Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Information

N-Succinimidyl 3-((4-(4-[^{18}F]fluorobutyl)-1H-1,2,3-triazol-1-yl)methyl)-5-(guanidinomethyl)benzoate ([^{18}F]SFBTMGMB): A Residualizing Label for ^{18}F-labeling of internalizing biomolecules

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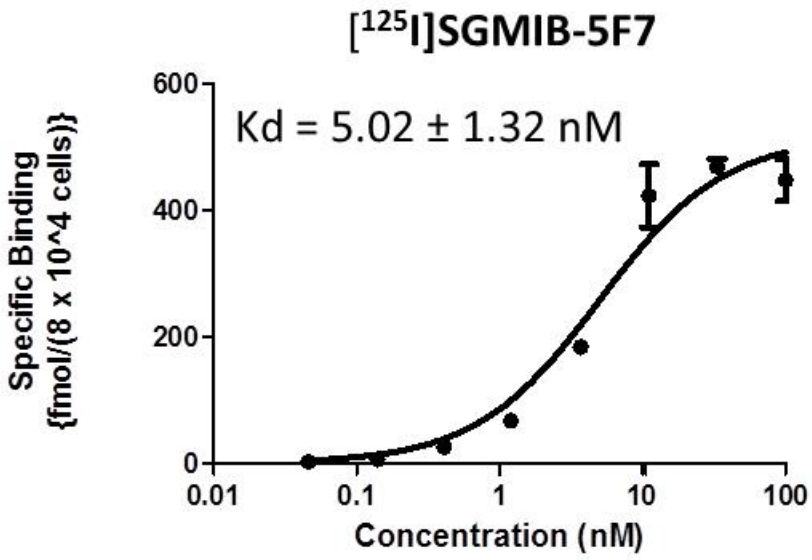
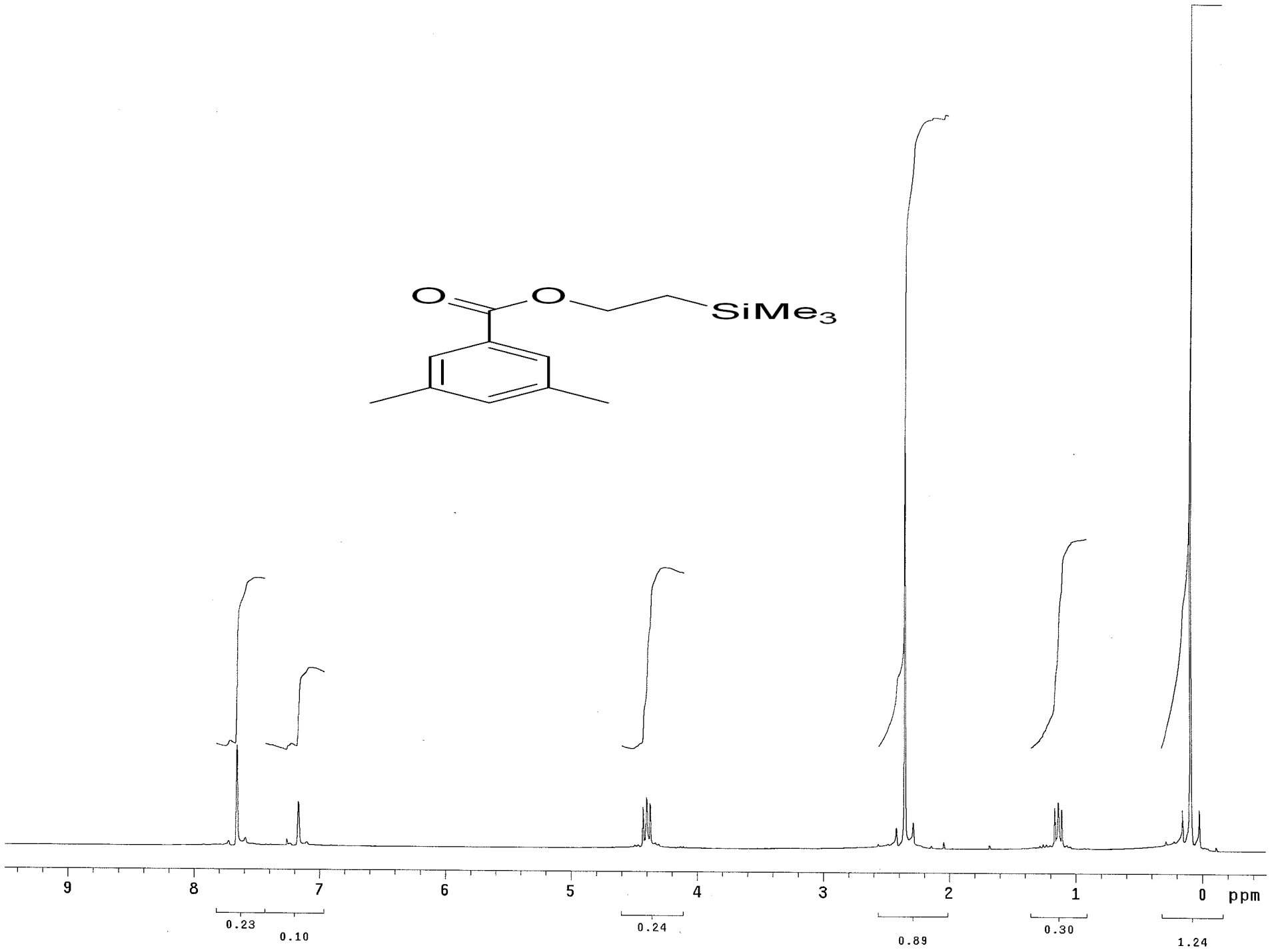
Formation of 6-(hex-5-yn-1-yloxy)hex-1-yne (12) during the synthesis of 6-fluorohex-1-yne from hex-5-yn-1-yl 4-methylbenzenesulfonate. Potassium fluoride (1.73 g, 29.7 mmol) was added to a solution of hex-5-yn-1-yl 4-methylbenzenesulfonate (2.5 g, 9.91 mmol) in THF (100 mL) and the mixture was stirred at 50°C for 17 h. The reaction mixture was cooled to 20^{o}C and partitioned between diethyl ether and water. The ethereal solution was dried over anhydrous sodium sulfate, filtered, and the filtrate concentrated to dryness by rotary evaporation. The residue was purified by silica gel chromatography using 5:1 hexanes:ethyl acetate as the mobile phase to afford 99 mg (10%) of 6-fluorohex-1-yne as a pale yellow oil and 605 mg (34%) of 6-(hex-5-yn-1-yloxy)hex-1-yne as a clear oil.

Figure S1. Saturation binding curve obtained for [^{125}I]SGMIB-5F7 using BT474M1 cells.

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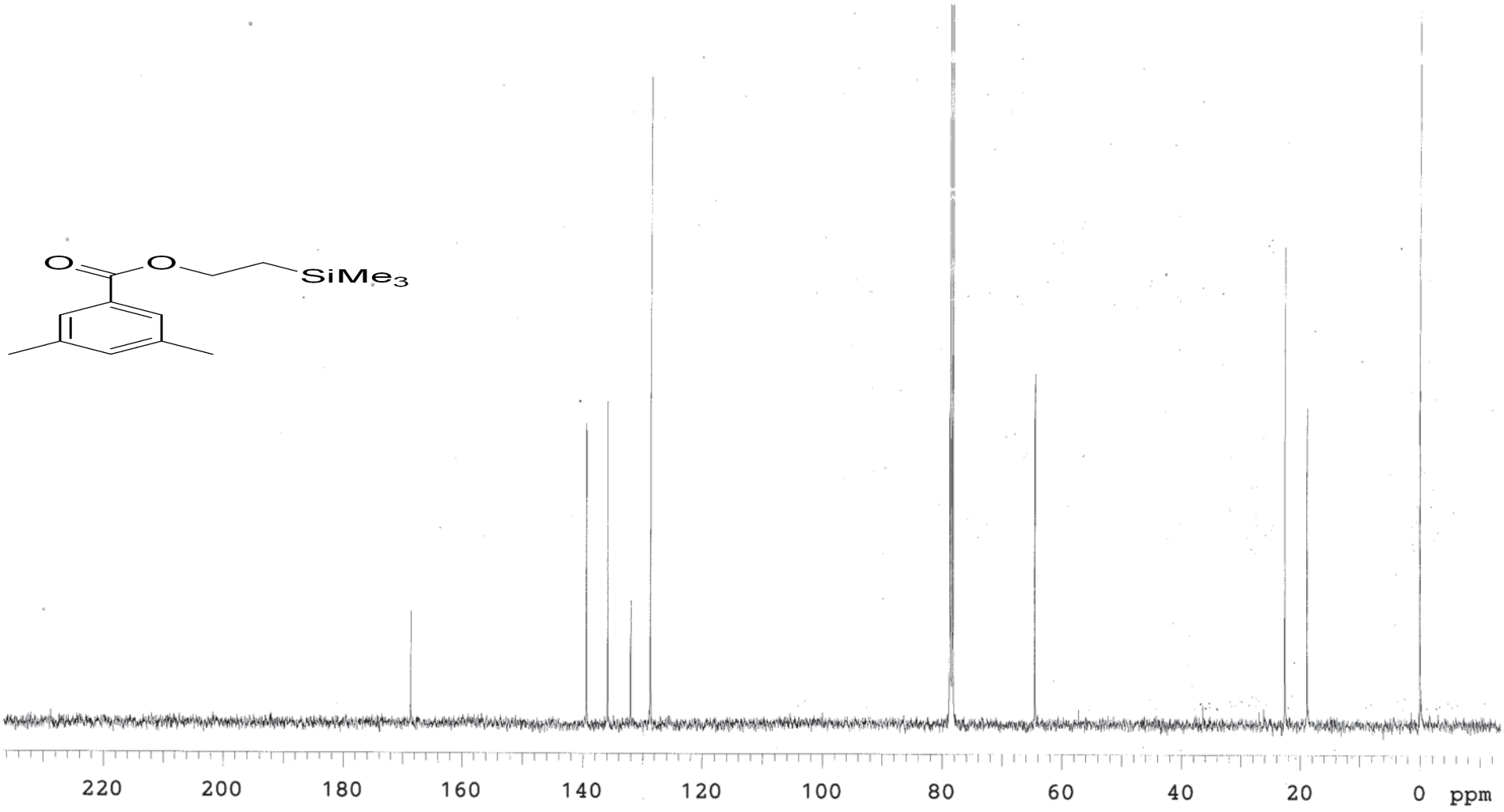
0.89
0.30
1.24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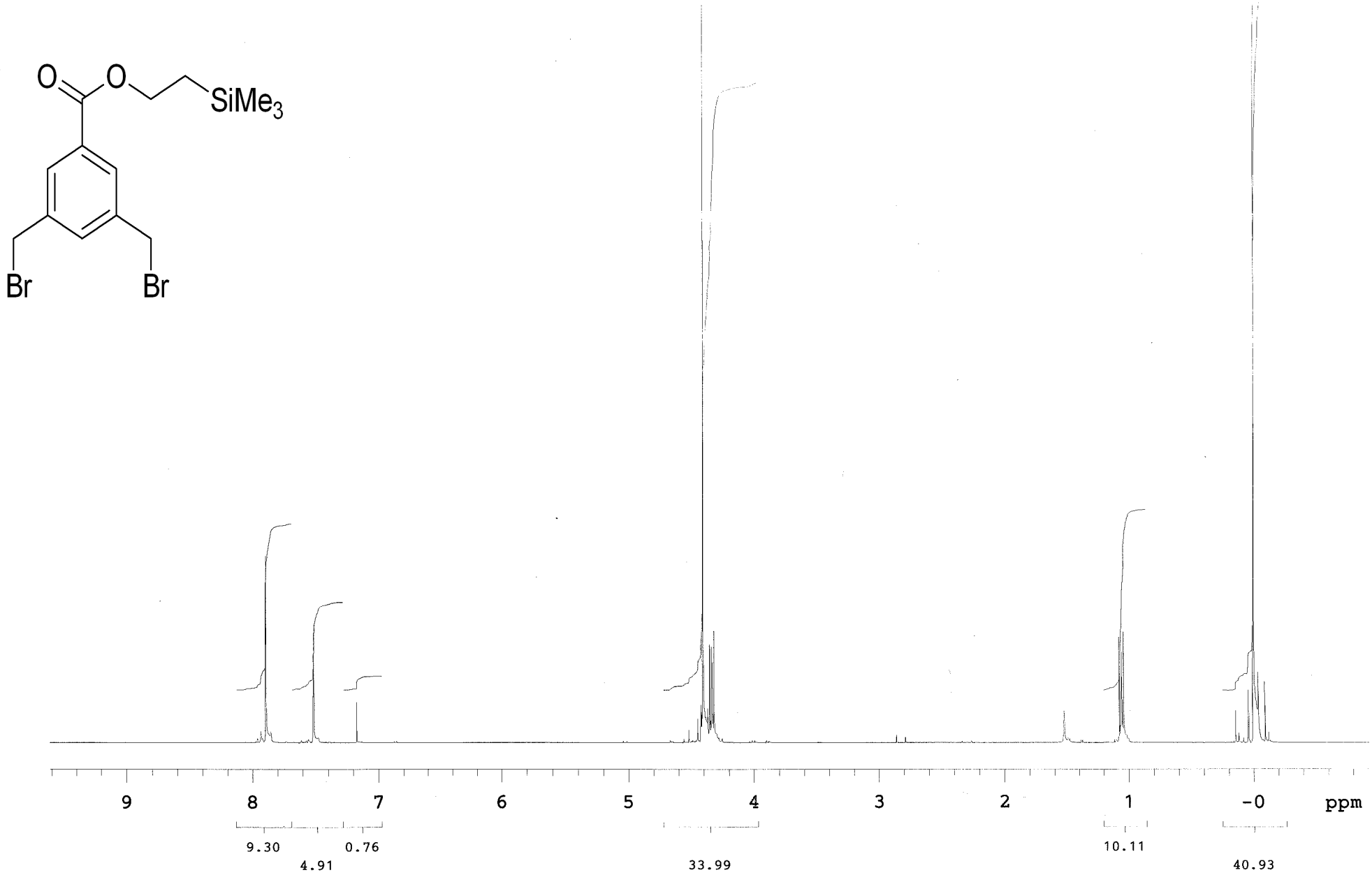
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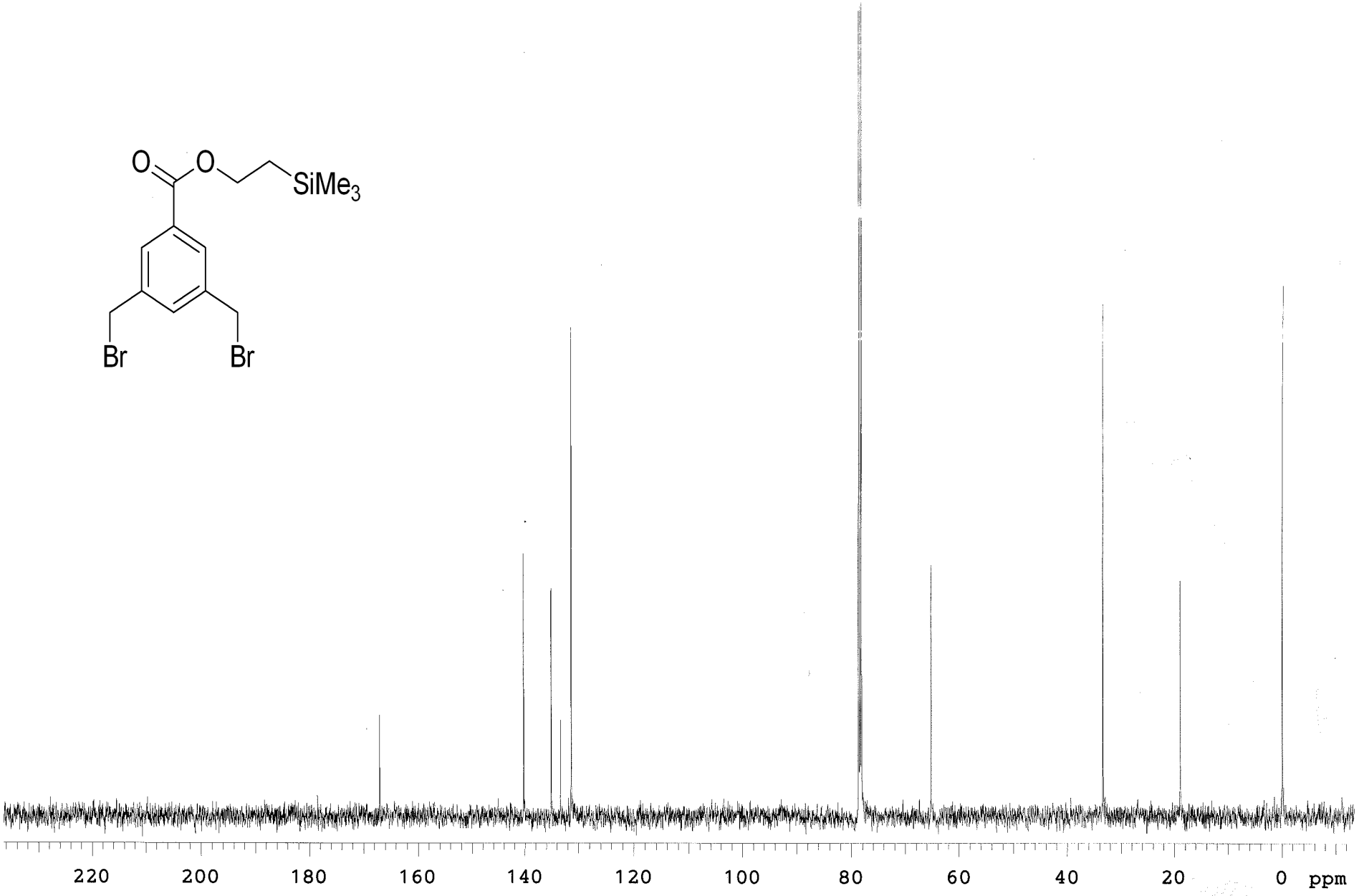
40.93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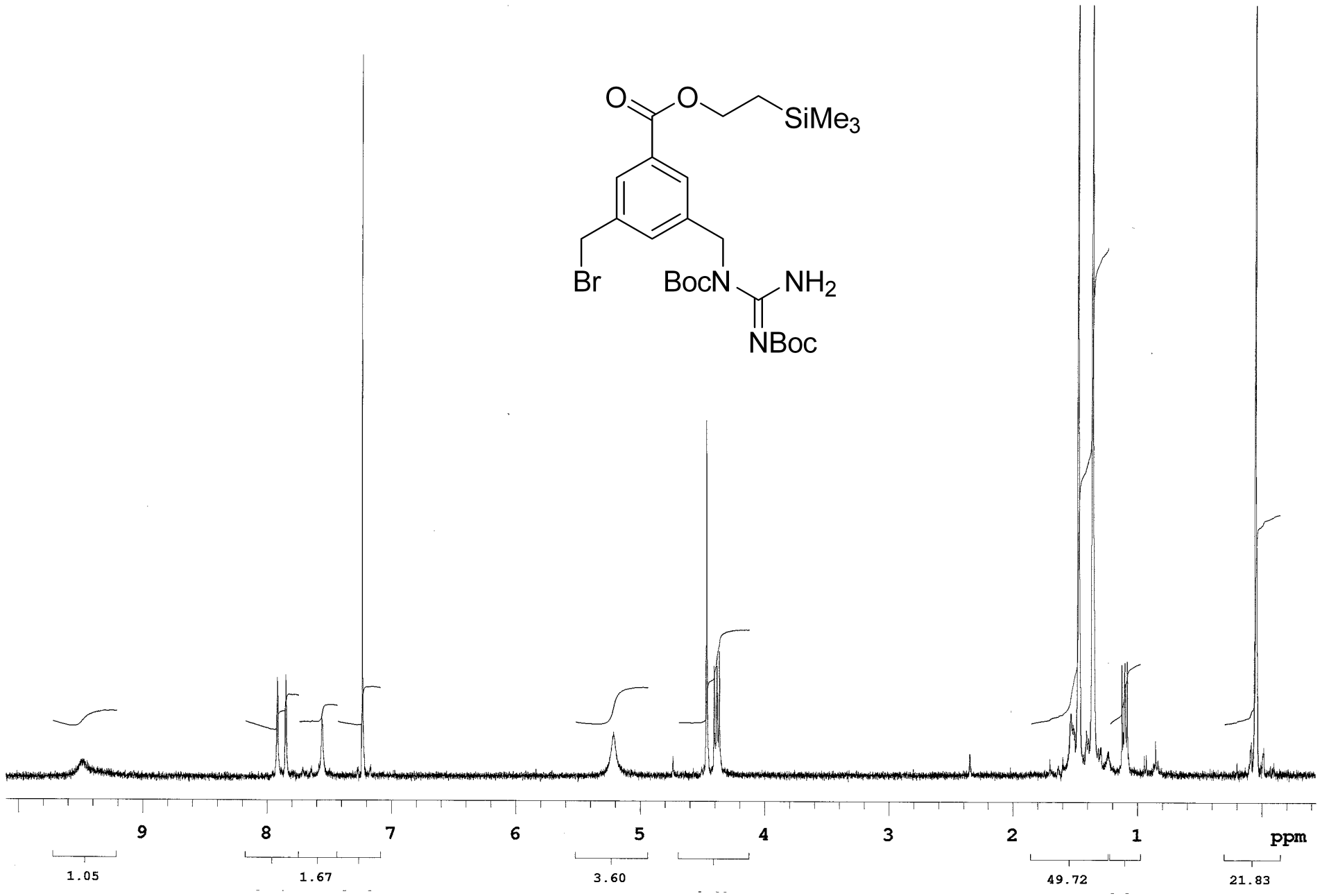
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NH2
NBoc
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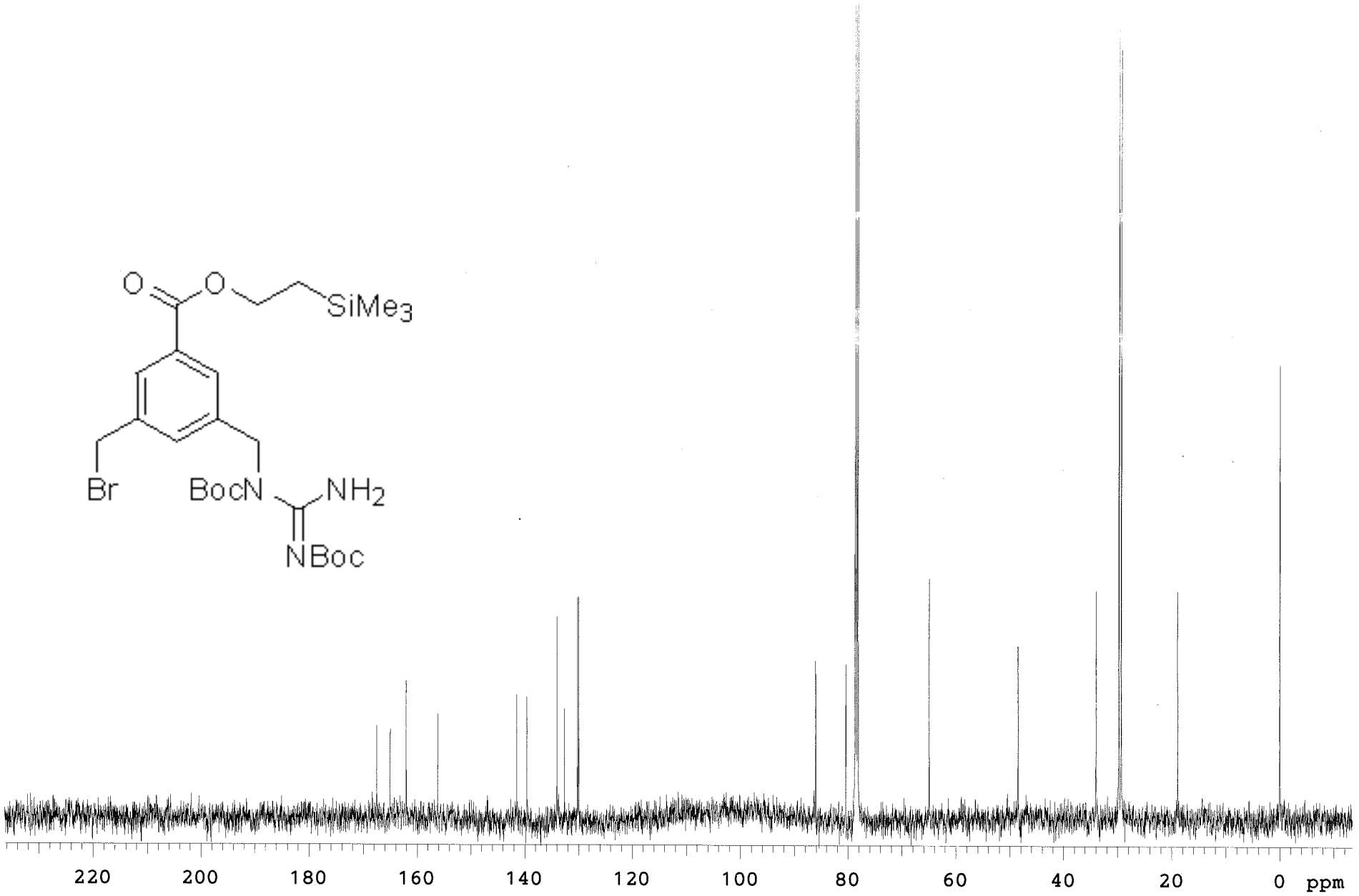
21.83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NH2
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100
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60
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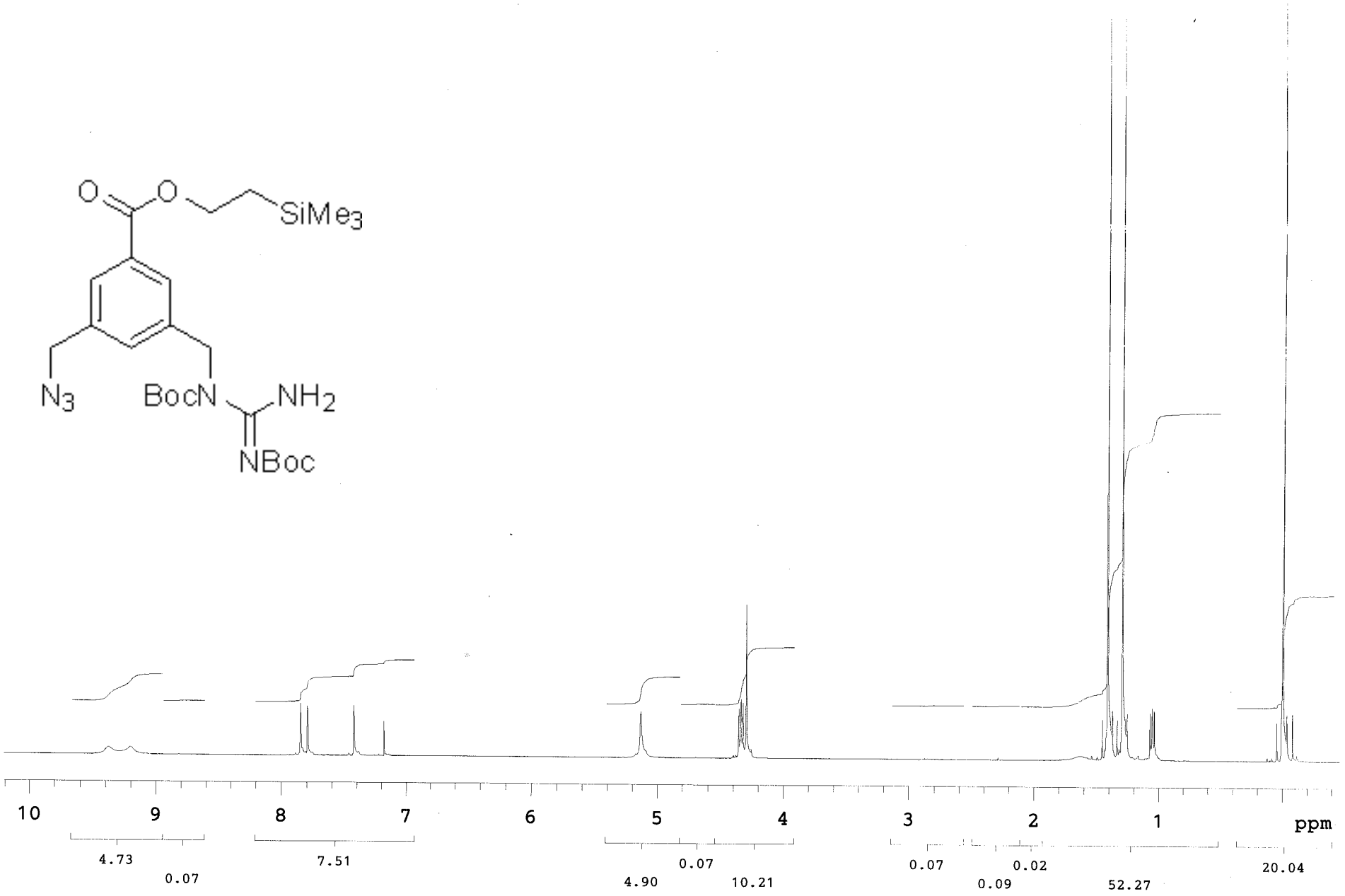
20
0
ppm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0.02
52.27
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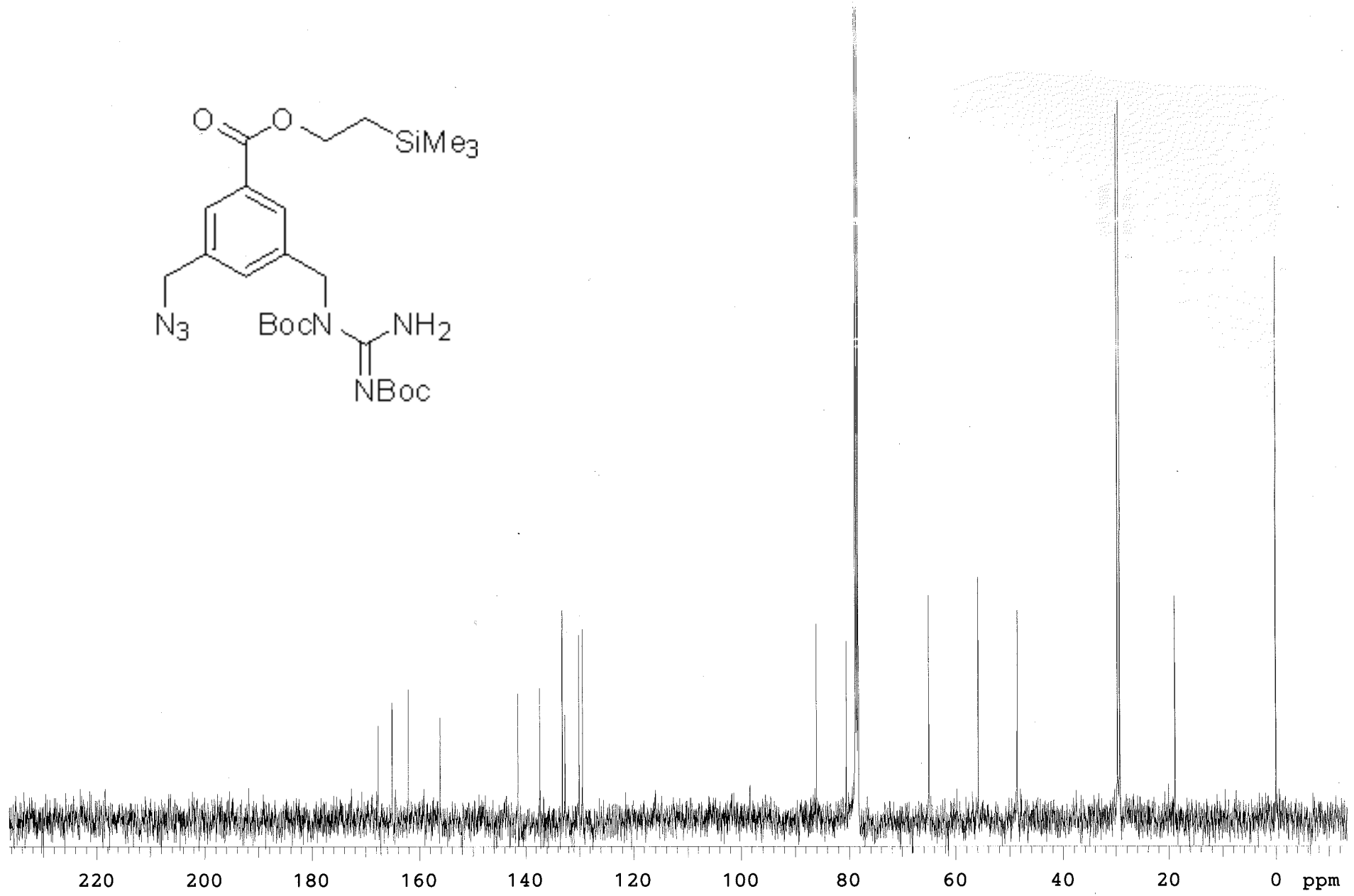
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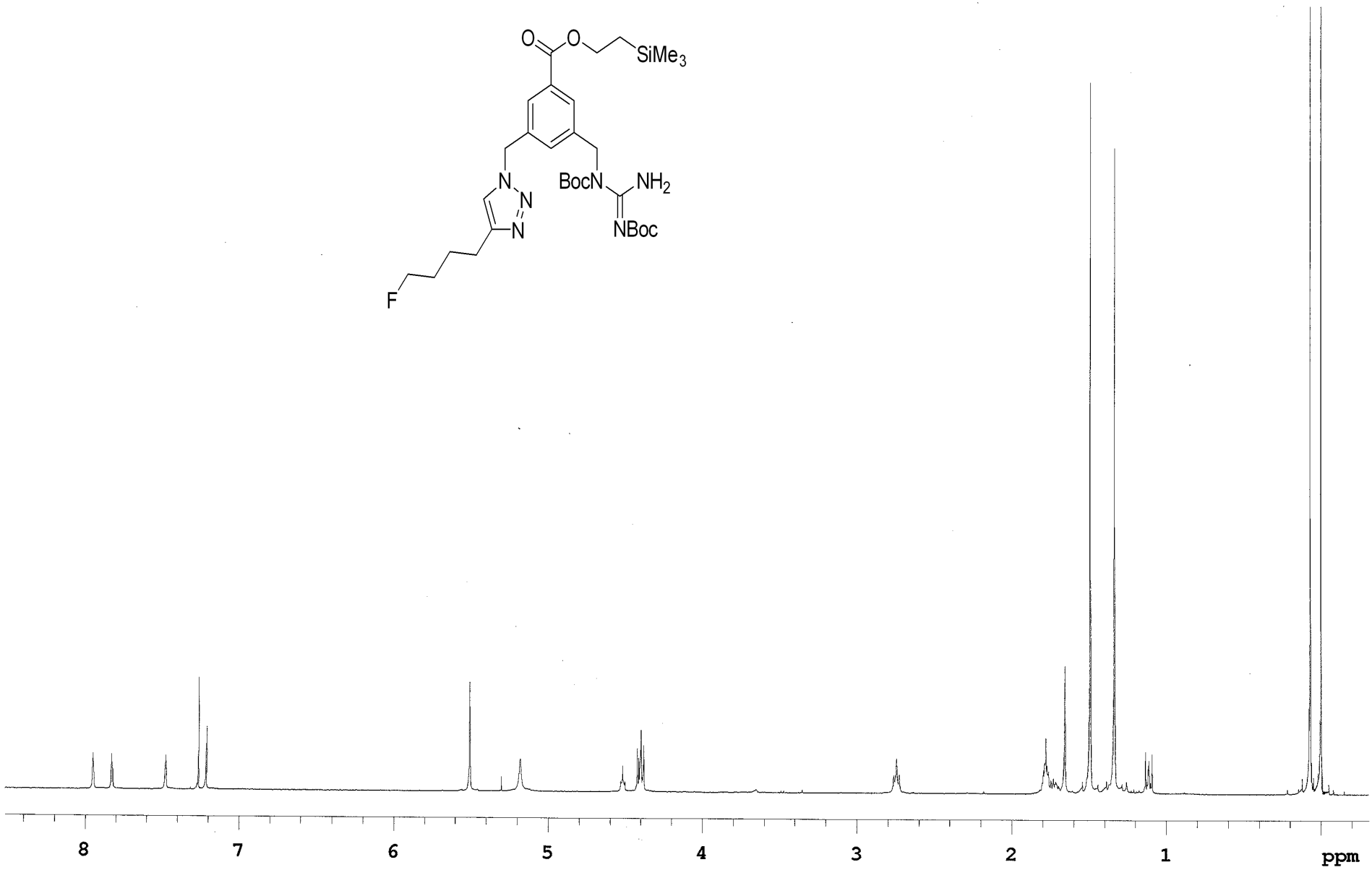
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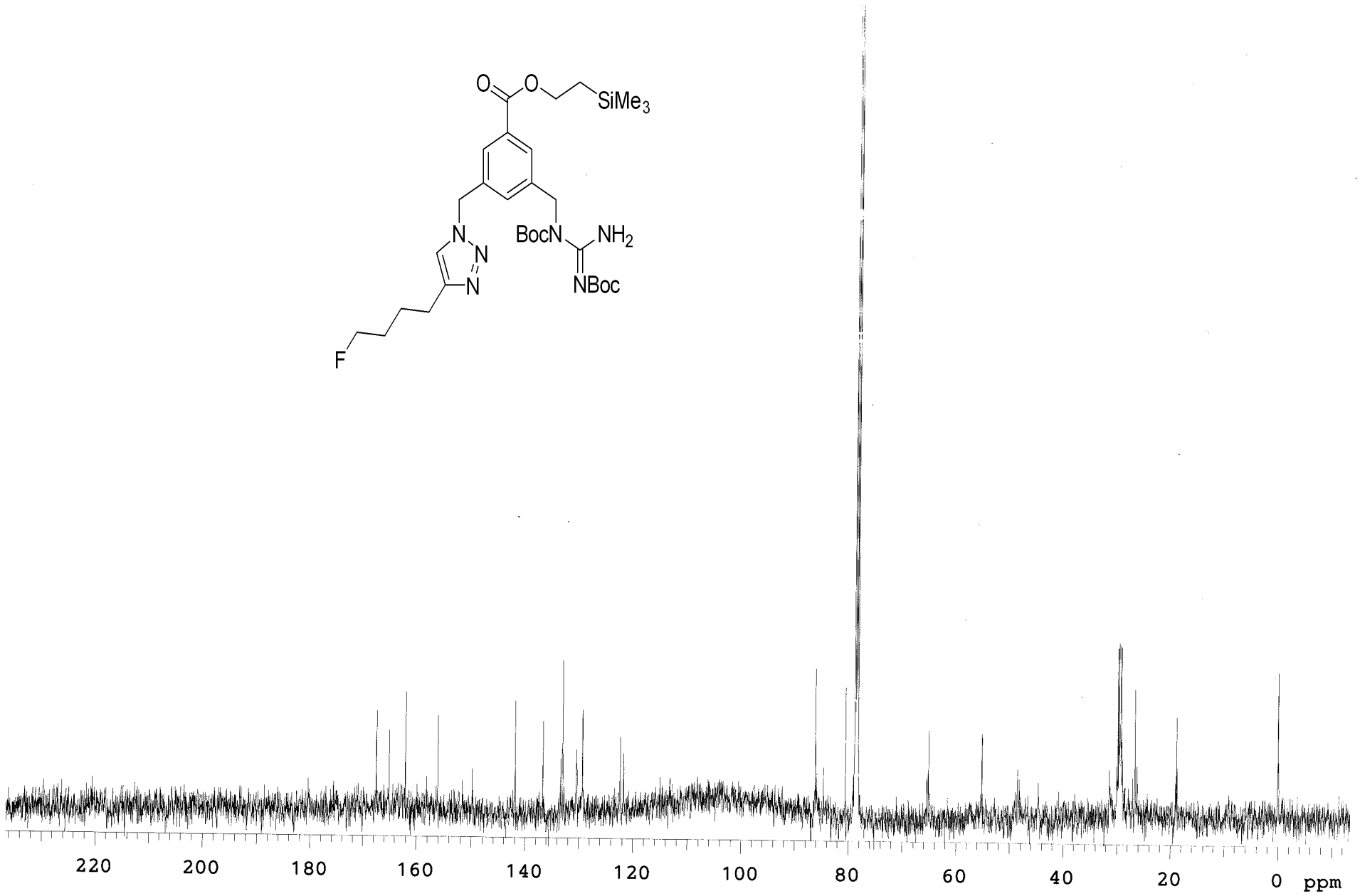
ppm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40
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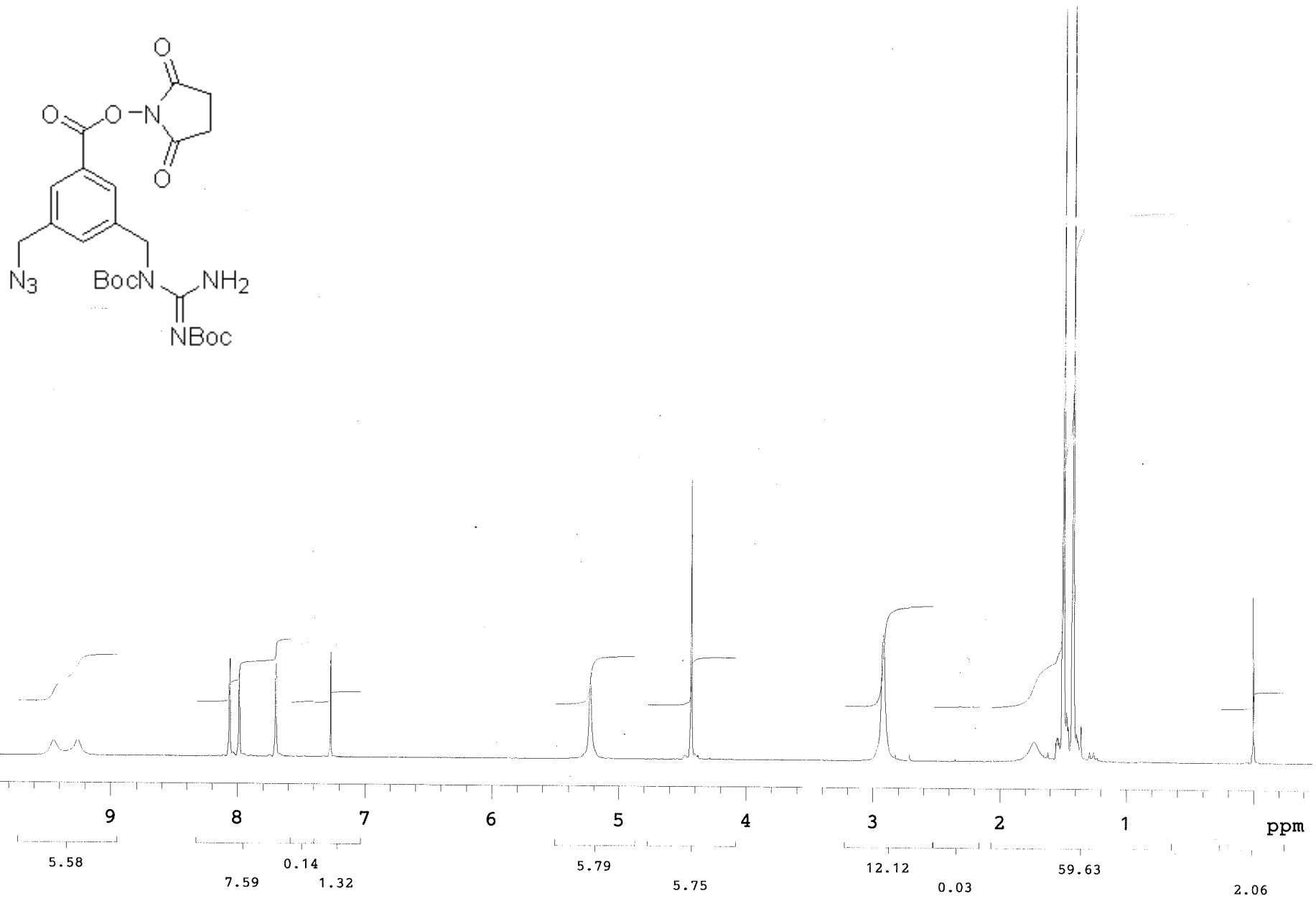
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N3
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NH2
NBoc
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6
5
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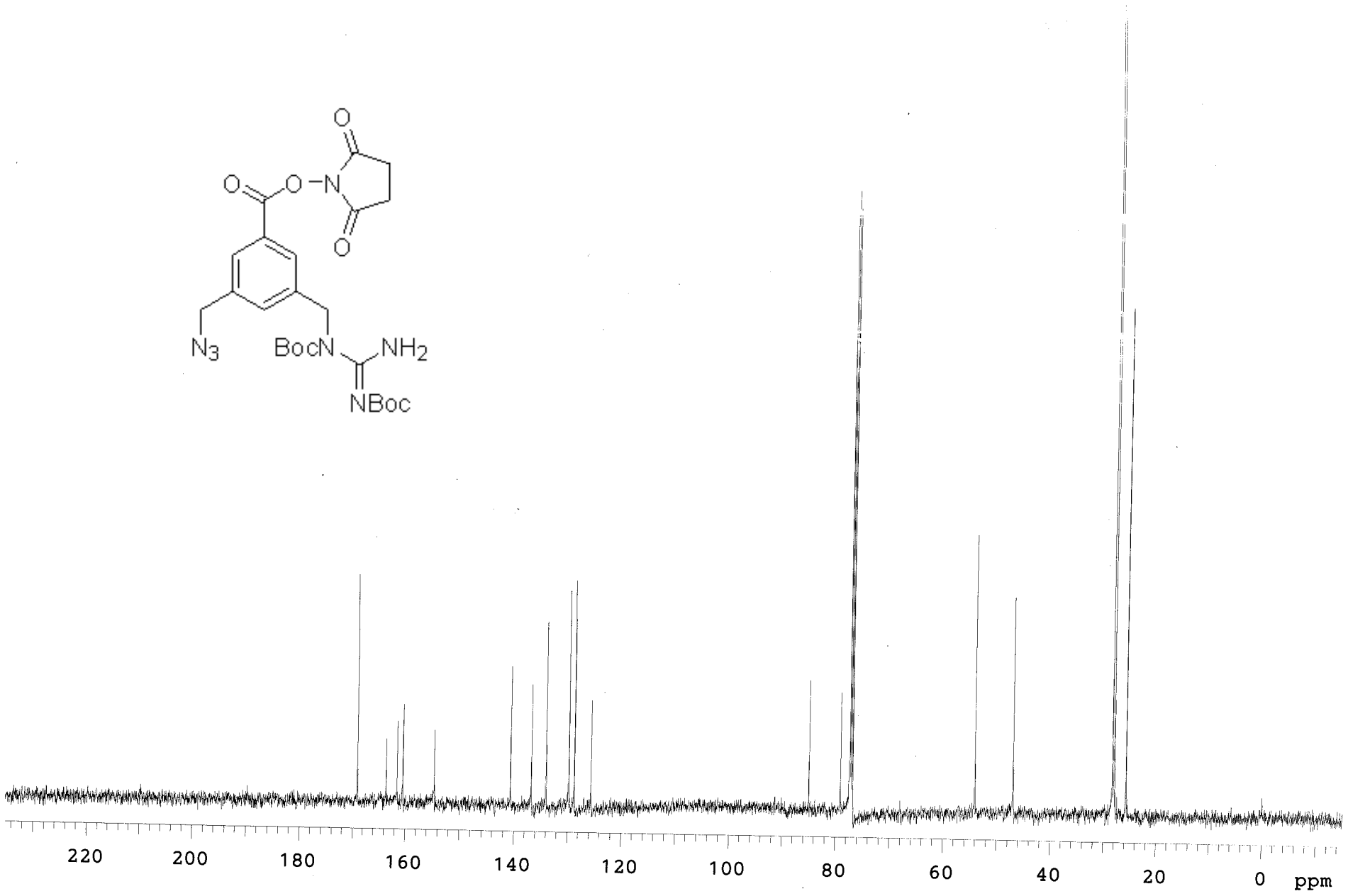
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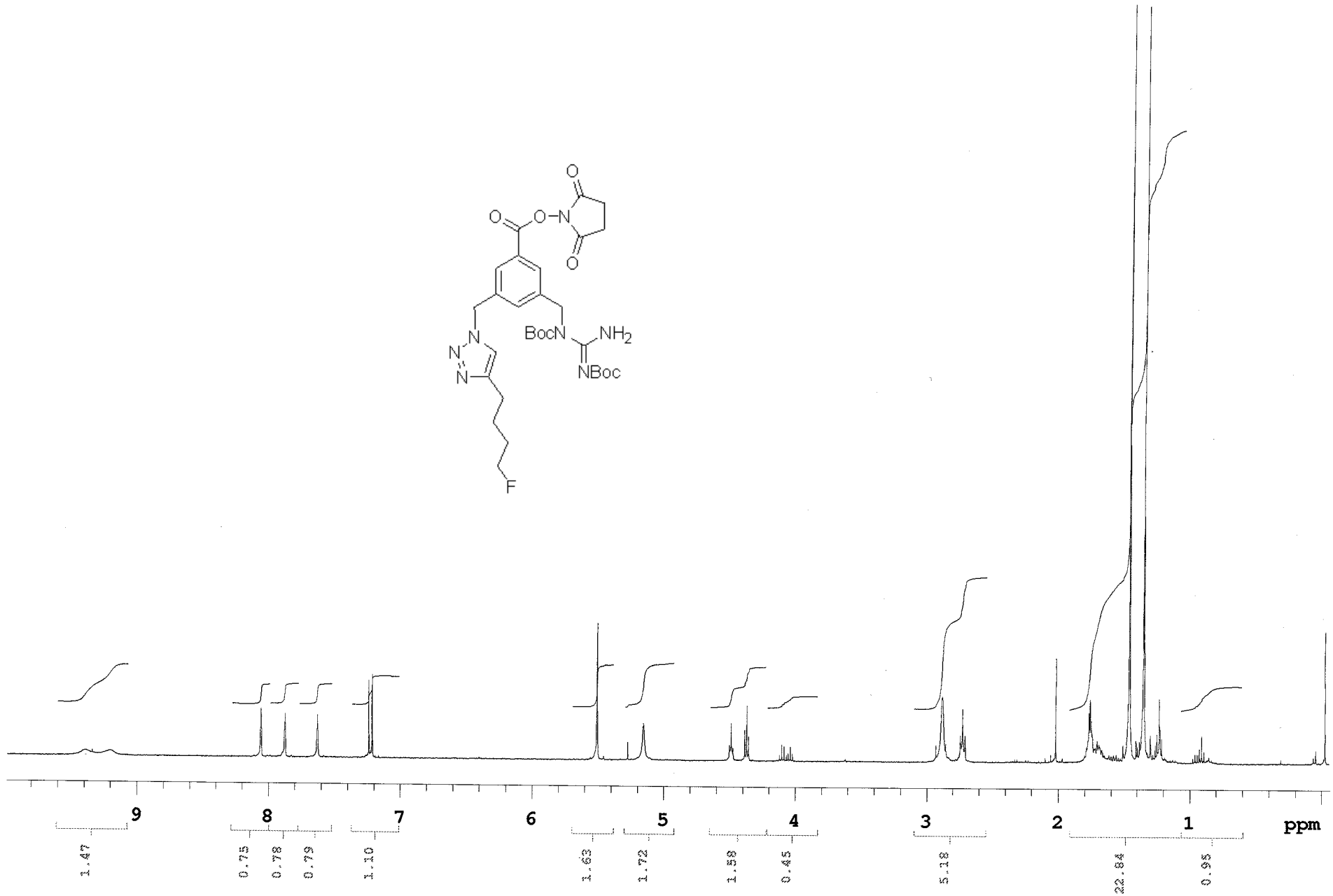
ppm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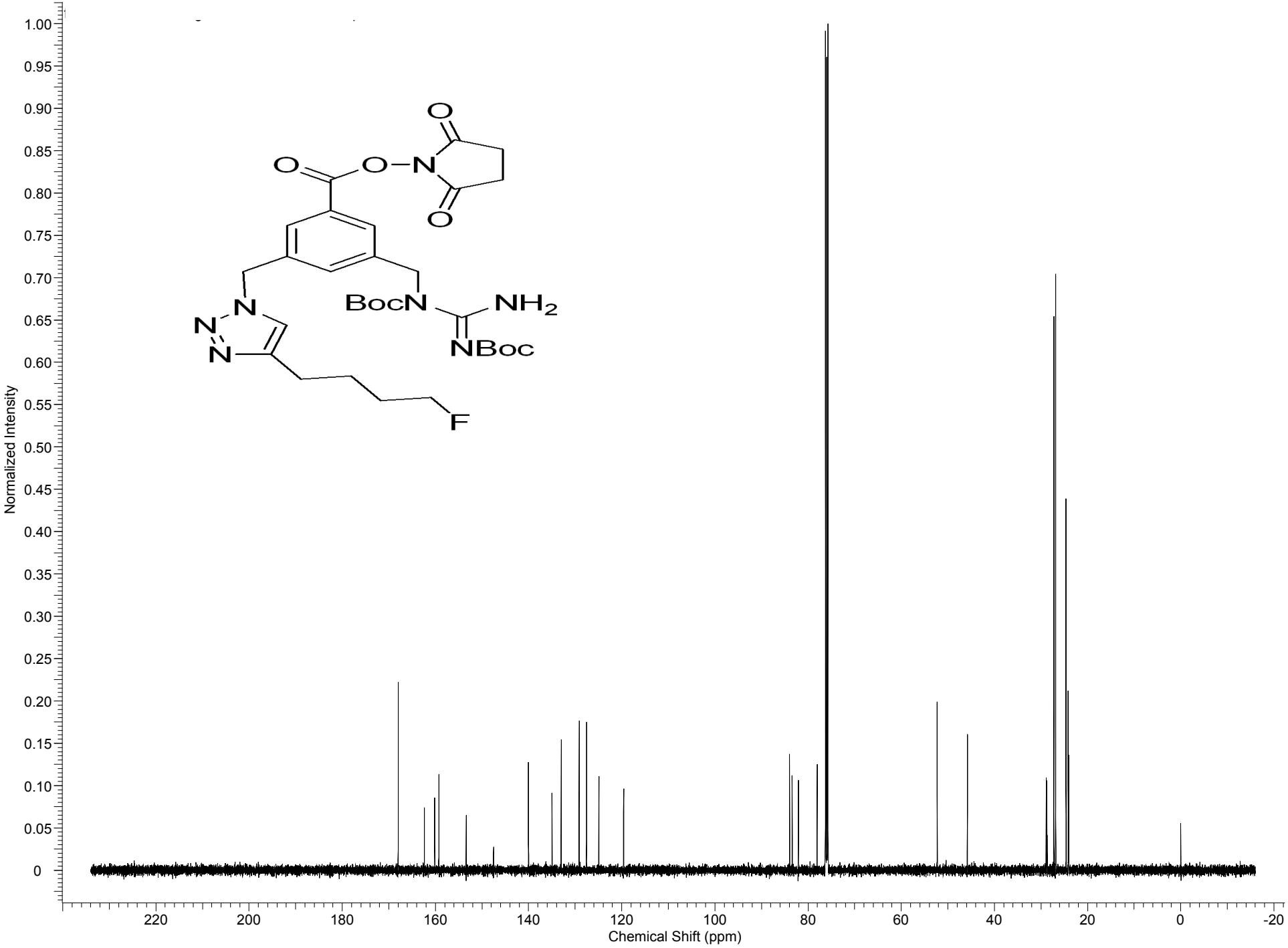
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0.40
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0.25
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0.15
0.10
0.05
0
220
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180
160
140
120
100
80
60
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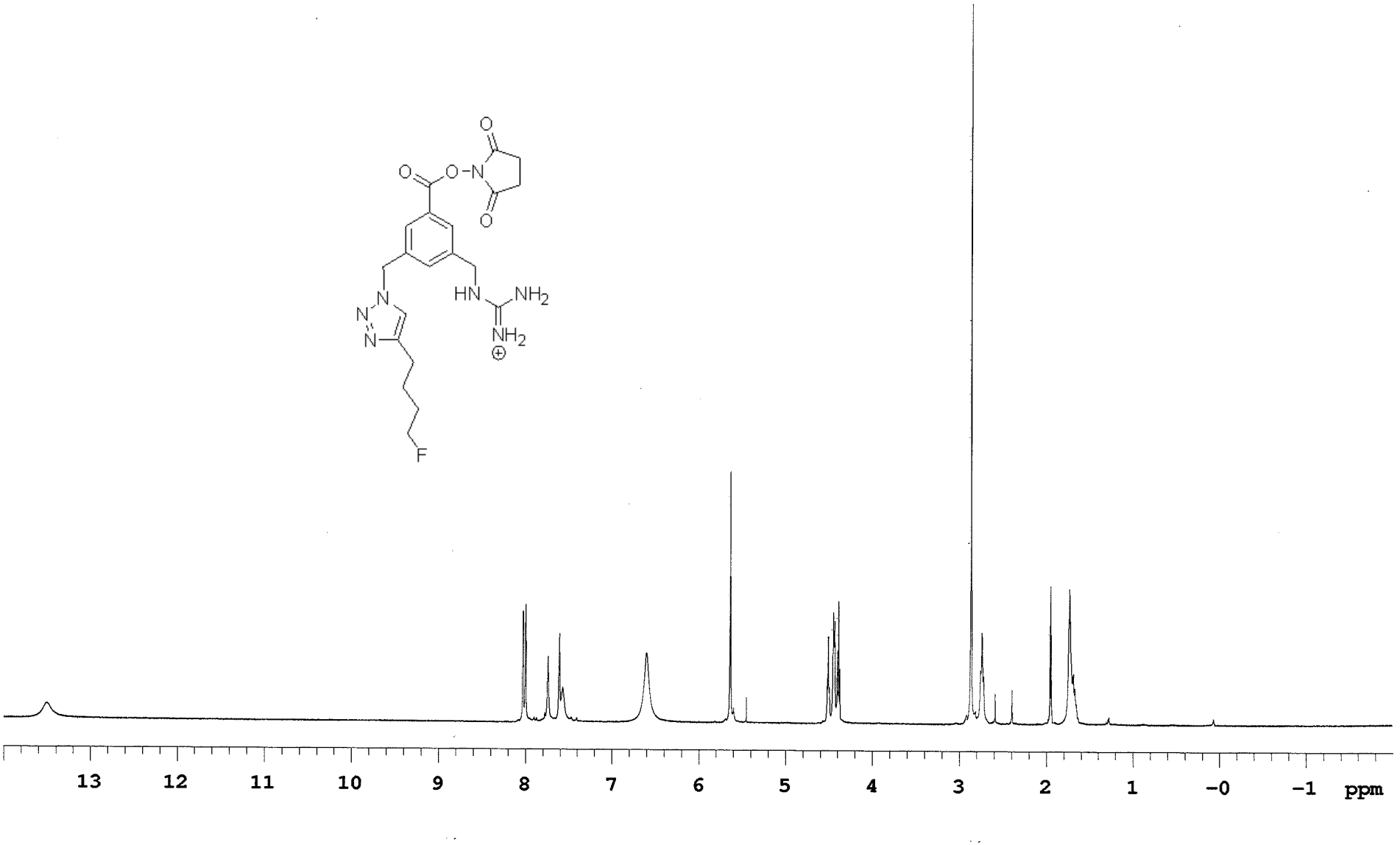
N
N
N
BocN
NH2
NBoc
F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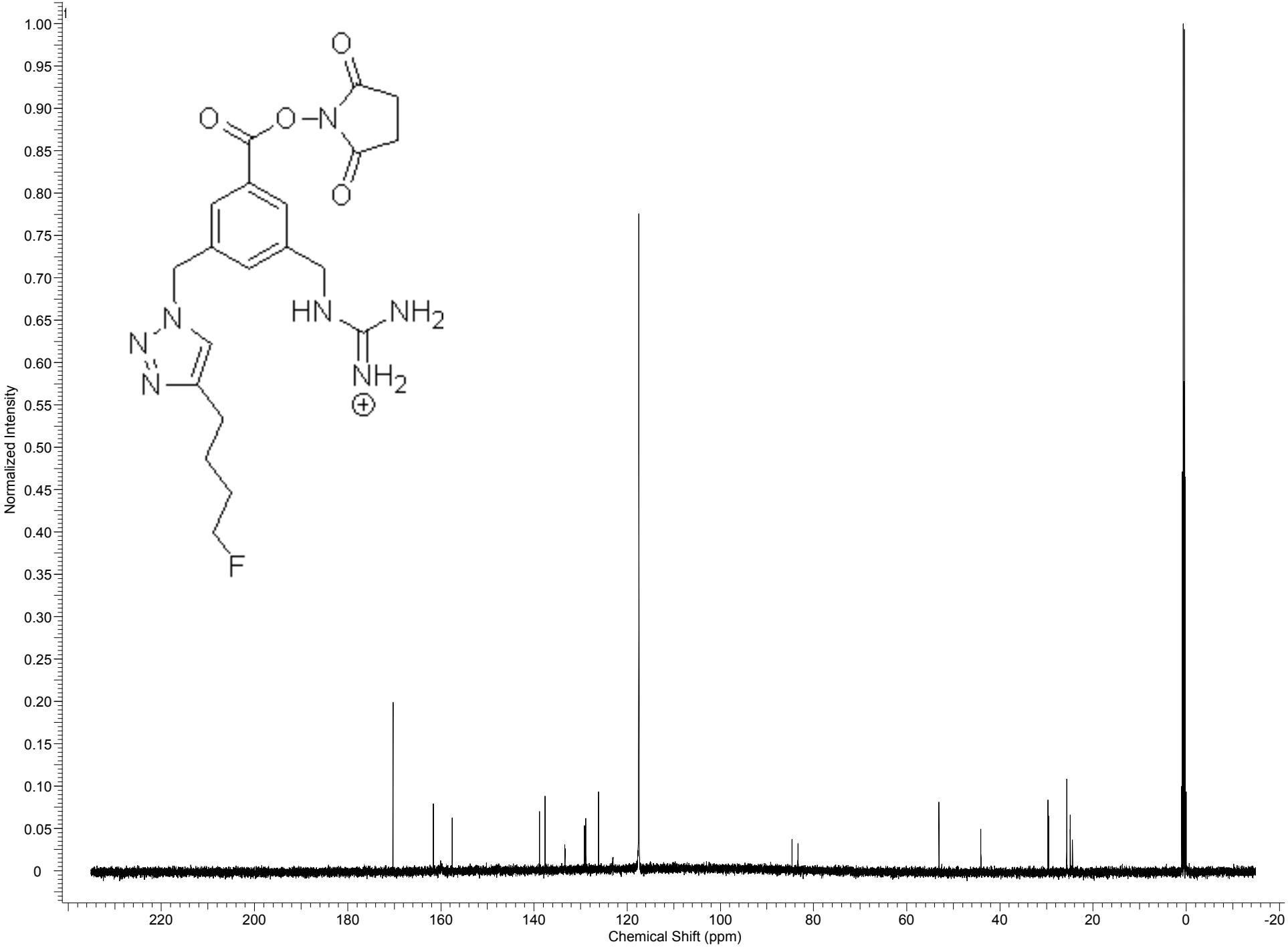
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0.10
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O
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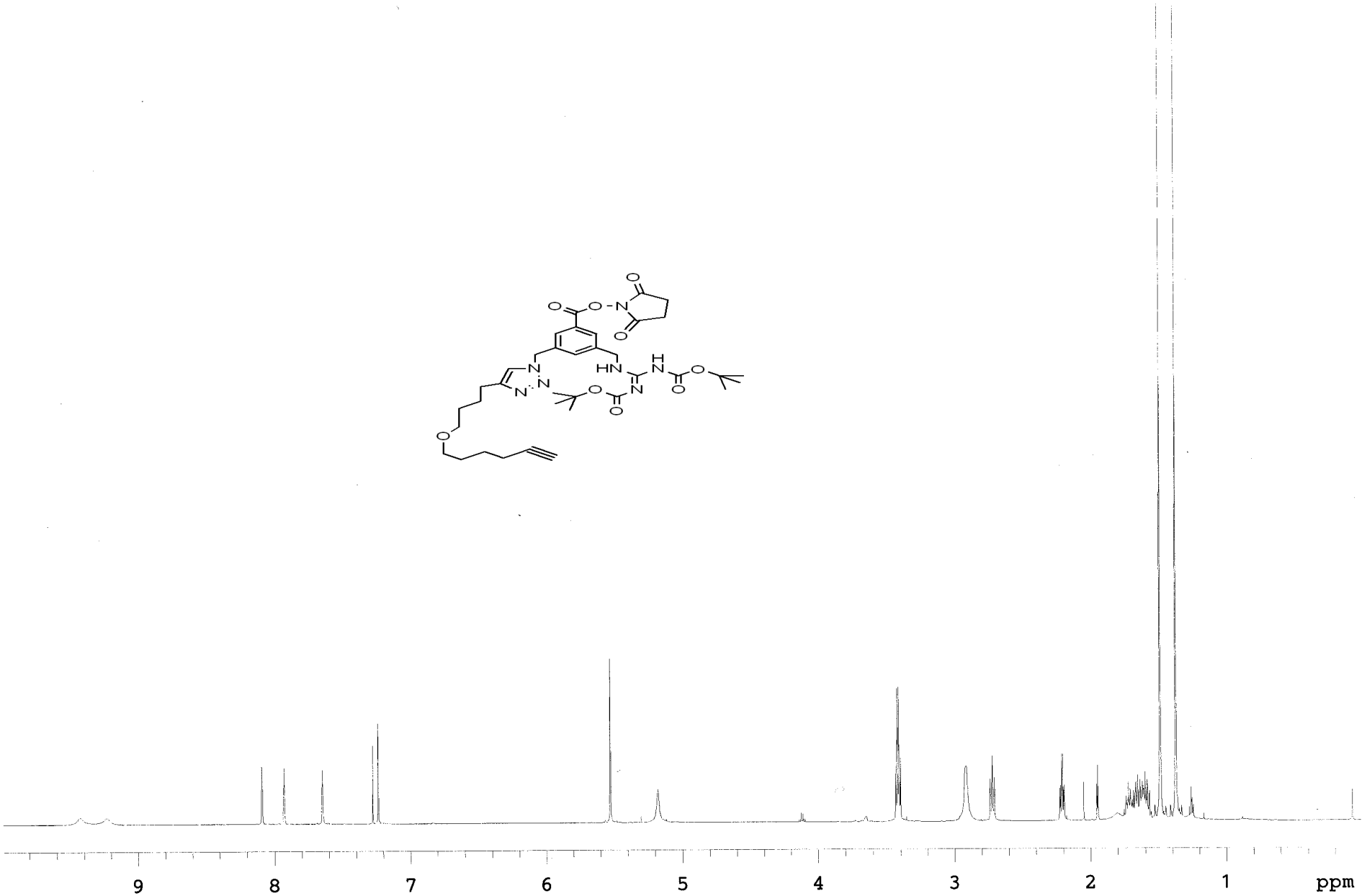
HN
NH2
NH2
N
N
N
F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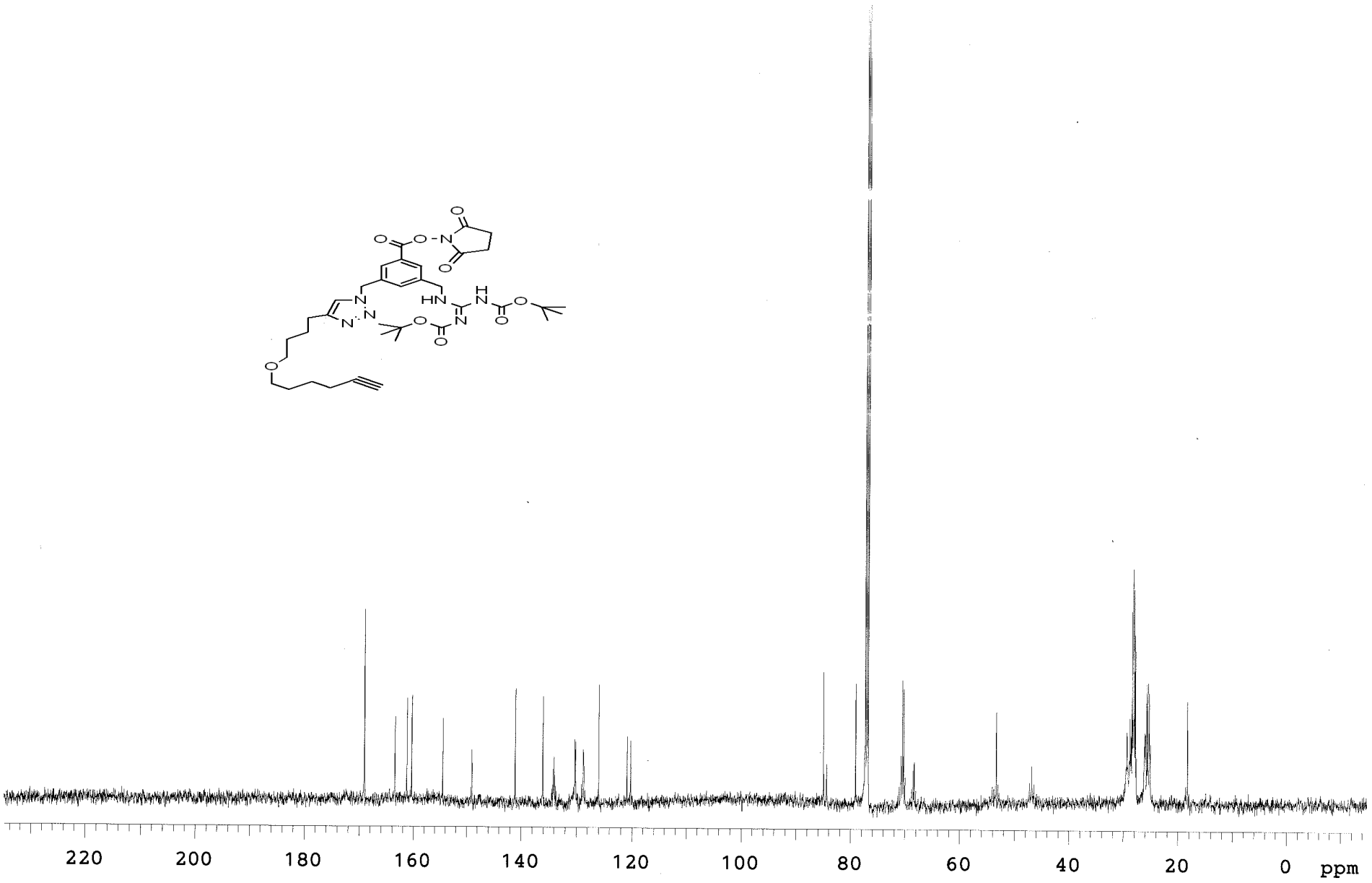
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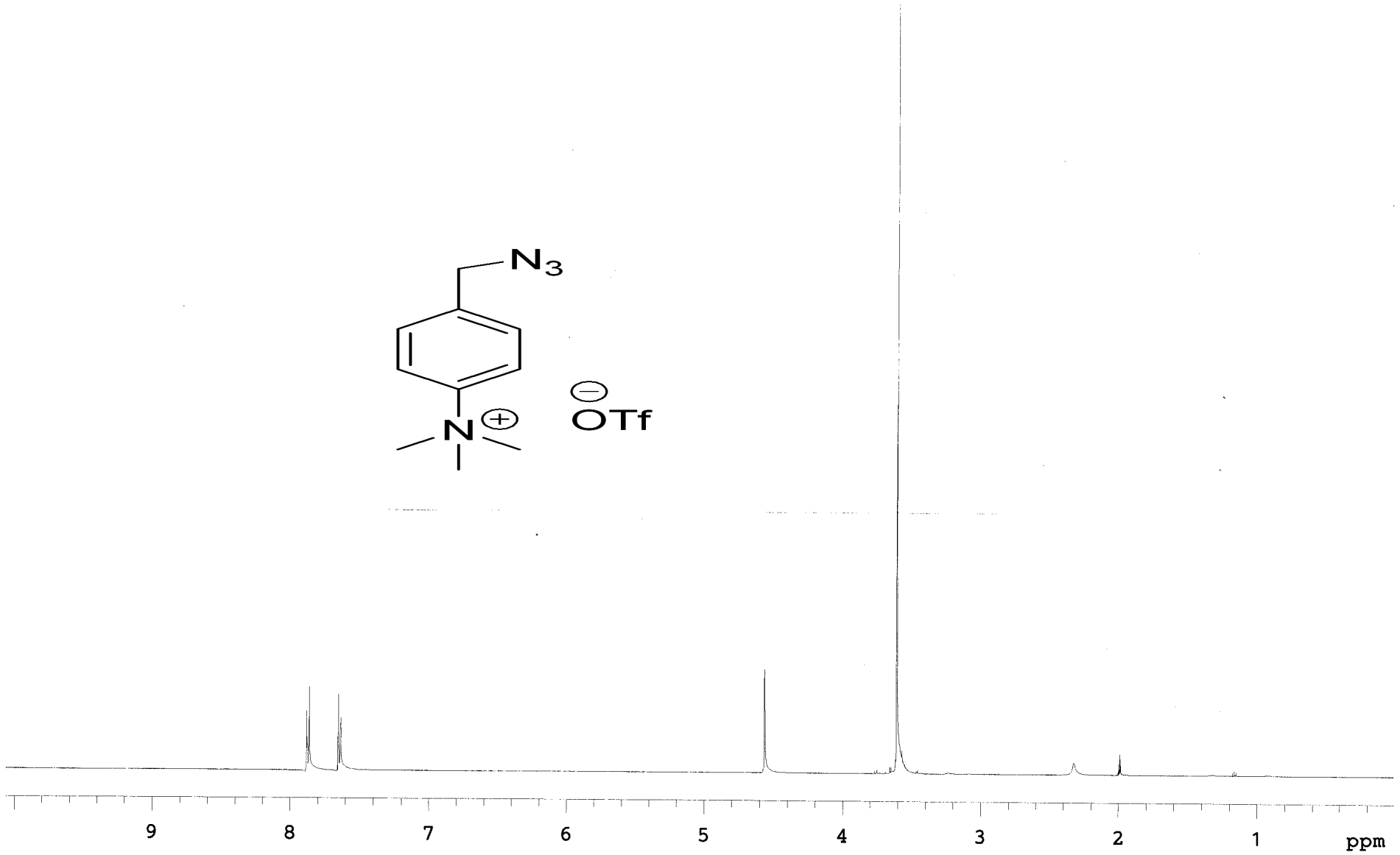
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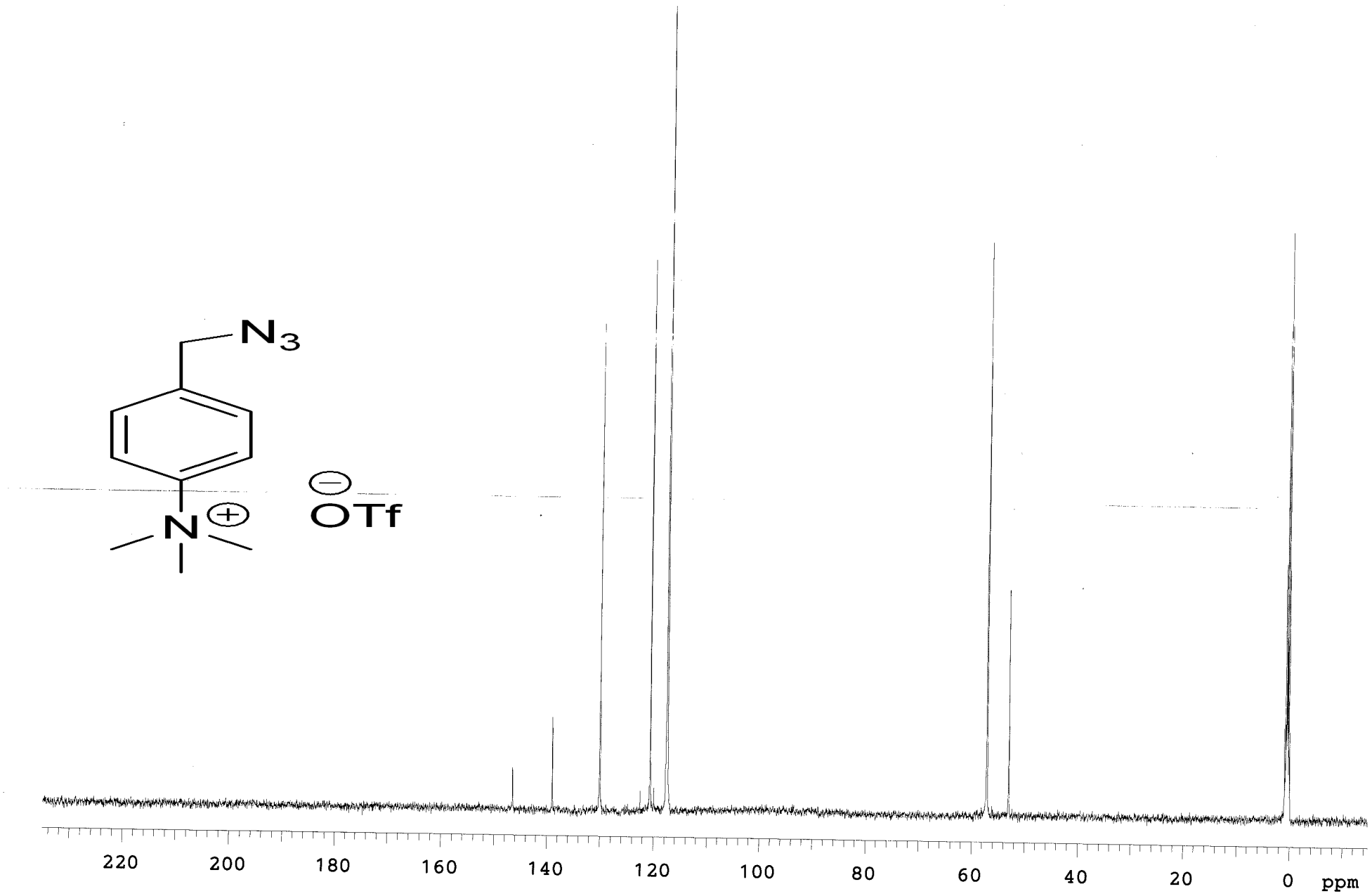
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