

Supporting Information

Cu(I)-catalyzed Chemical Fixation of CO₂ with 2-Alkynylaniline into 4-Hydroxyquinolin-2(1H)-one

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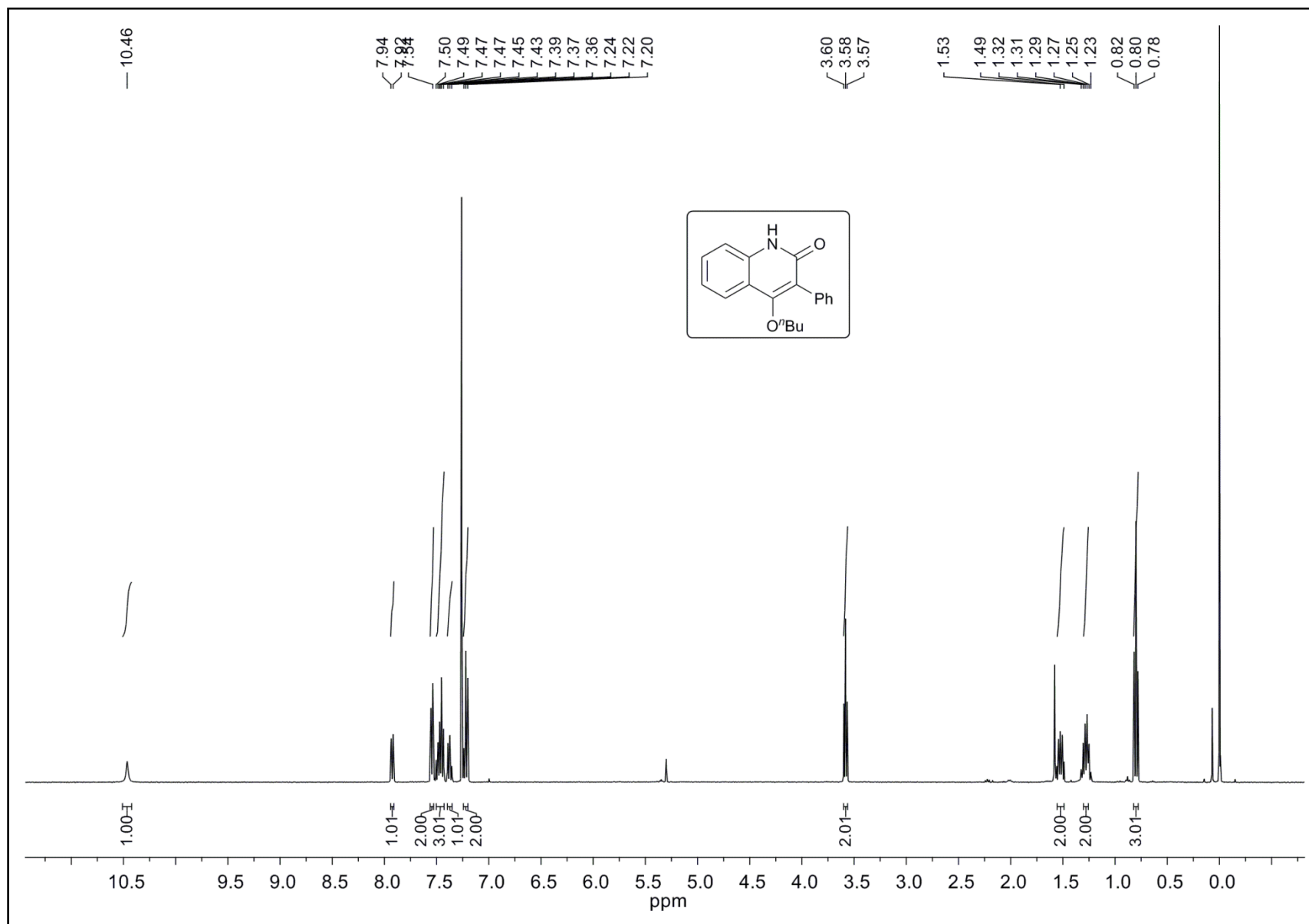
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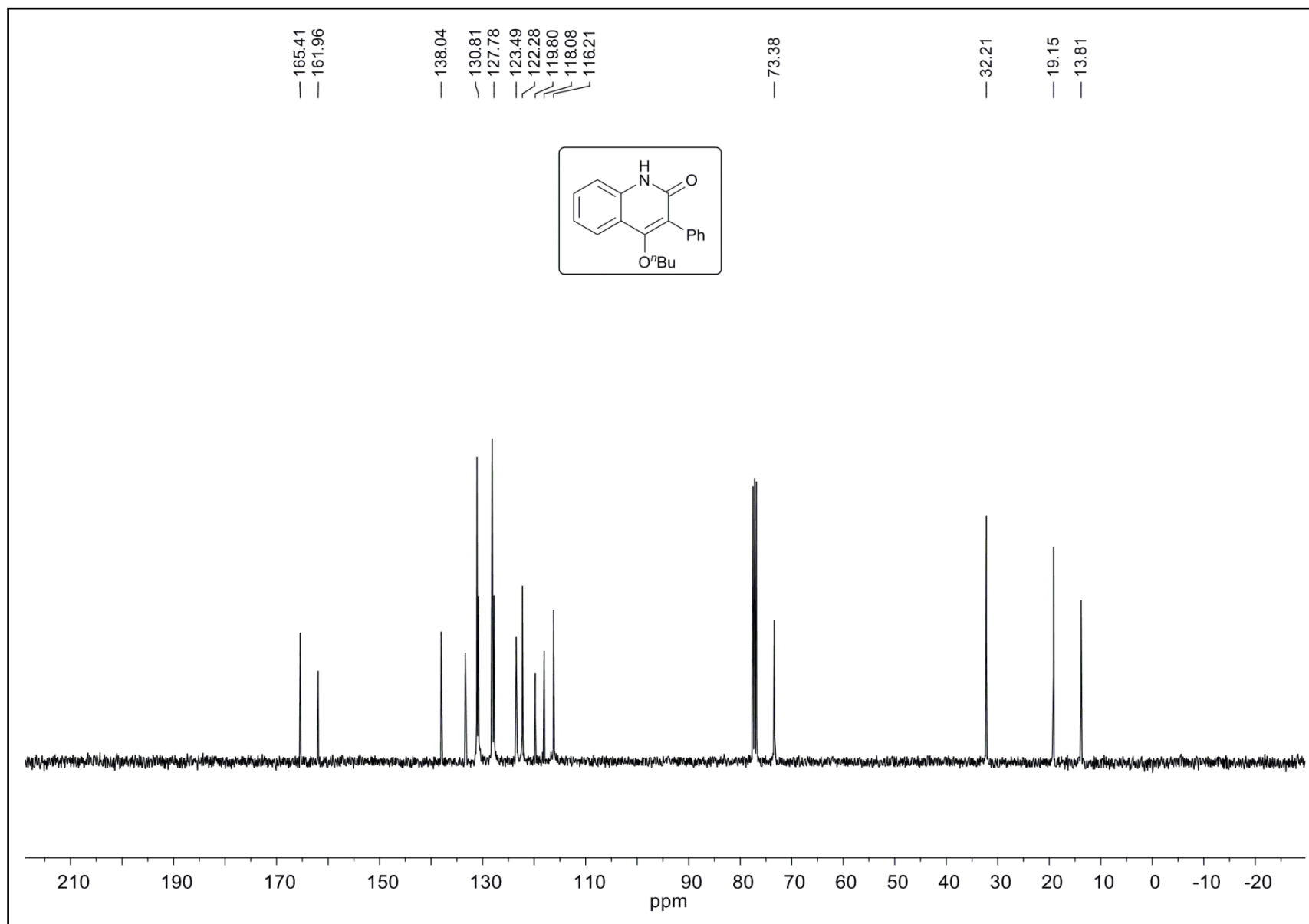
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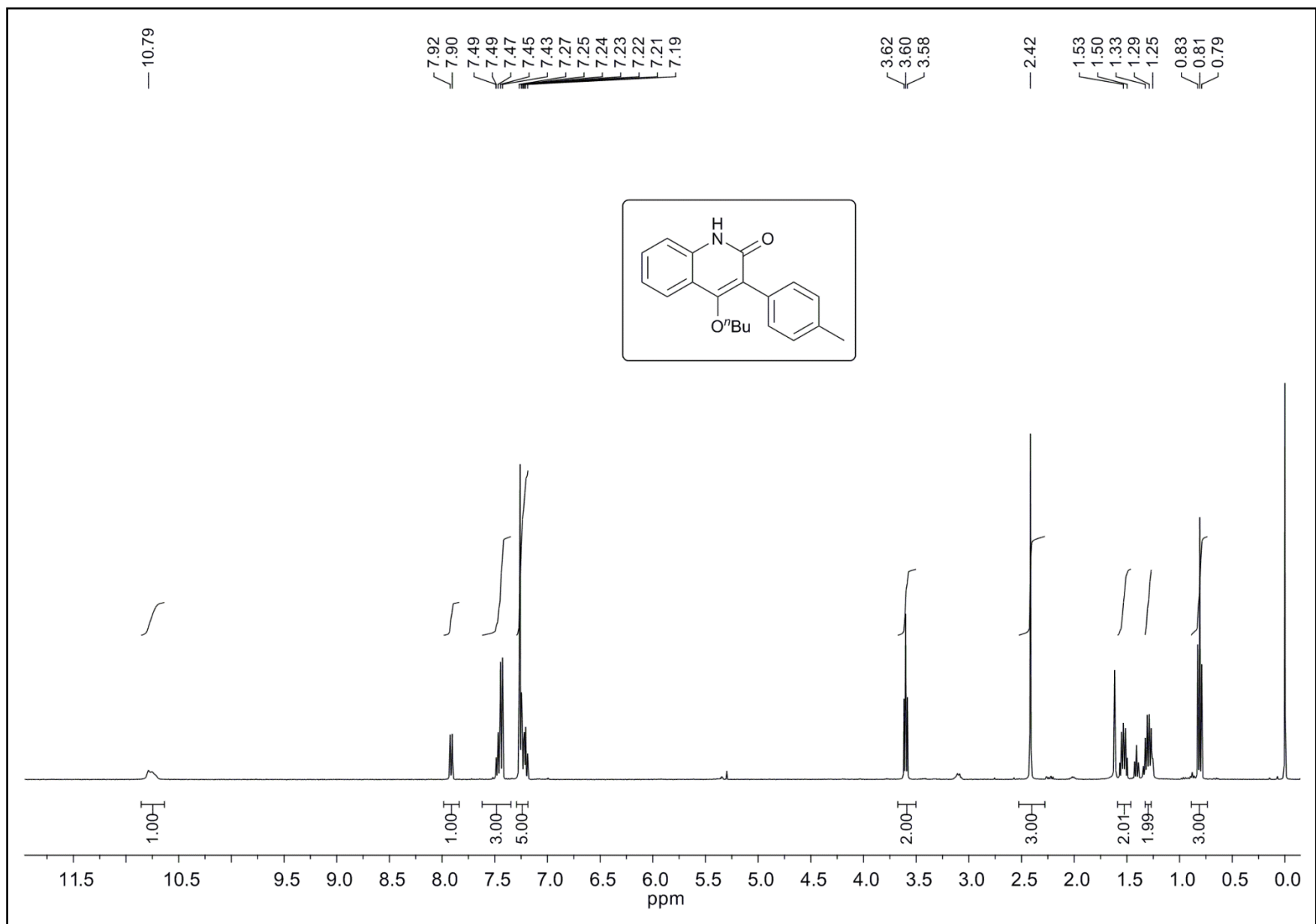
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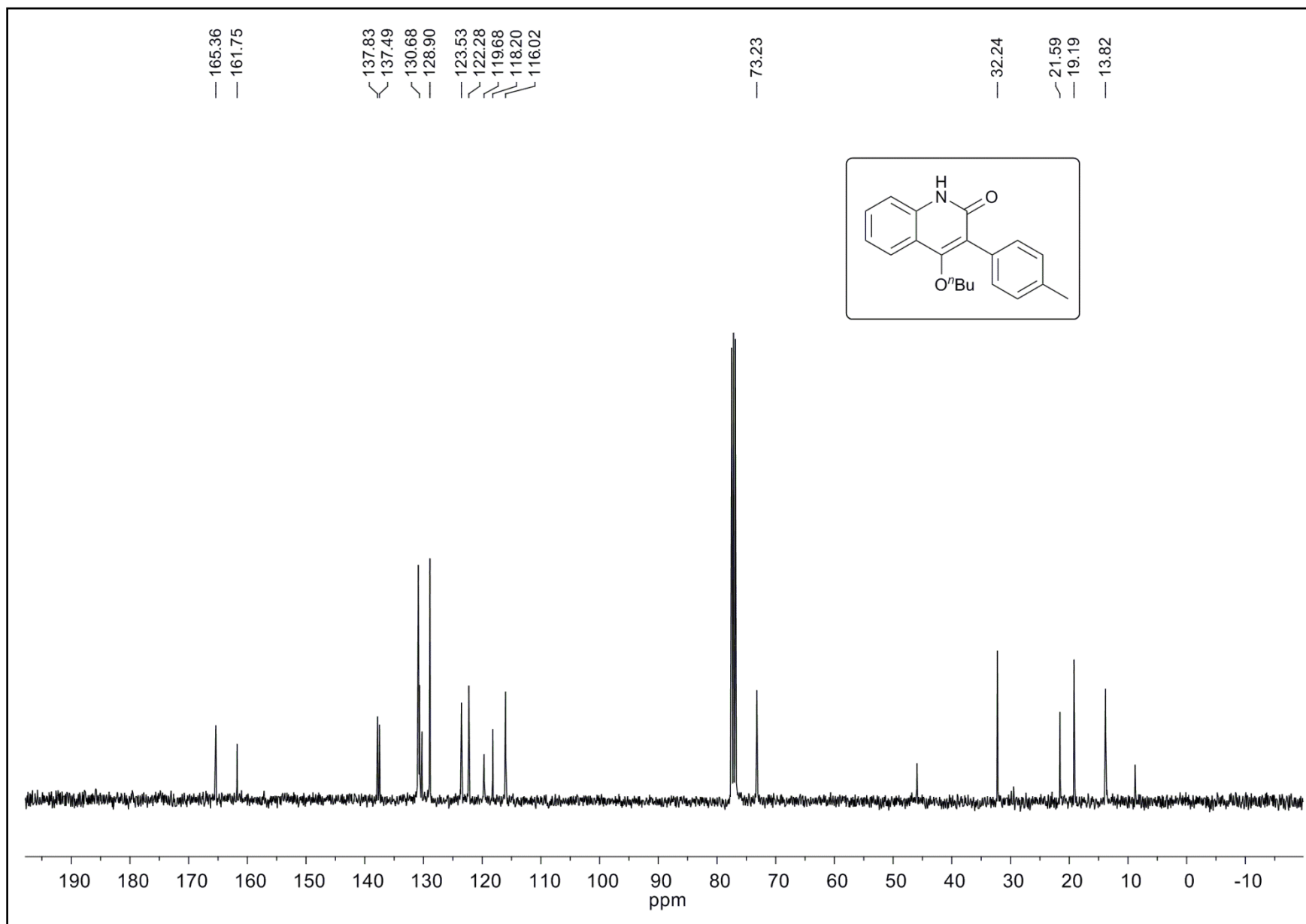
Table S1. Crystallographic data for **2q** and **2s**

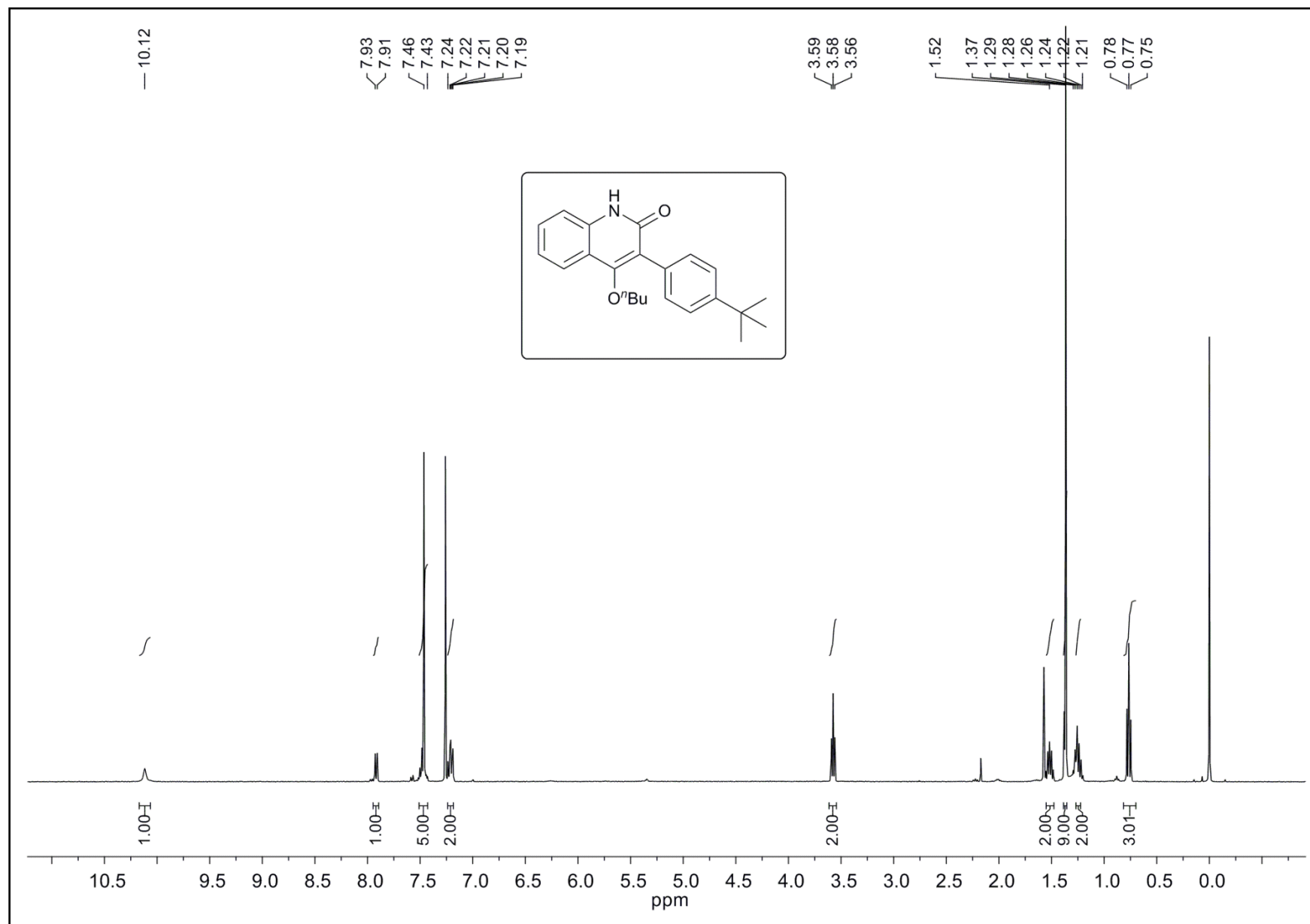
	2q	2s
formula	C ₂₁ H ₂₃ NO ₂	C ₂₁ H ₂₀ F ₃ NO ₂
formula weight	321.40	375.38
color	white	white
crystal system	triclinic	triclinic
space group	<i>P</i> 1	<i>P</i> 1
<i>a</i> , Å	7.7051(4)	6.1860(5)
<i>b</i> , Å	10.8189(5)	9.6029(9)
<i>c</i> , Å	11.1726(5)	16.4251(11)
α , deg	75.918(3)	77.495(6)
β , deg	86.590(3)	80.955(6)
γ , deg	87.802(3)	87.557(7)
<i>V</i> , Å ³	901.49(7)	940.68(13)
<i>Z</i>	2	2
<i>T</i> , K	296(2)	296(2)
μ , mm ⁻¹	0.076	0.105
<i>F</i> (000)	344	392
θ range, deg	1.94 to 24.99	2.17 to 24.99
index ranges (<i>h</i> , <i>k</i> , <i>l</i>)	±9, ±12, -12 to 13	±7, -11 to 10, ±19
reflections collected	6207	5416
independent reflections / <i>R</i> _{int}	3156/0.0170	3279/0.0279
obsd reflections (<i>I</i> > 2 σ (<i>I</i>))	2539	1579
data/restraints/parameters	3156/0/217	3279/0/244
<i>R</i> 1/ <i>wR</i> 2 (<i>I</i> > 2 σ (<i>I</i>))	0.0469/0.1415	0.0993/0.2961
<i>R</i> 1/ <i>wR</i> 2 (all data)	0.0573/0.1522	0.1723/0.3474
GOF (on <i>F</i> ²)	1.080	1.047

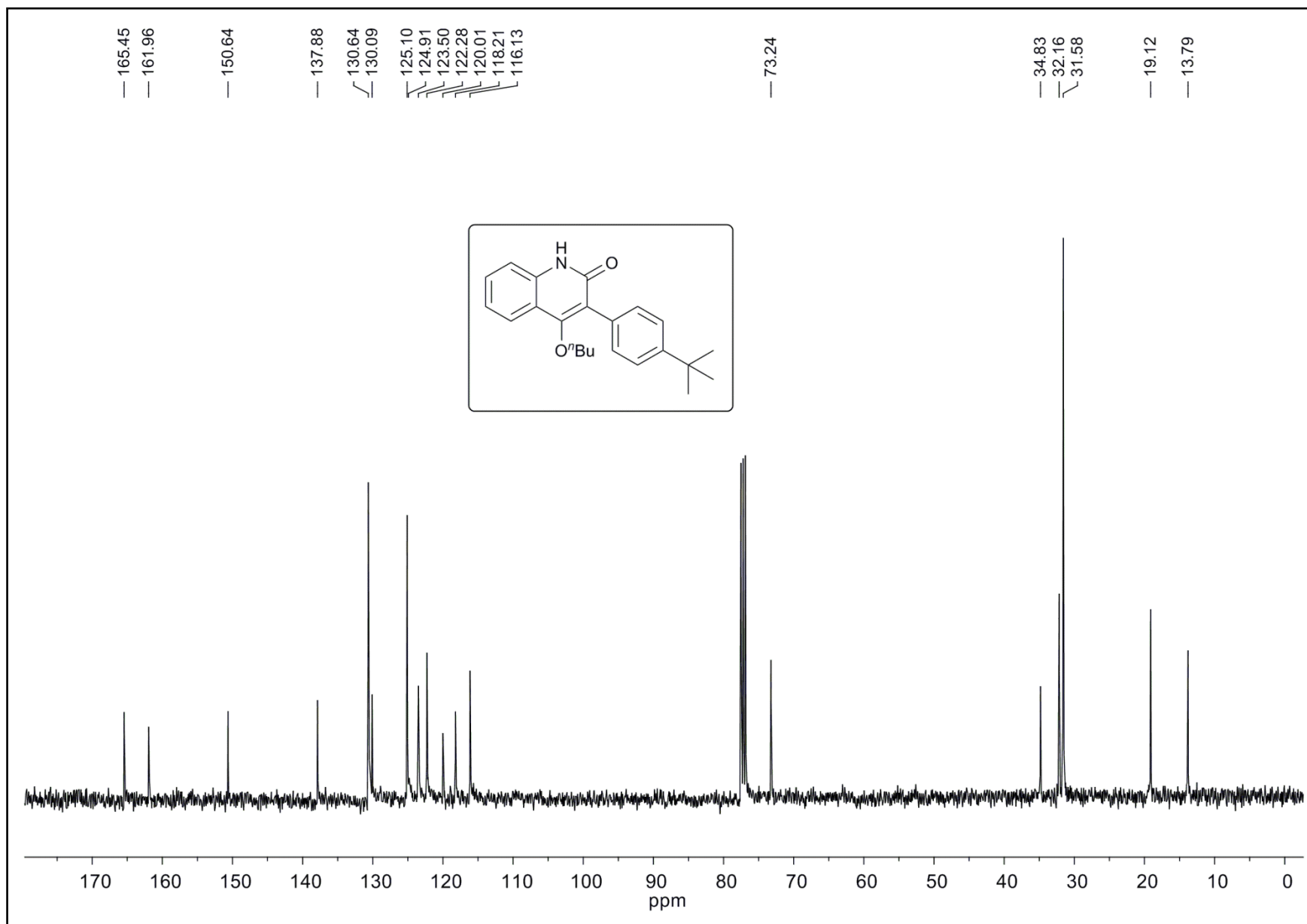


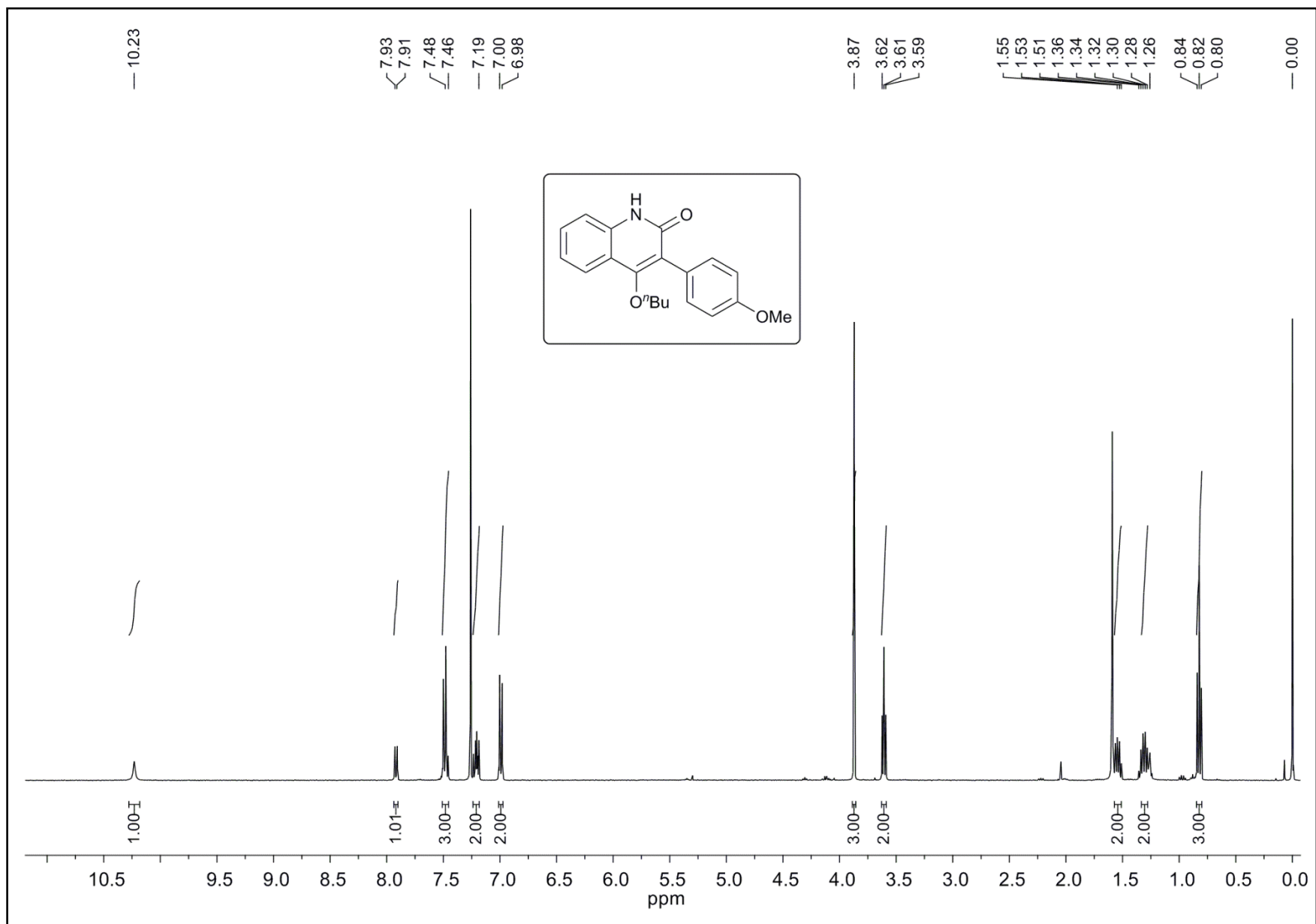


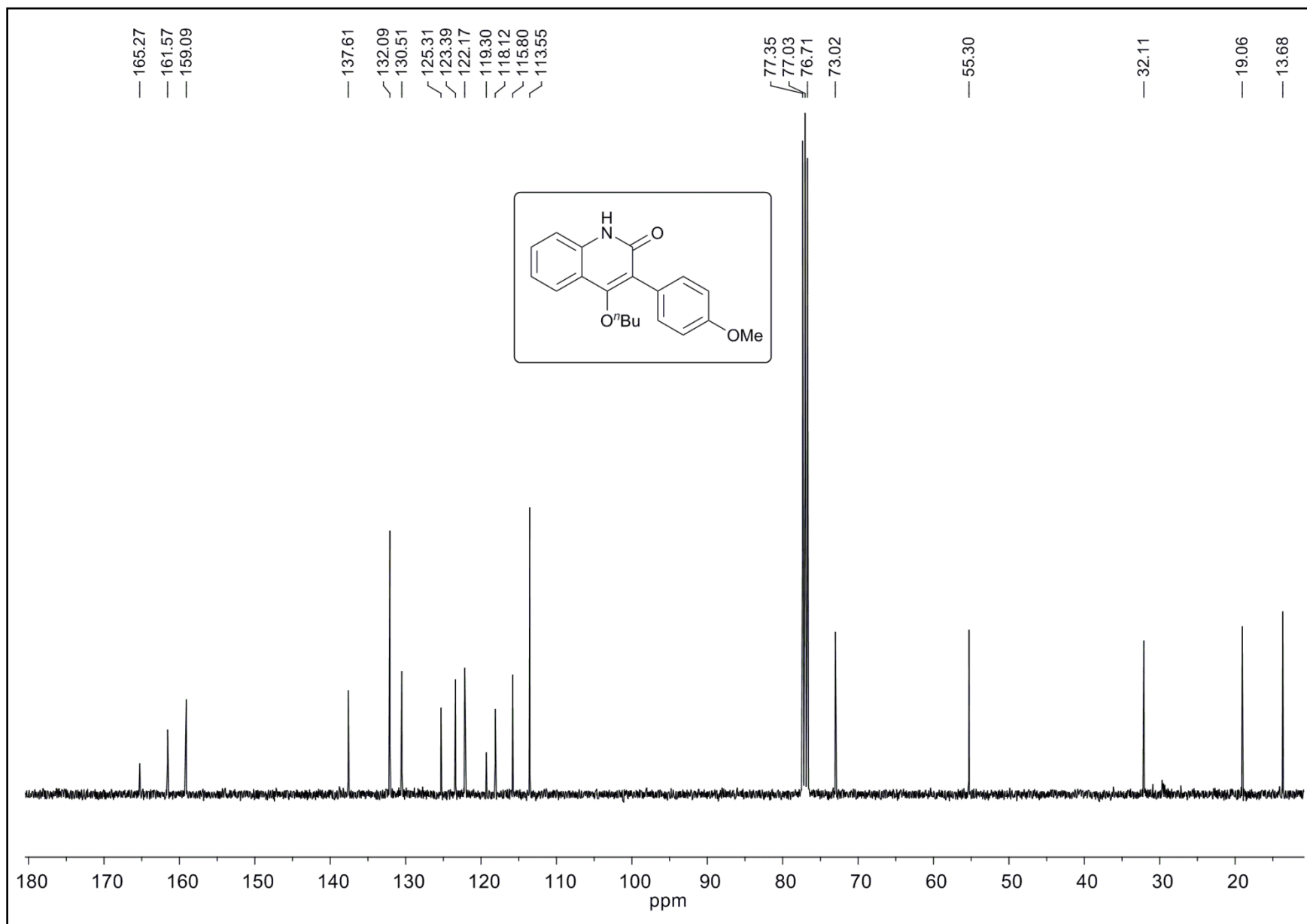


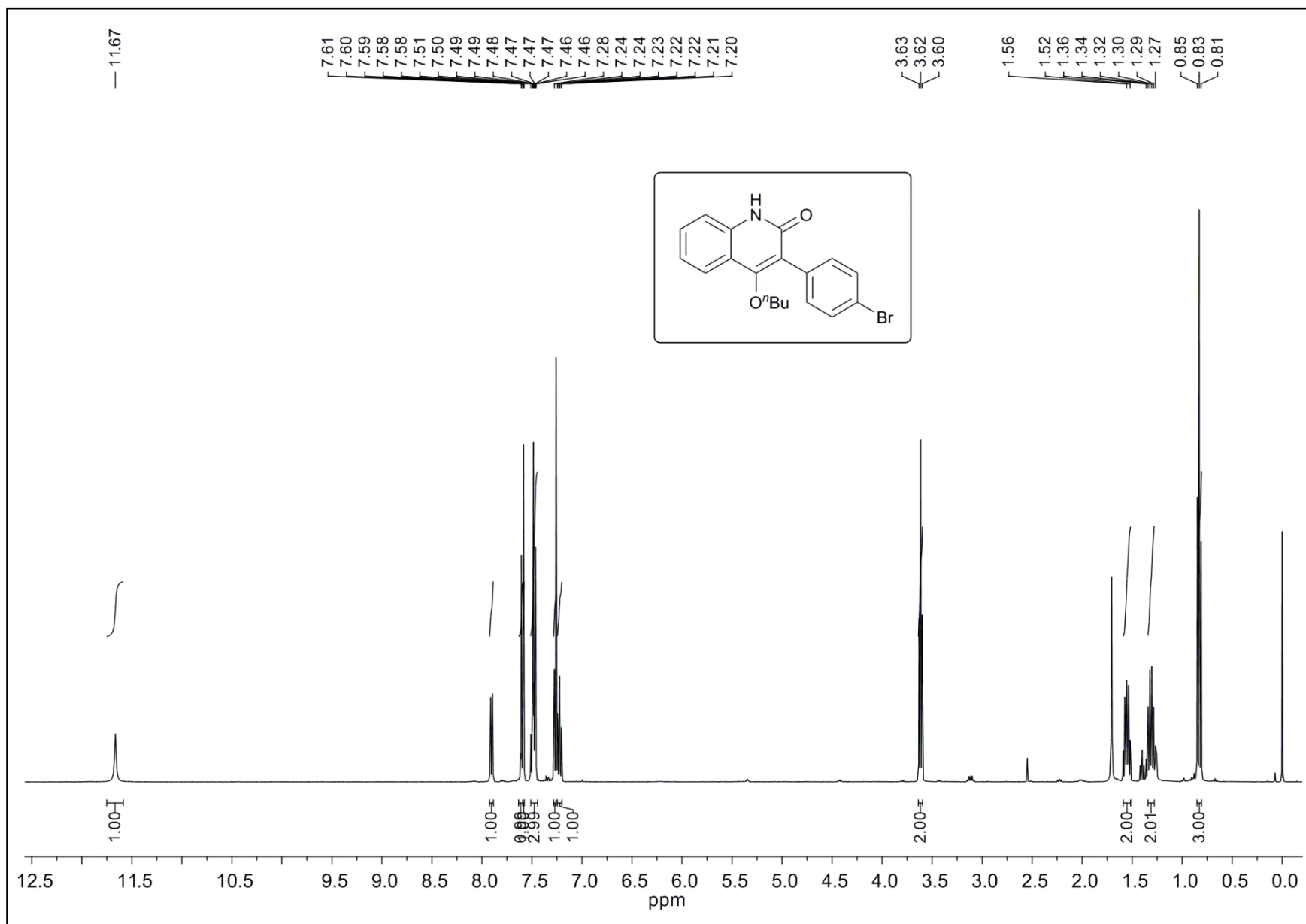


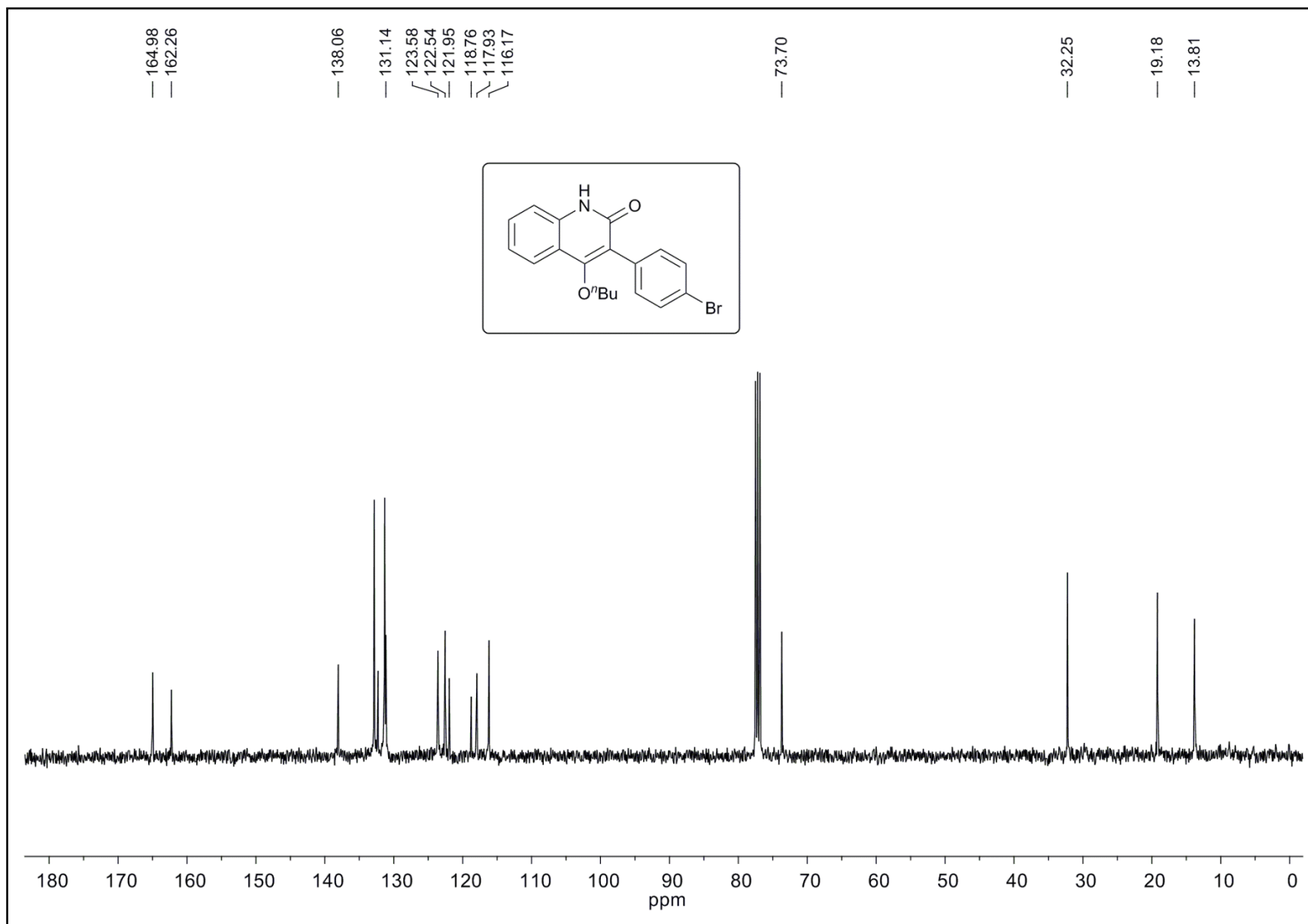


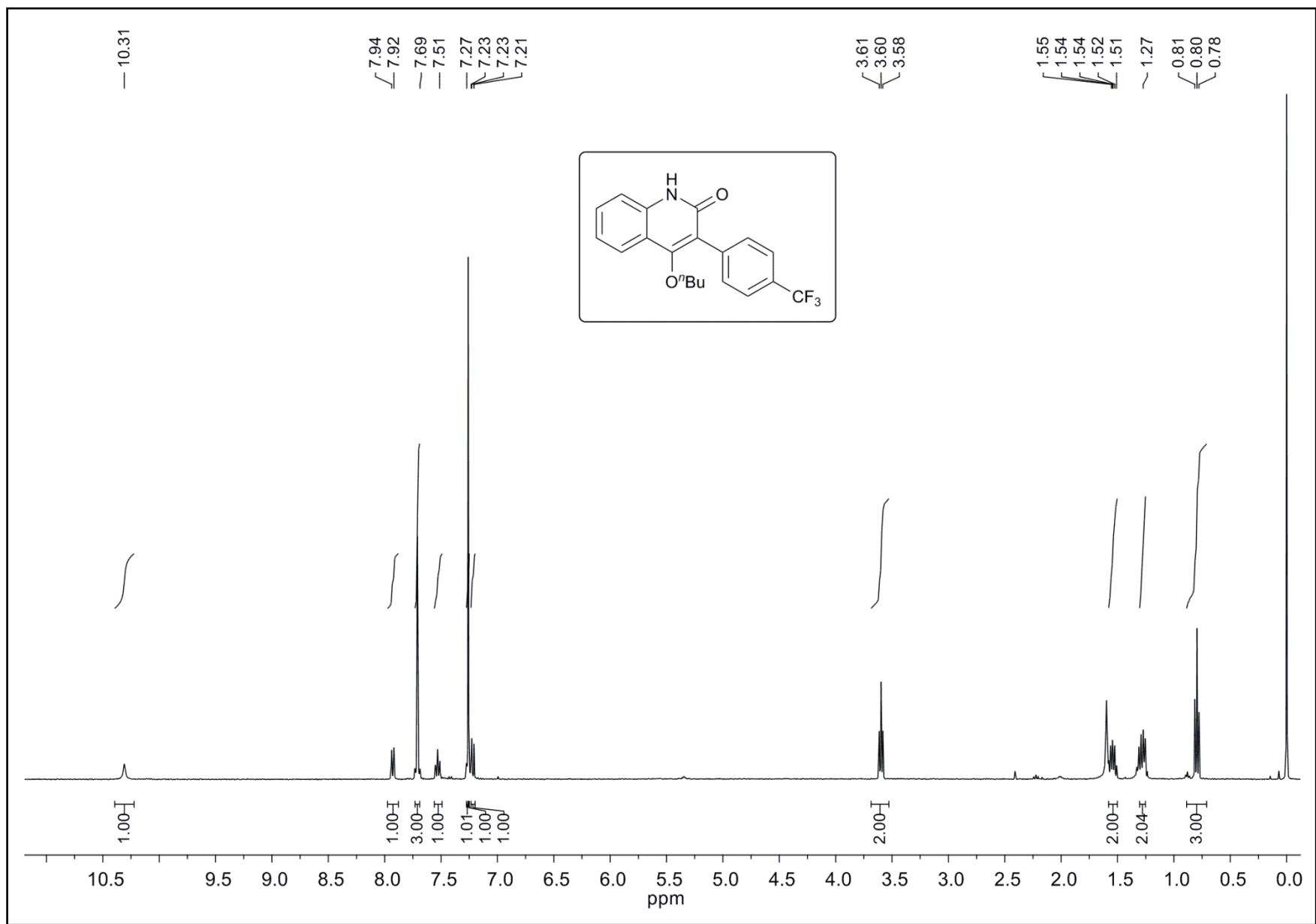


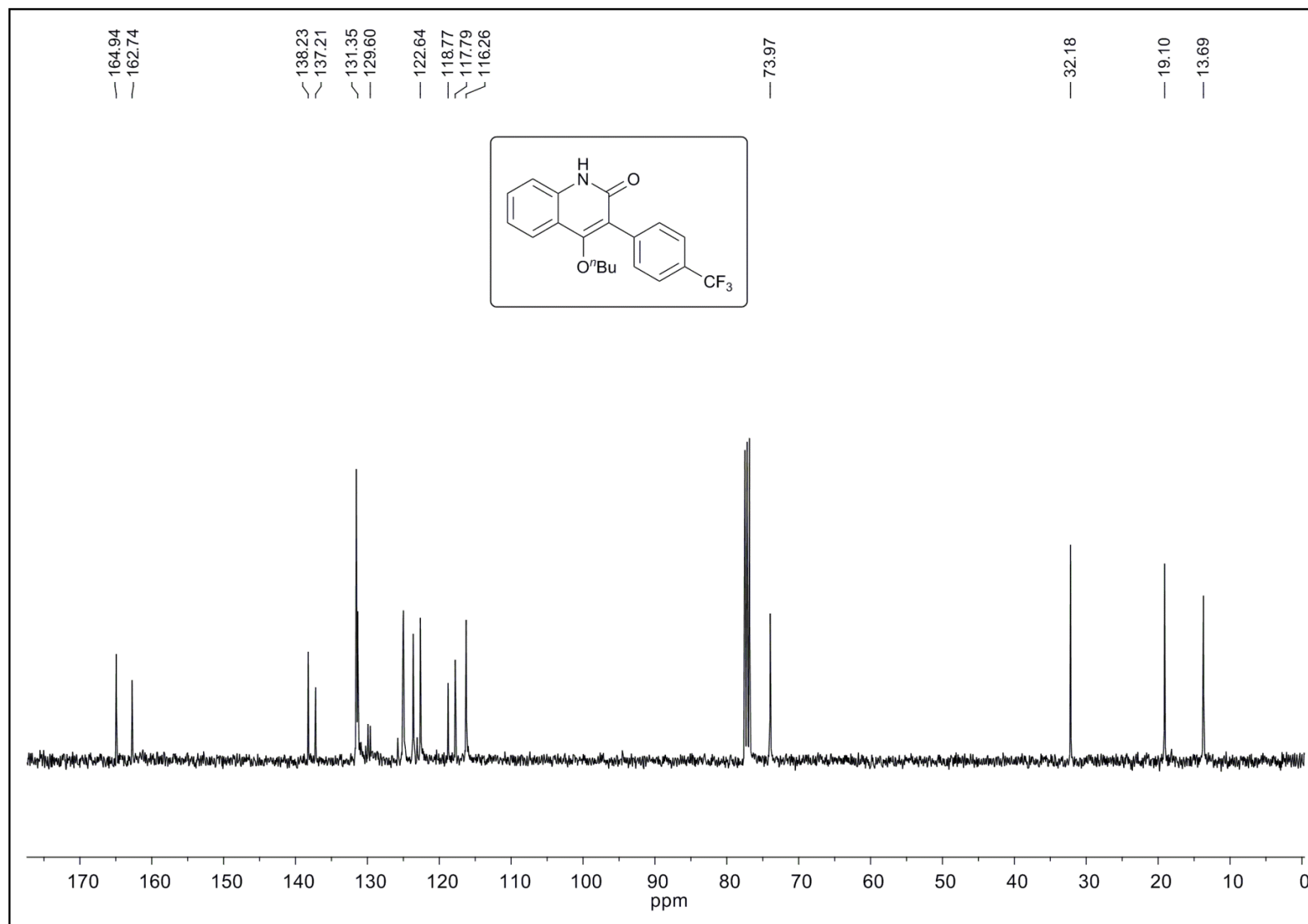


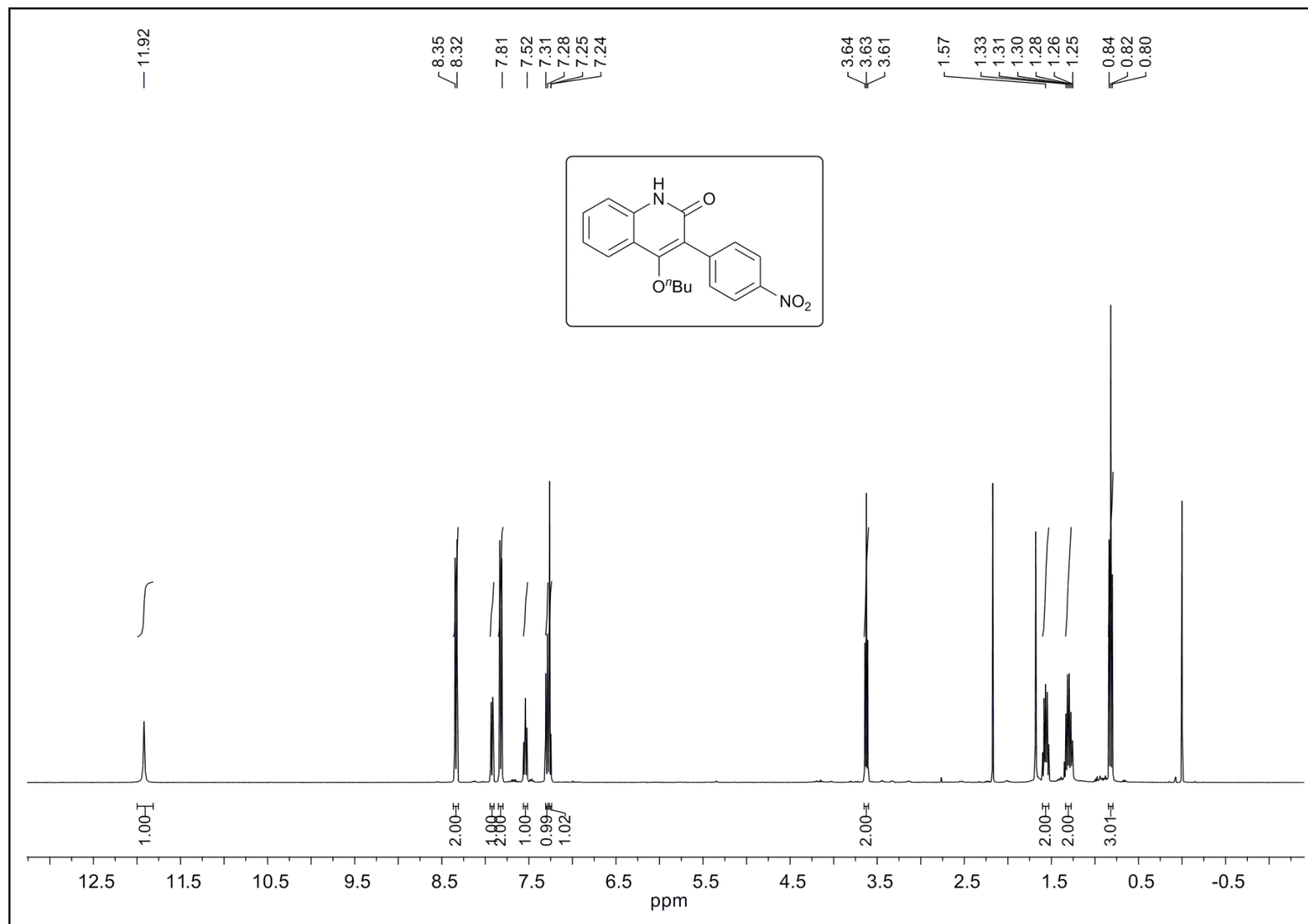


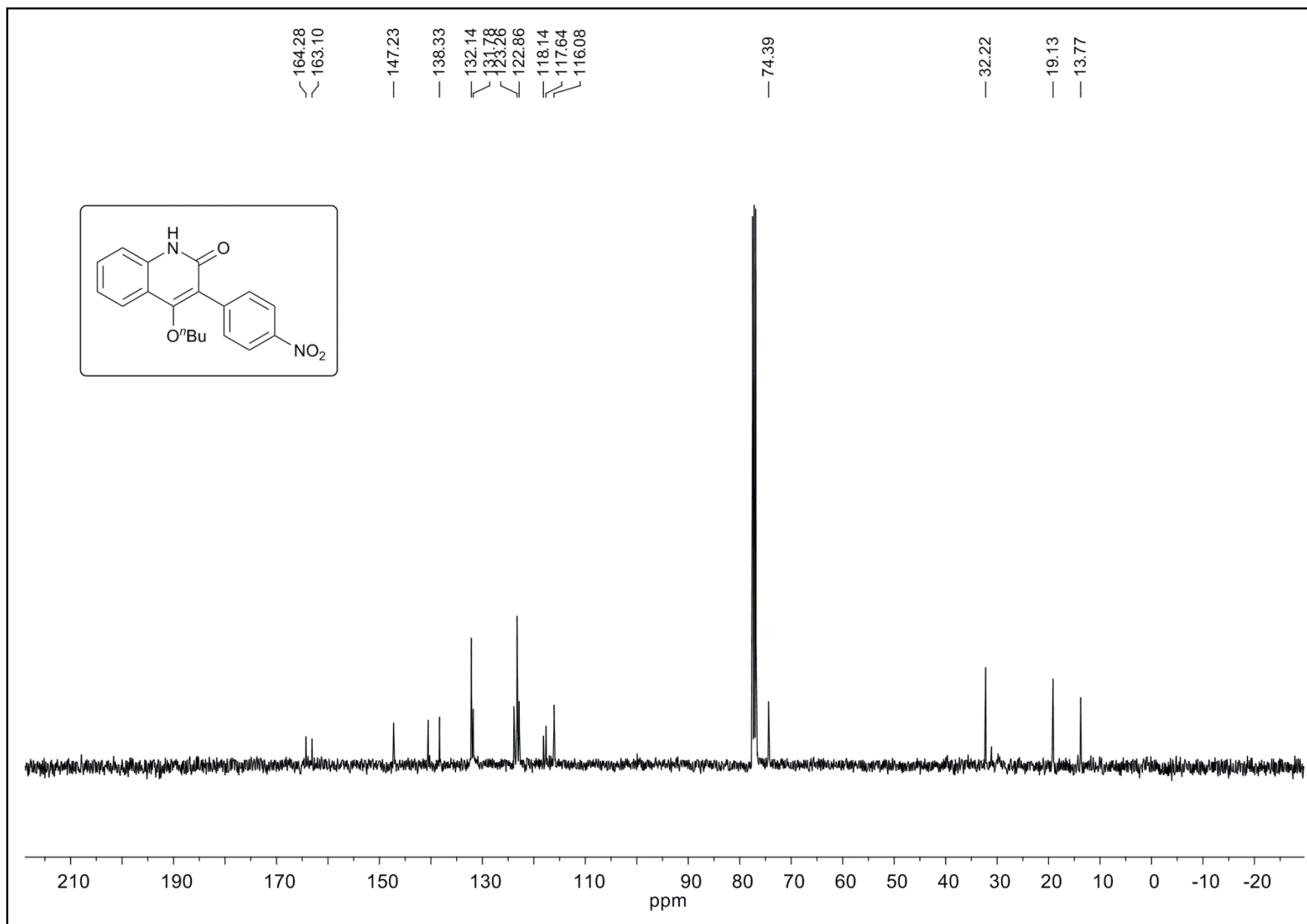


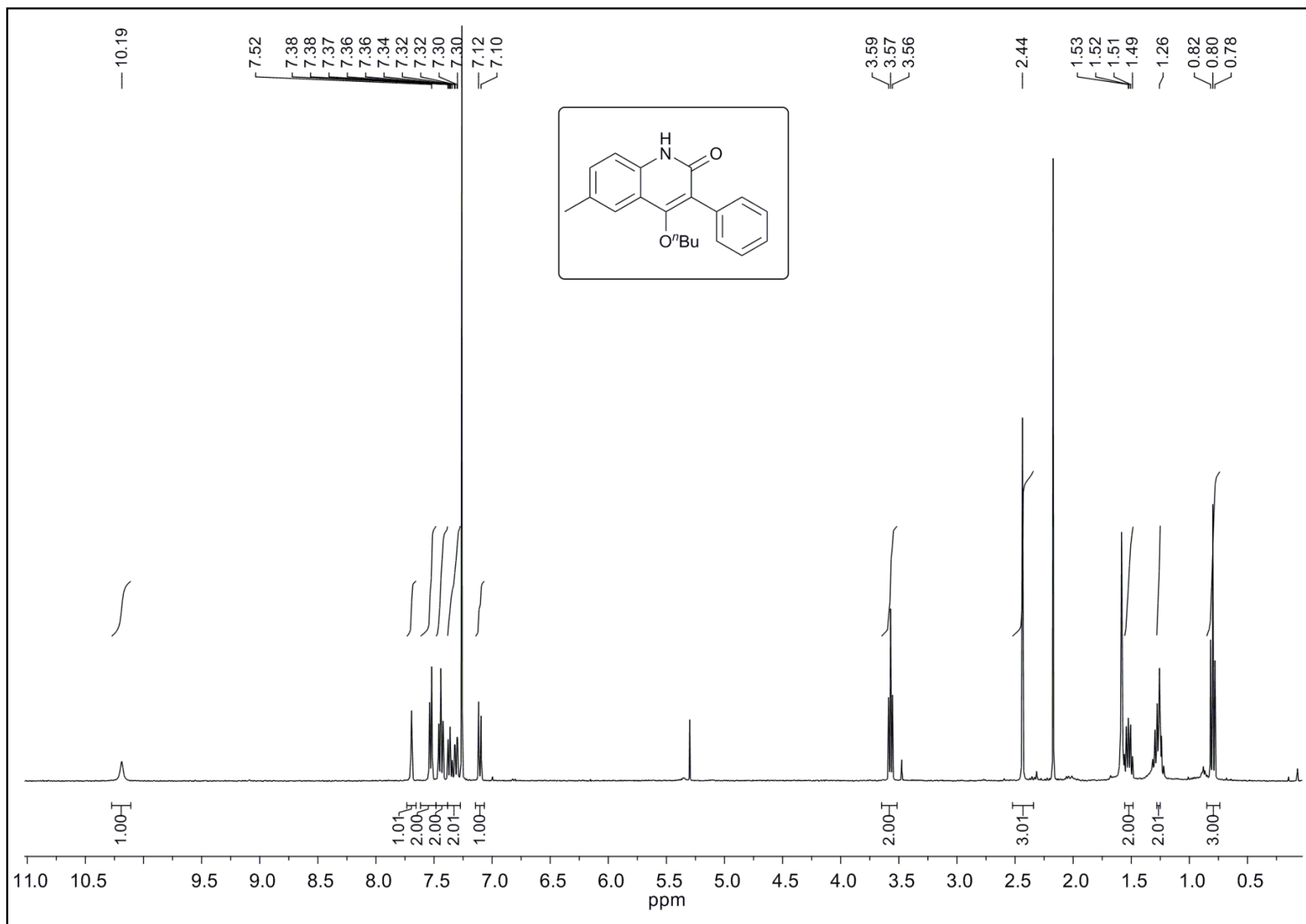


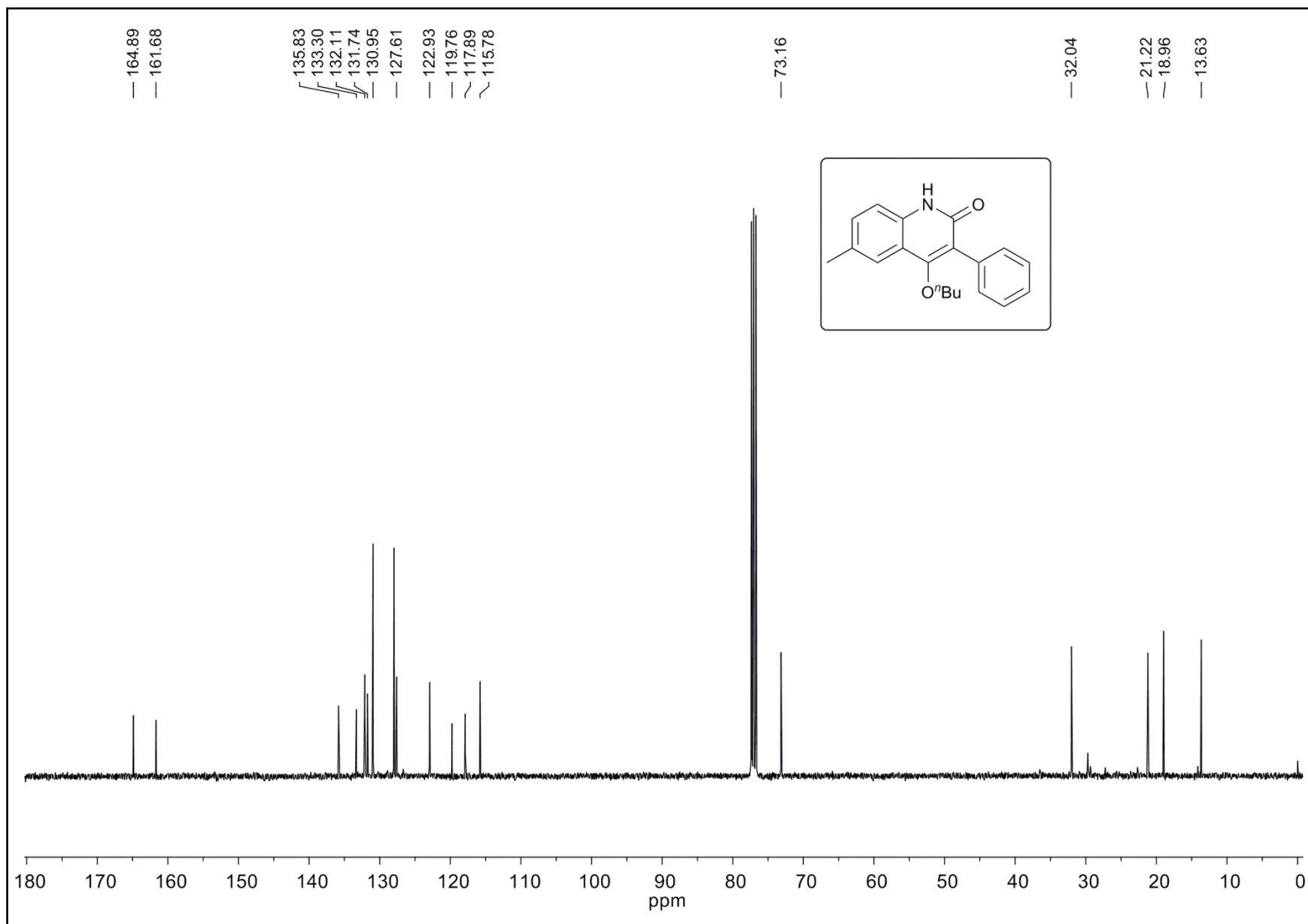


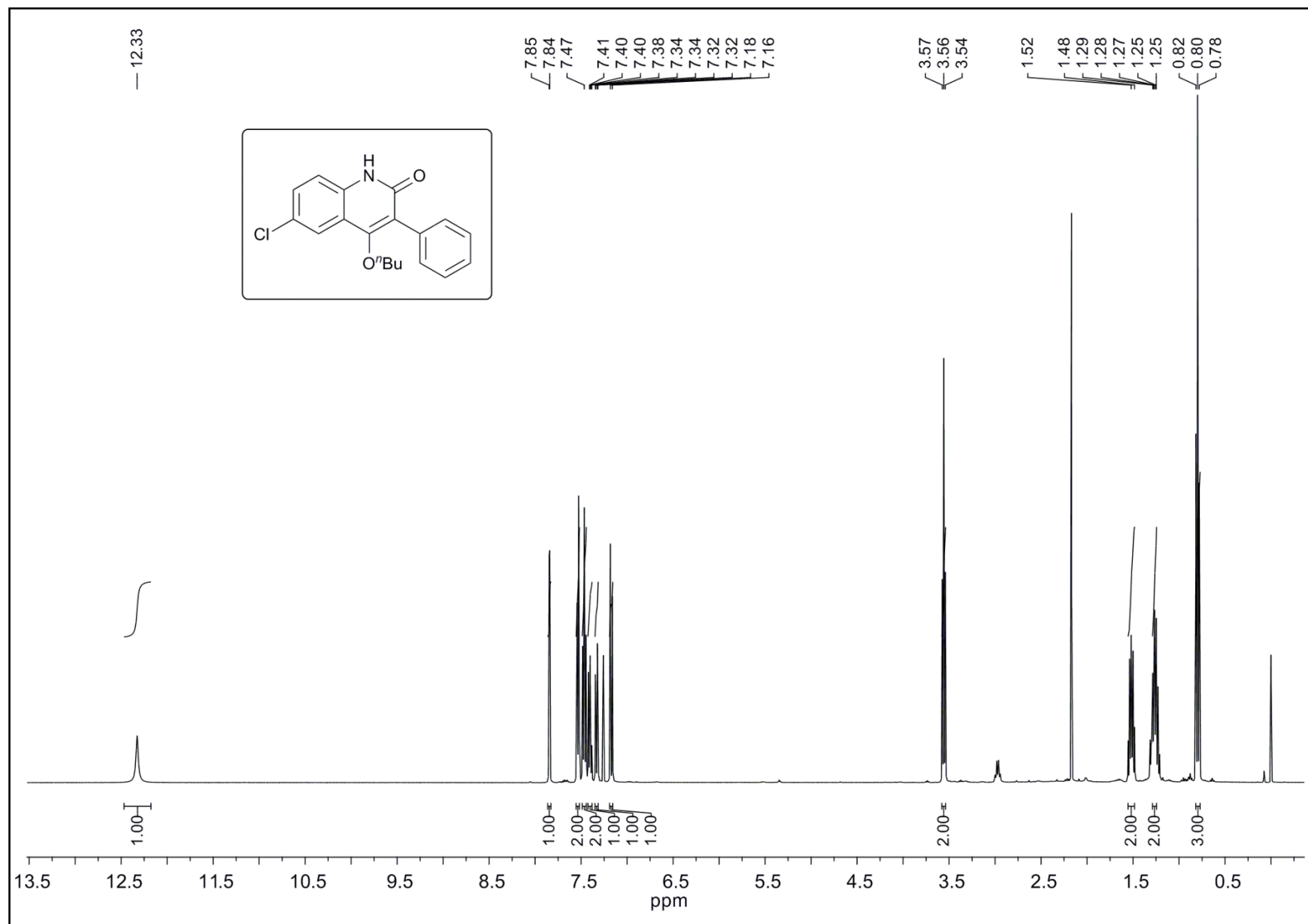


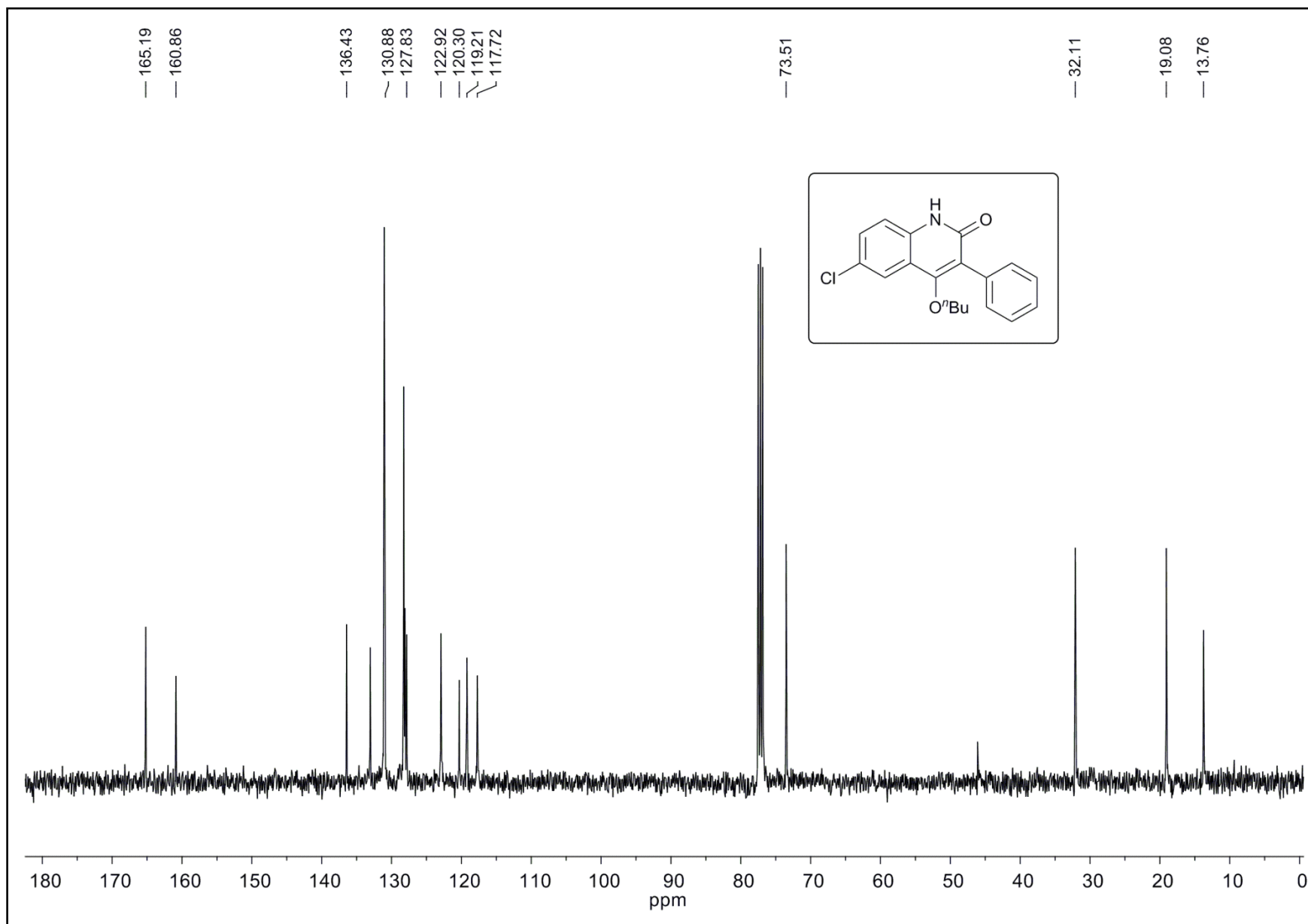


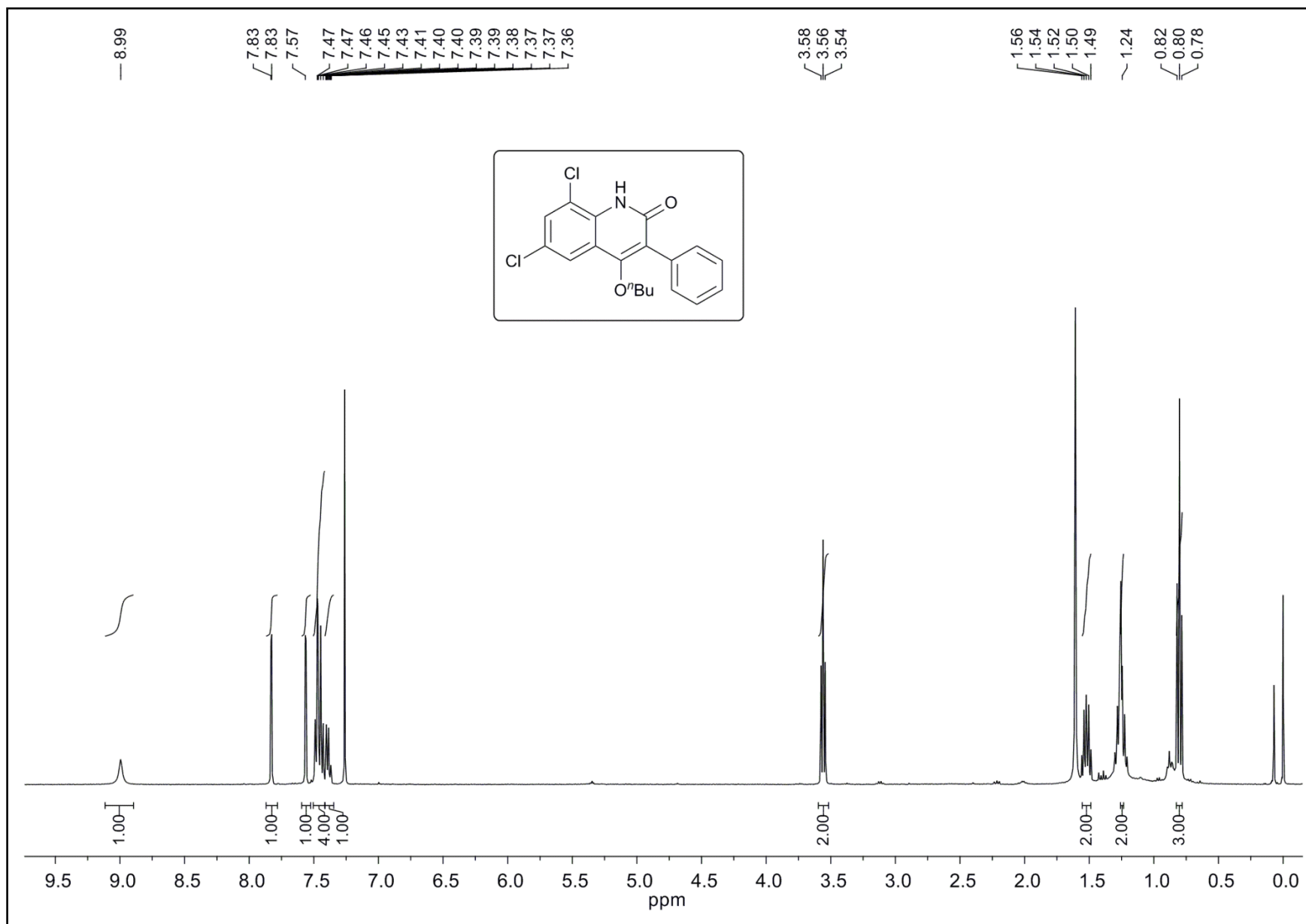


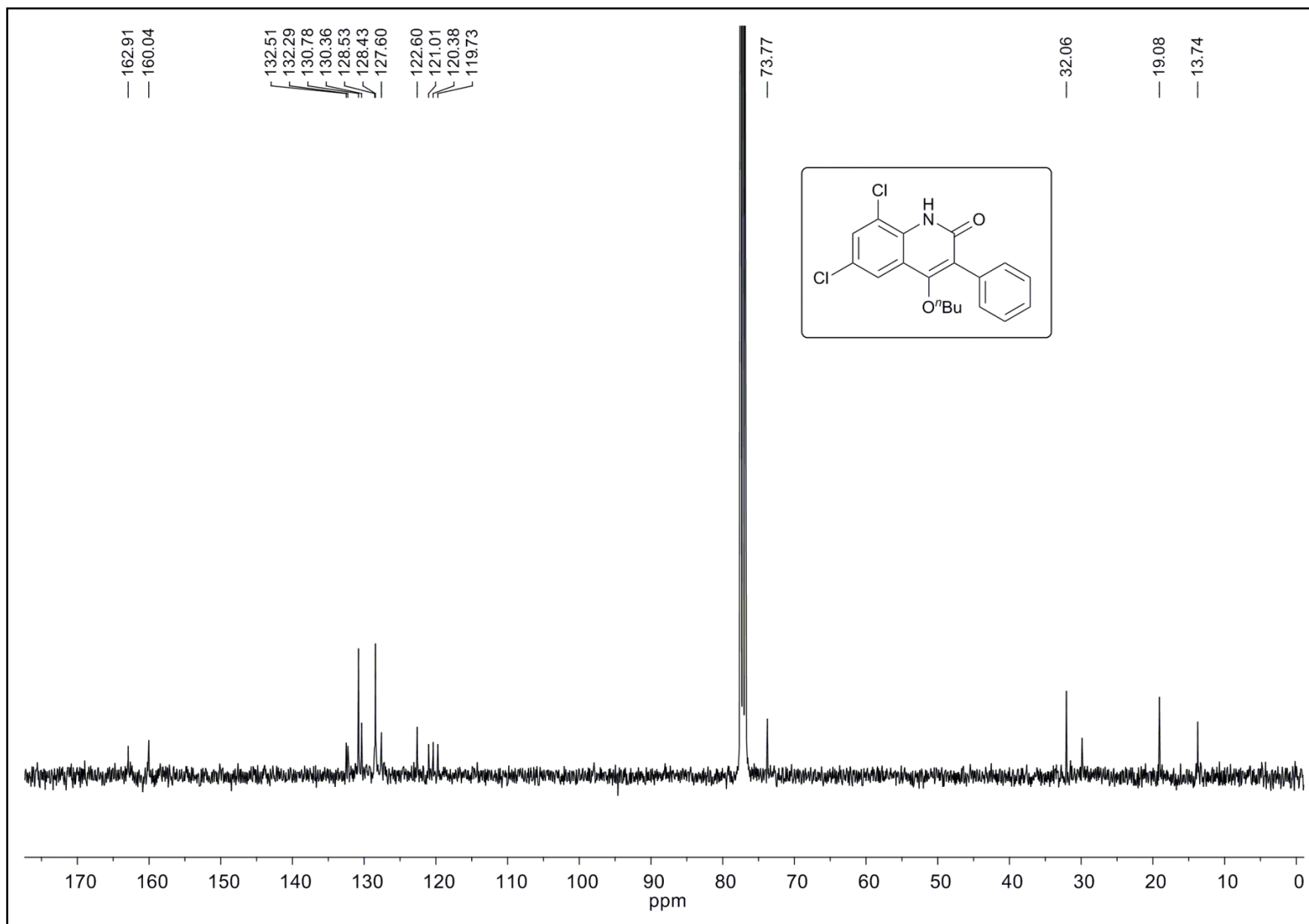


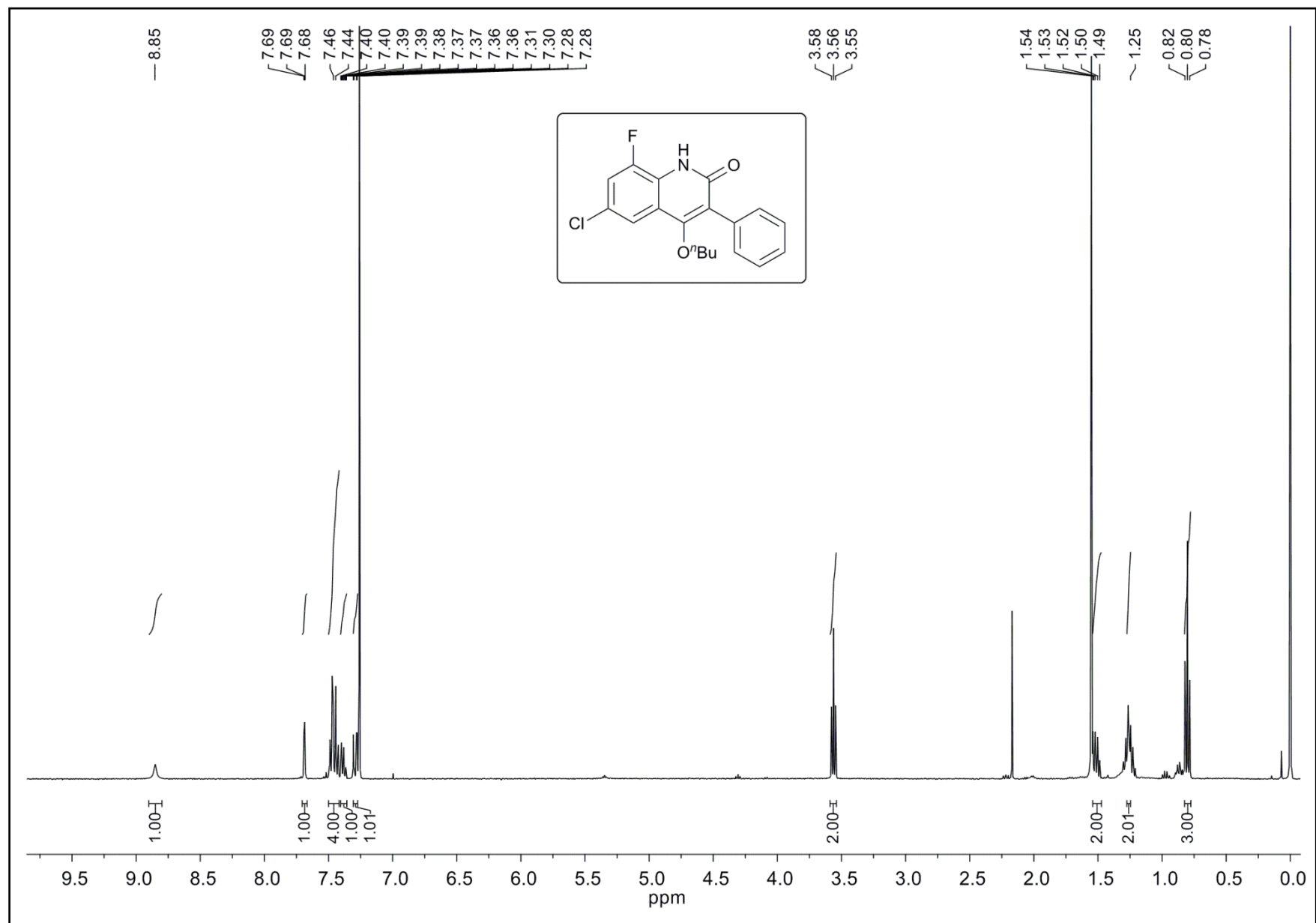


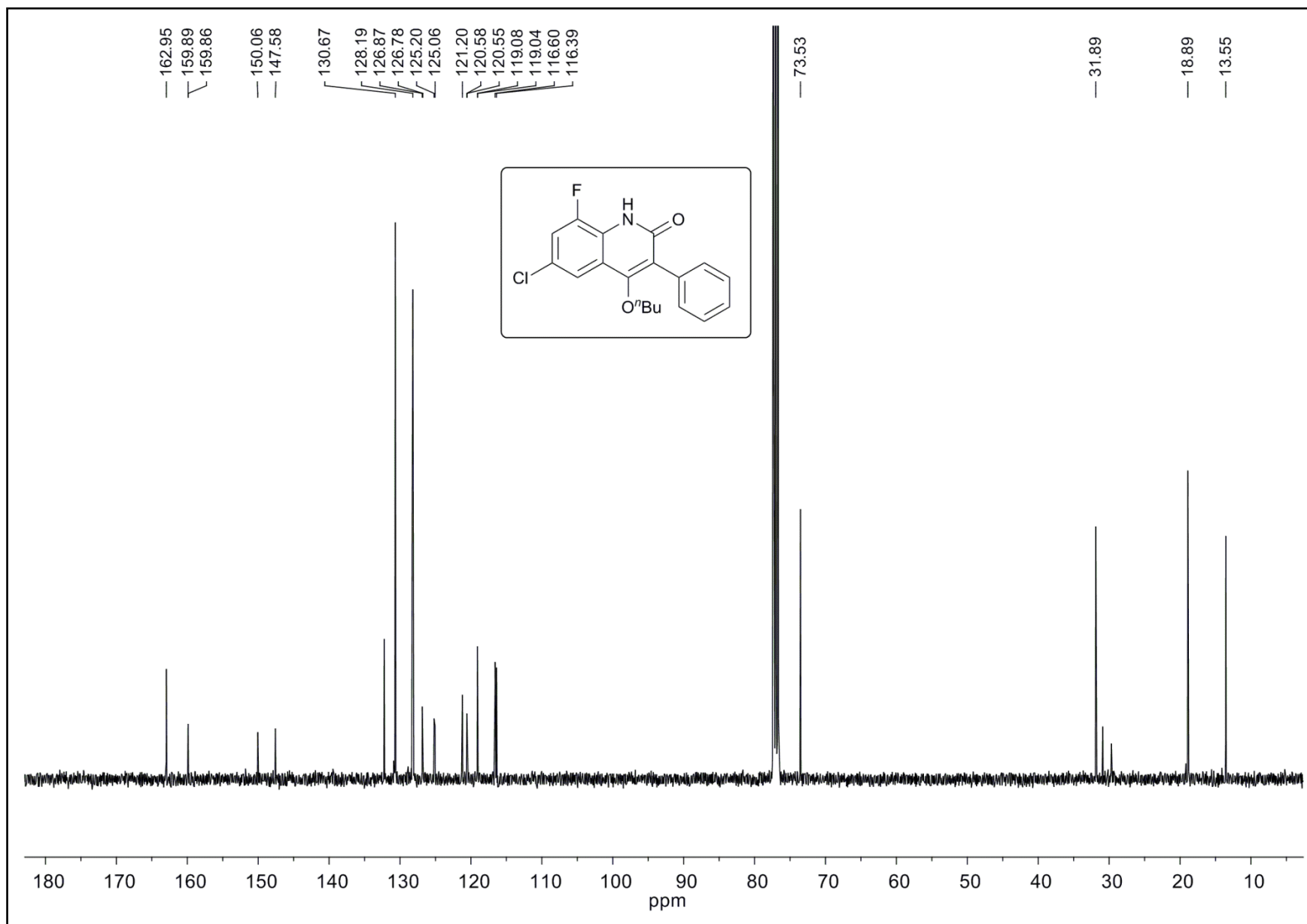


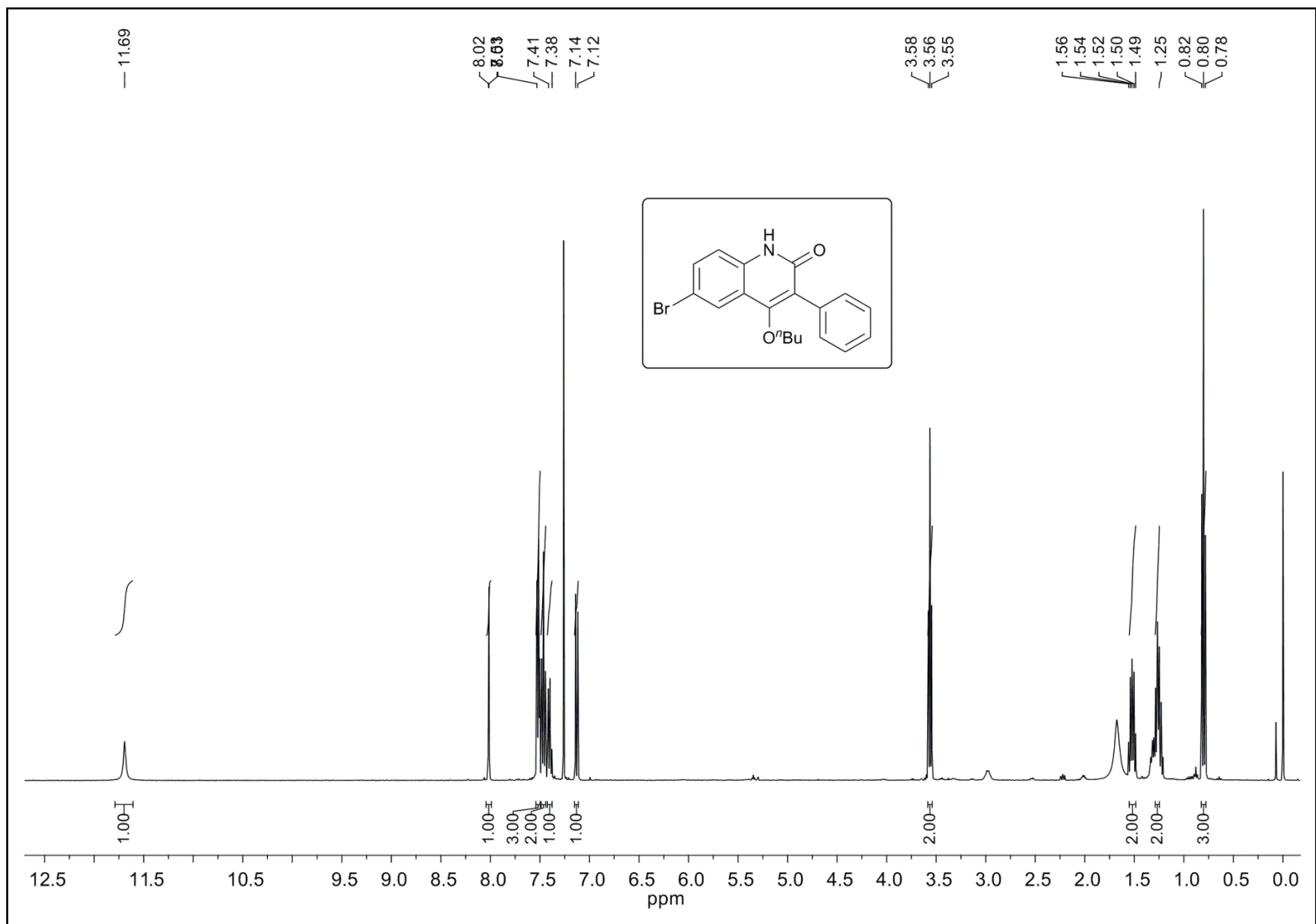


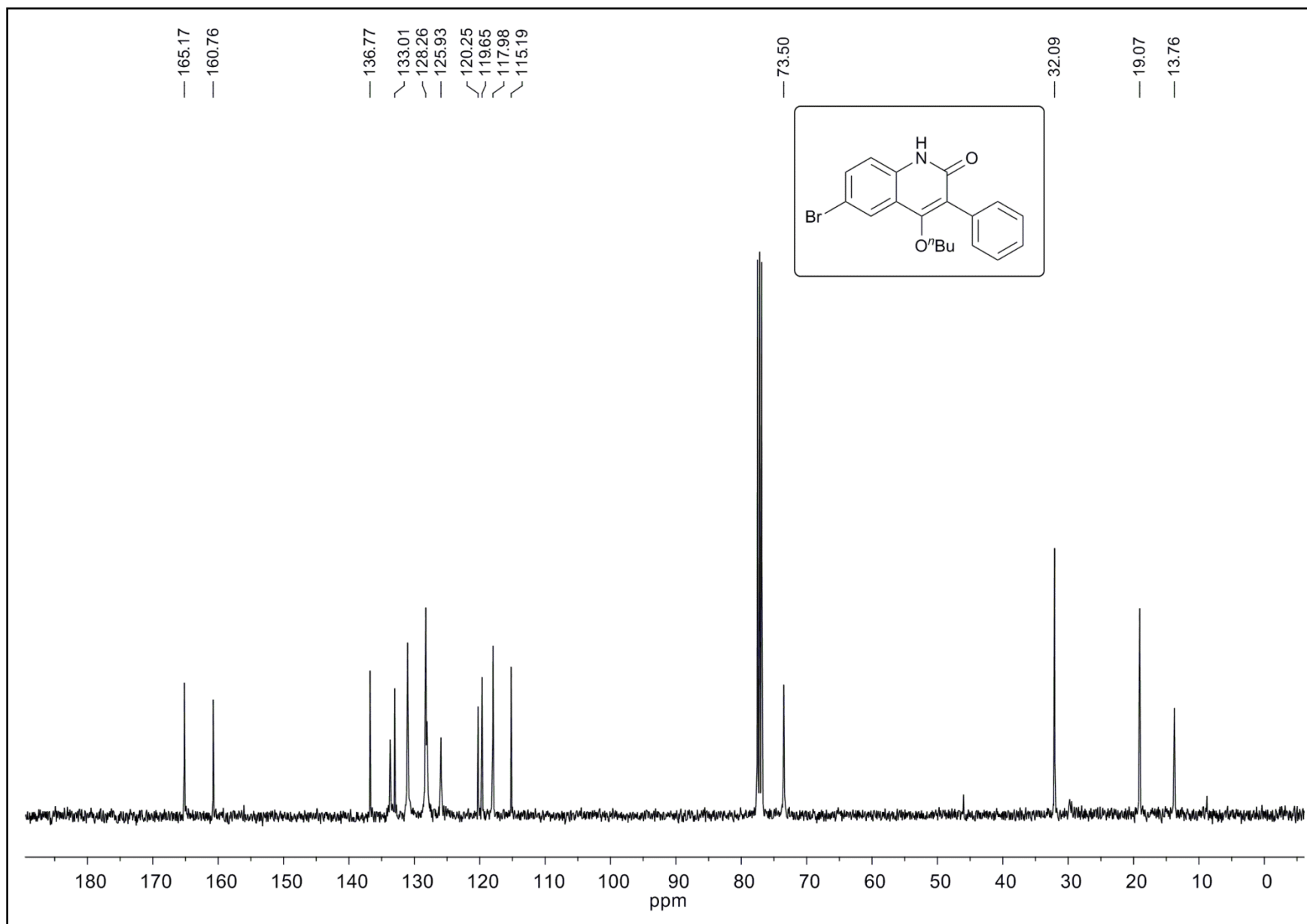


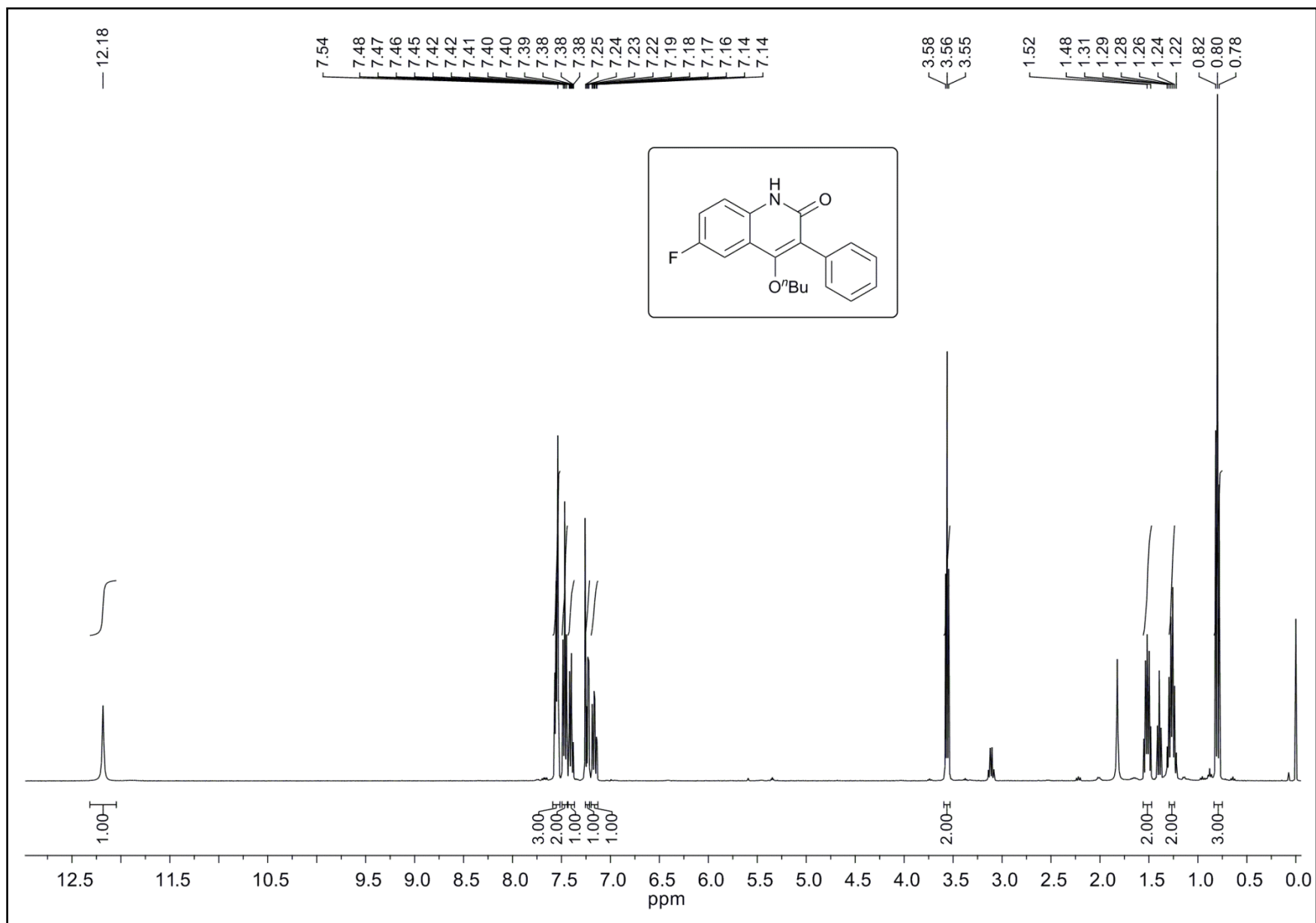


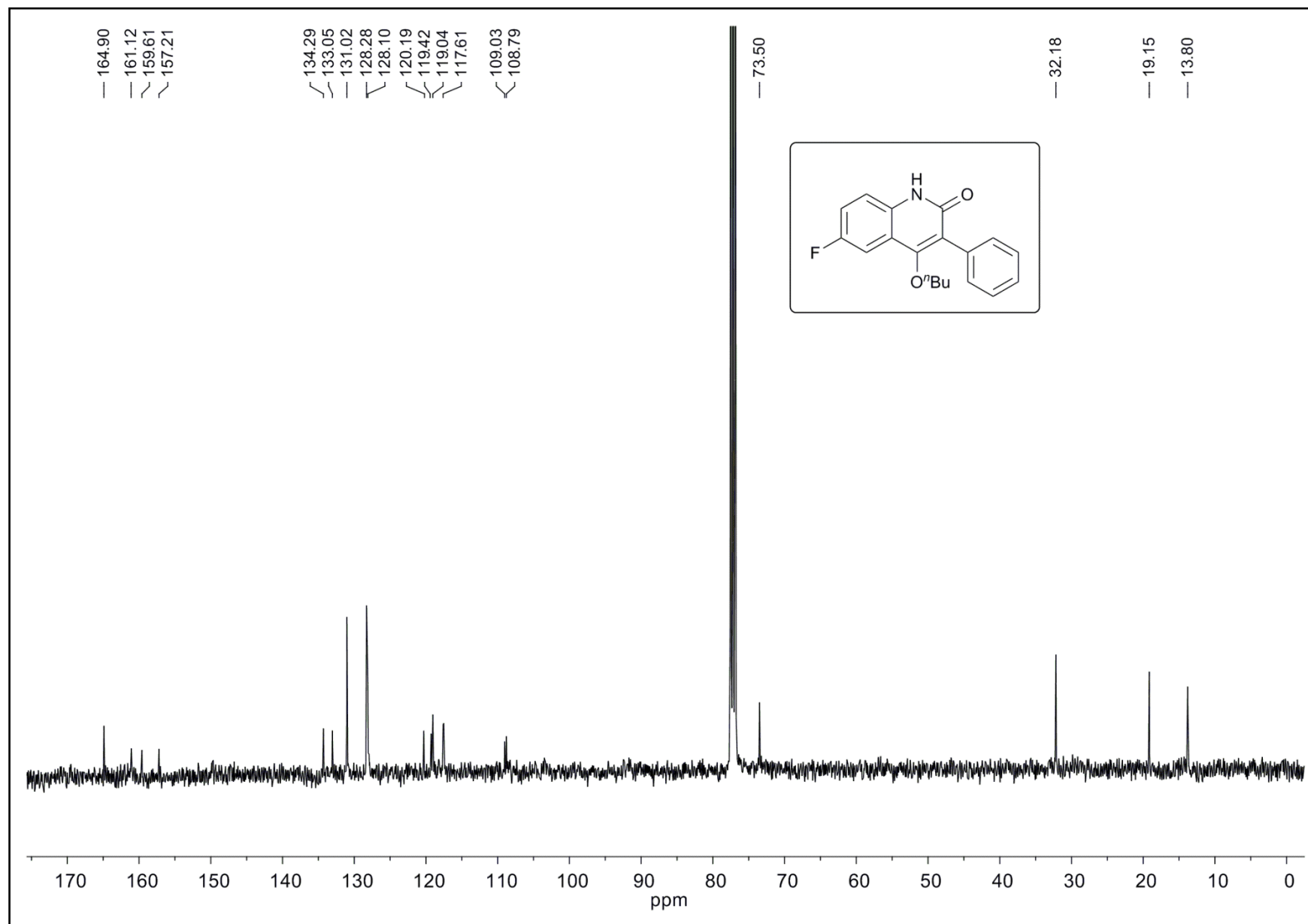


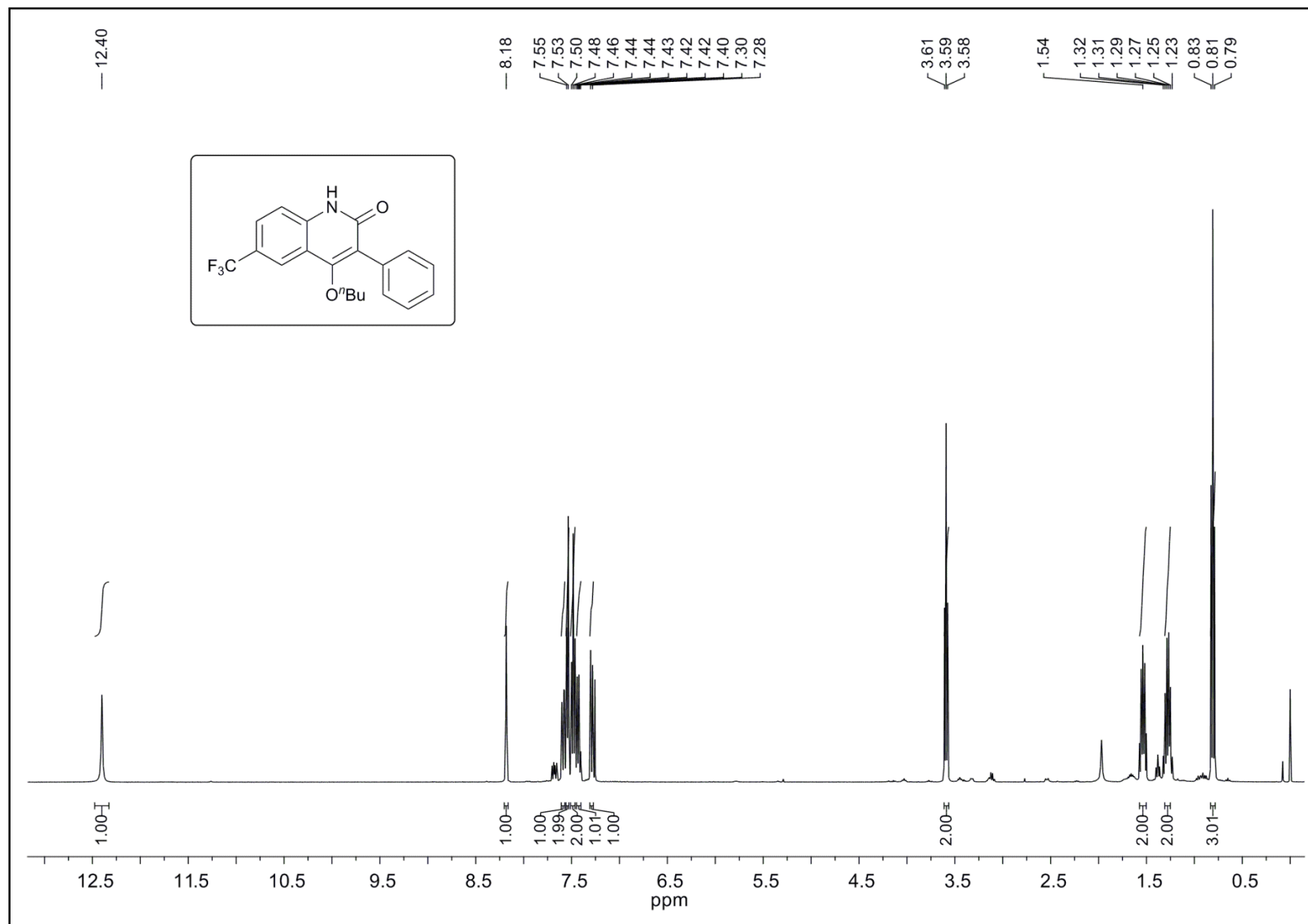


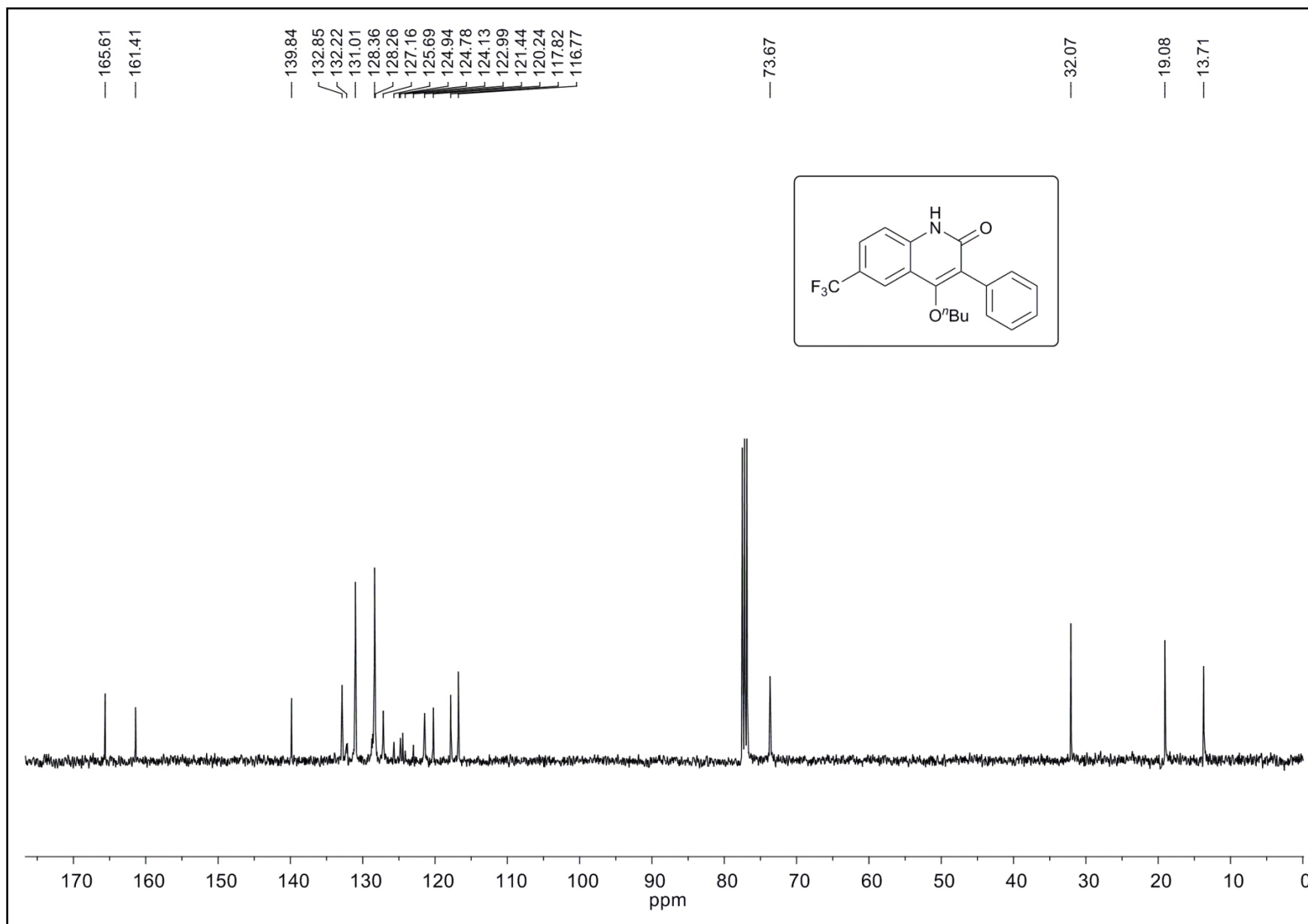


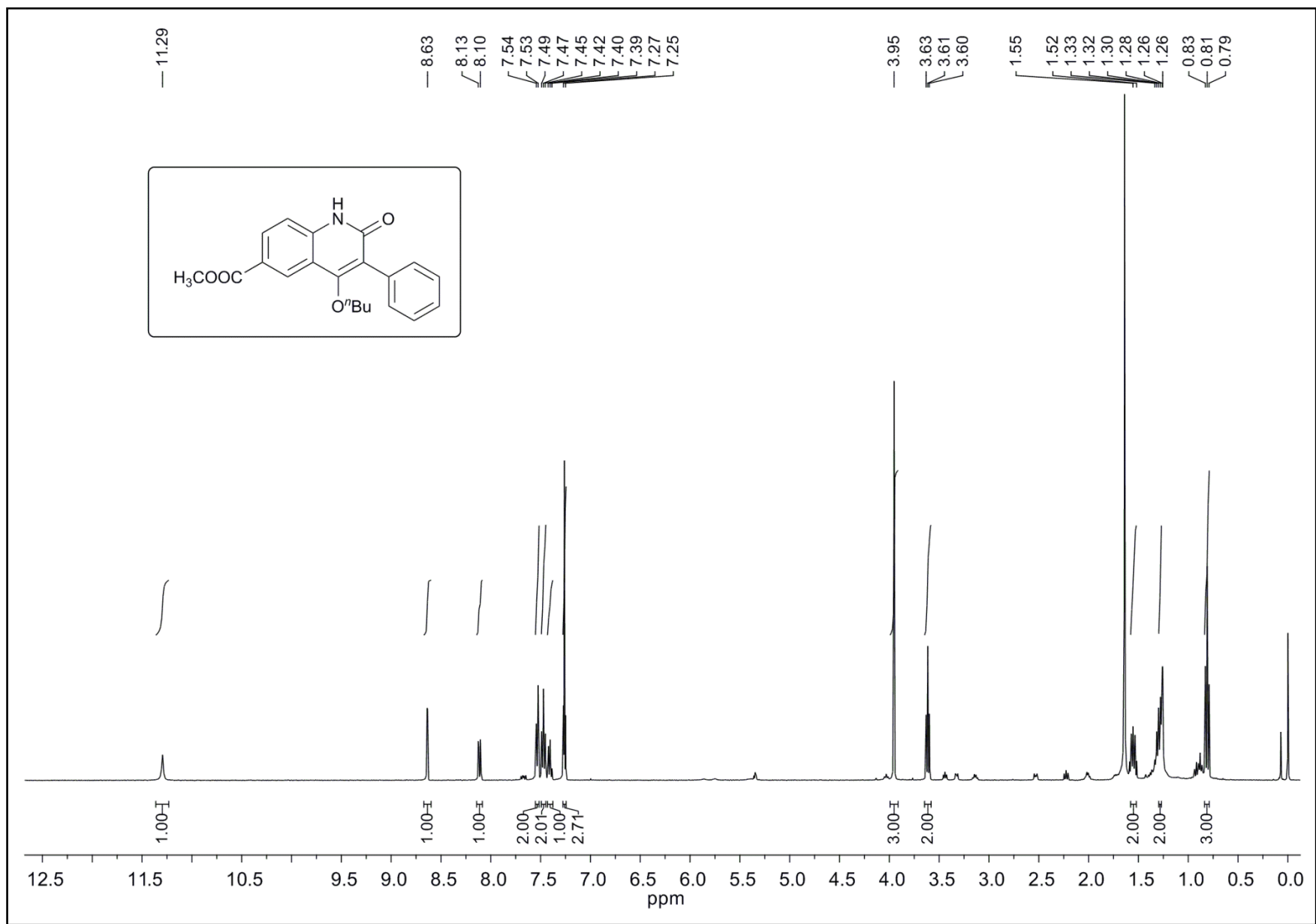


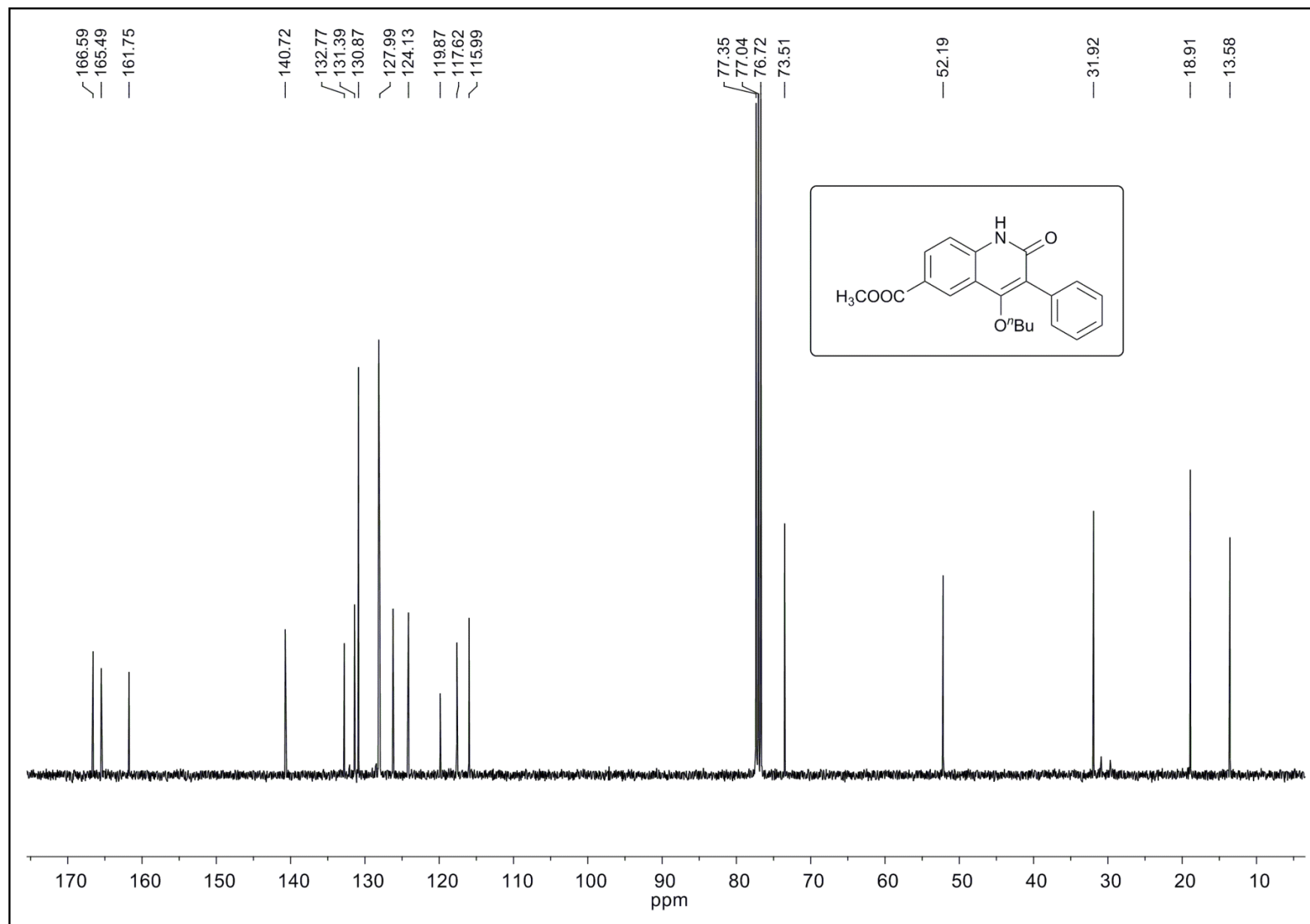


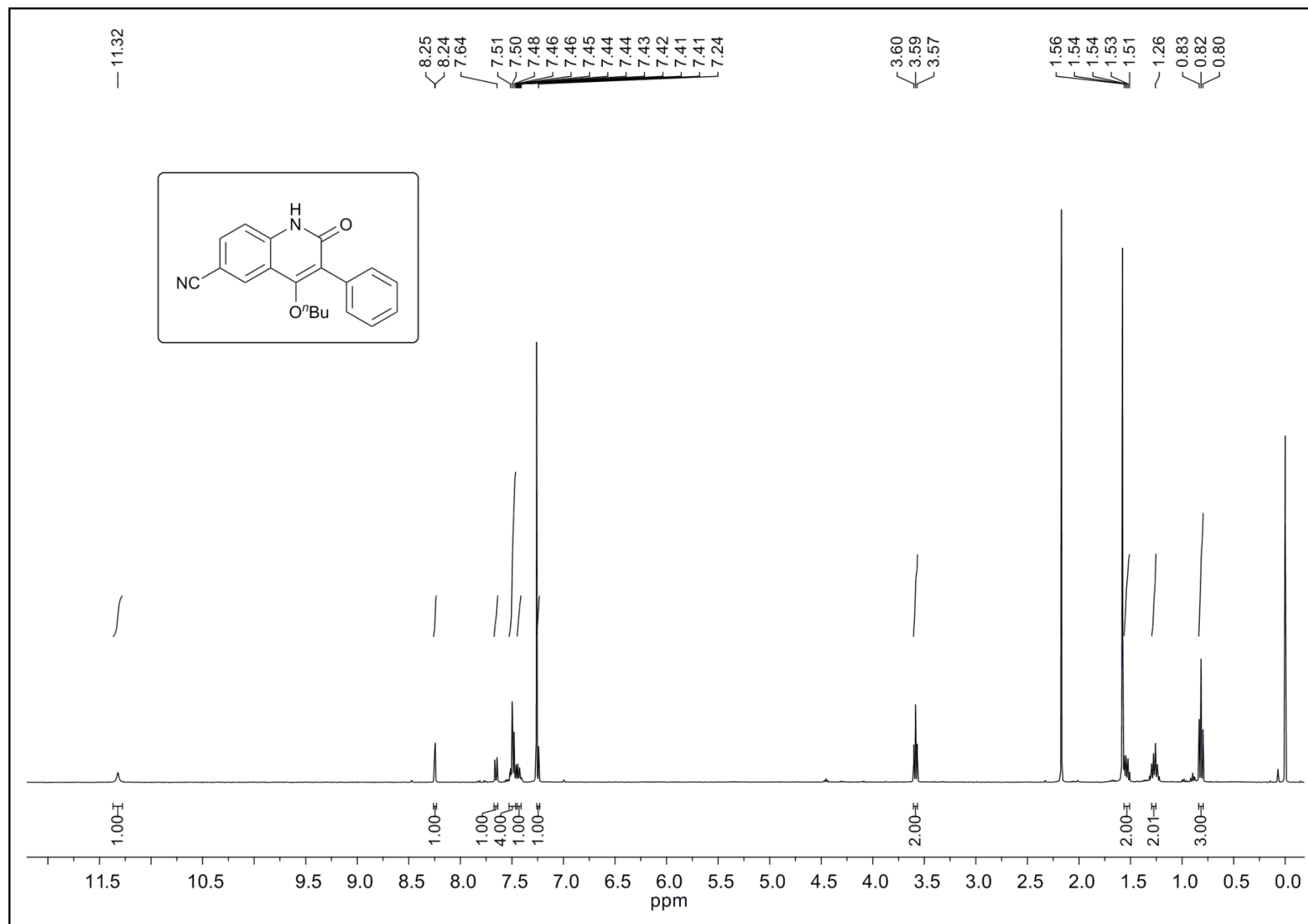


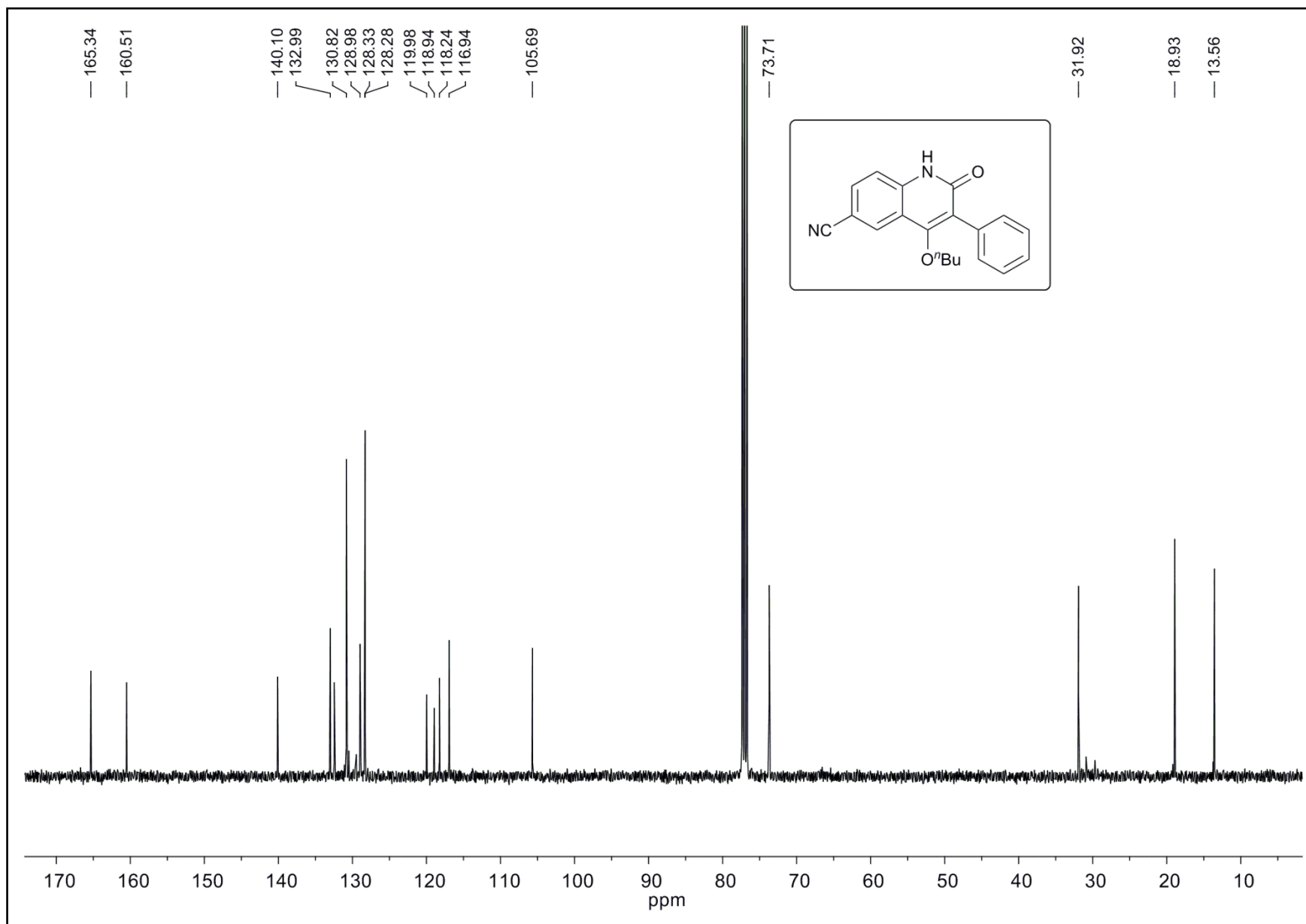


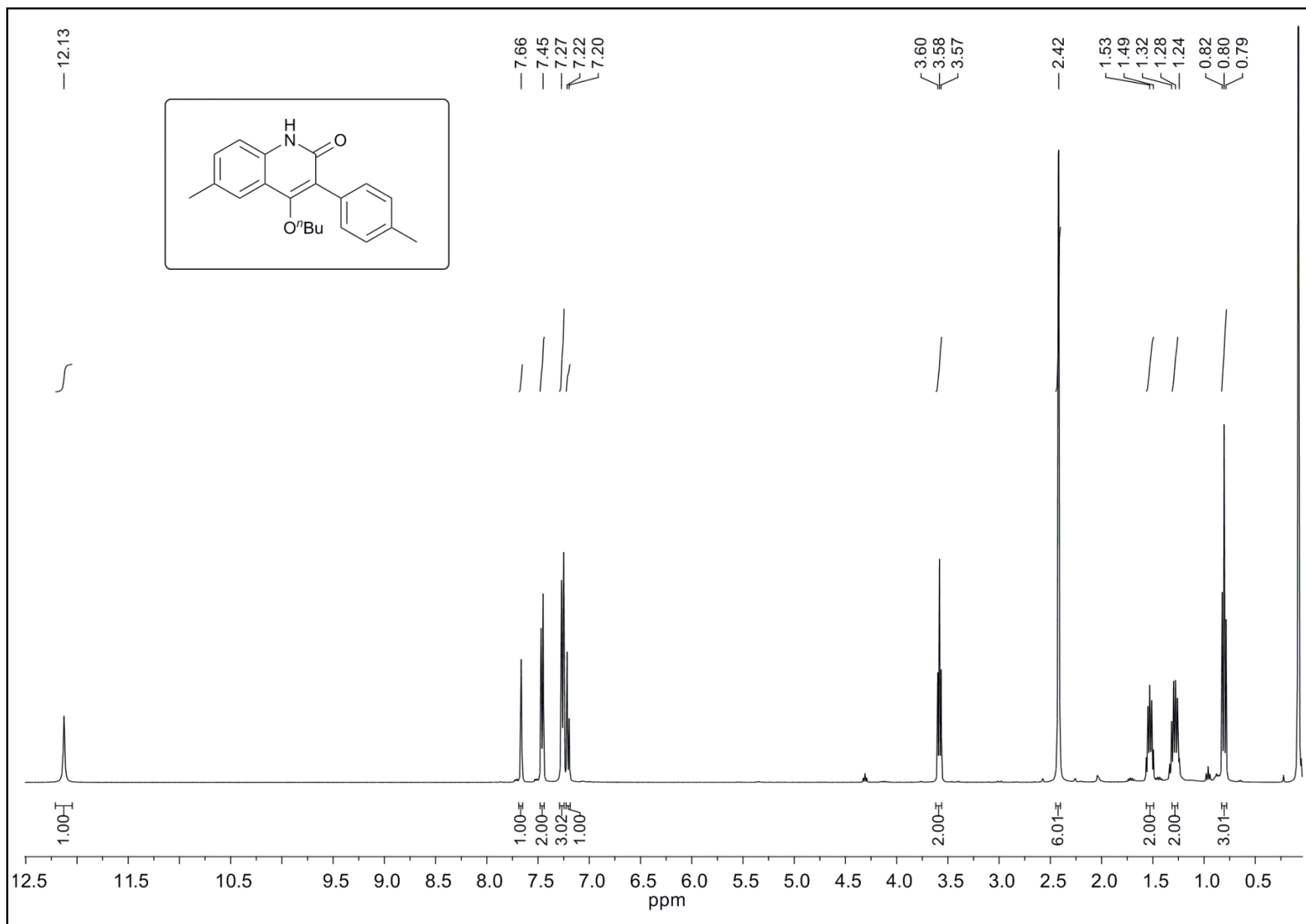


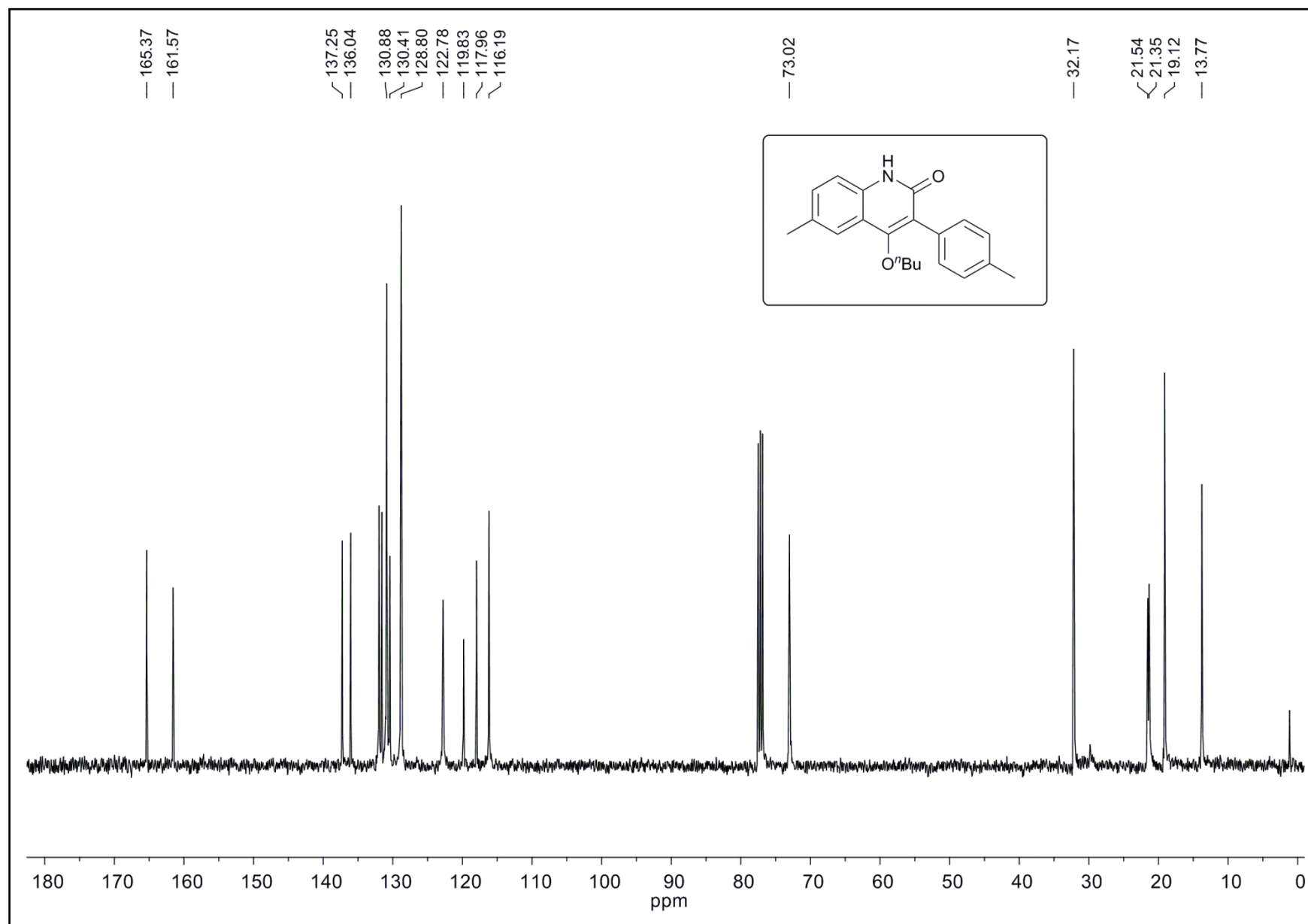


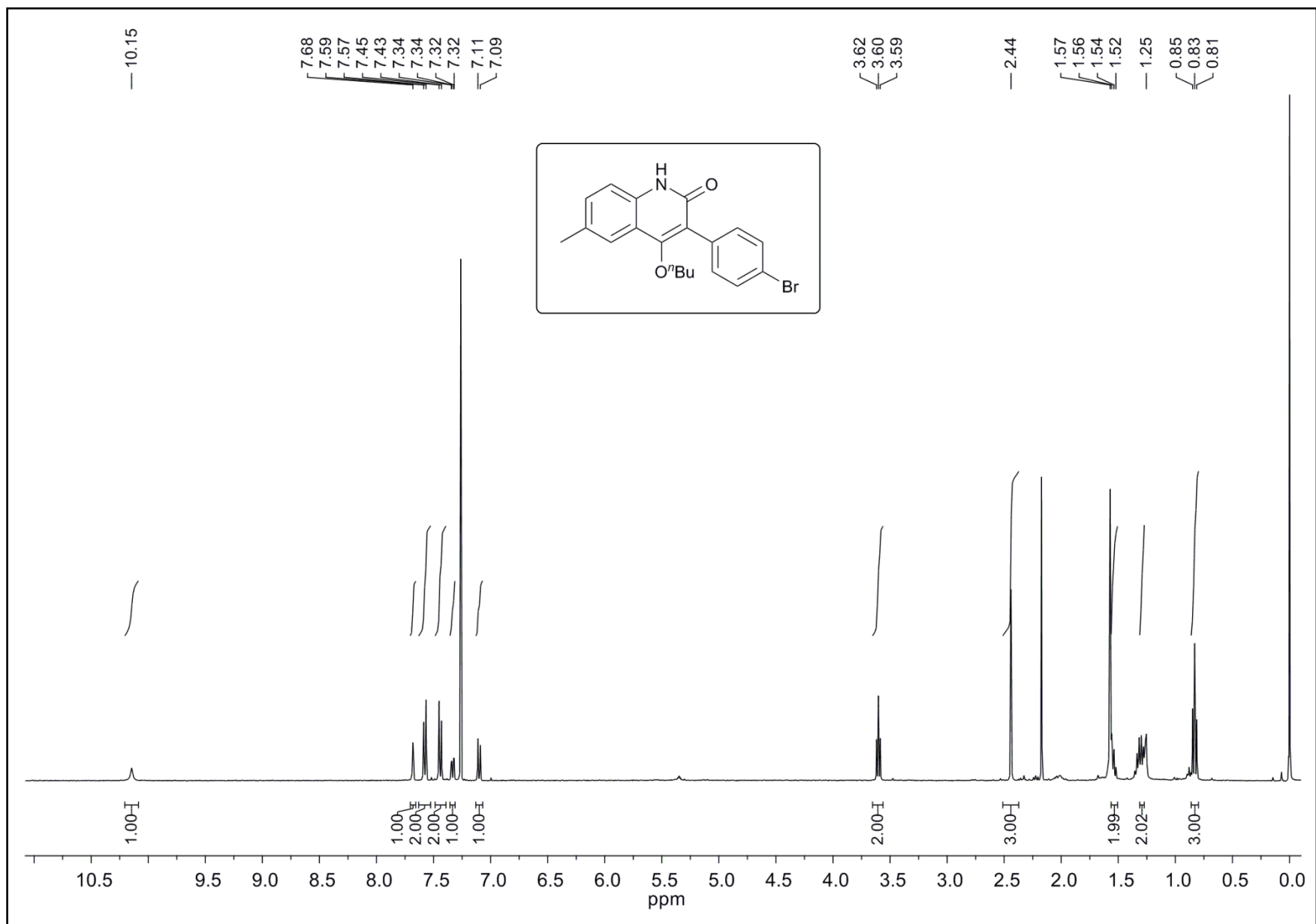


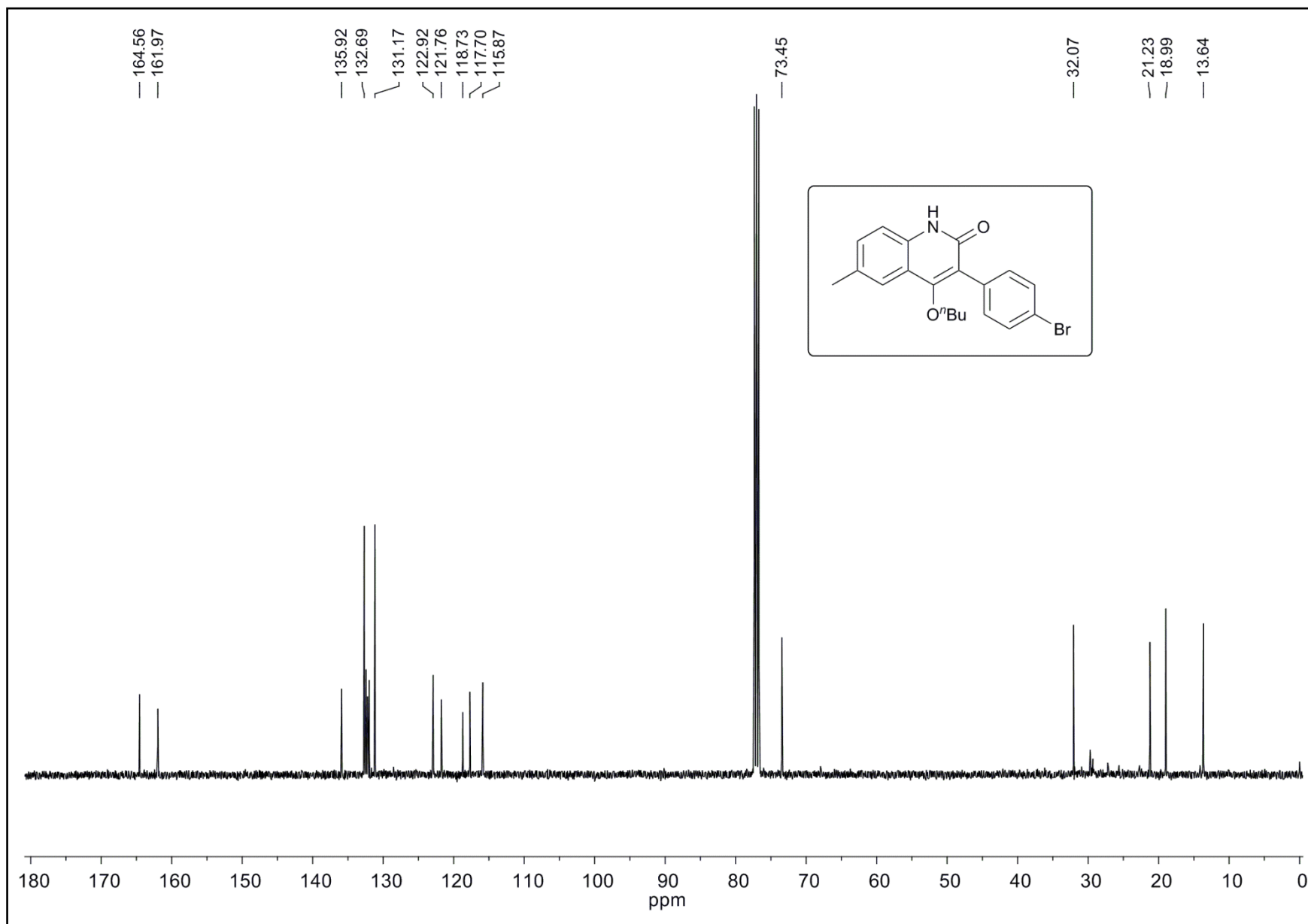


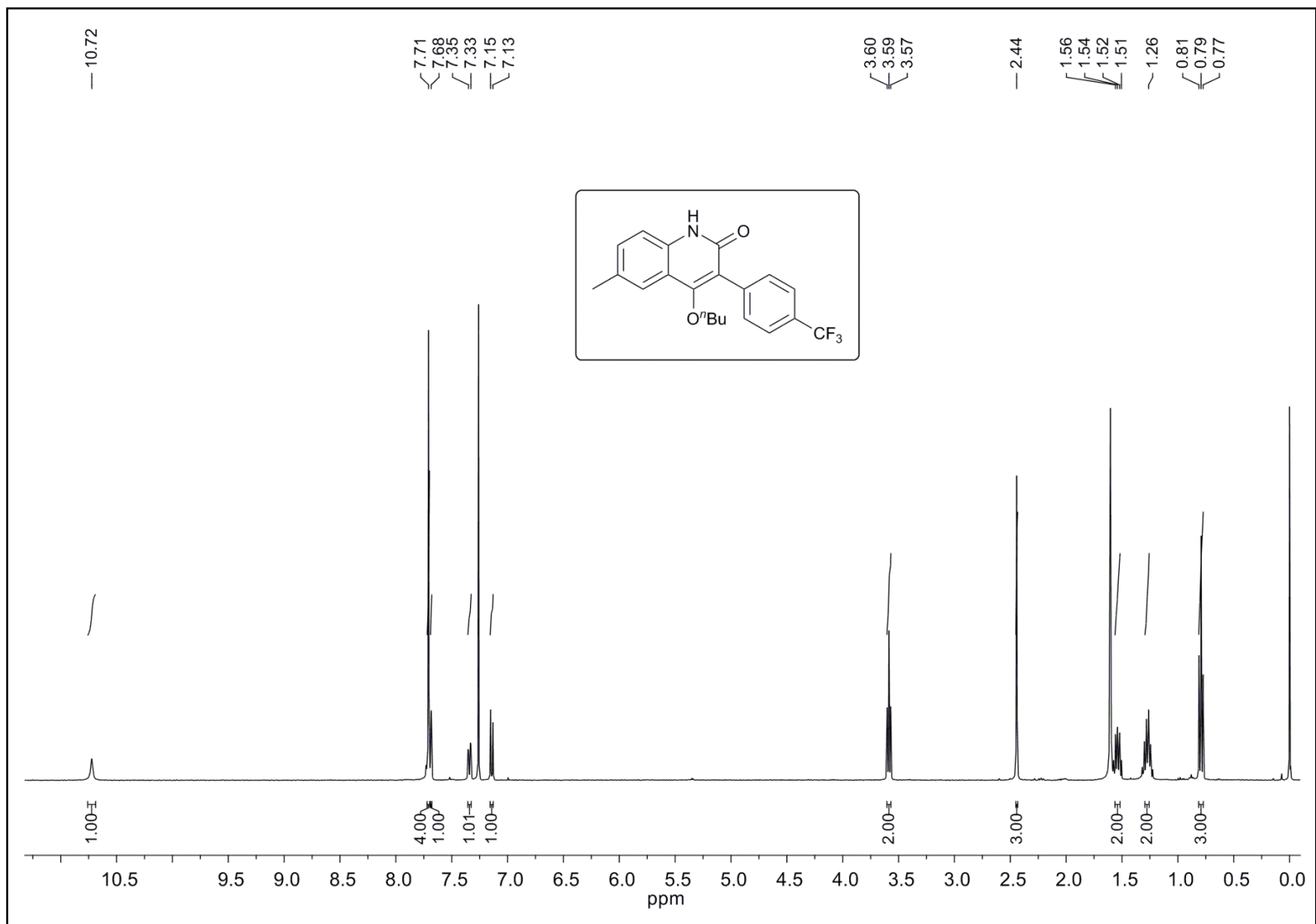


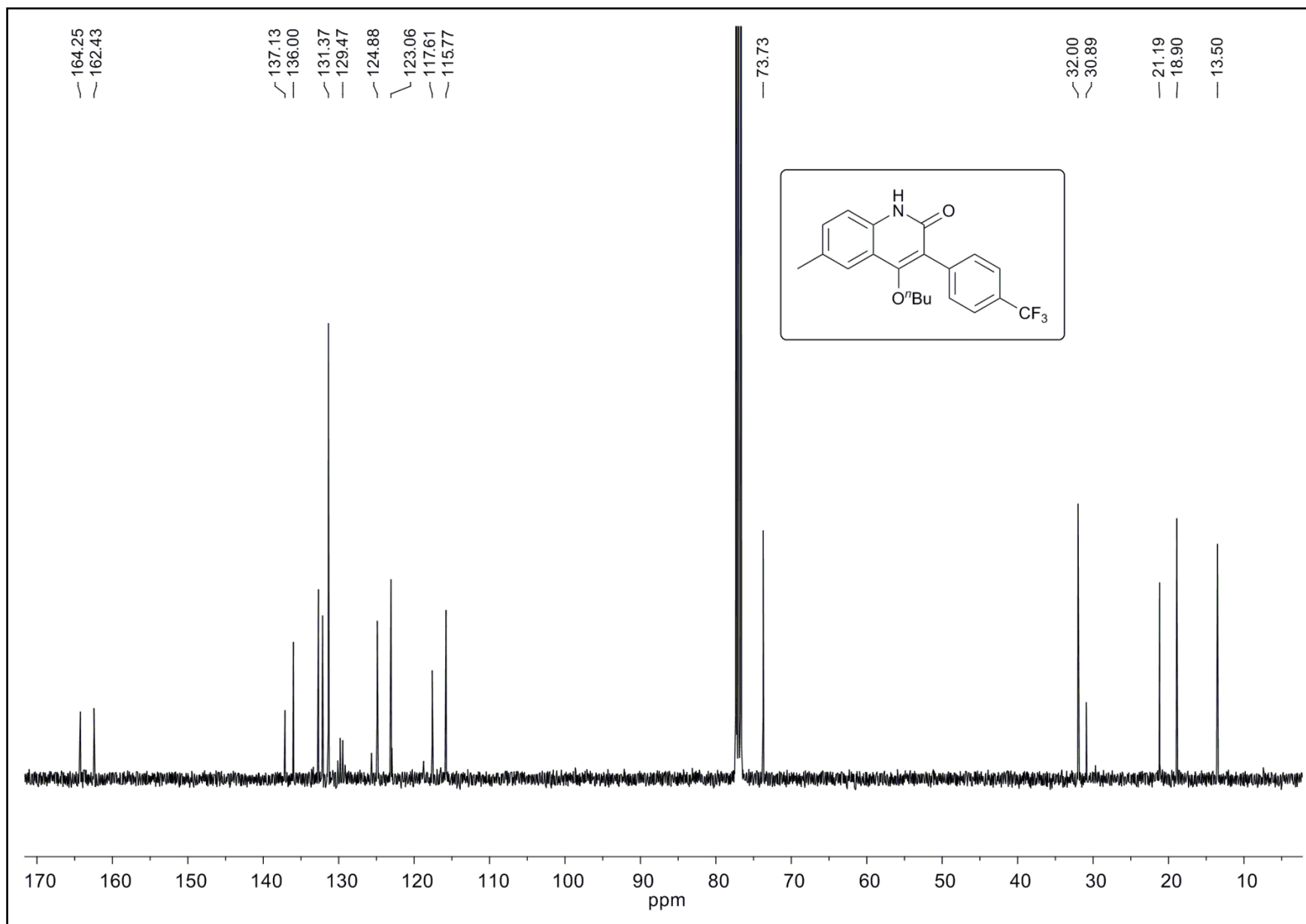












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162.43

137.13
136.00
131.37
129.47
124.88
123.06
117.61
115.77

73.73

32.00
30.89

21.19
18.90
13.50

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm