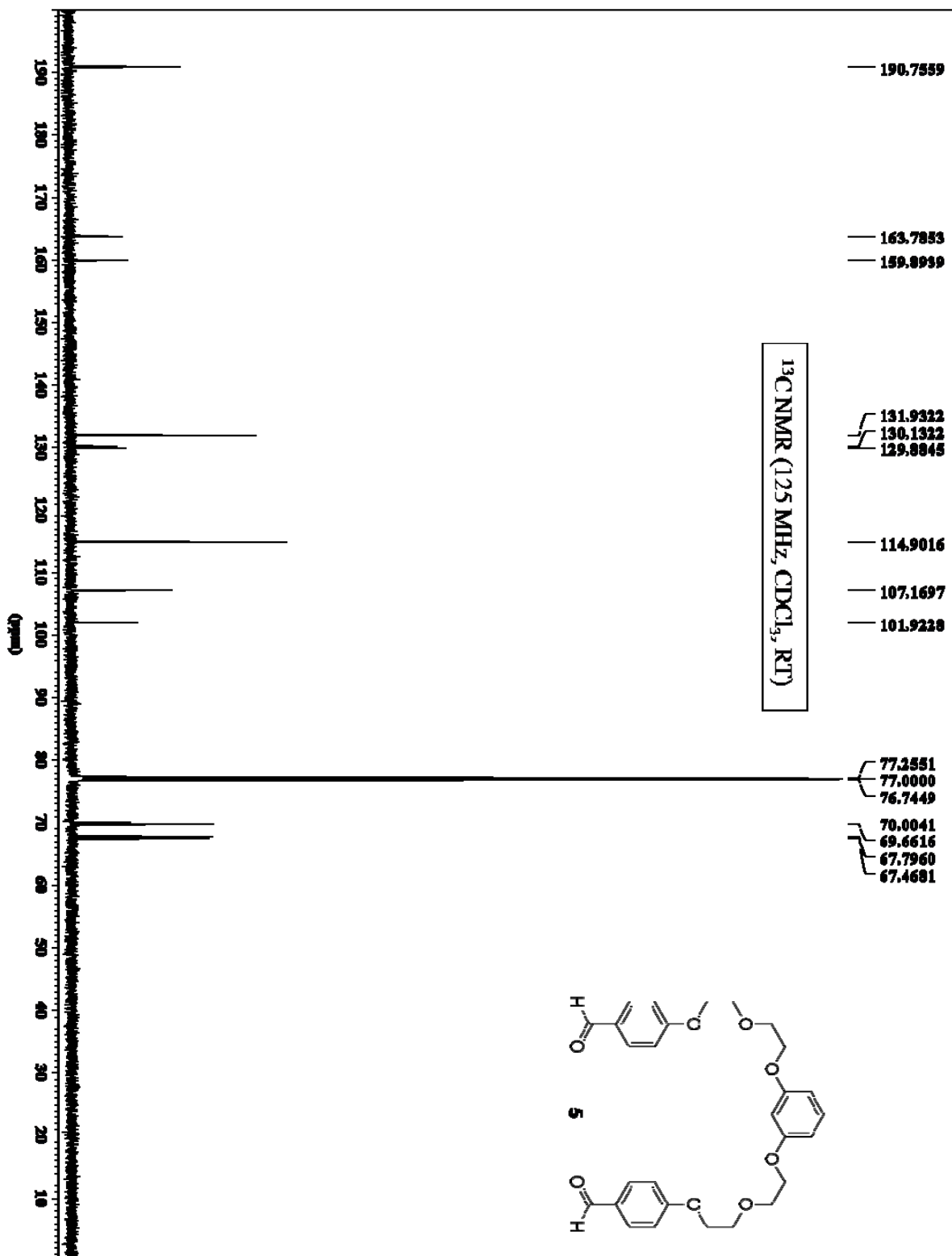


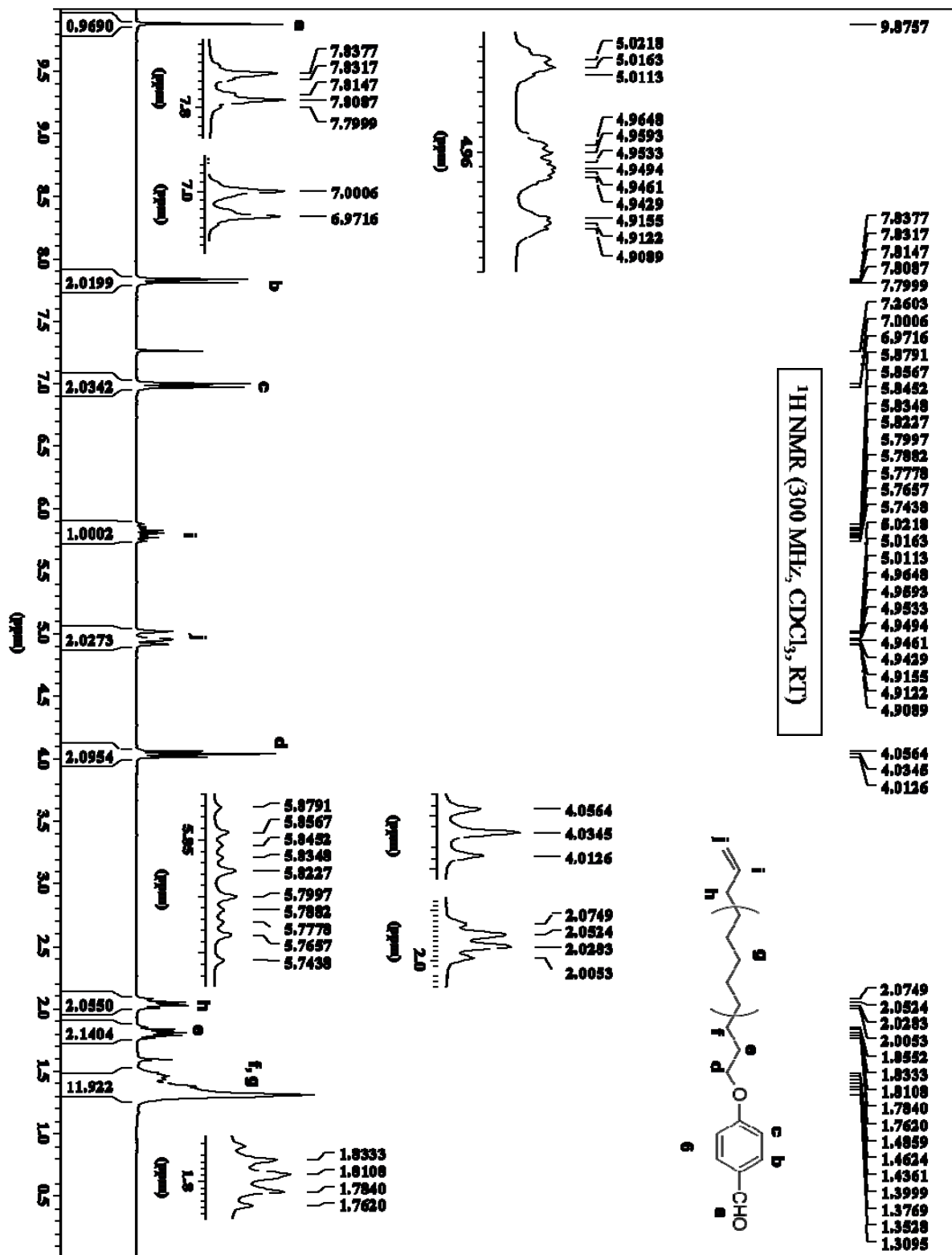


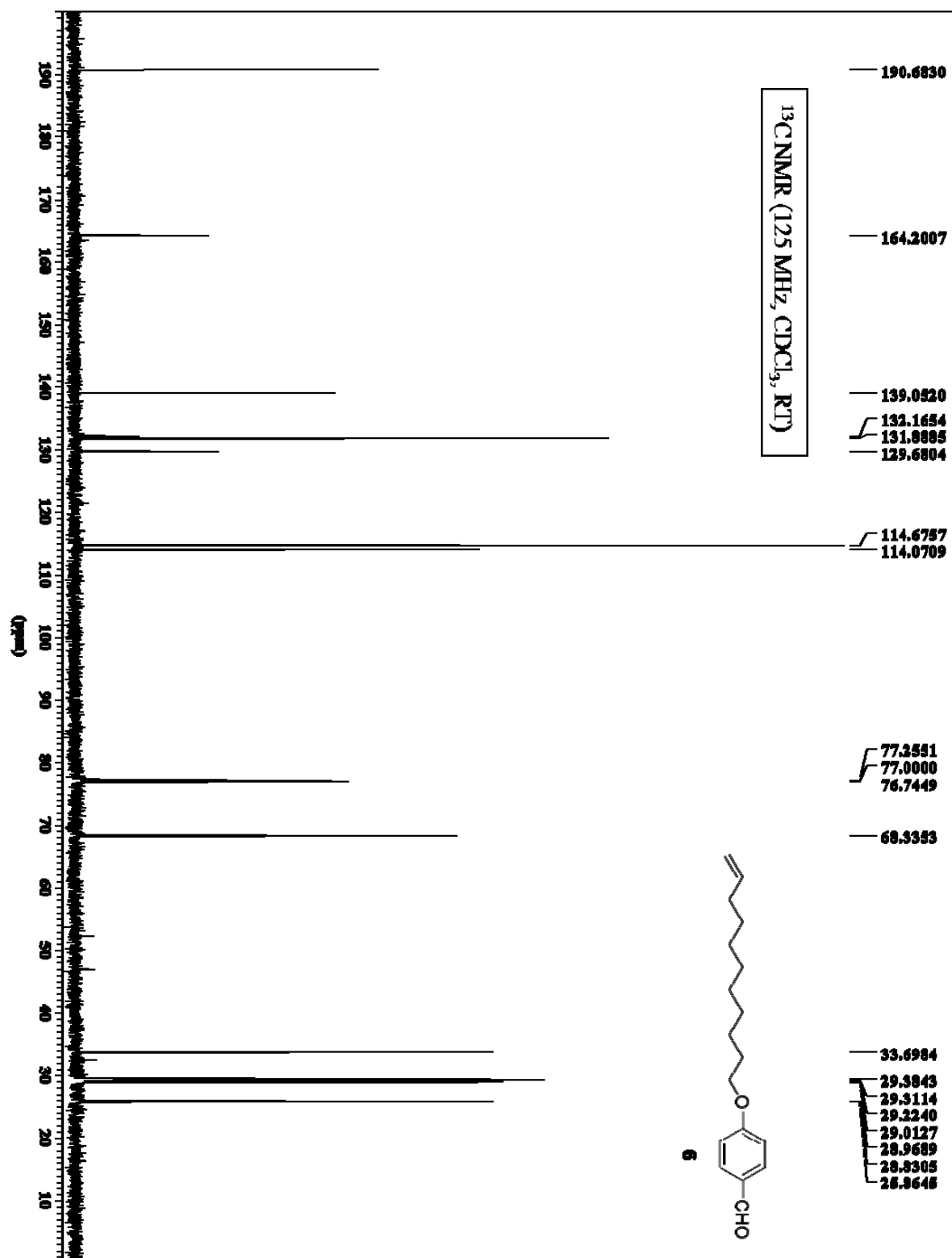


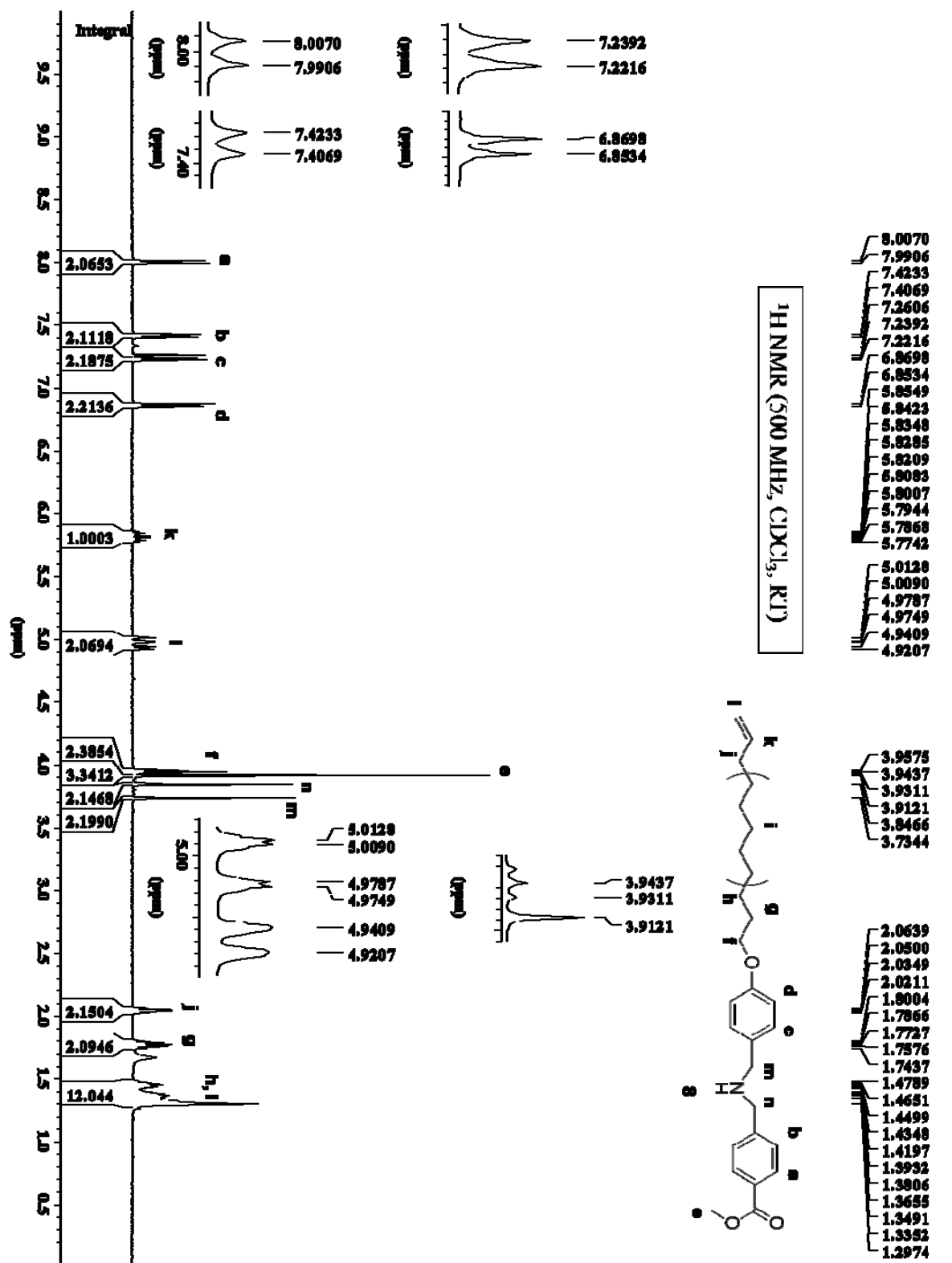


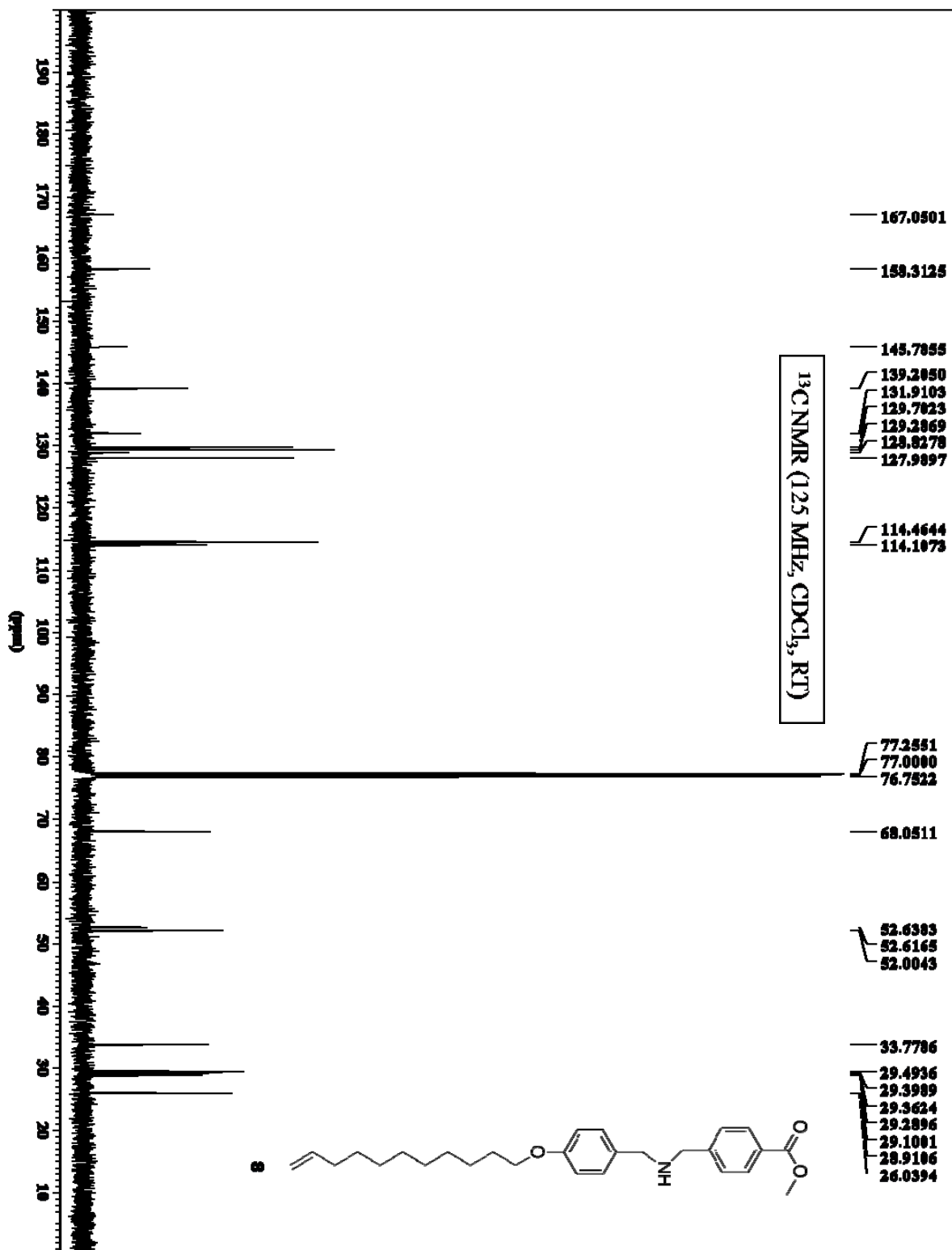


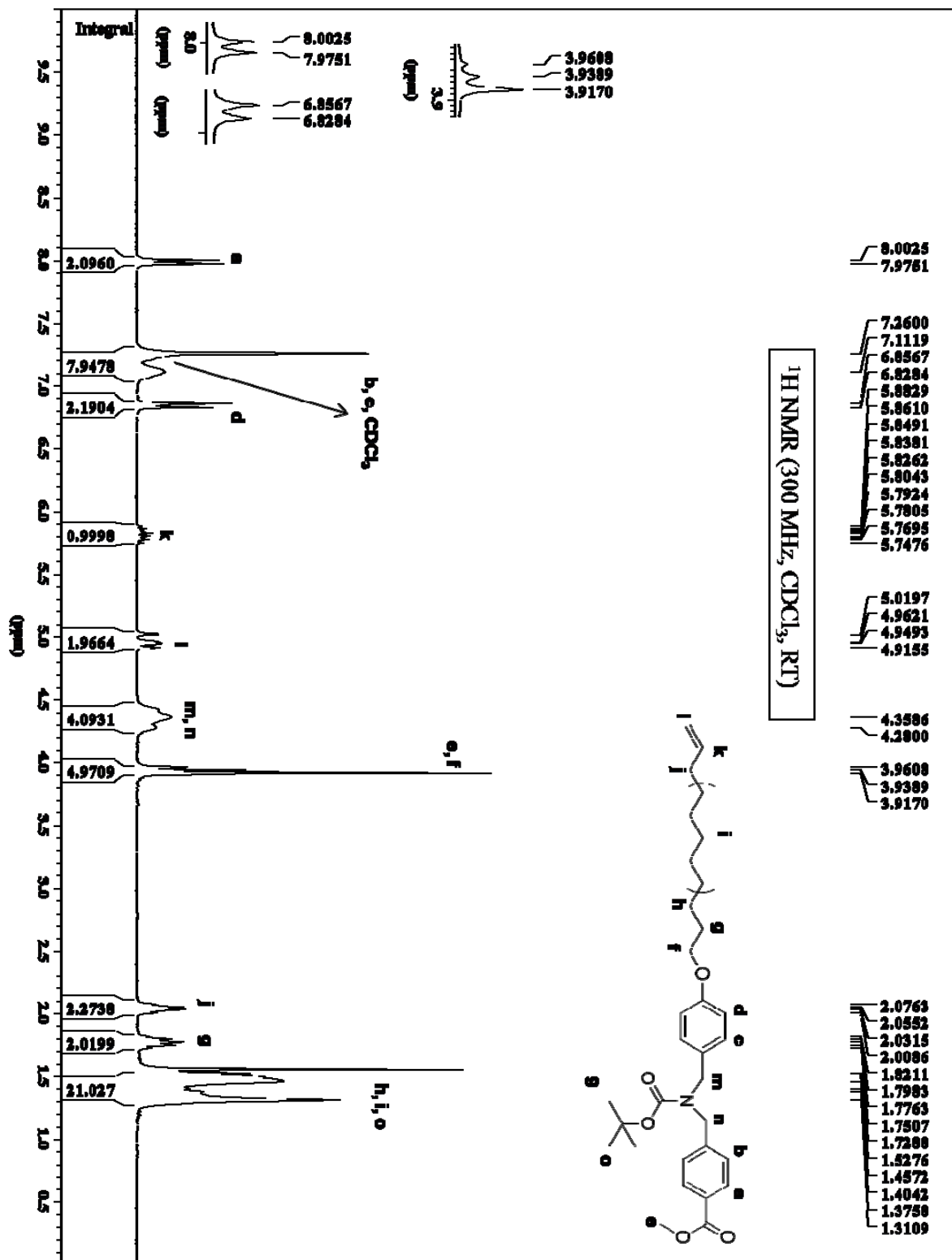


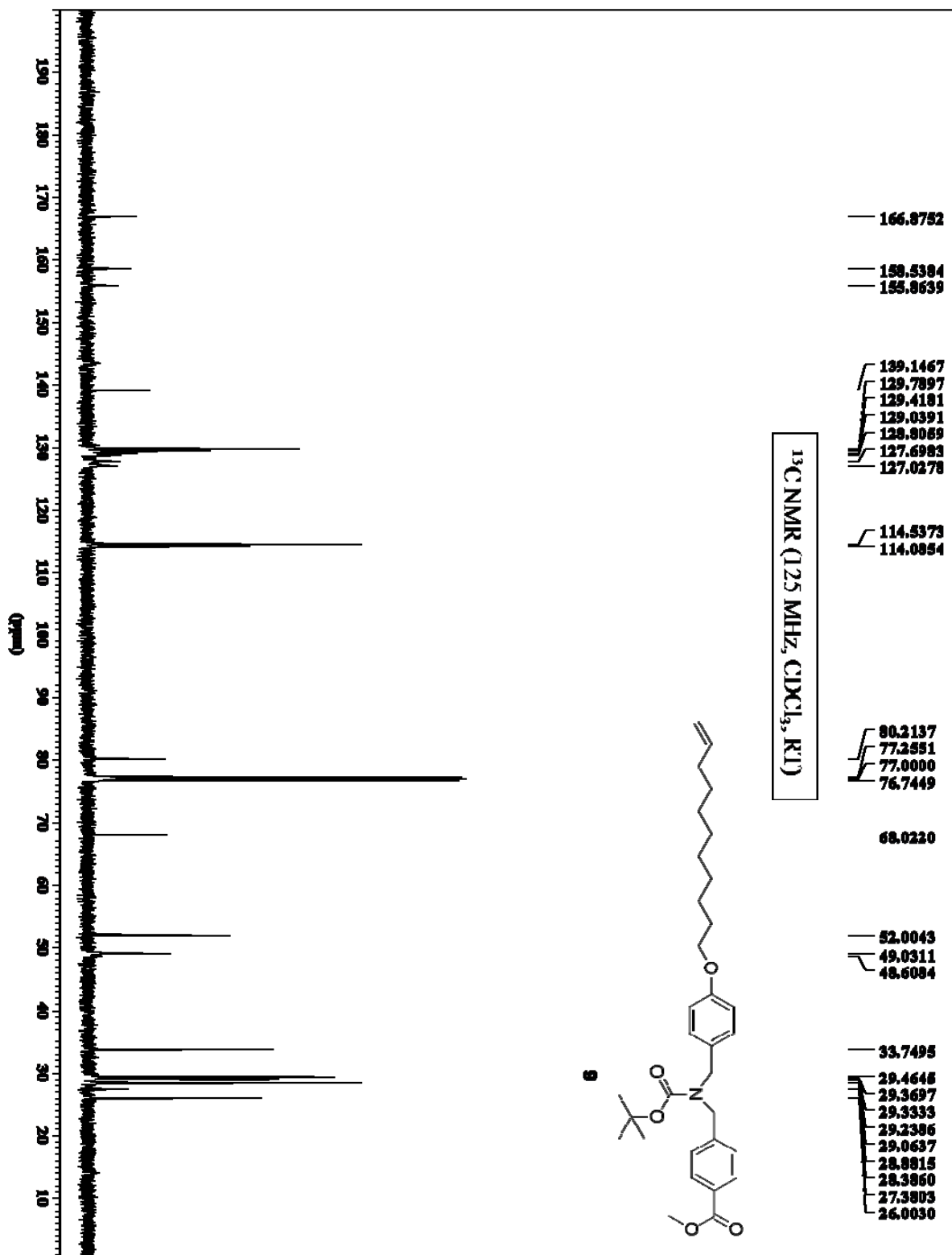


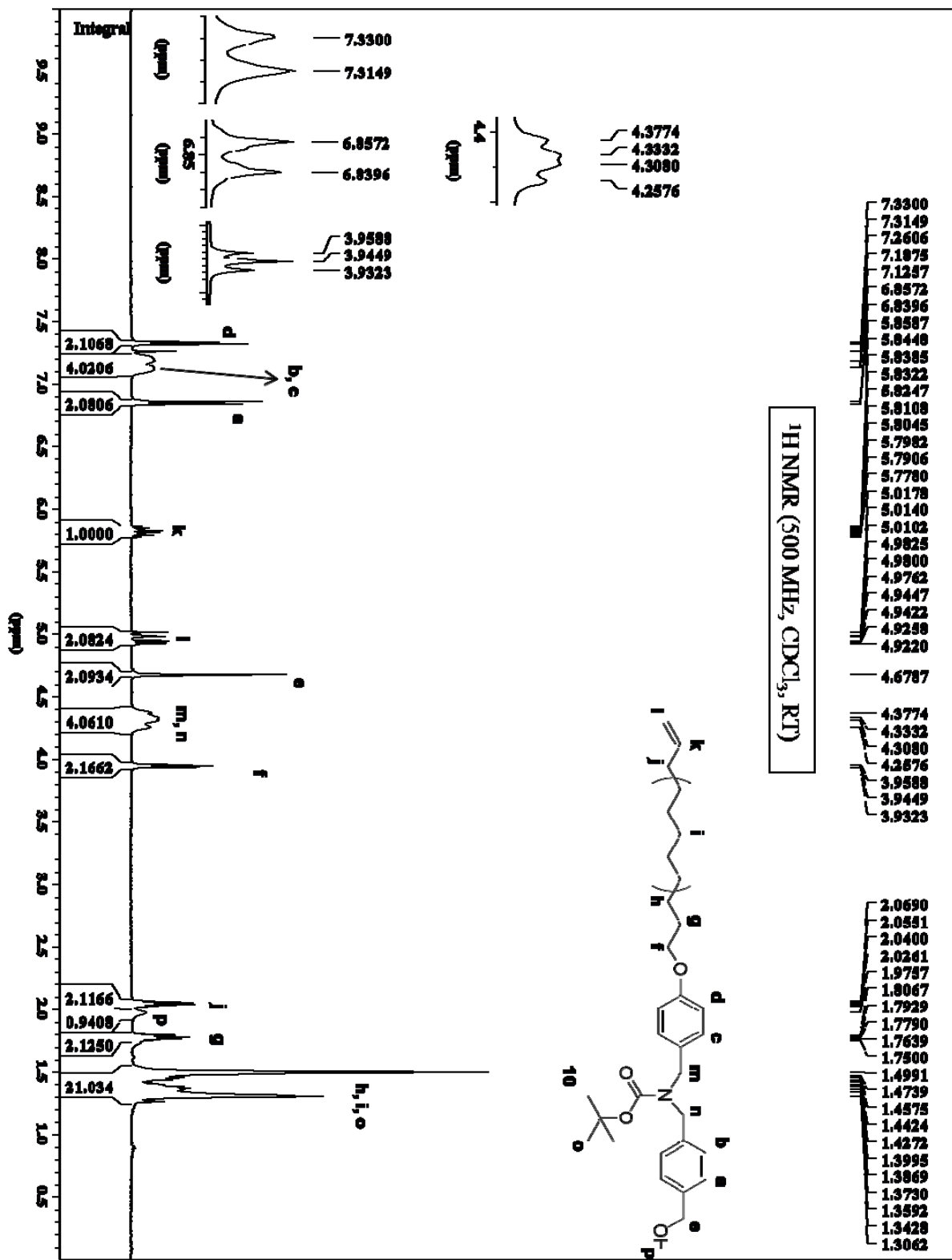


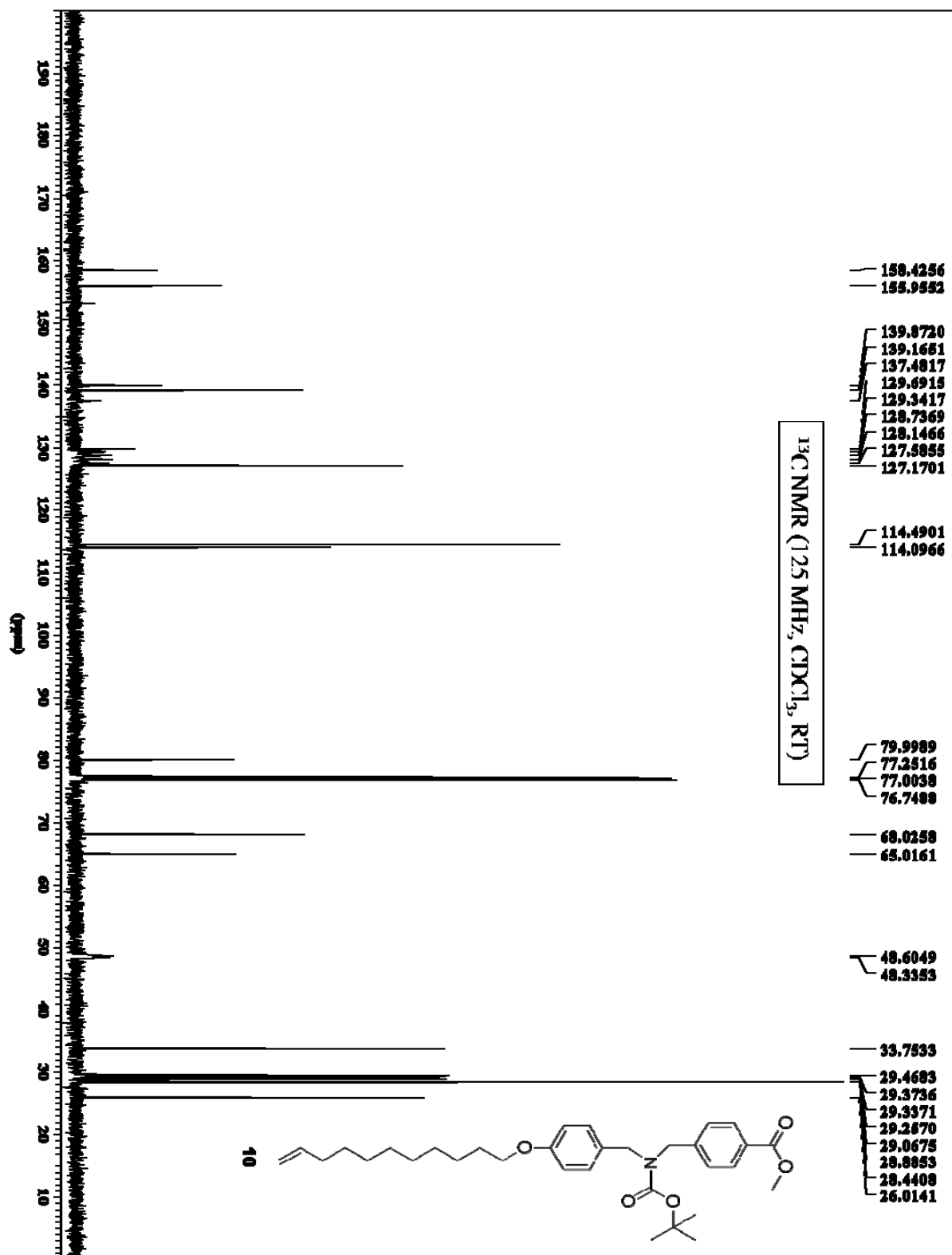


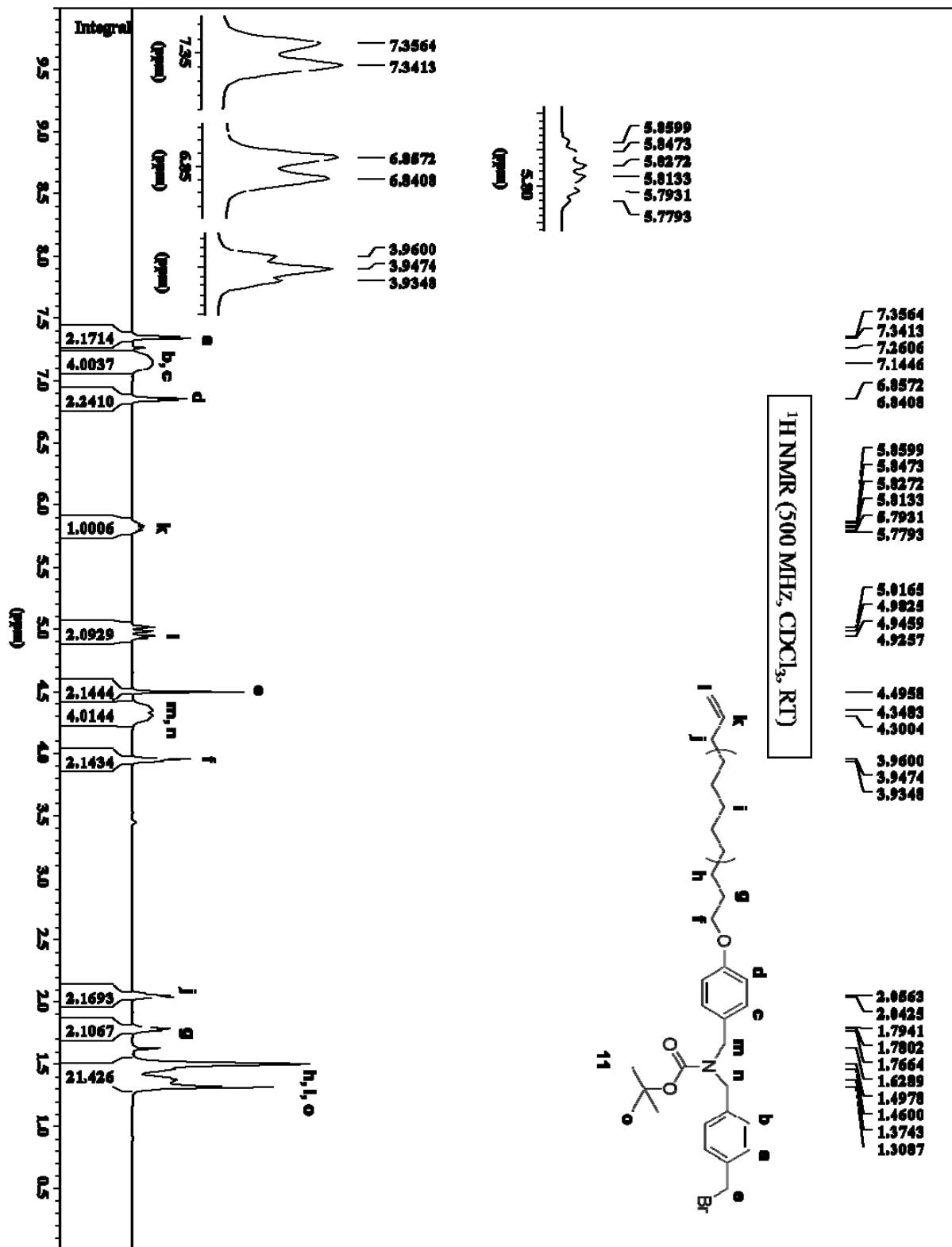


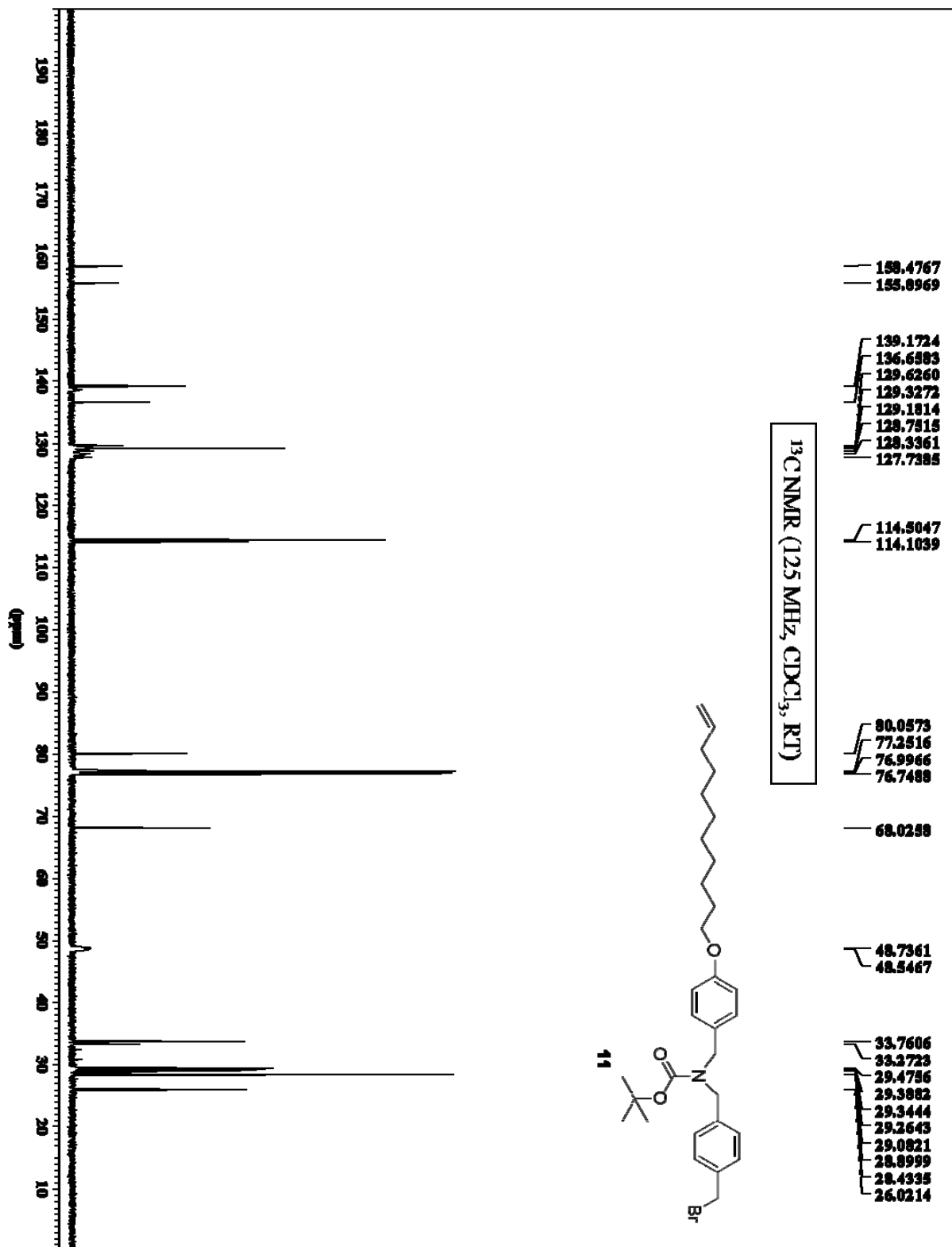


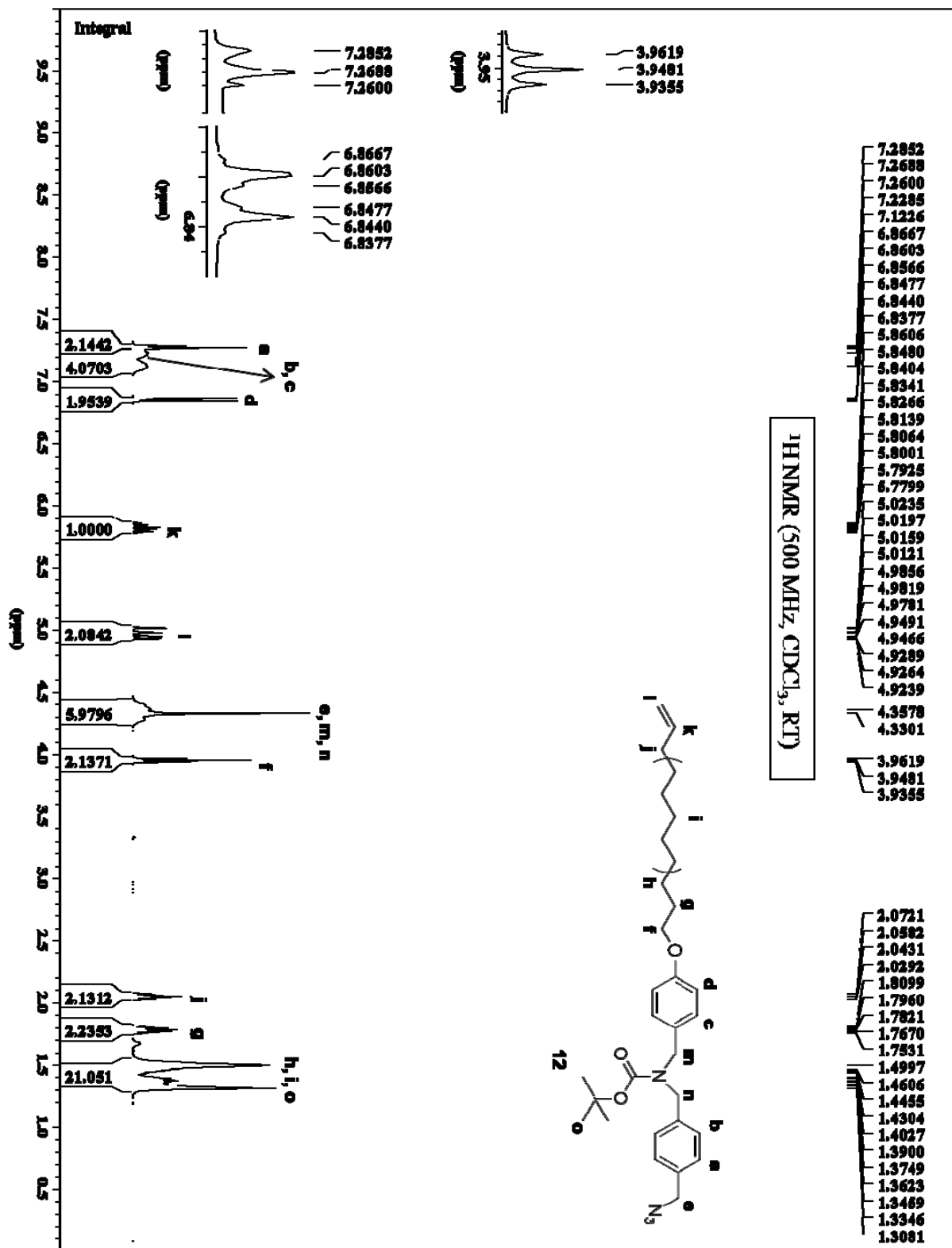


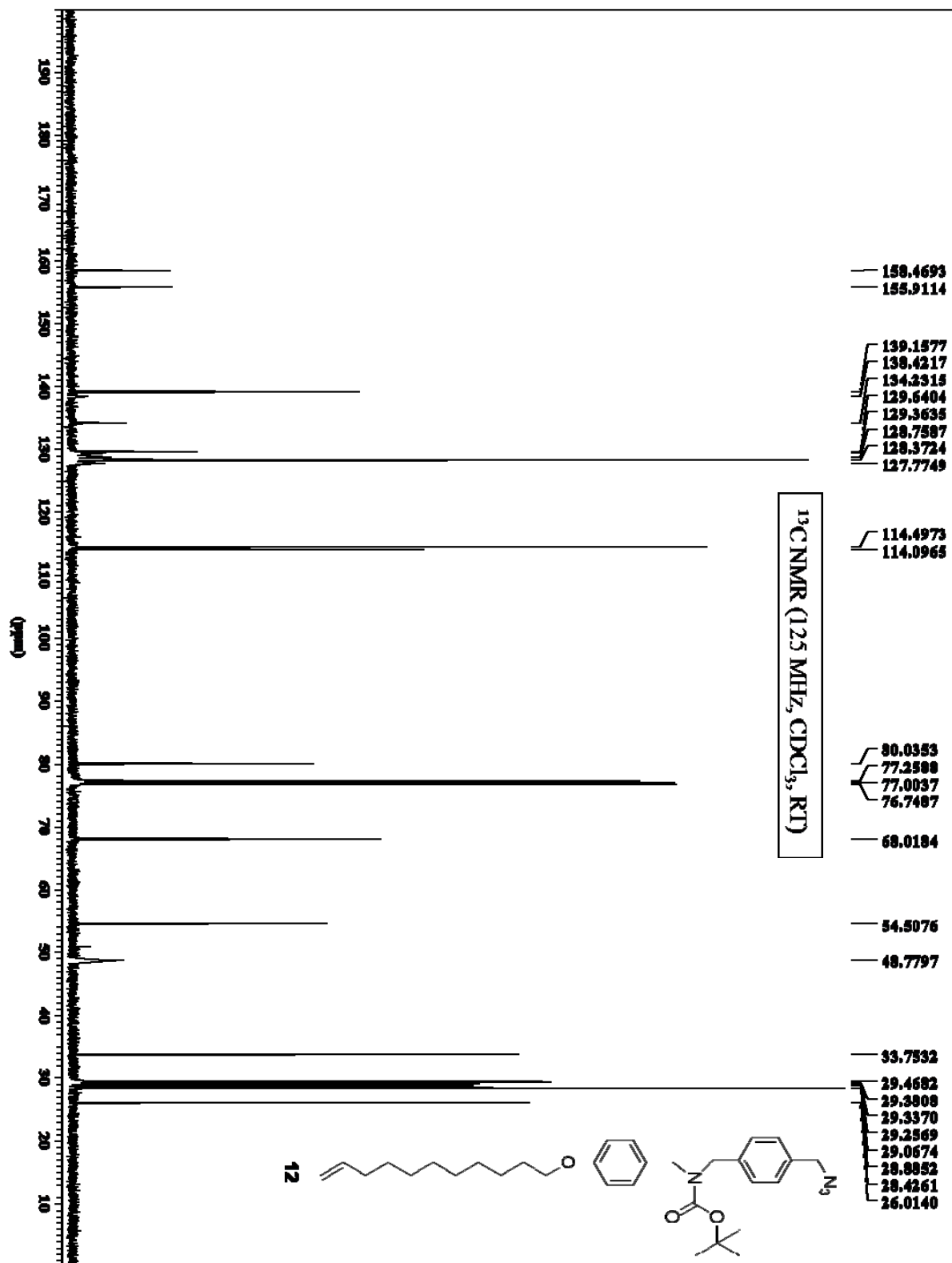


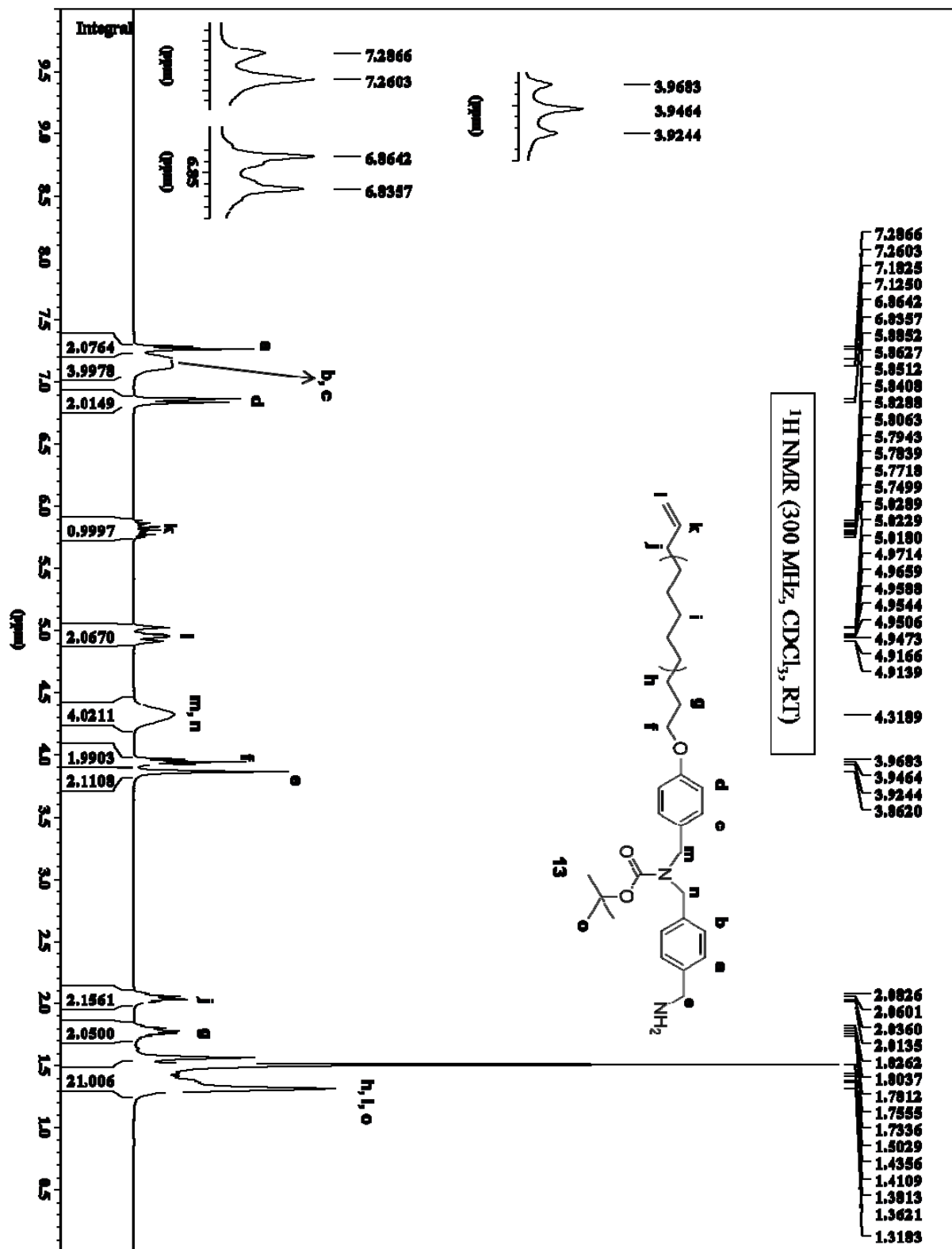


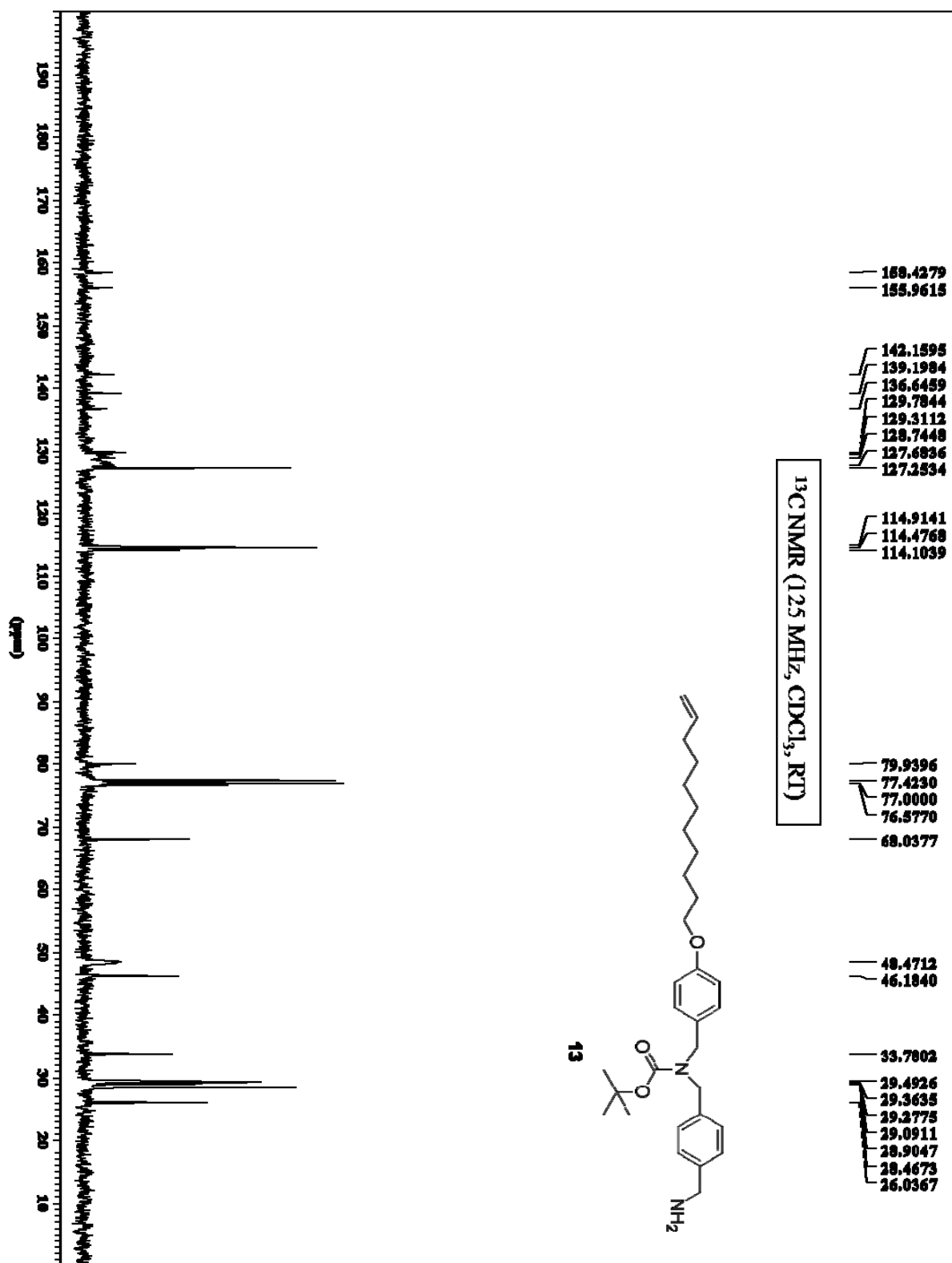


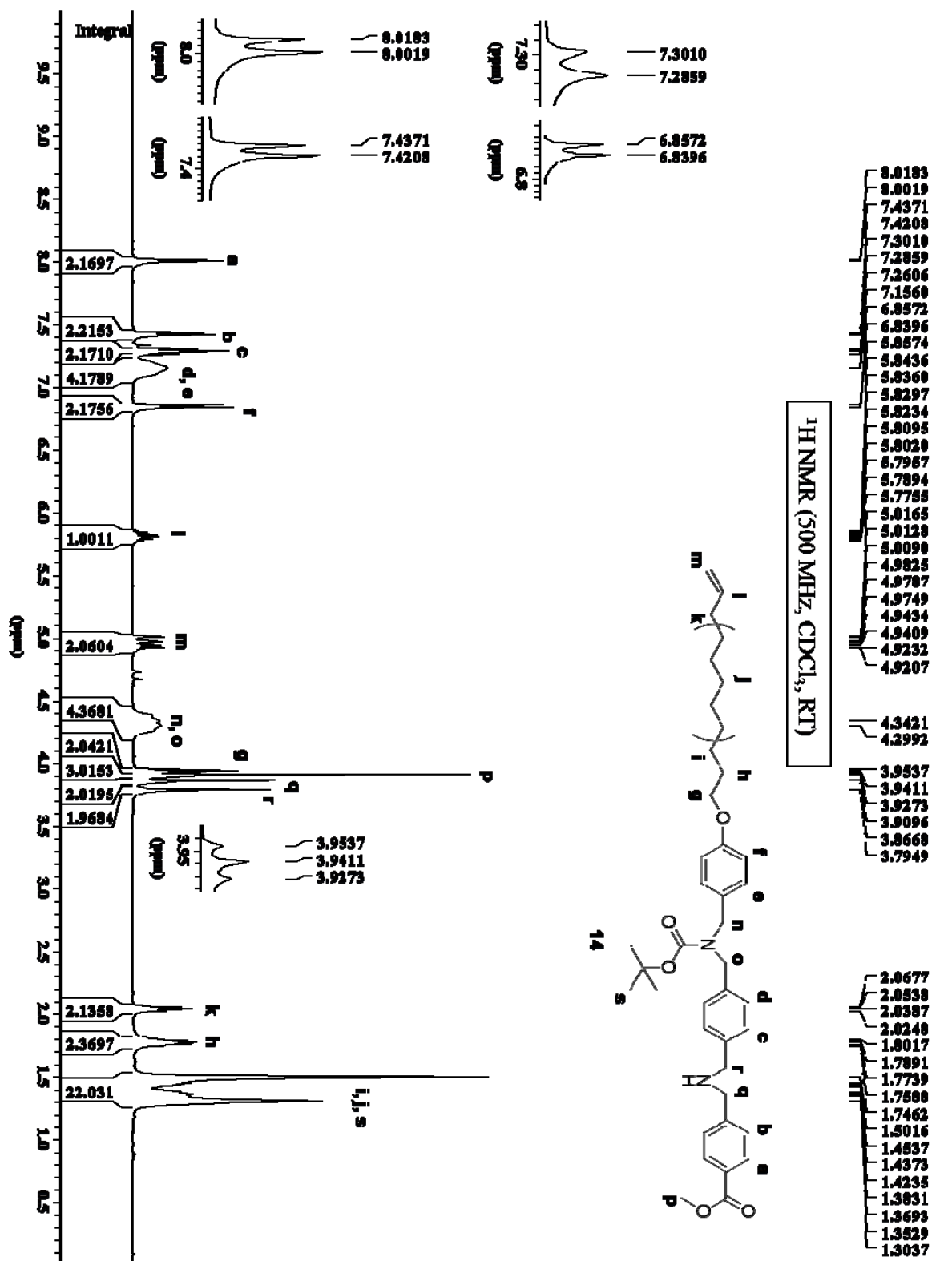


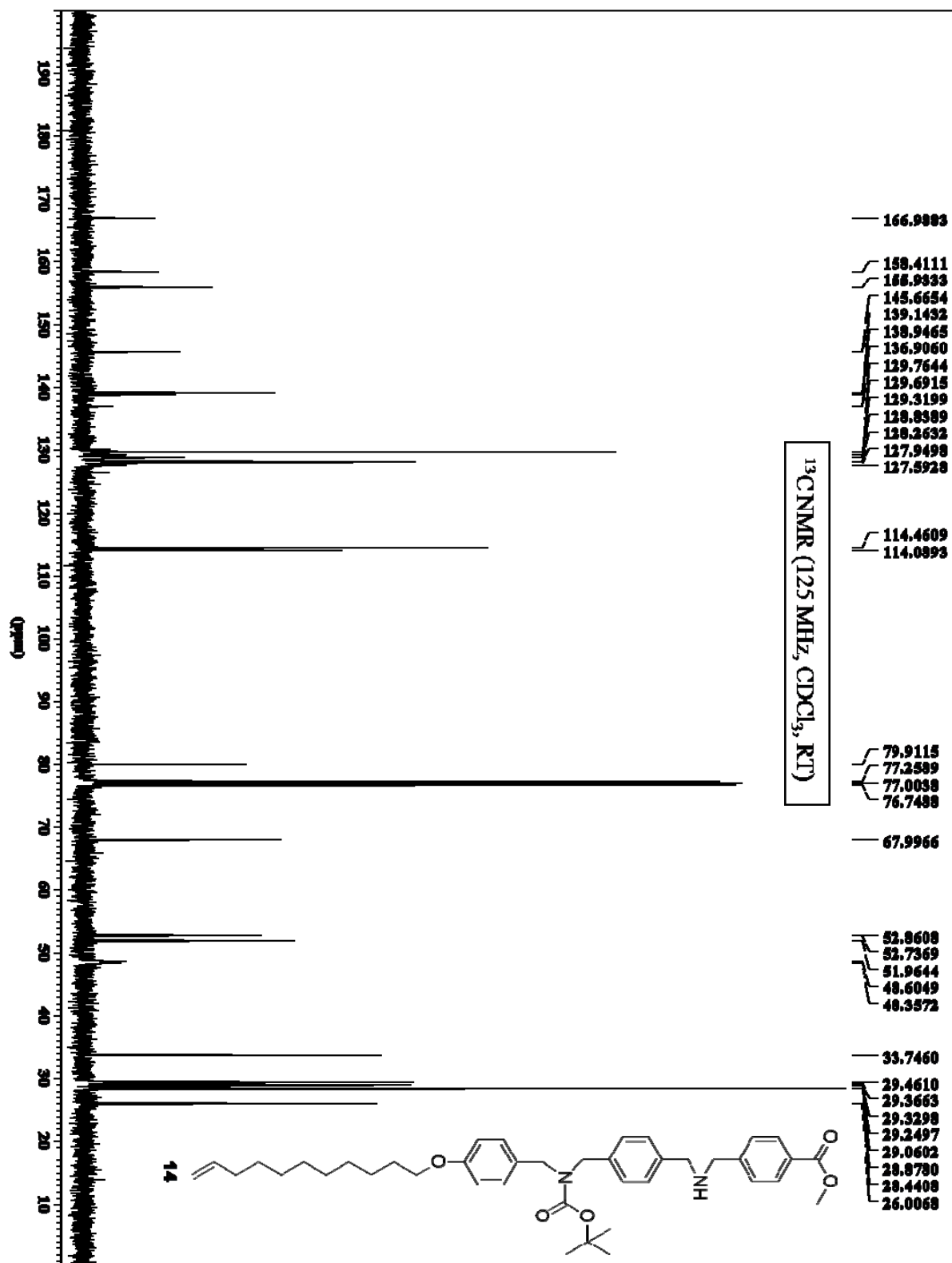


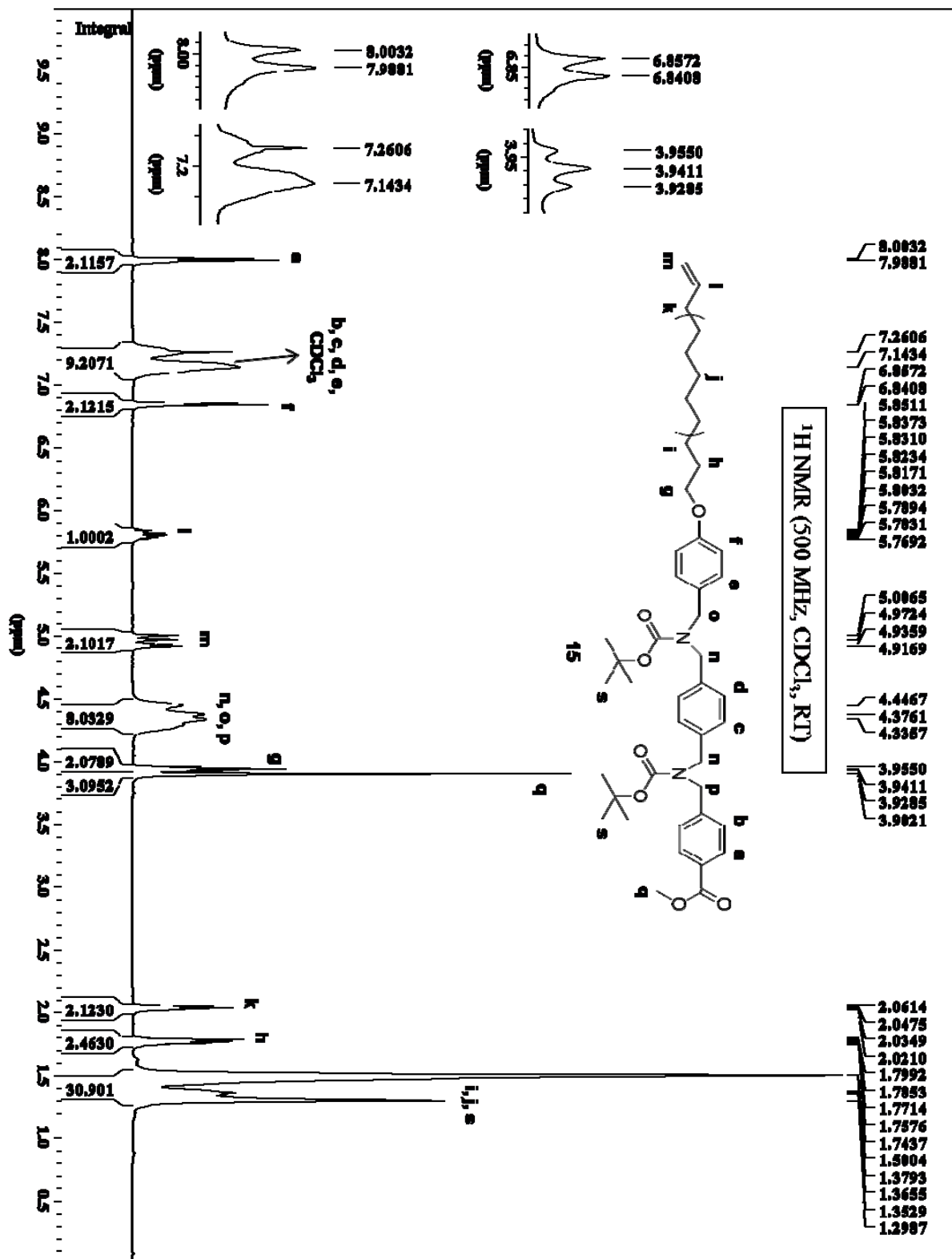


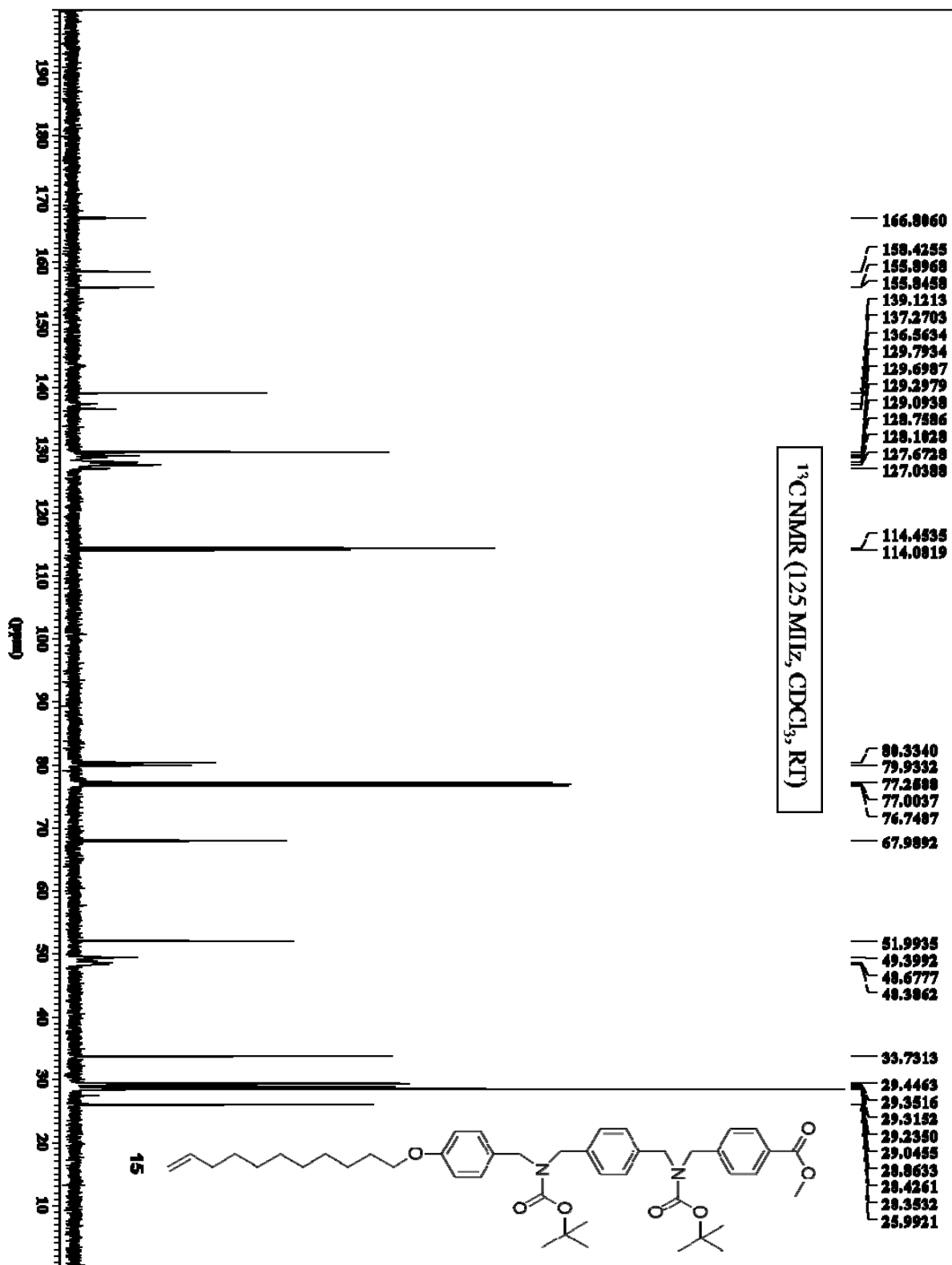


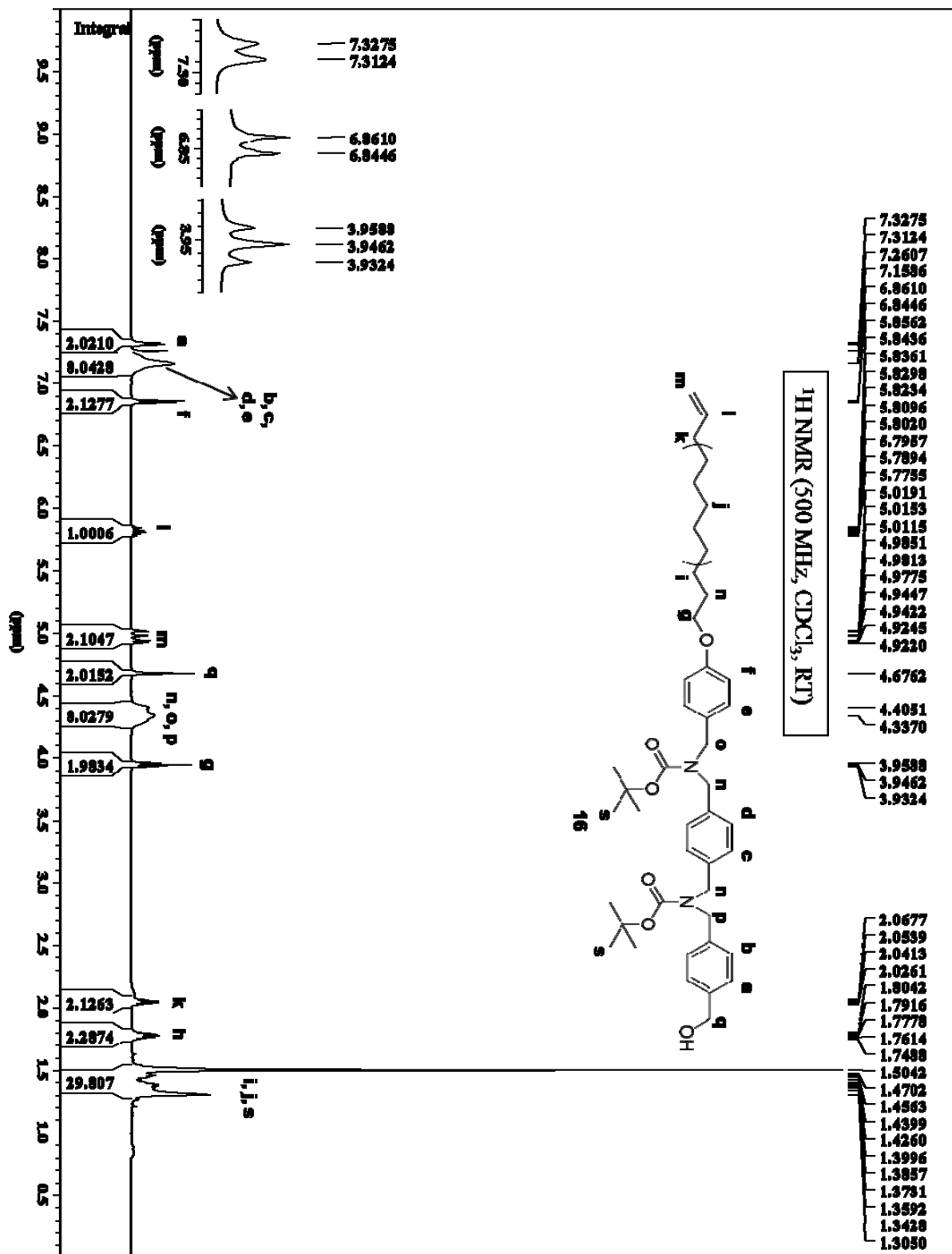


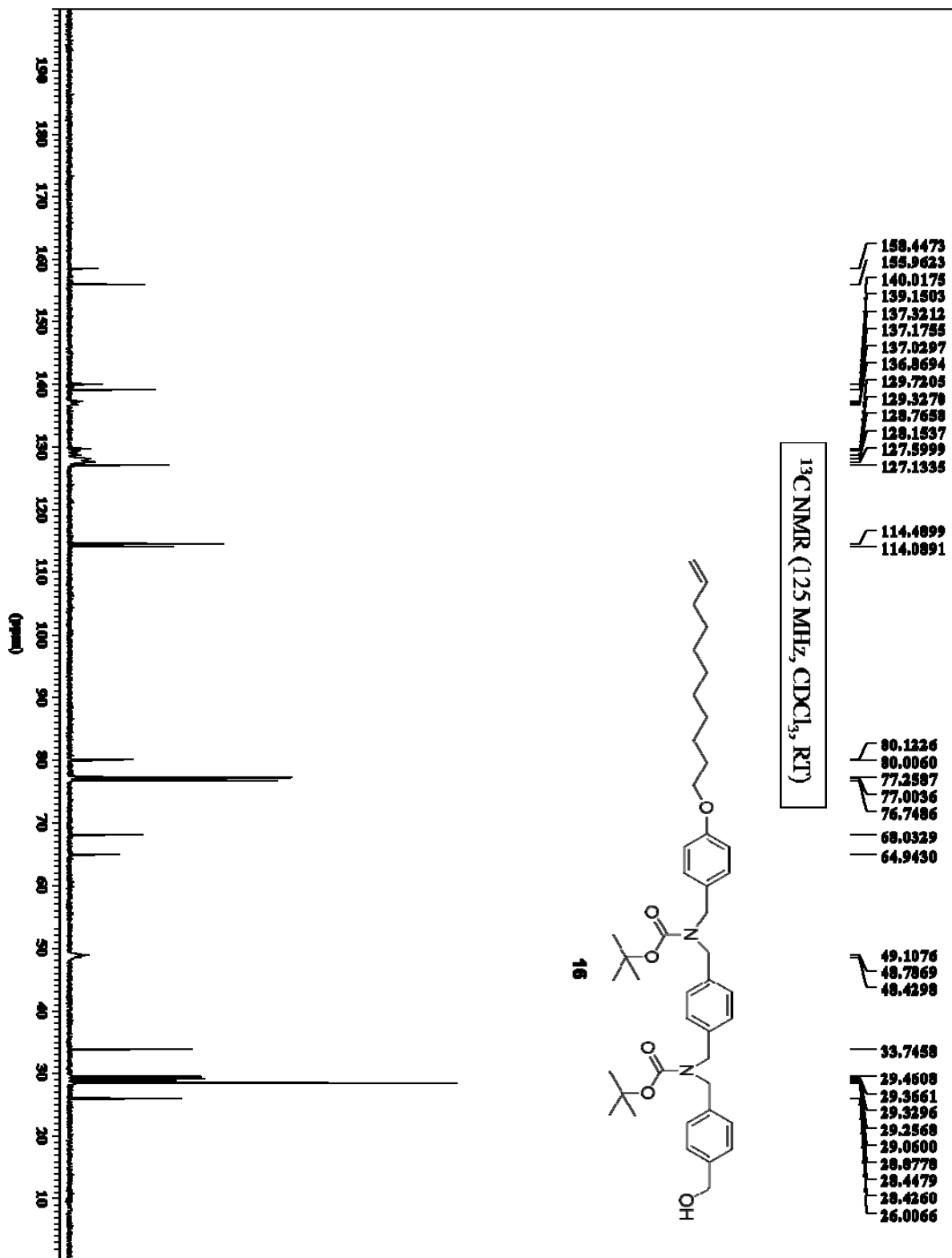


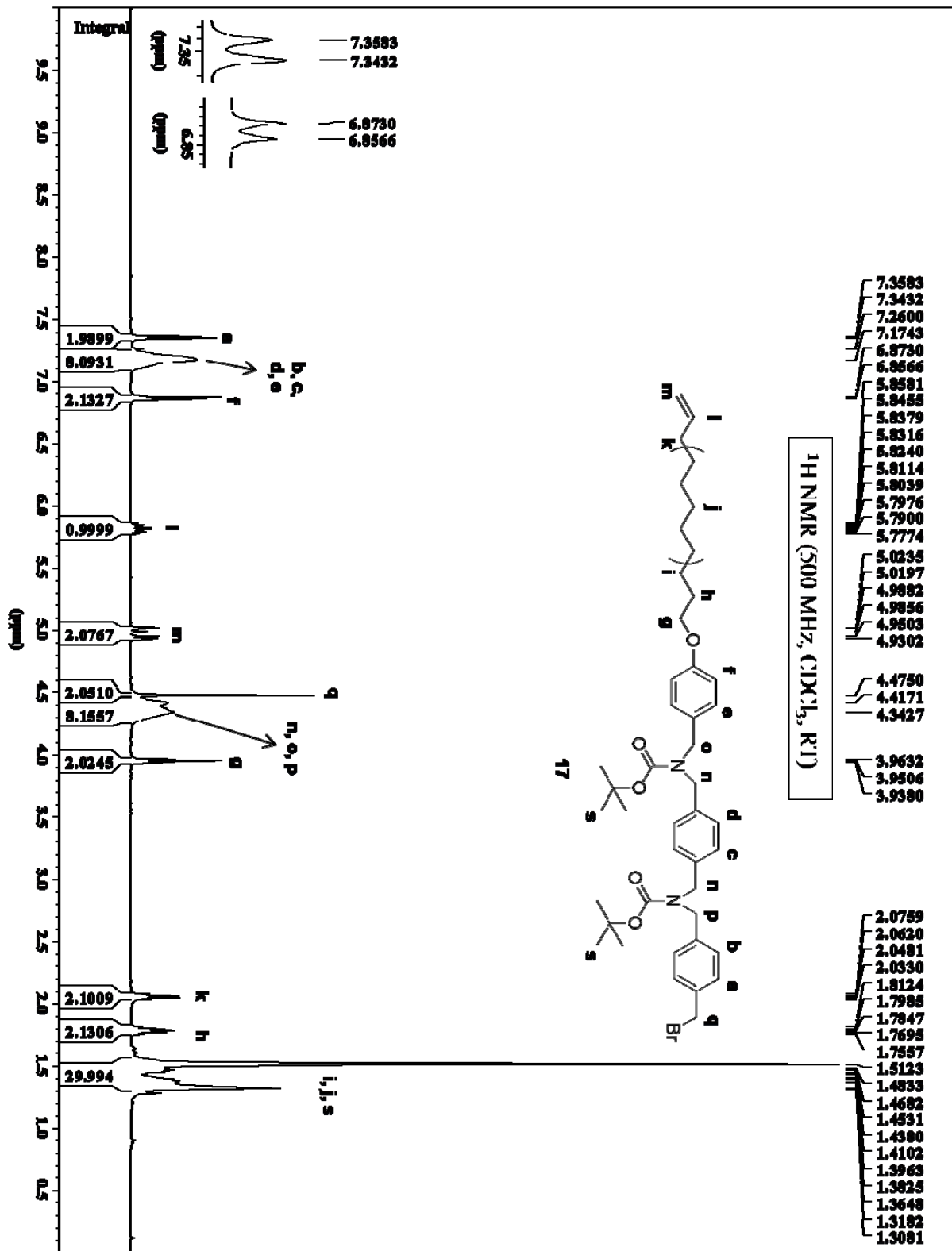


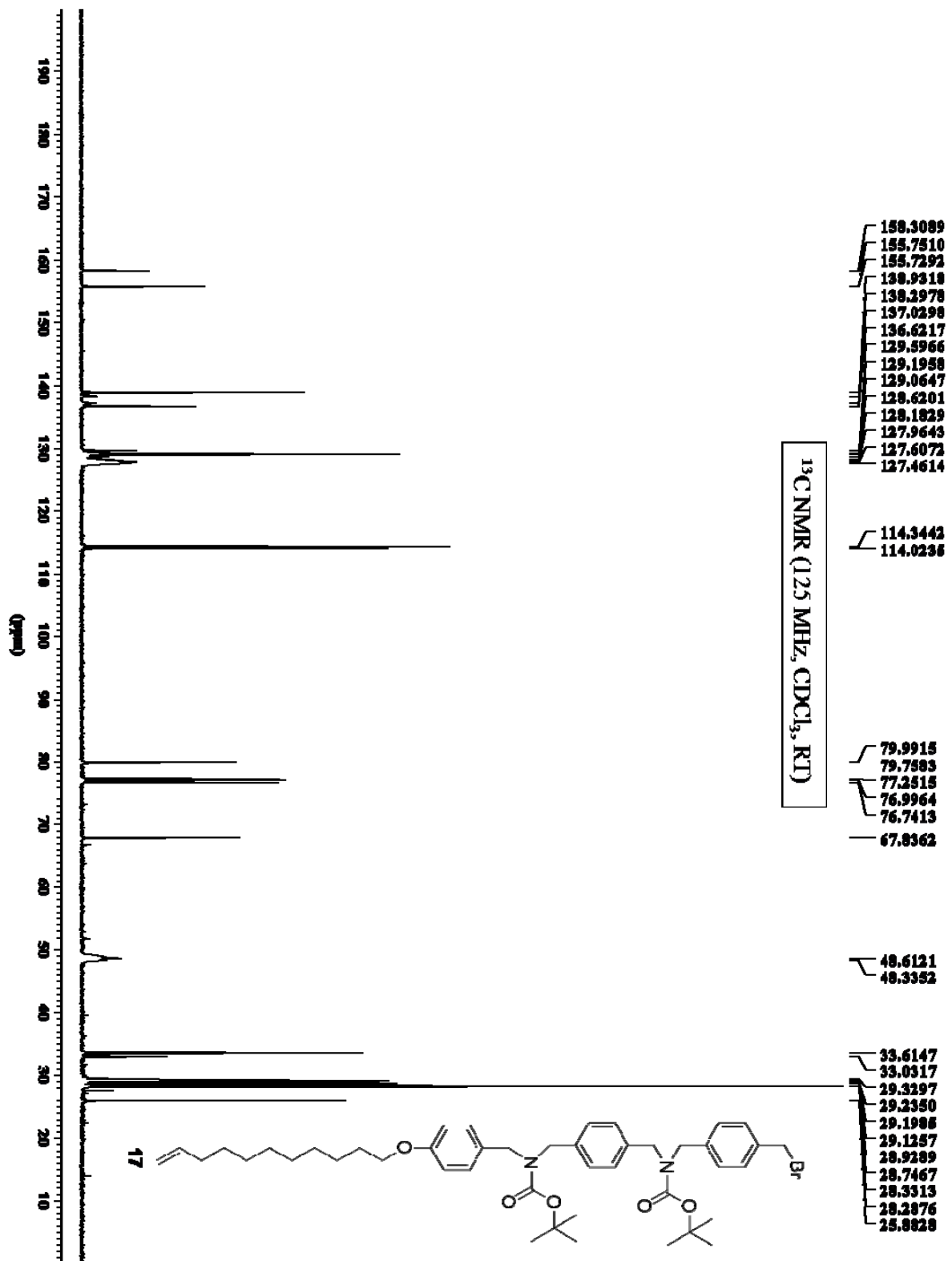


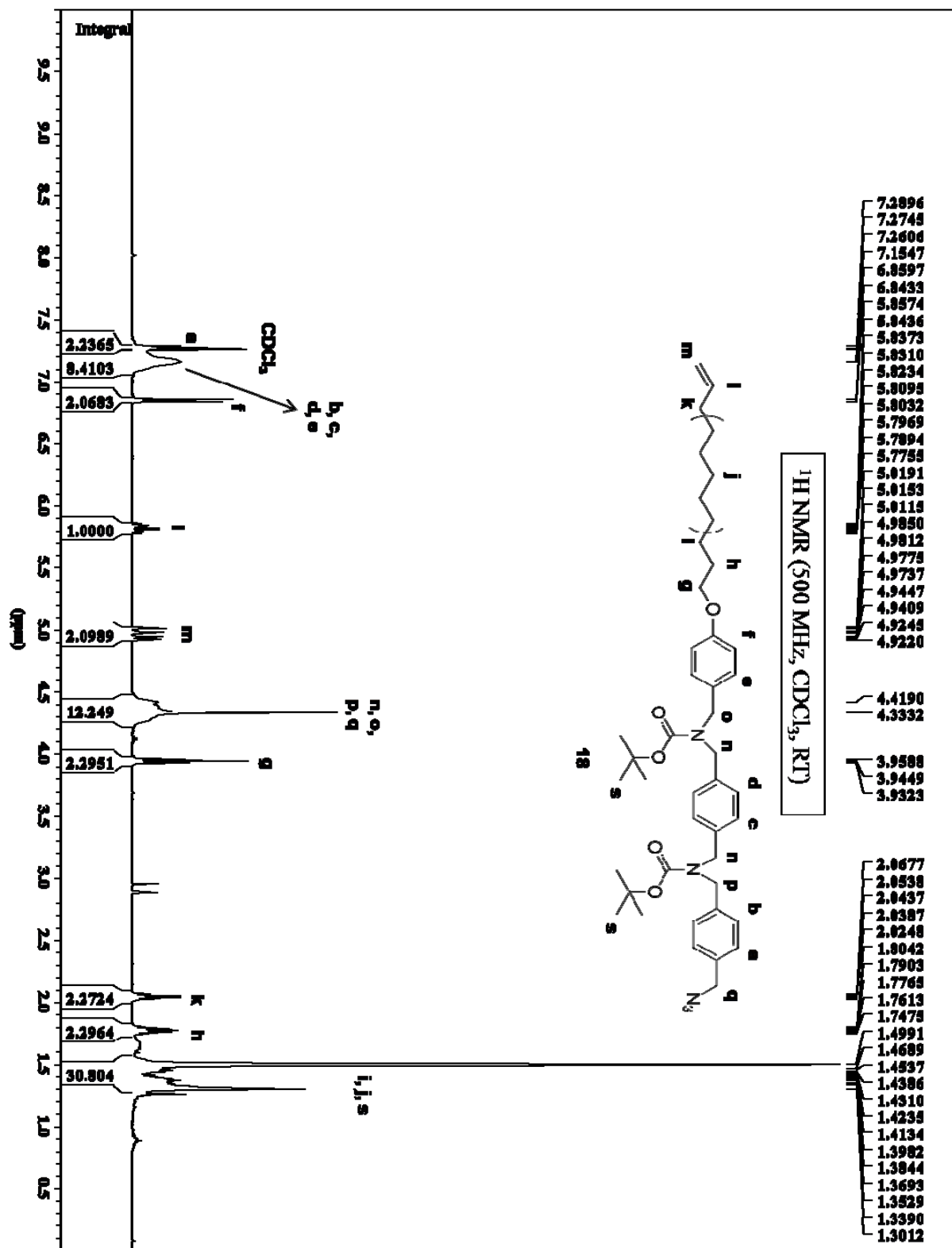


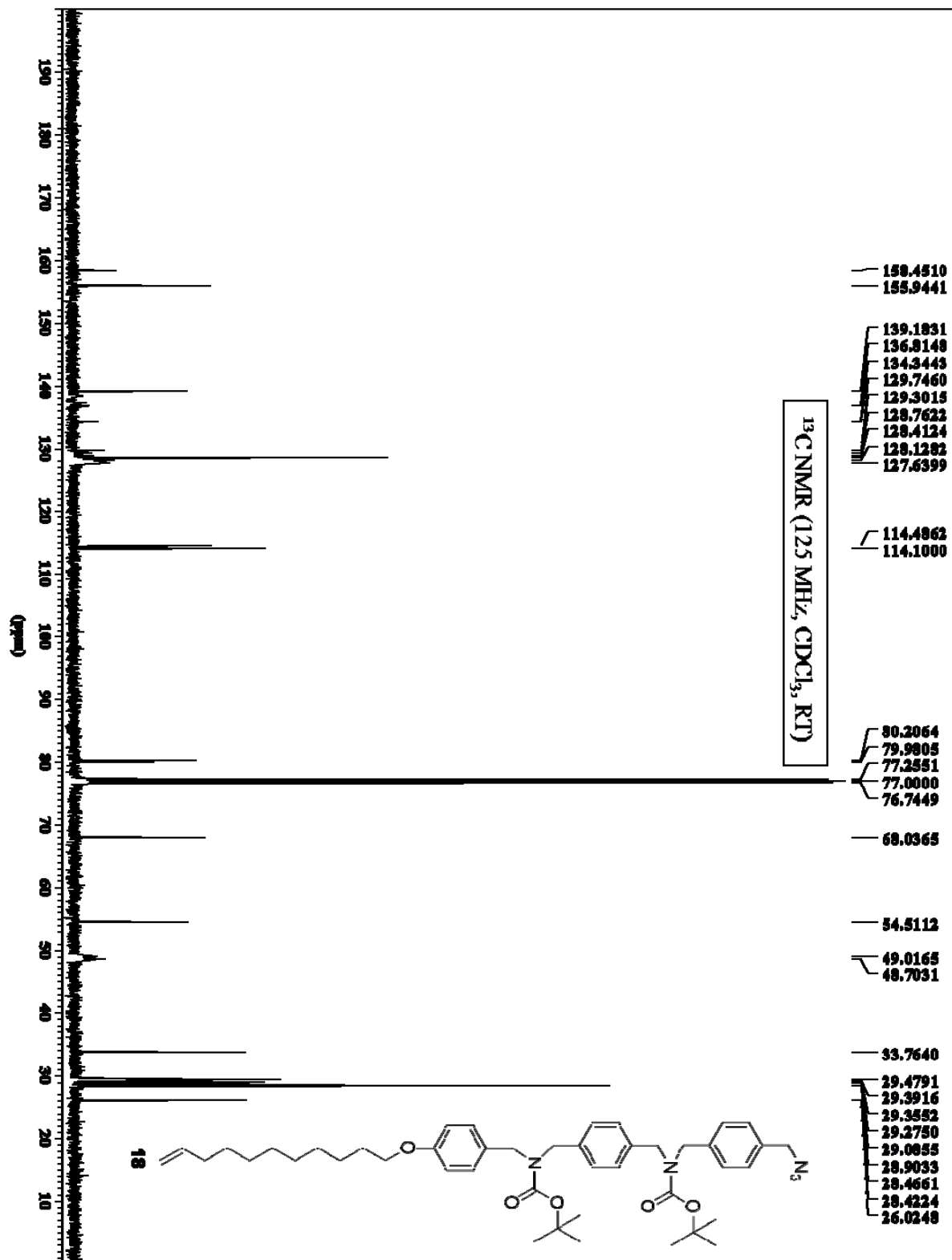


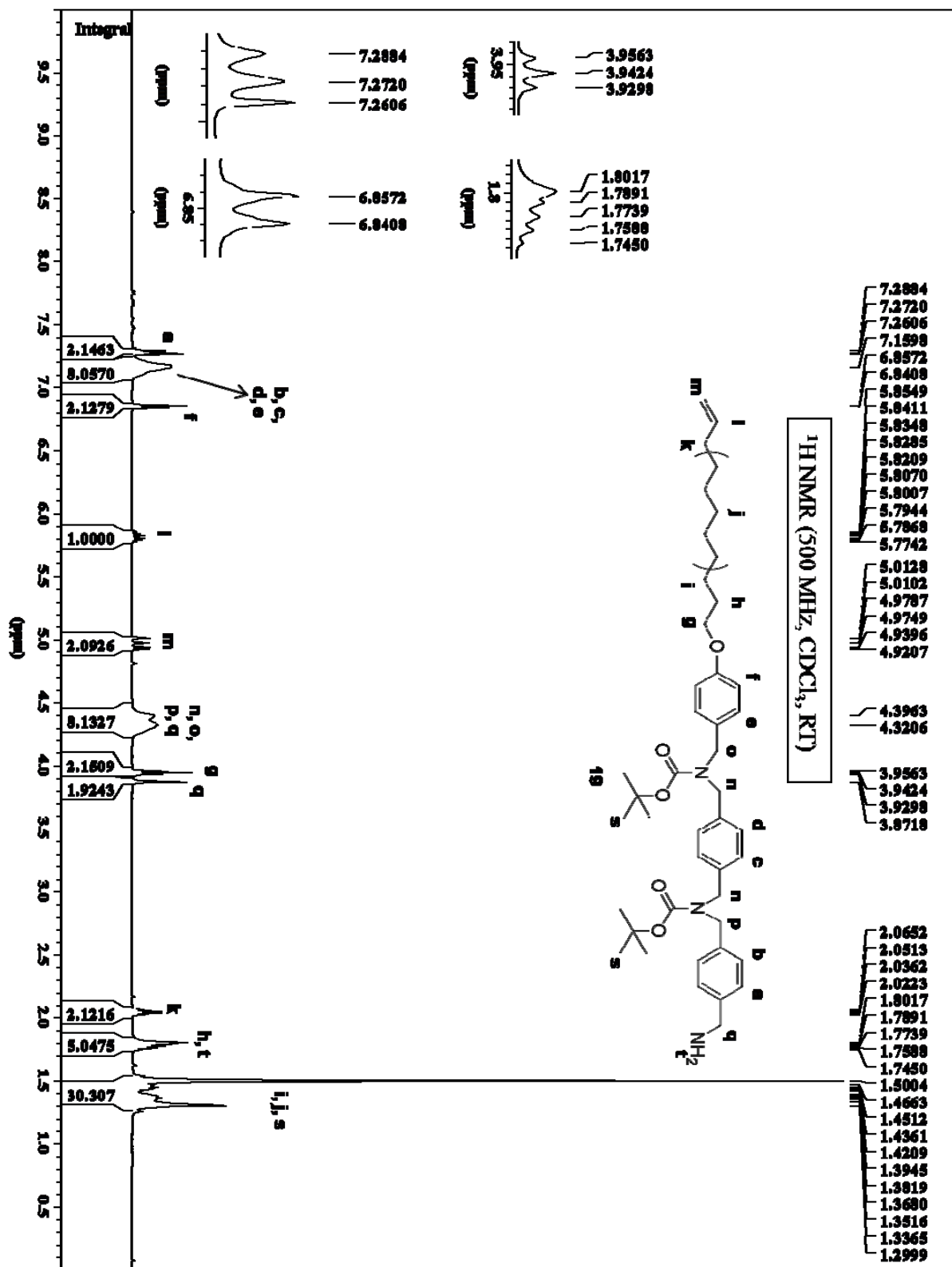


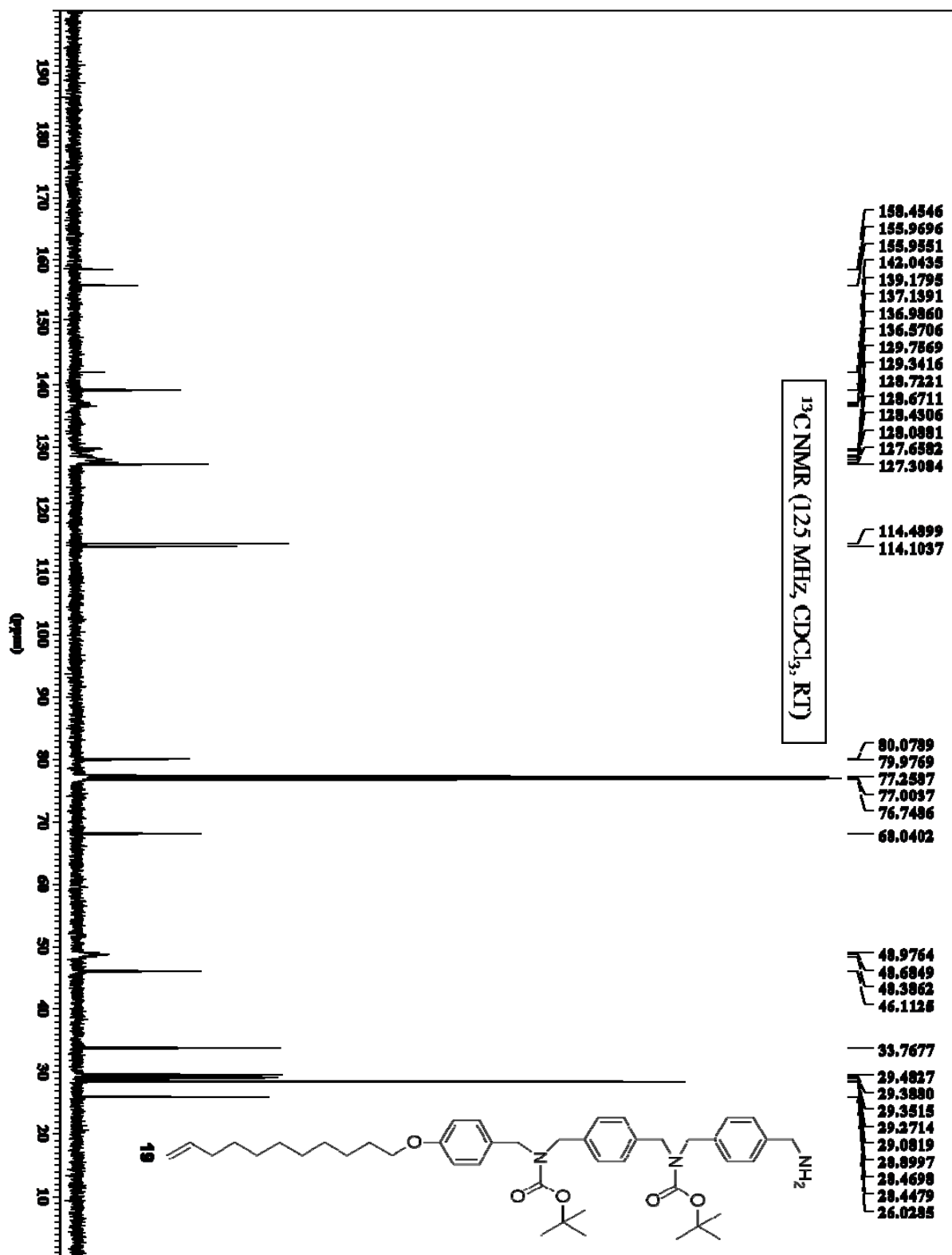


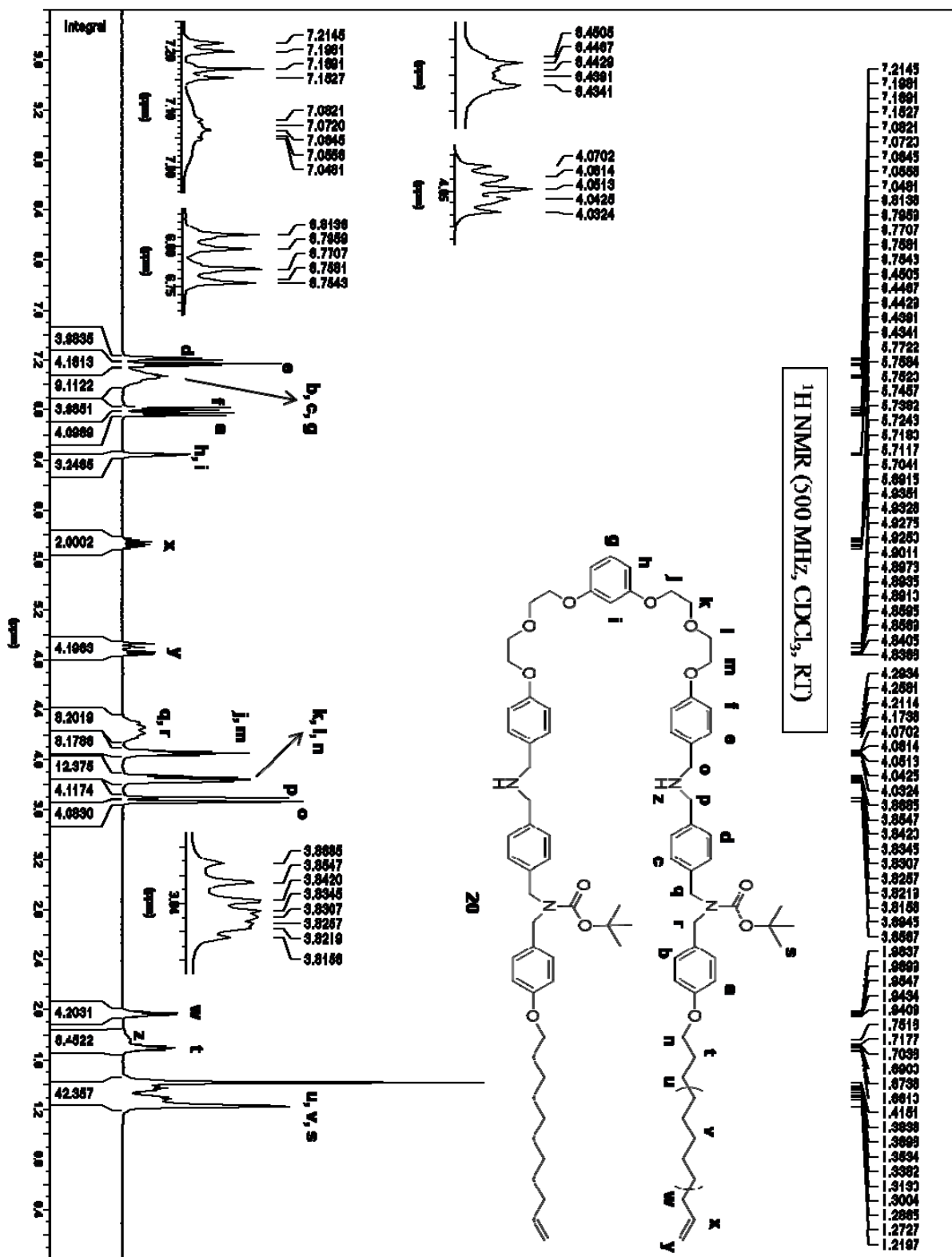


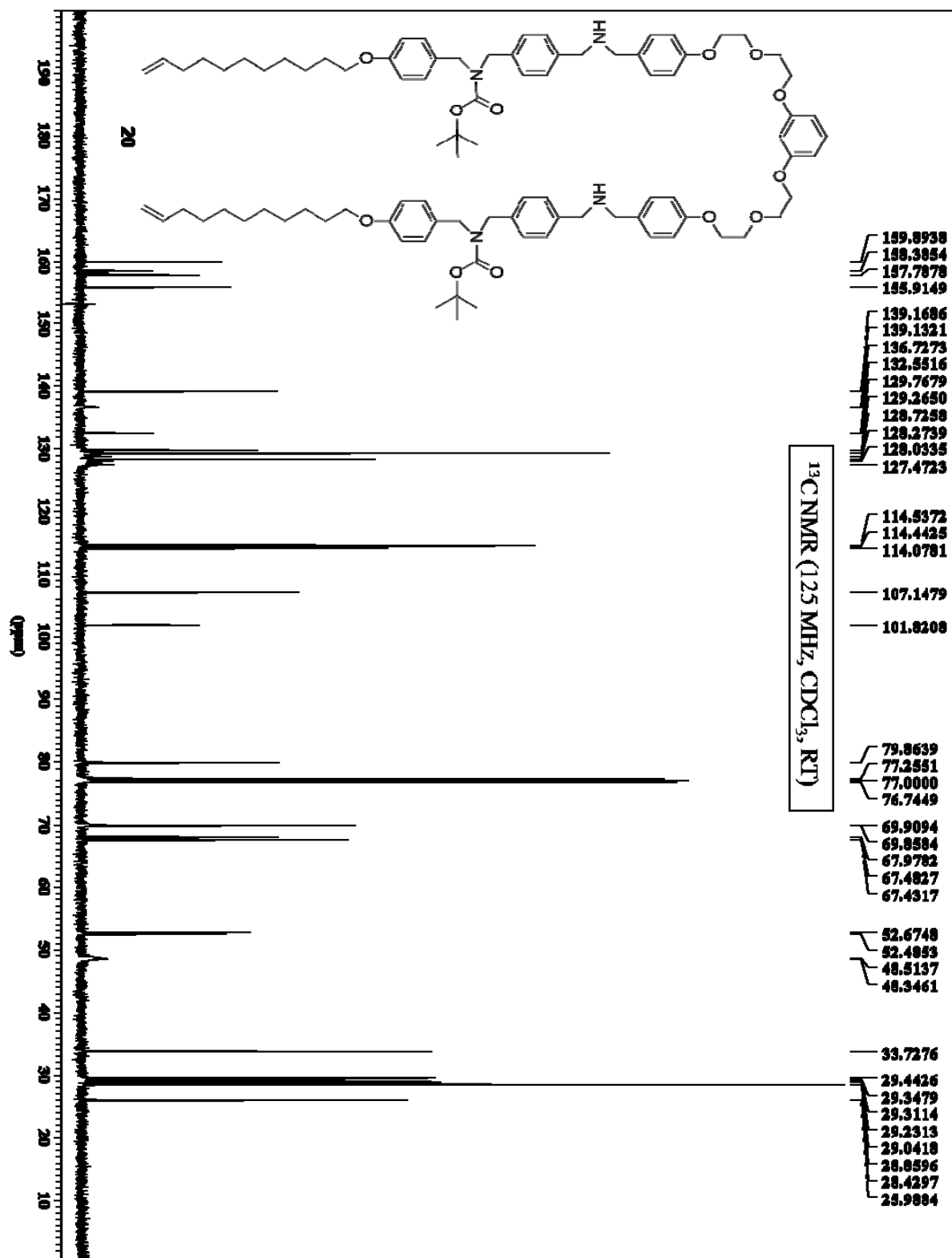


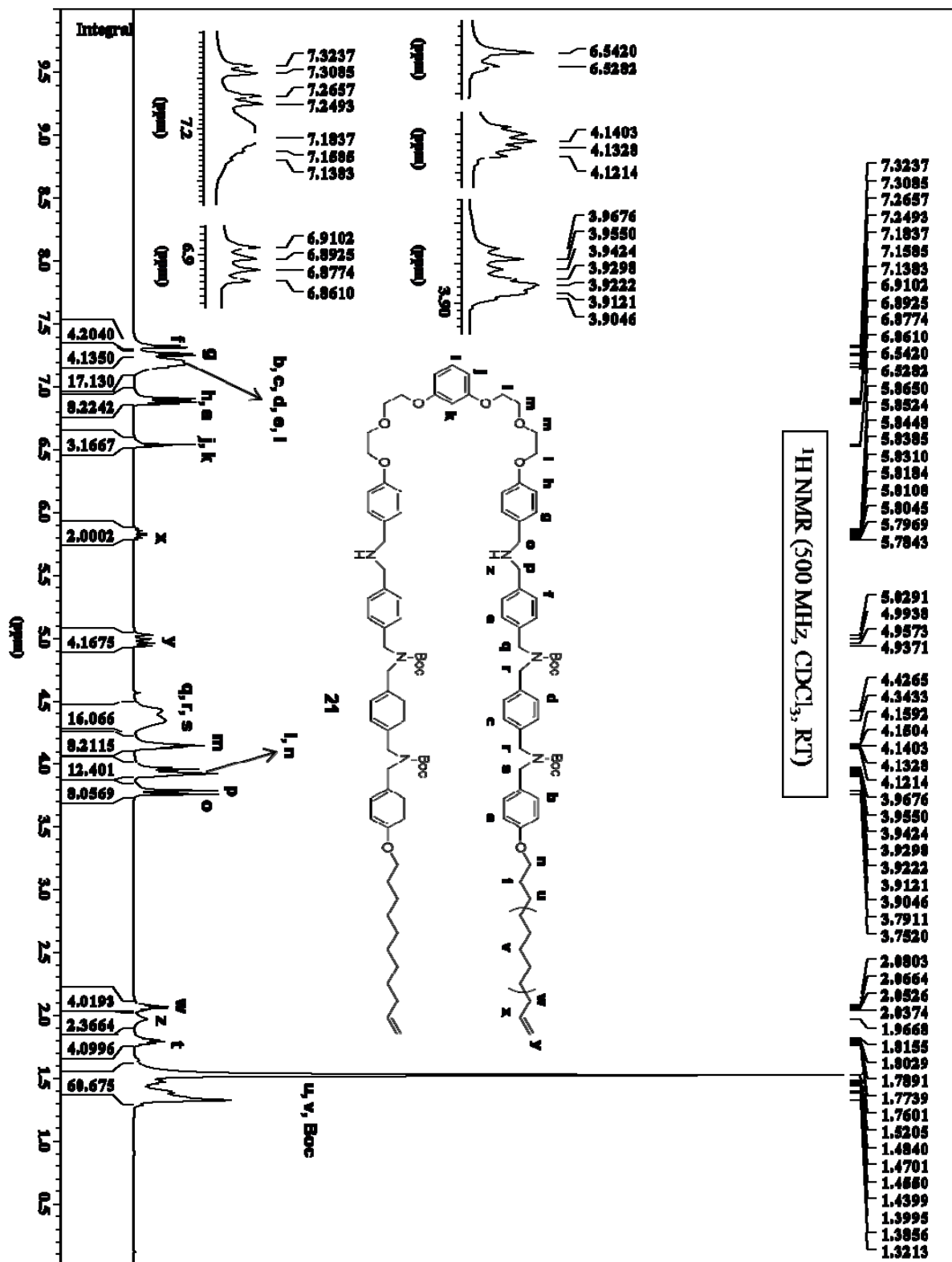


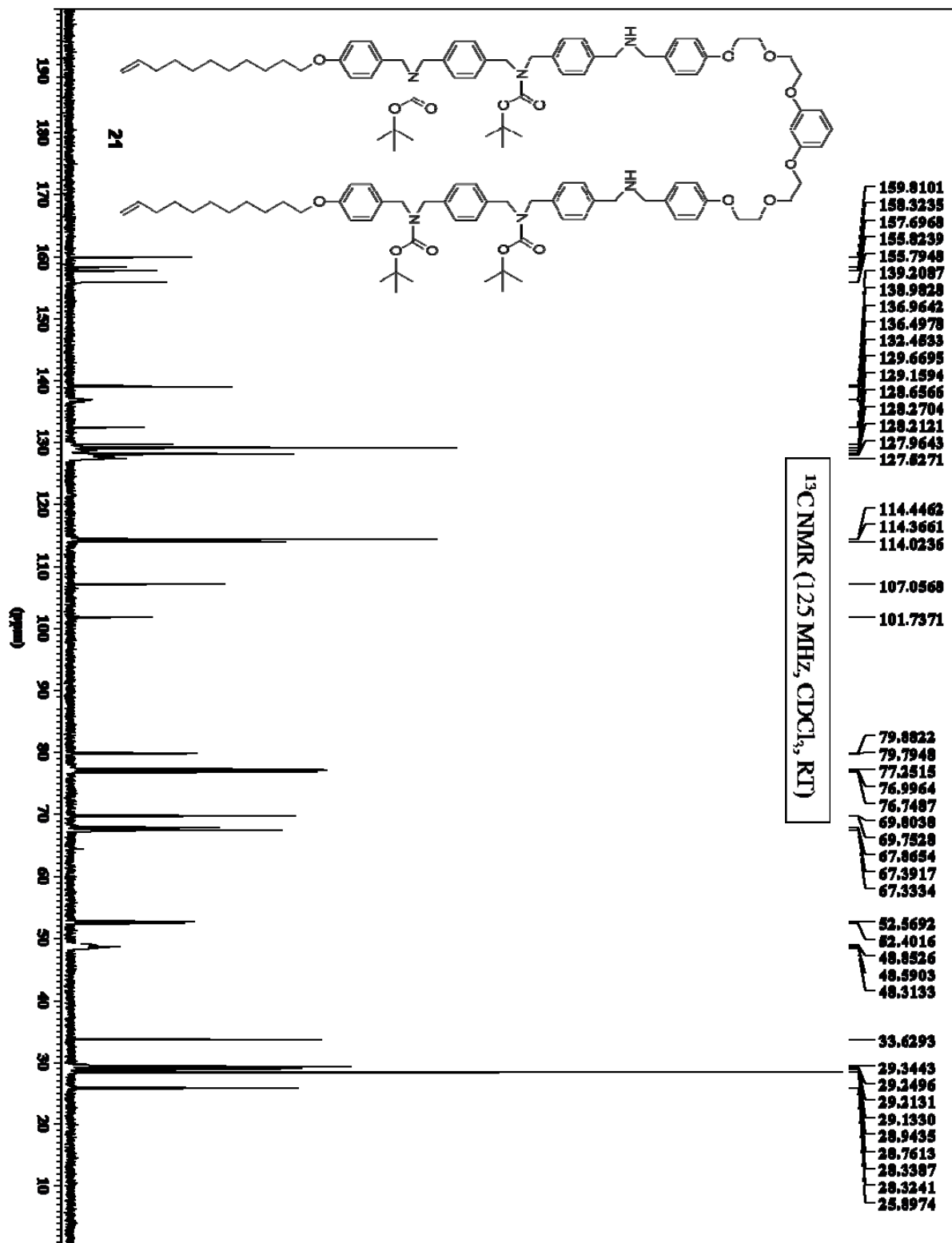


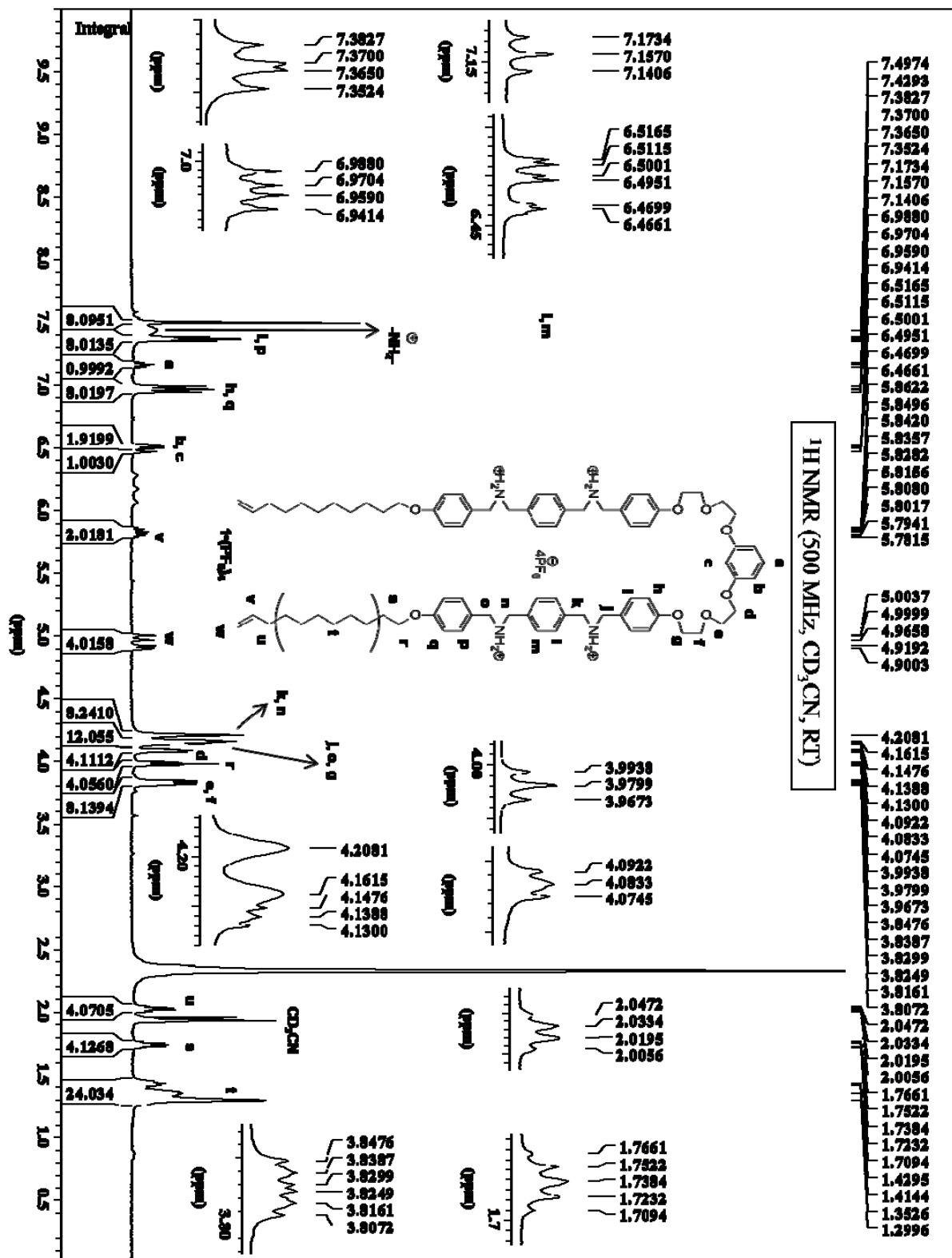


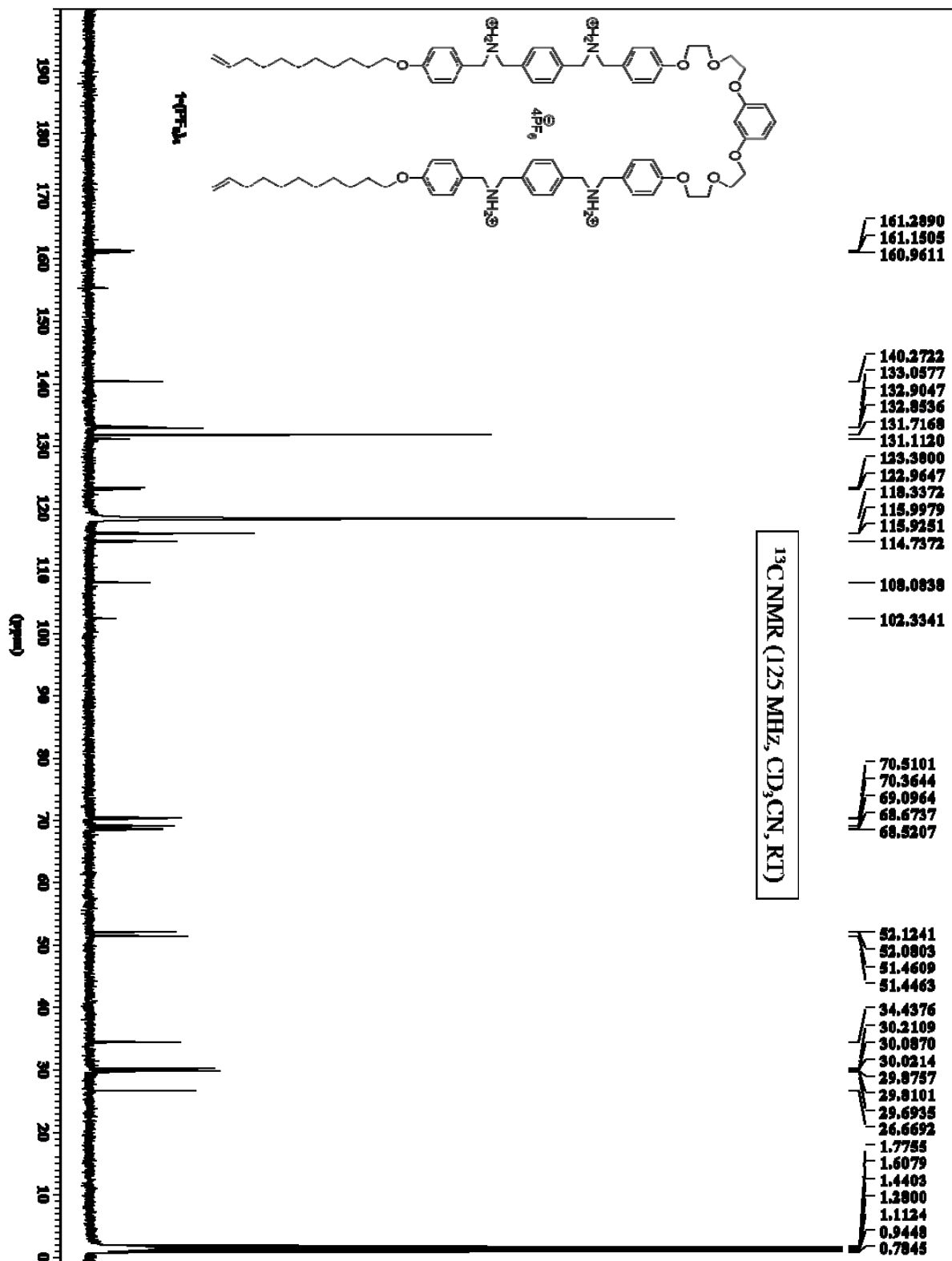


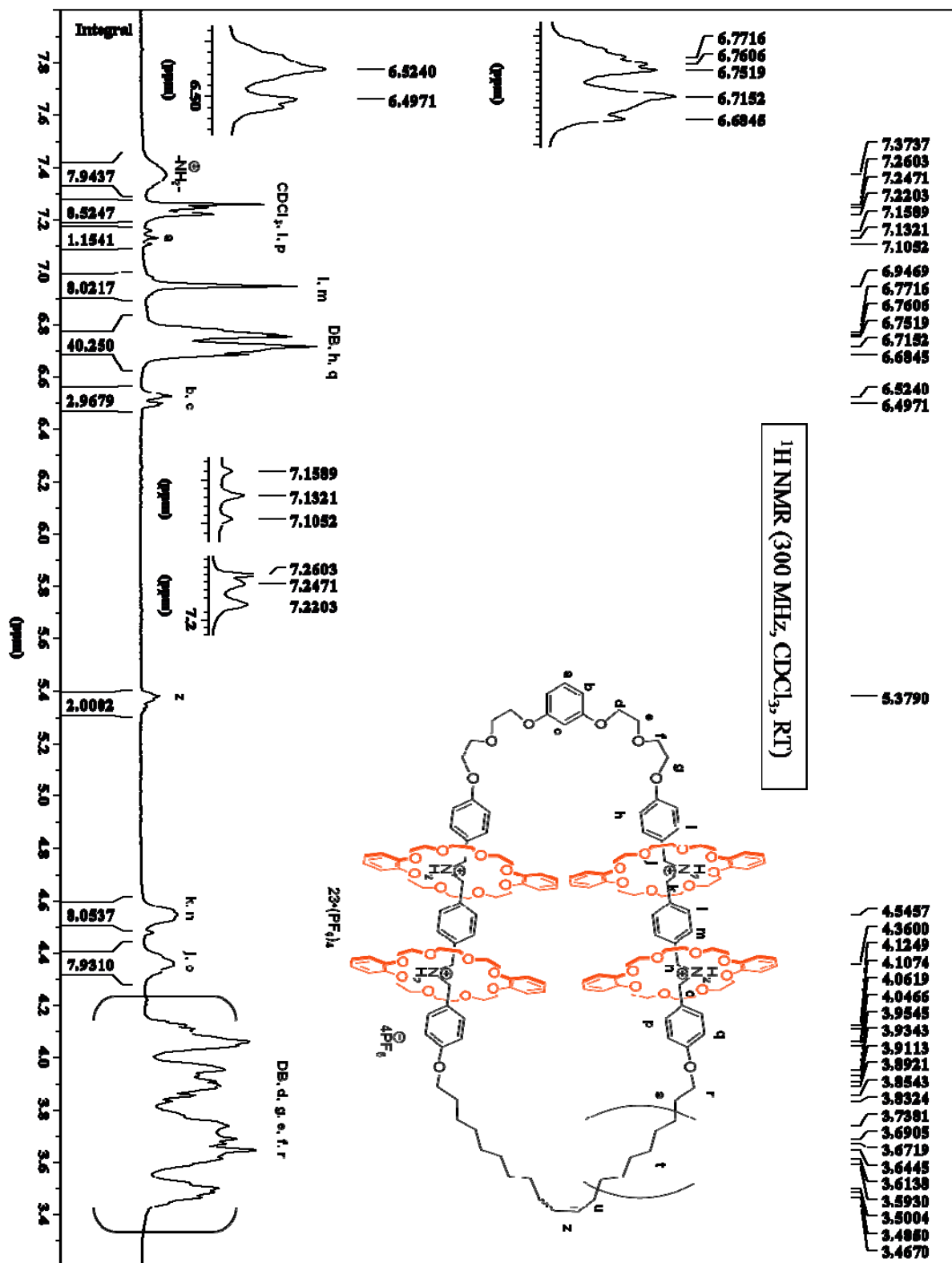


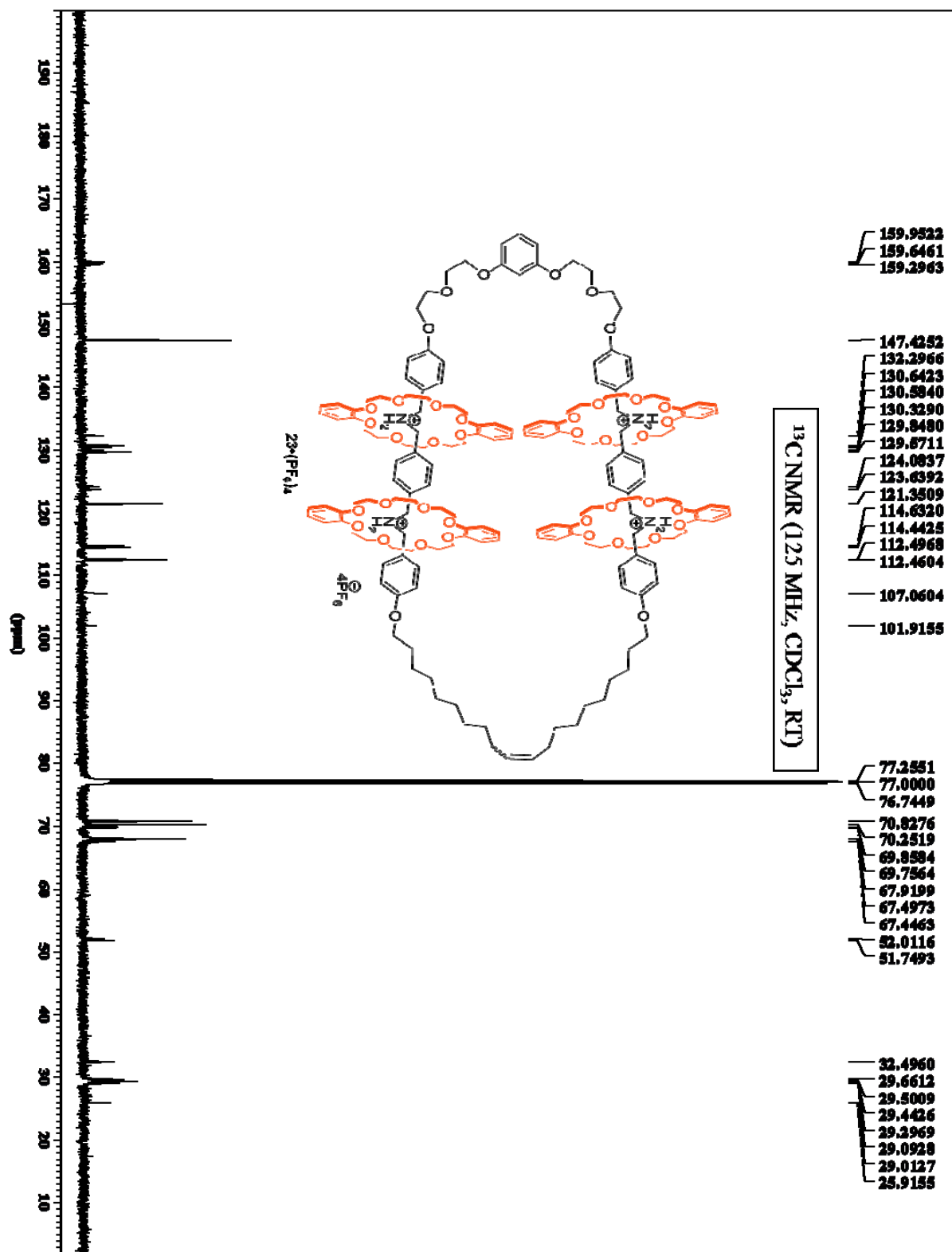


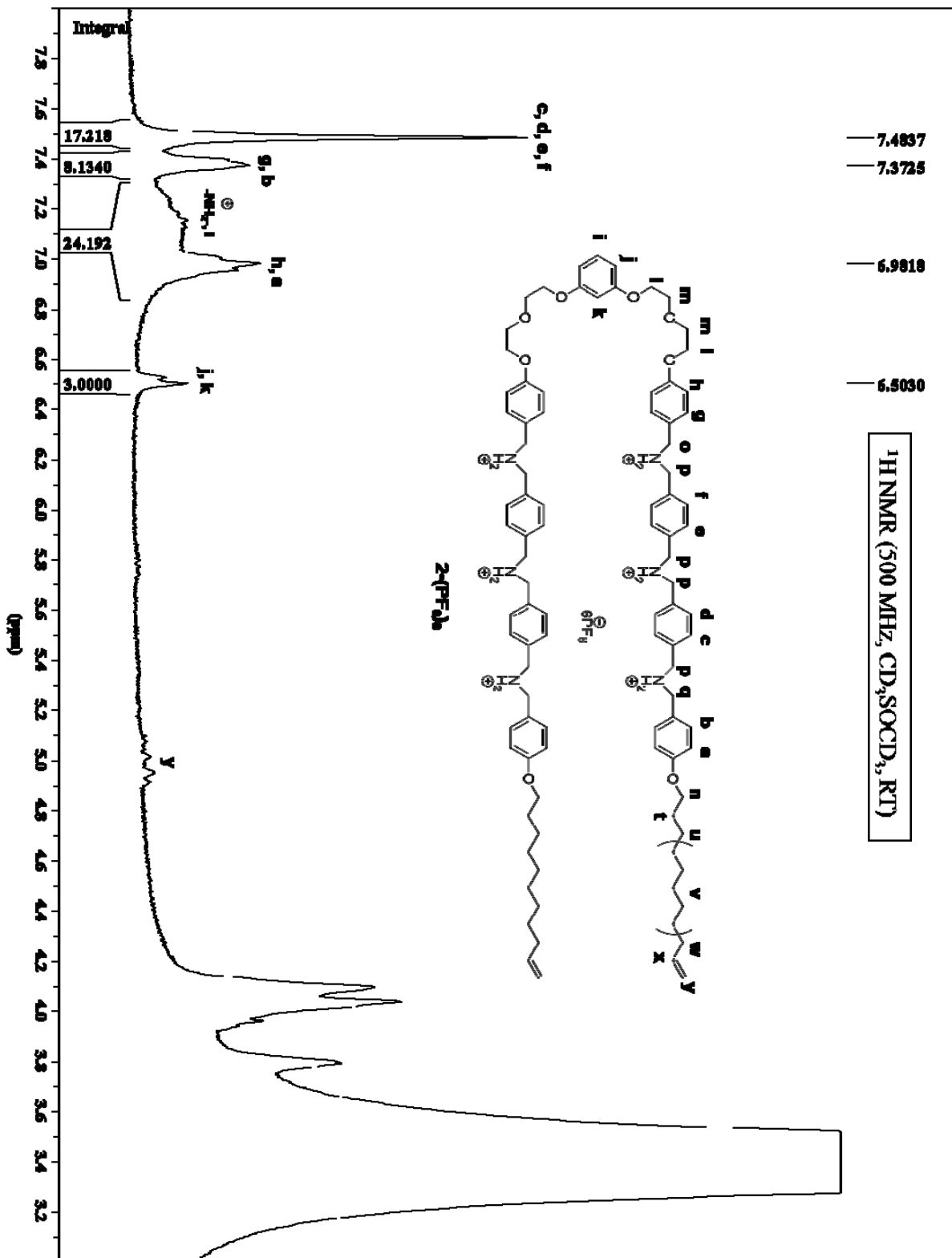


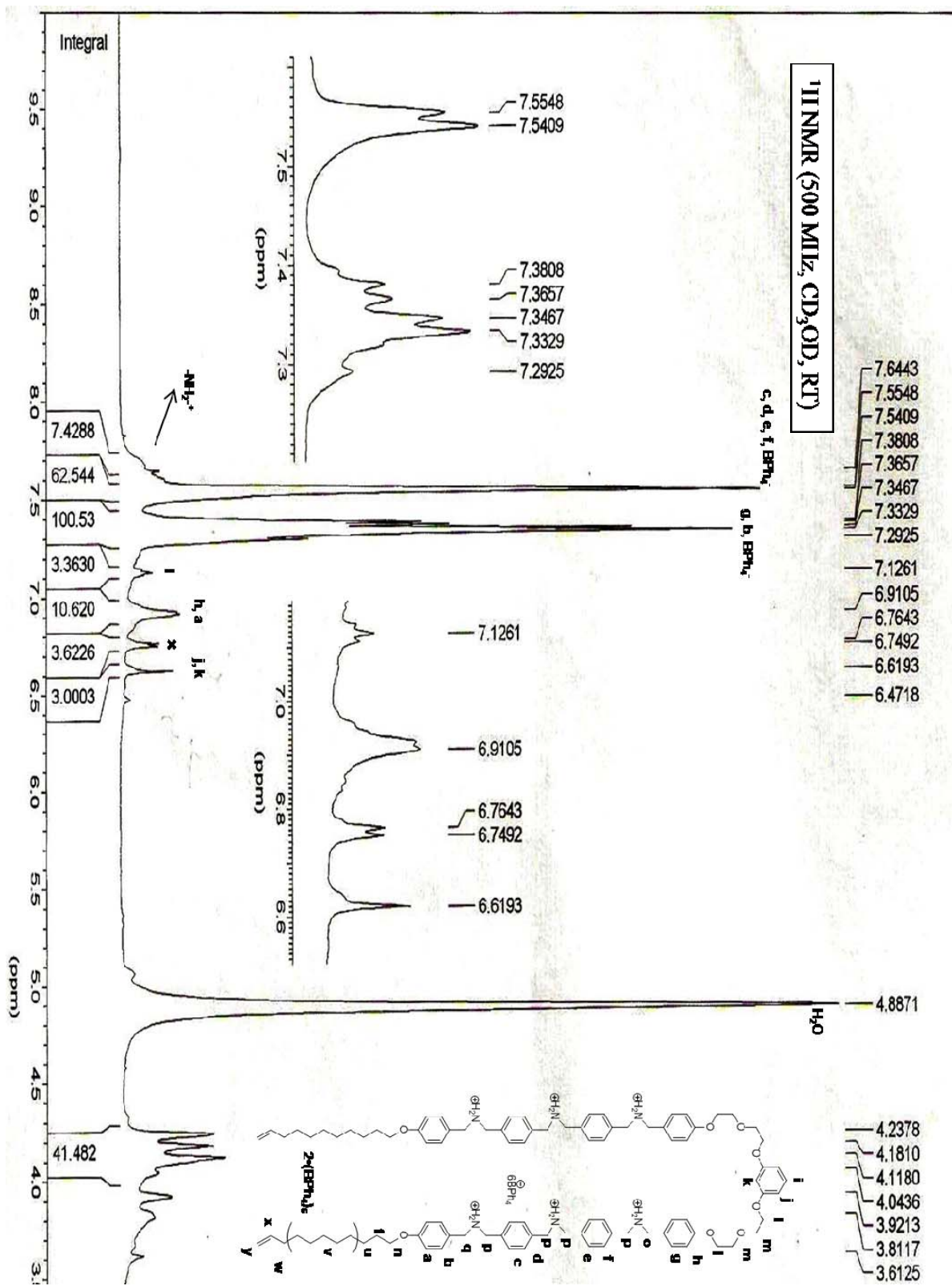


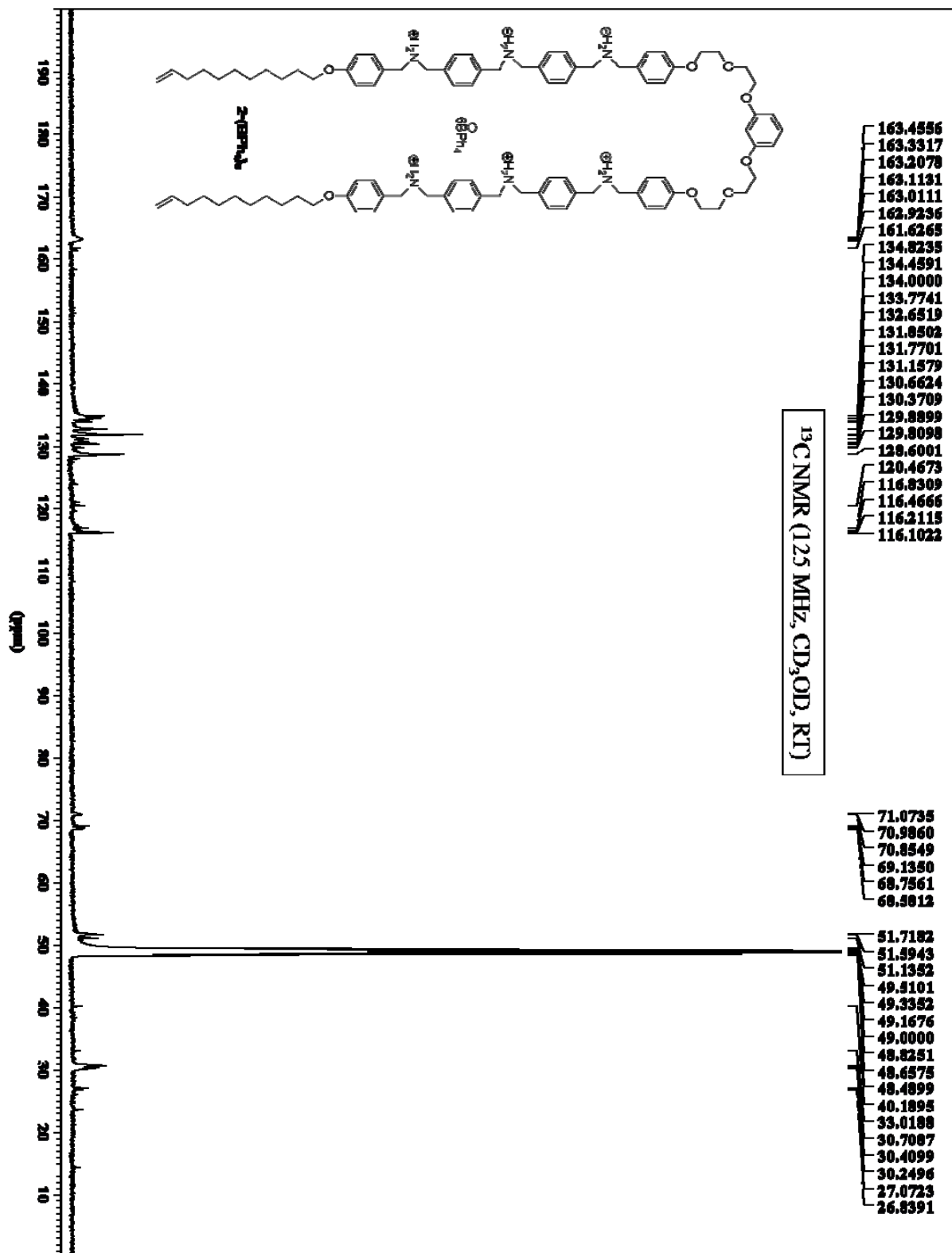












2. 2D COSY and 2D NOESY NMR spectra of [5]Molecular Necklace

^1H - ^1H correlation spectroscopy (COSY) experiment for $23\cdot(\text{PF}_6)_4$ (dissolved in $\text{C}_2\text{D}_2\text{Cl}_4$) was performed on Bruker AMX500 at 500 MHz to investigate the connectivity of neighbouring protons of interest. This basically helps us to confirm the structure of the thread. As expected H_j , H_n , H_k , H_o correlates with the ammonium ion reiterating our claim that the upfield shifted broad peak (typically observed in threading) originates from benzyl (methylene) protons adjacent to ammonium ions (Figure S1). Furthermore H_a correlating with H_b , H_i with H_n and H_p with H_q goes on to confirm our peak assignment.

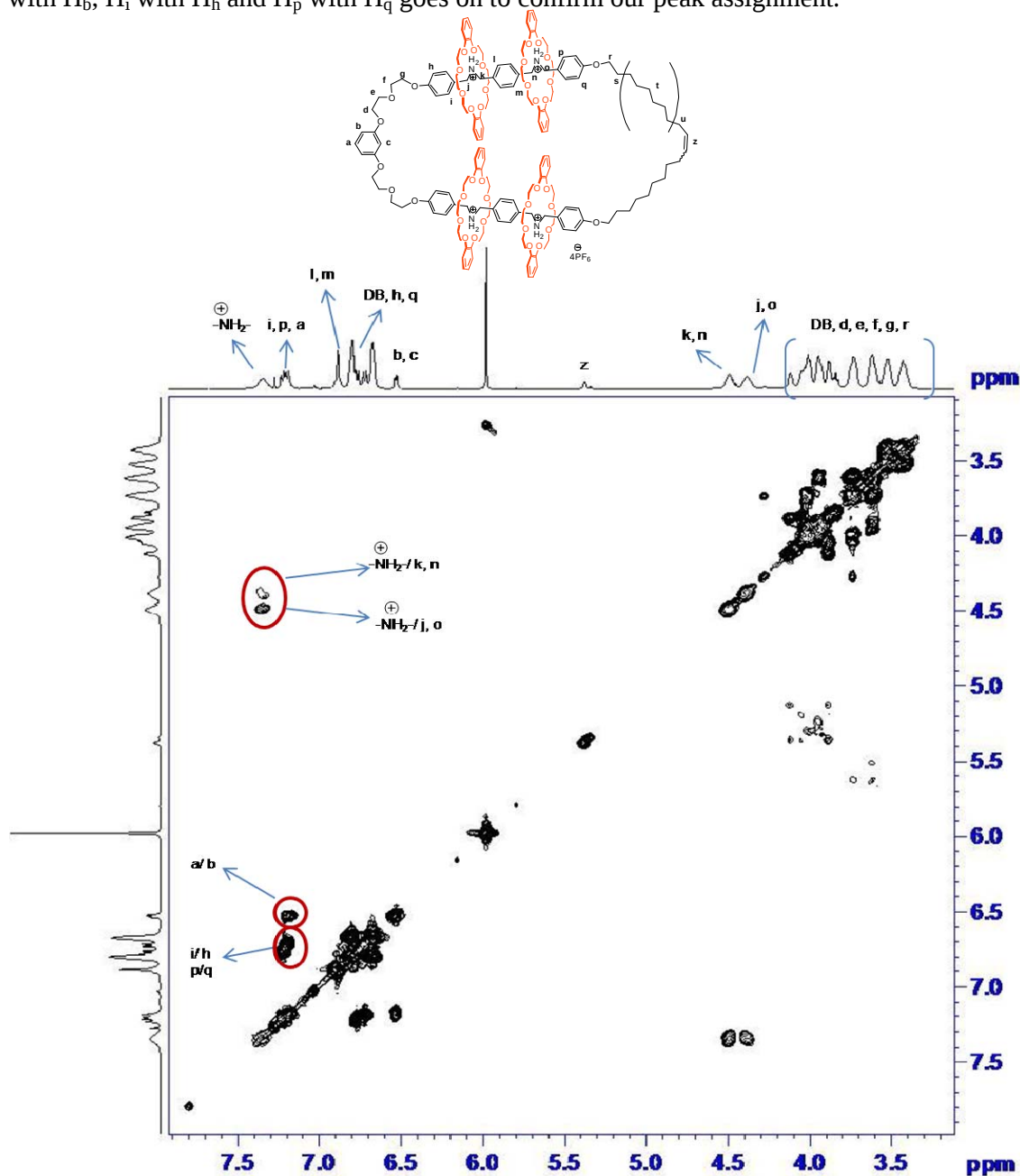


Figure S1. 500 MHz ^1H - ^1H COSY NMR spectrum of $23\cdot(\text{PF}_6)_4$ in $\text{C}_2\text{D}_2\text{Cl}_4$.

NOESY (Nuclear Overhauser effect Spectroscopy) spectra for $23 \cdot (\text{PF}_6)_4$ (dissolved in $\text{C}_2\text{D}_2\text{Cl}_4$) was obtained from Bruker AMX500 at 500 MHz. NOESY spectra correlates protons not separated by more than 5 Angstroms through space. Therefore, this technique is ideally suited for analysing mechanical bonds in supramolecular assemblies. In our case the NOESY spectra decisively proves that DB24C8 (referred as DB in spectral assignment) strongly correlates with the aromatic protons (H_l , H_m , H_i , H_p , H_h , H_q), benzyl (methylene) protons (H_k , H_n , H_j , H_o) and ammonium protons as expected from the structure elucidated for [5]MN $23 \cdot (\text{PF}_6)_4$ (Figure S2). Hence, the one-dimensional (1D), two-dimensional (2D), variable temperature ^1H NMR spectroscopy along with ESI mass spectroscopy confirms the formation of the desired [5]MN.

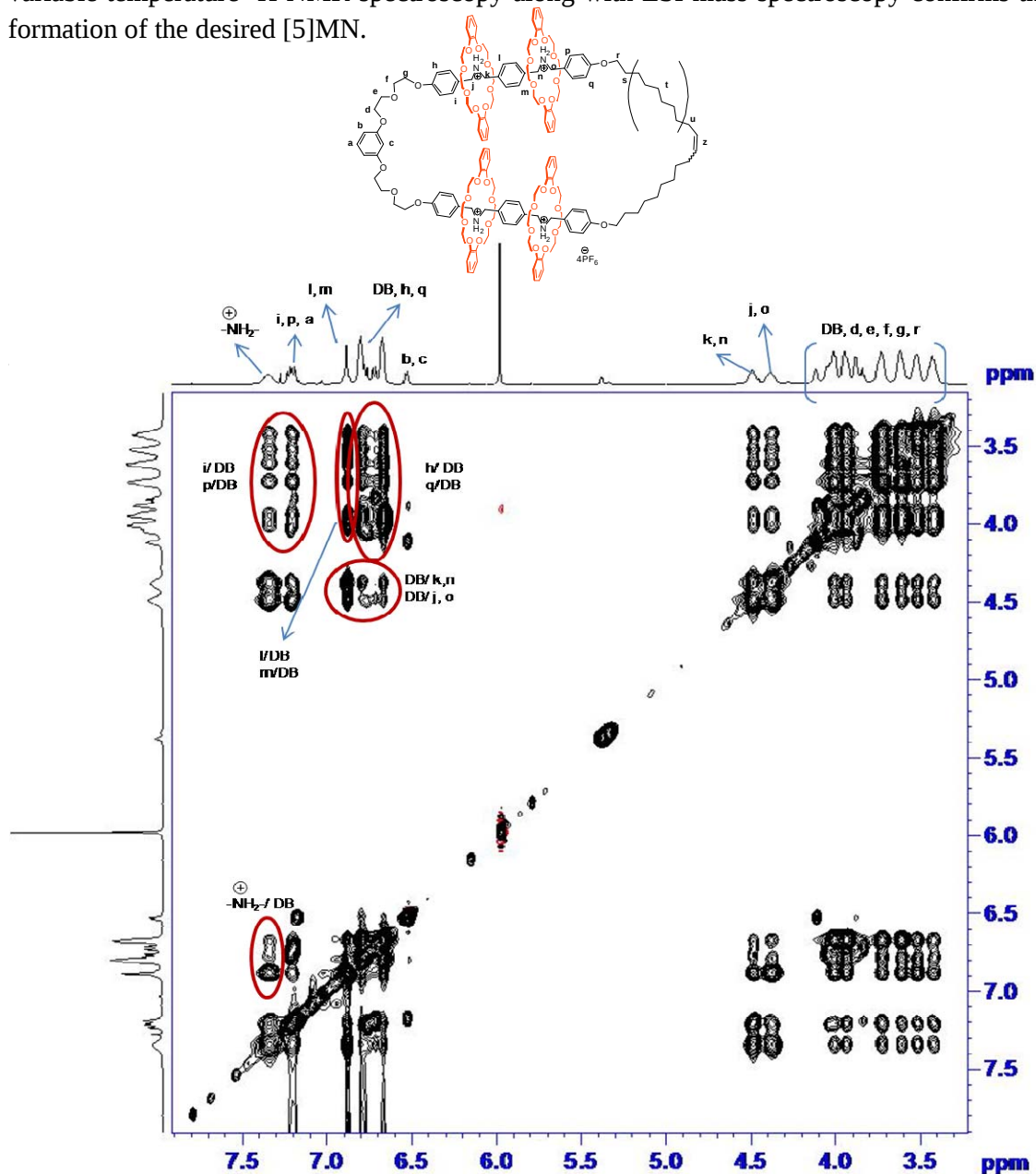


Figure S2. 500 MHz NOESY NMR spectrum of $23 \cdot (\text{PF}_6)_4$ in $\text{C}_2\text{D}_2\text{Cl}_4$.