

Transformation of a Metal Chelate into a “Catch and Anchor” Inhibitor of Botulinum A Protease

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Figure S1. Cytotoxicity of the PPO compounds

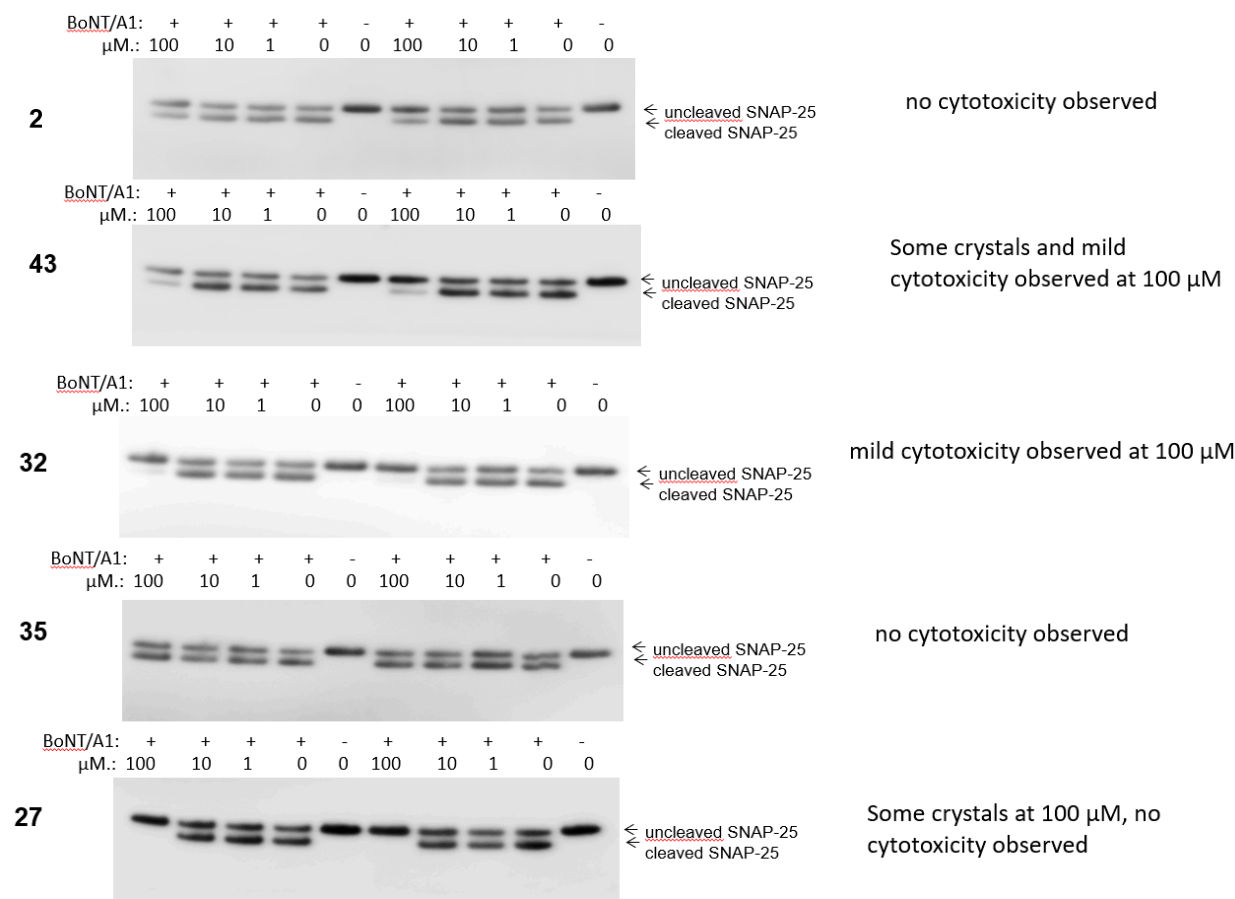
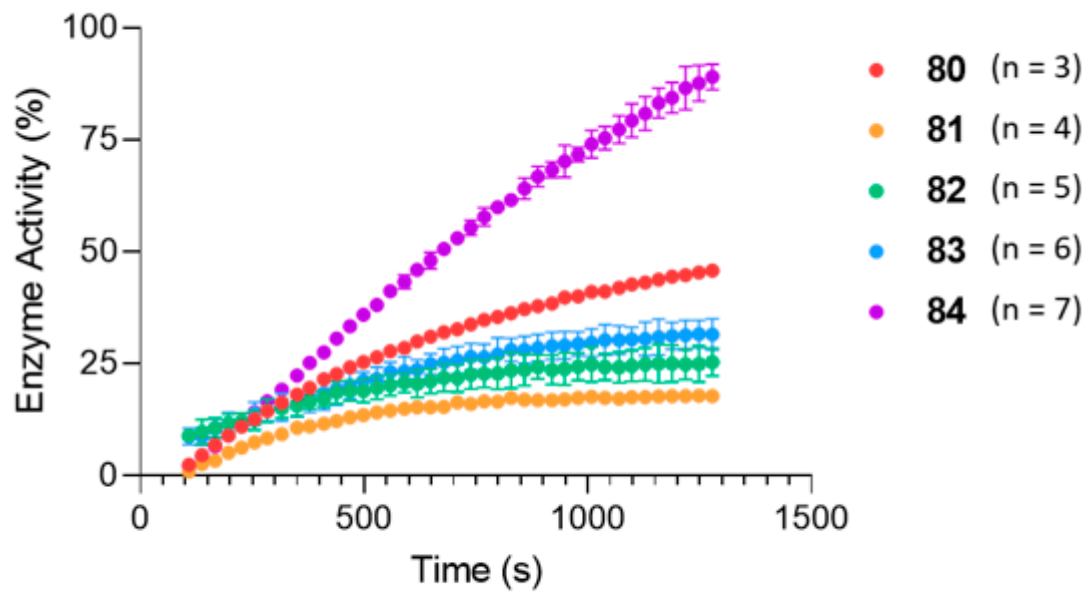
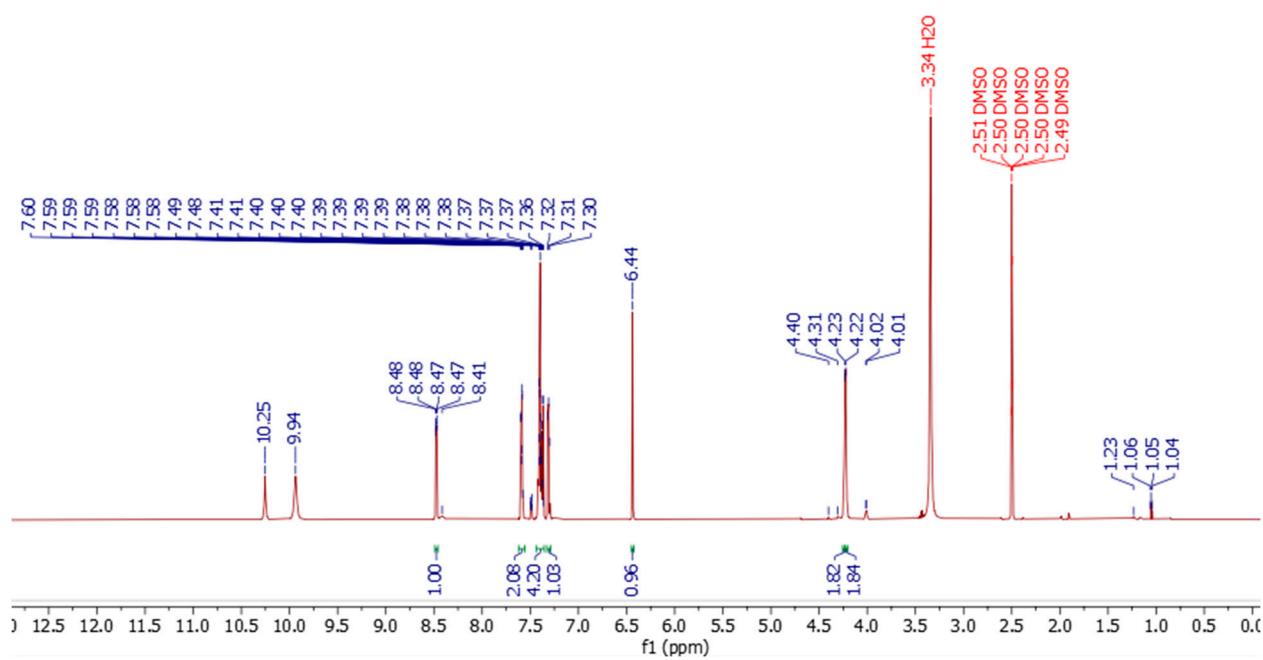
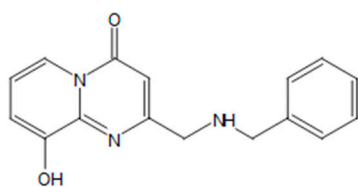


Figure S2. Activity Screen of Bifunctional inhibitors

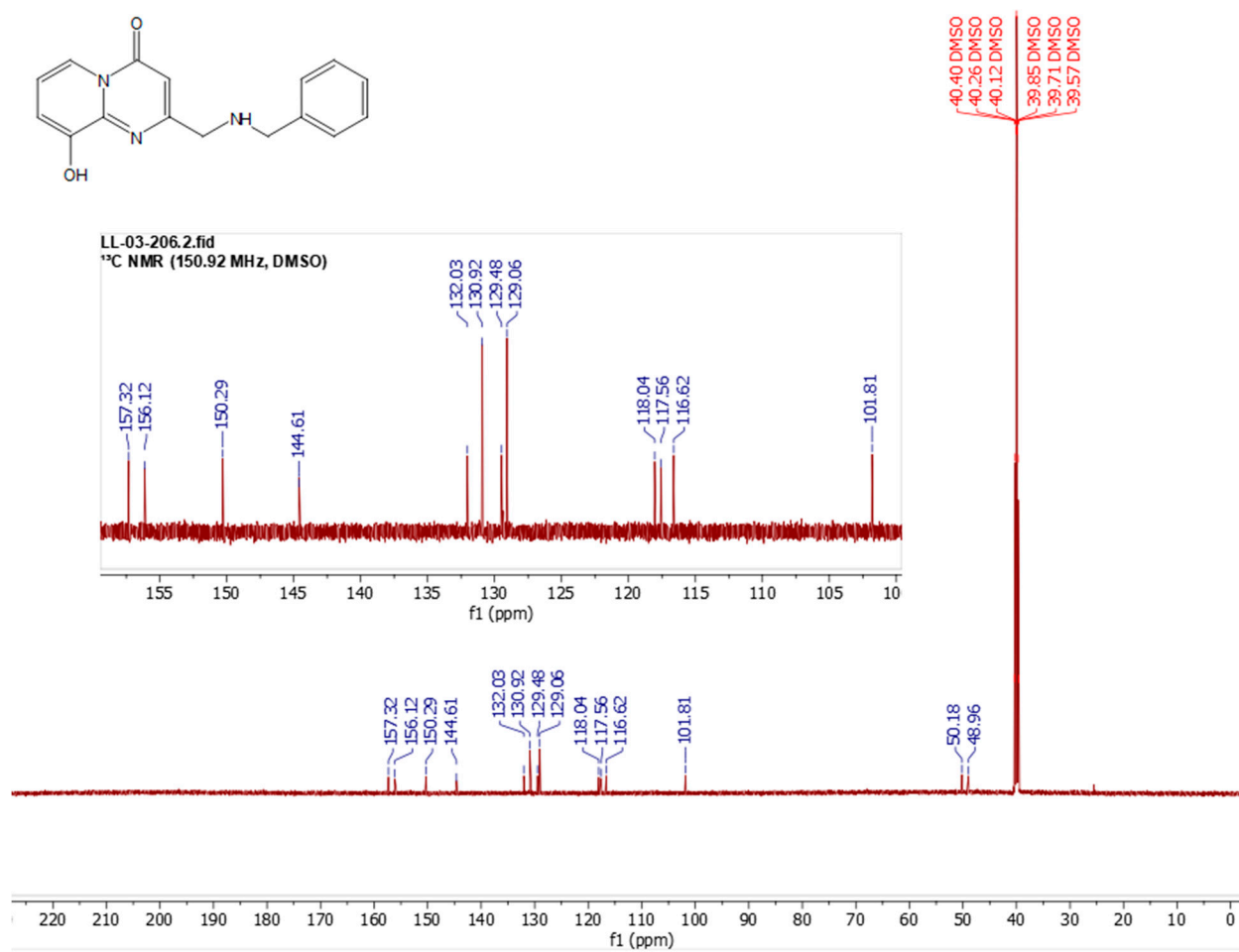
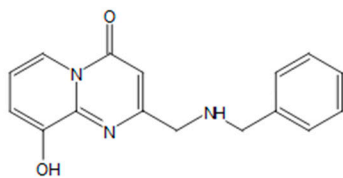


Screened at 4 μ M against 10 nM BoNT/A-LC, at 37°C

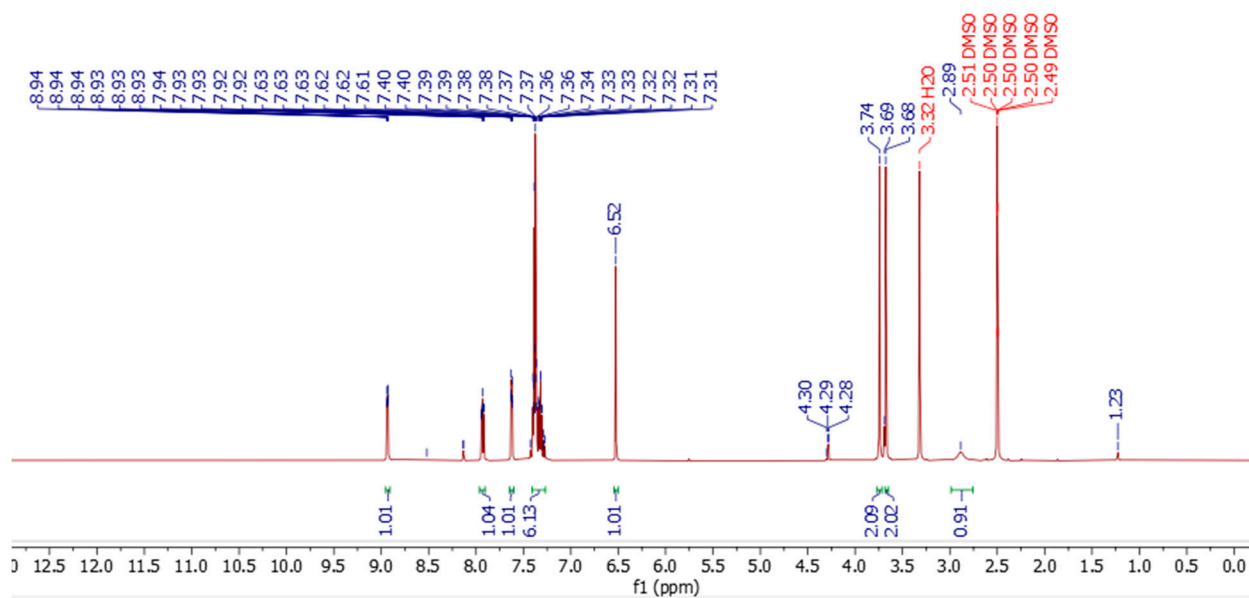
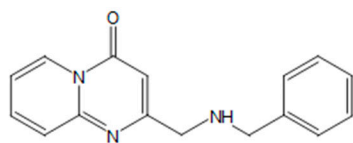
¹H NMR of **2**



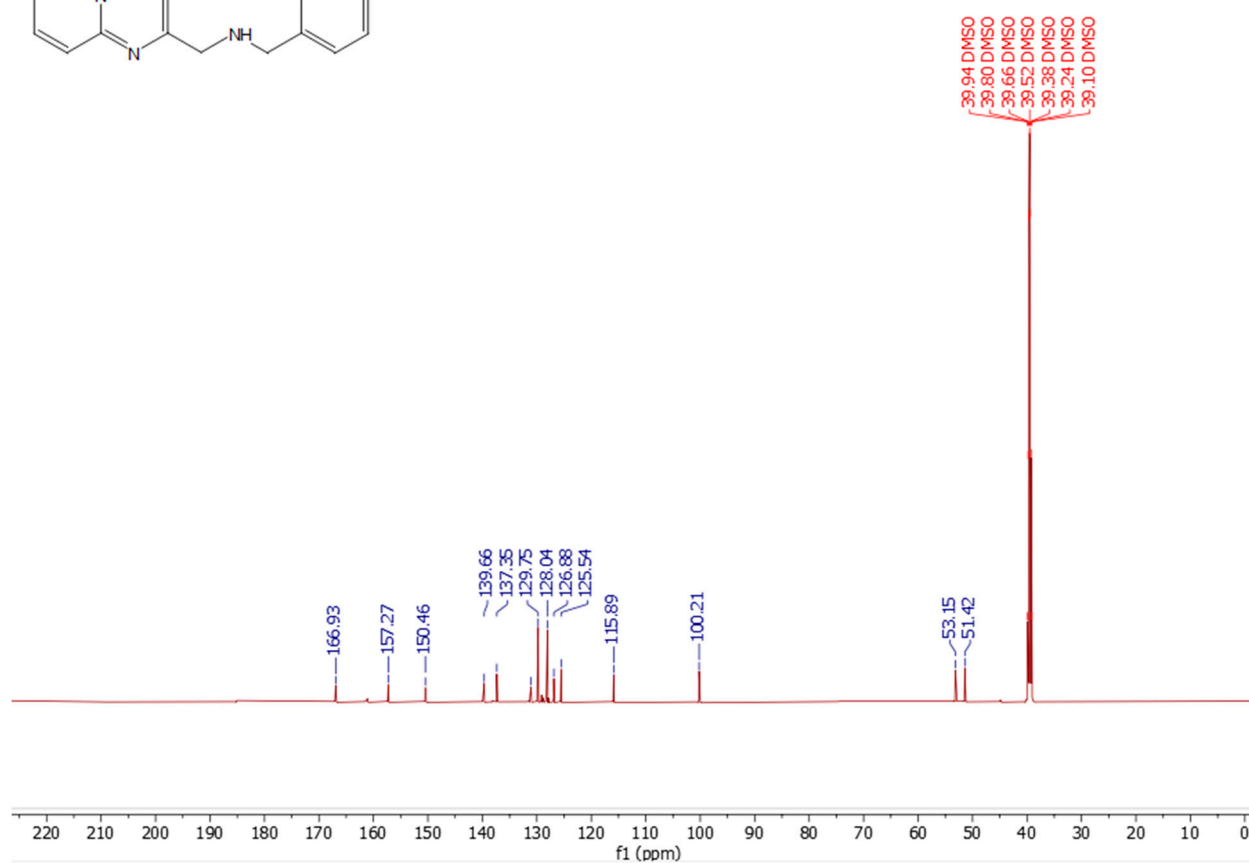
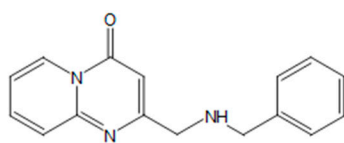
¹³C NMR of **2**



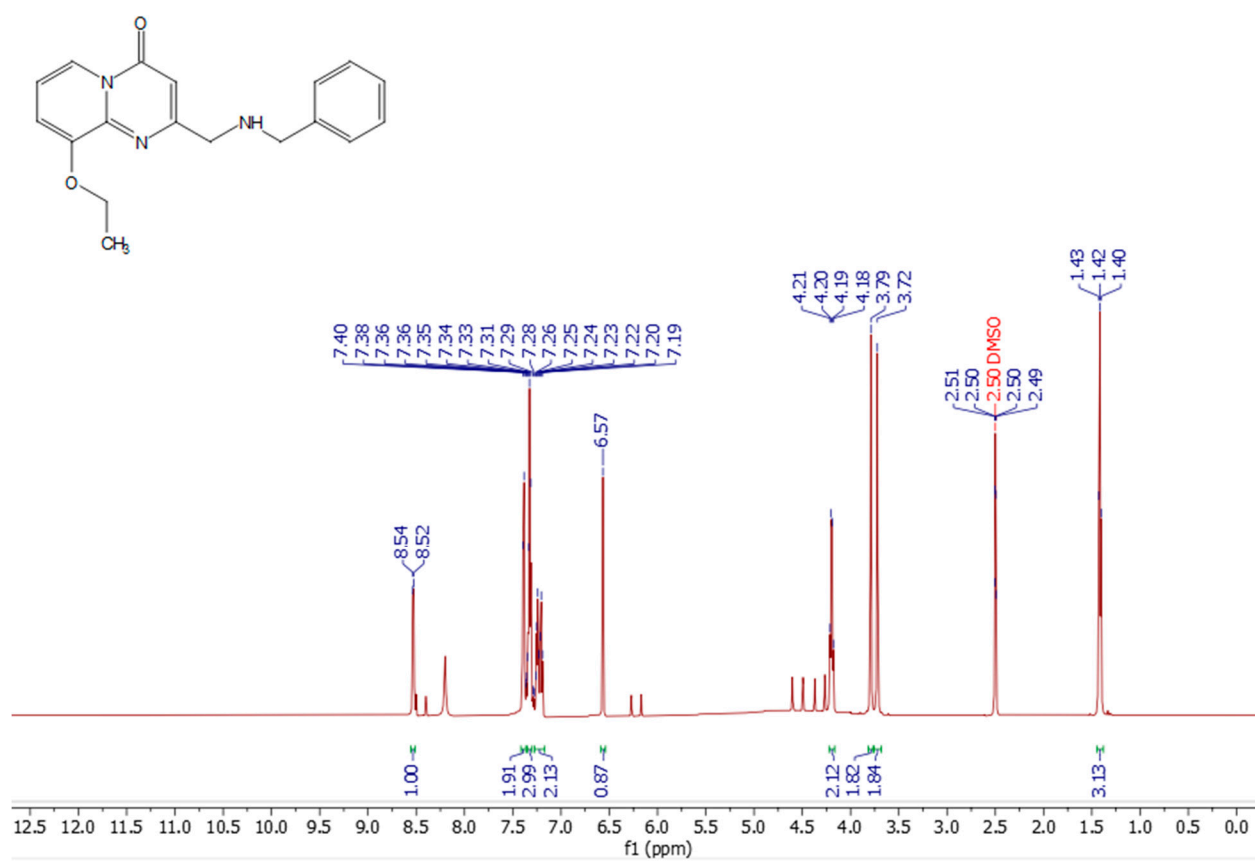
¹H NMR of 6



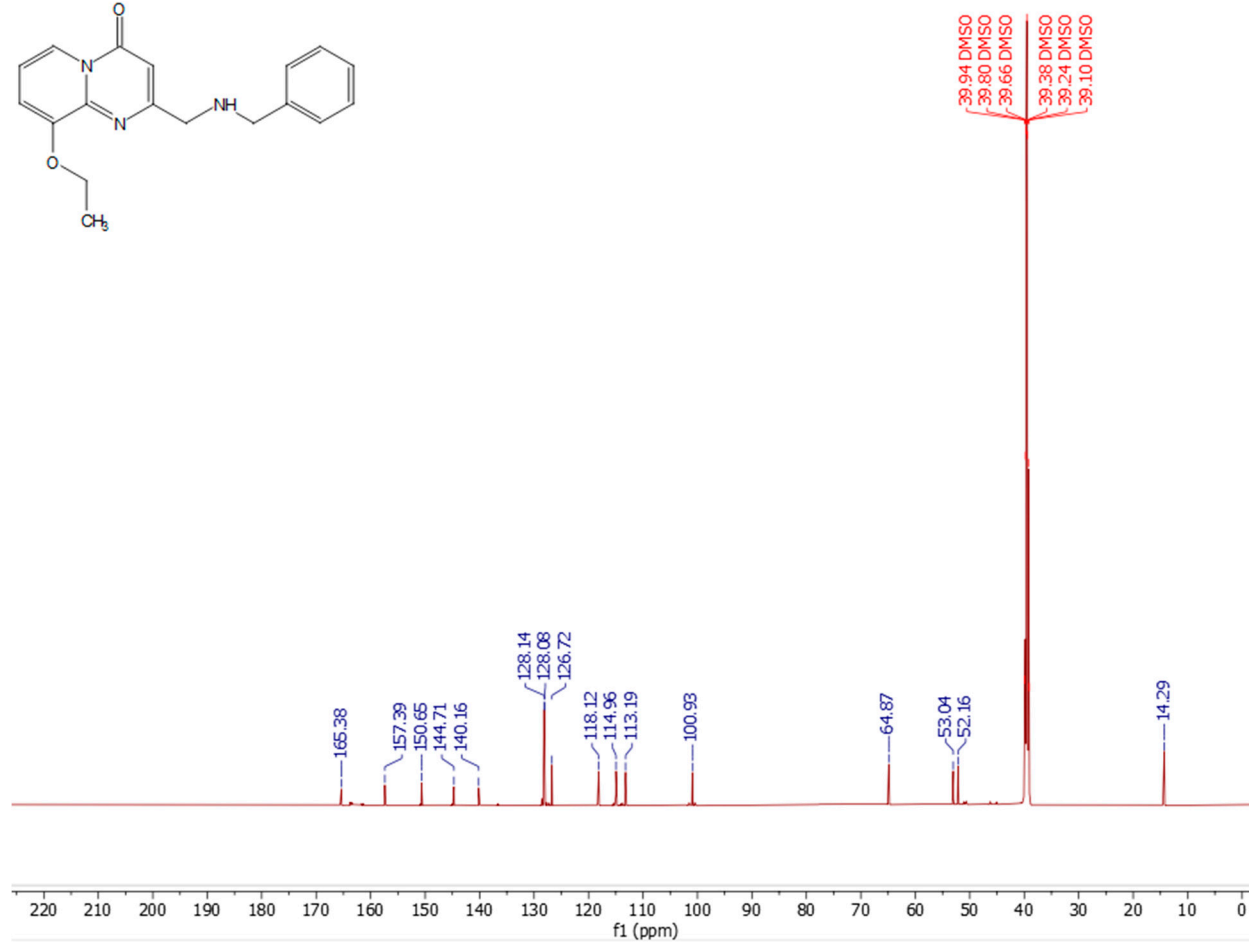
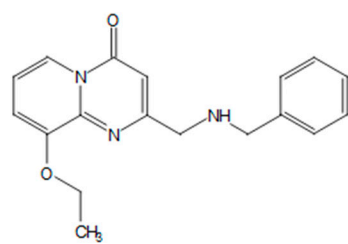
¹³C NMR of **6**



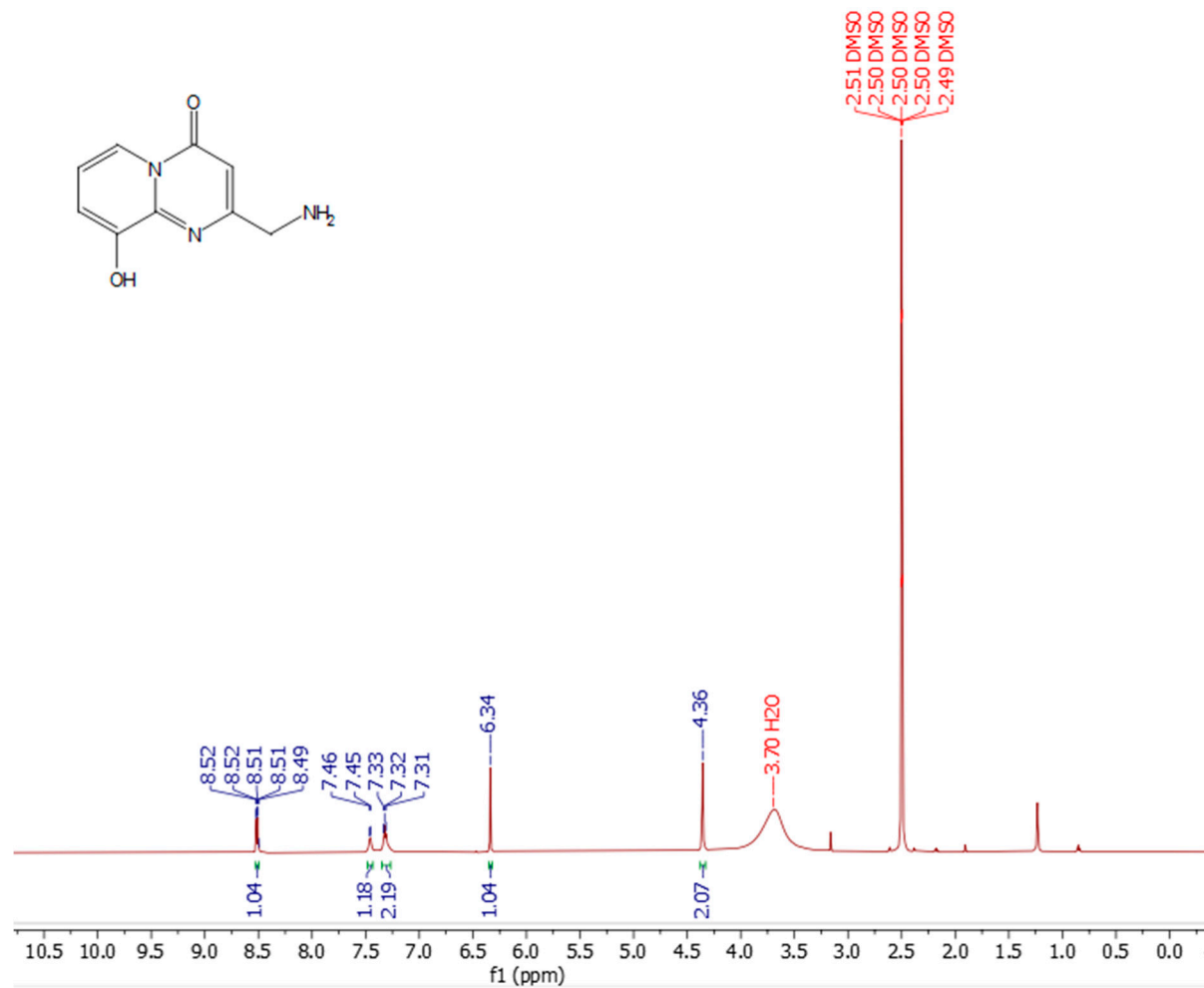
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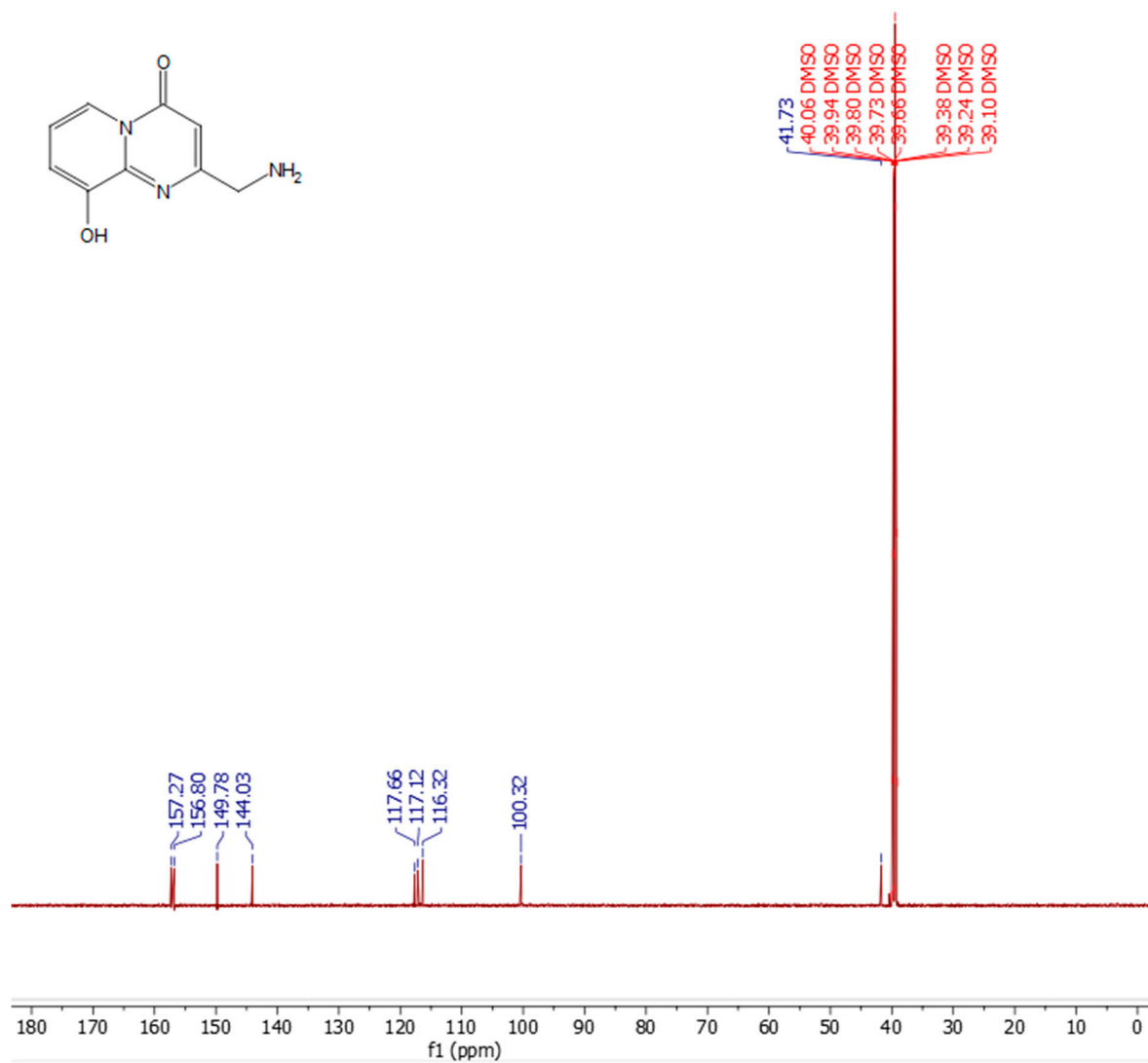
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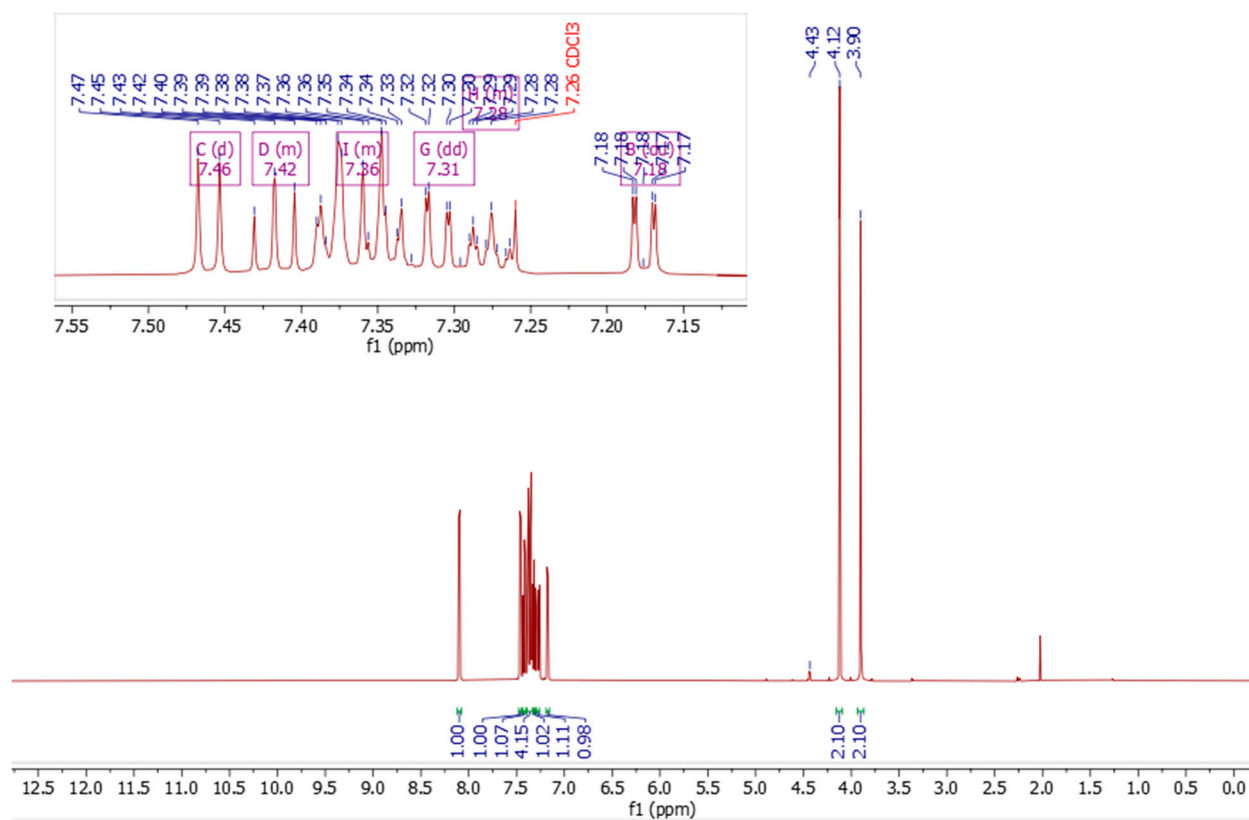
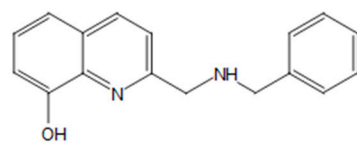
¹H NMR of **13**



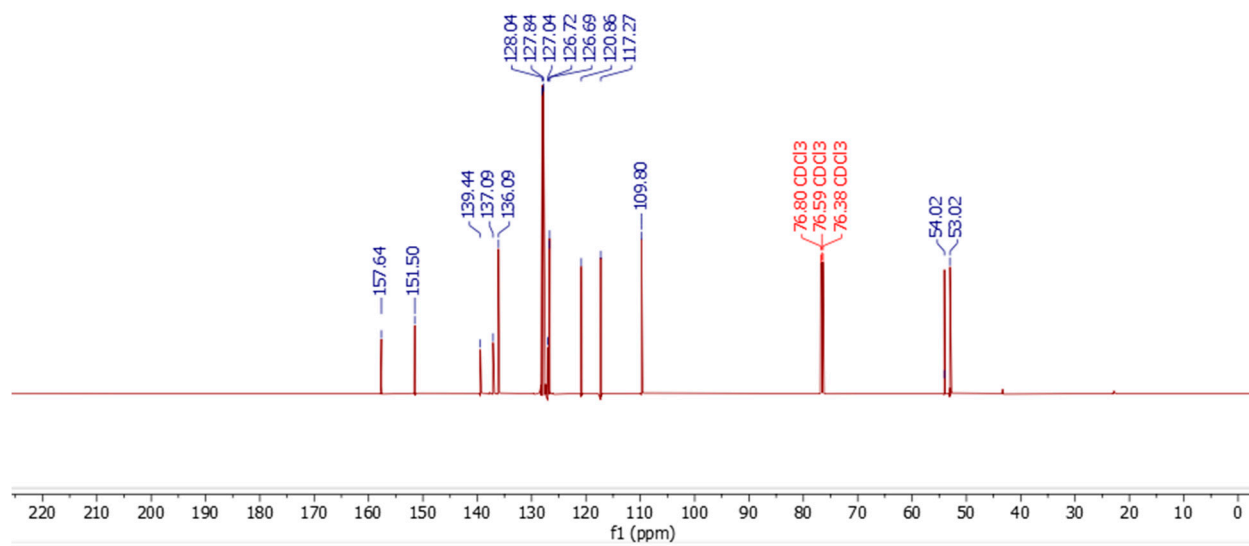
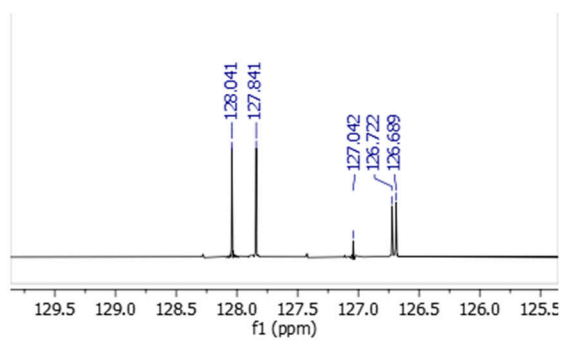
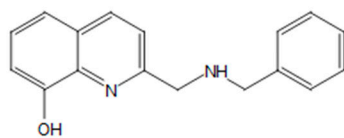
¹³C NMR of **13**



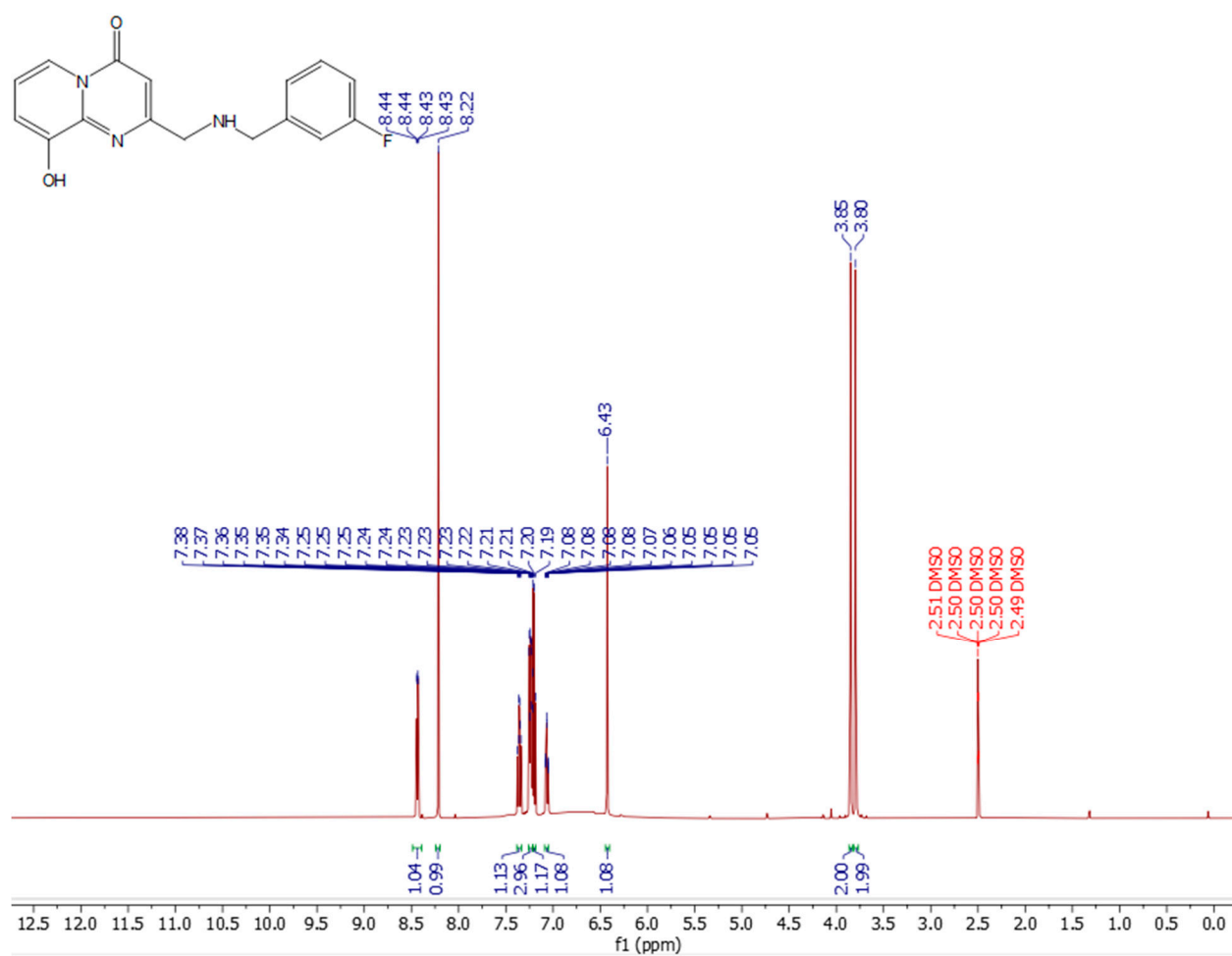
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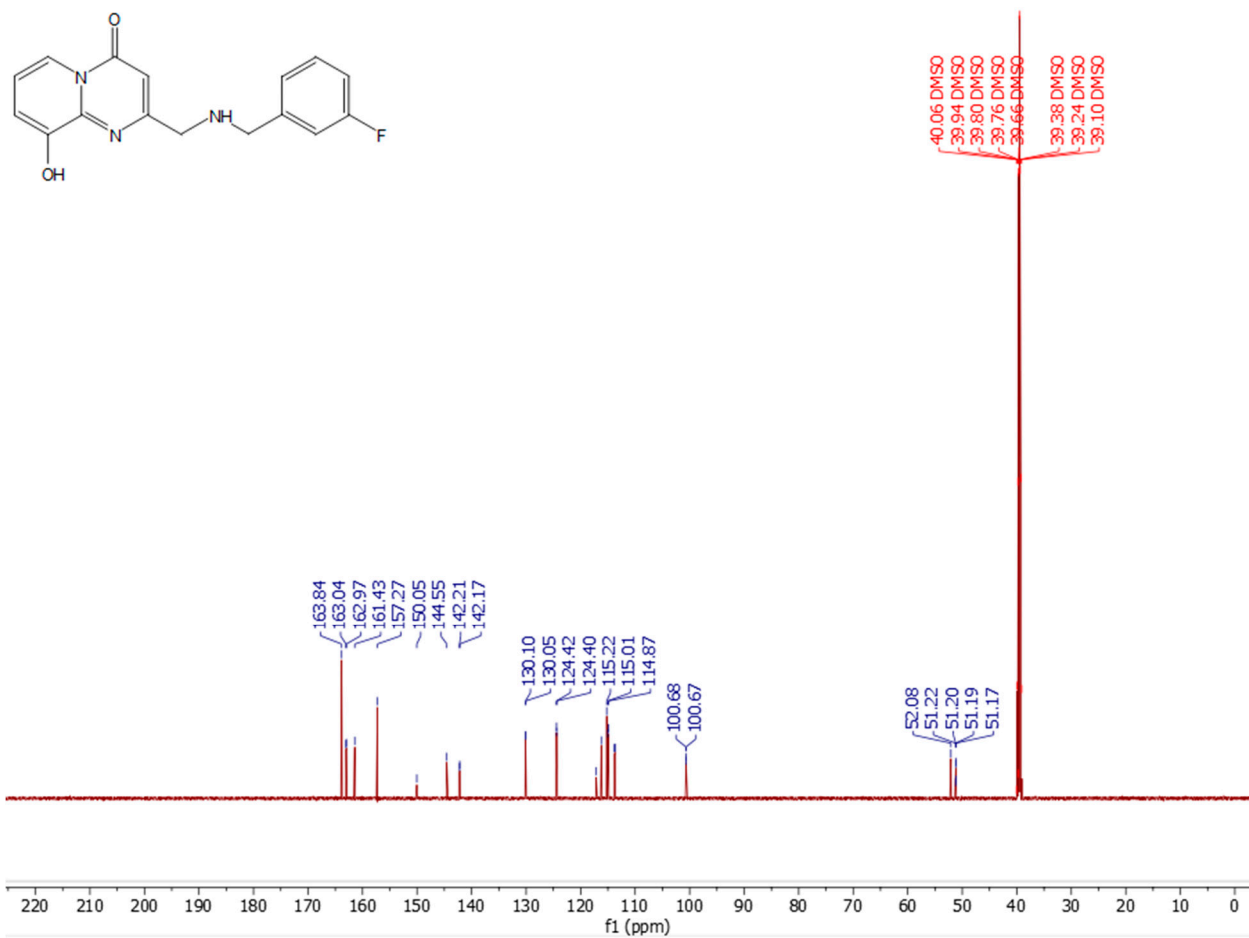
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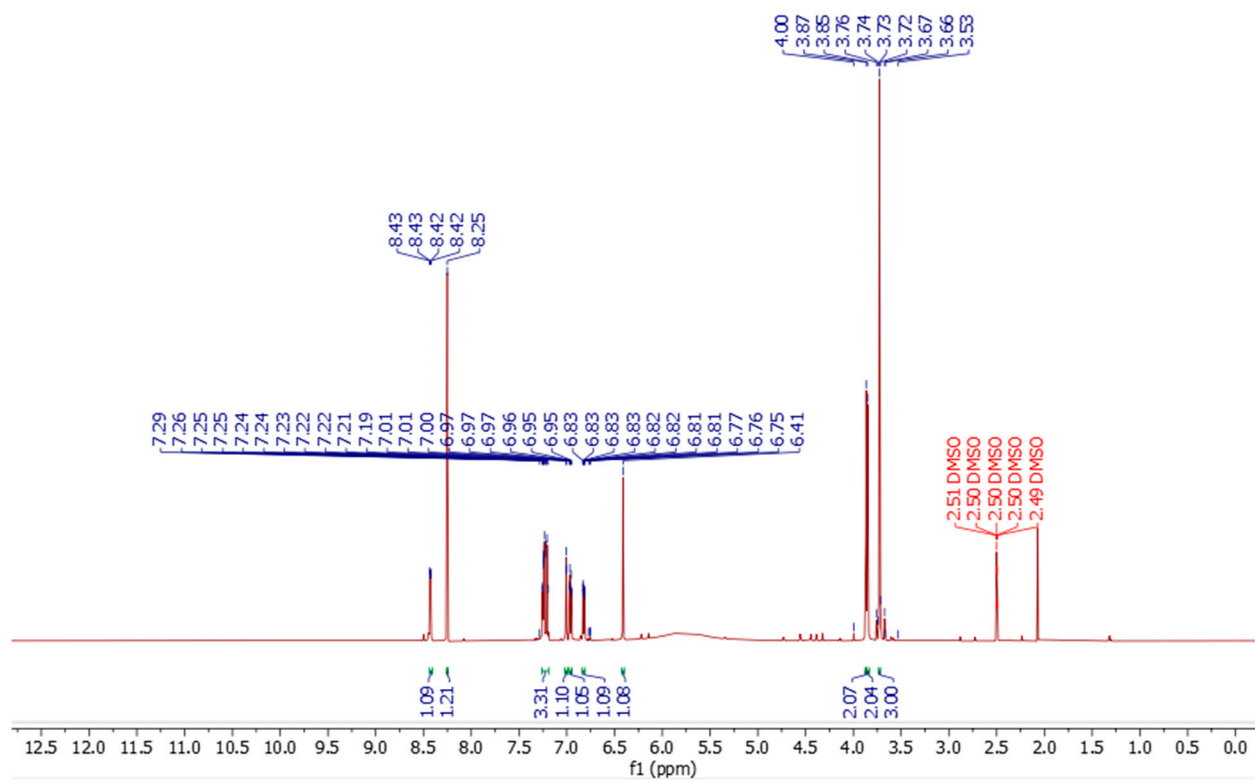
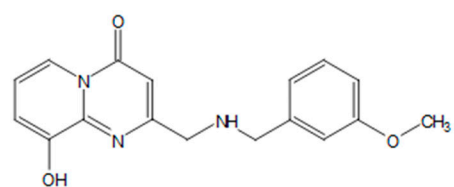


¹H NMR of **16**

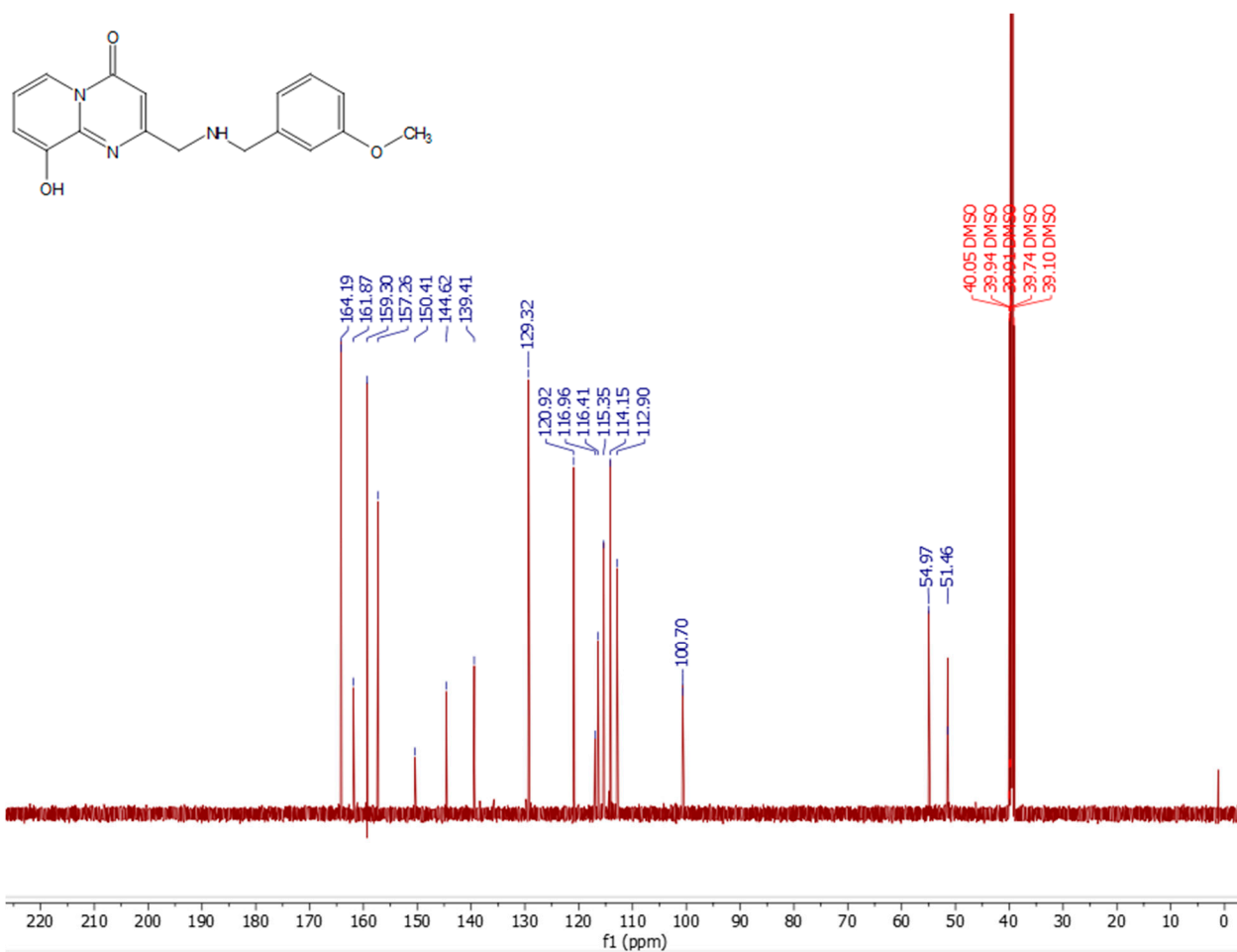


¹³C NMR of **16**

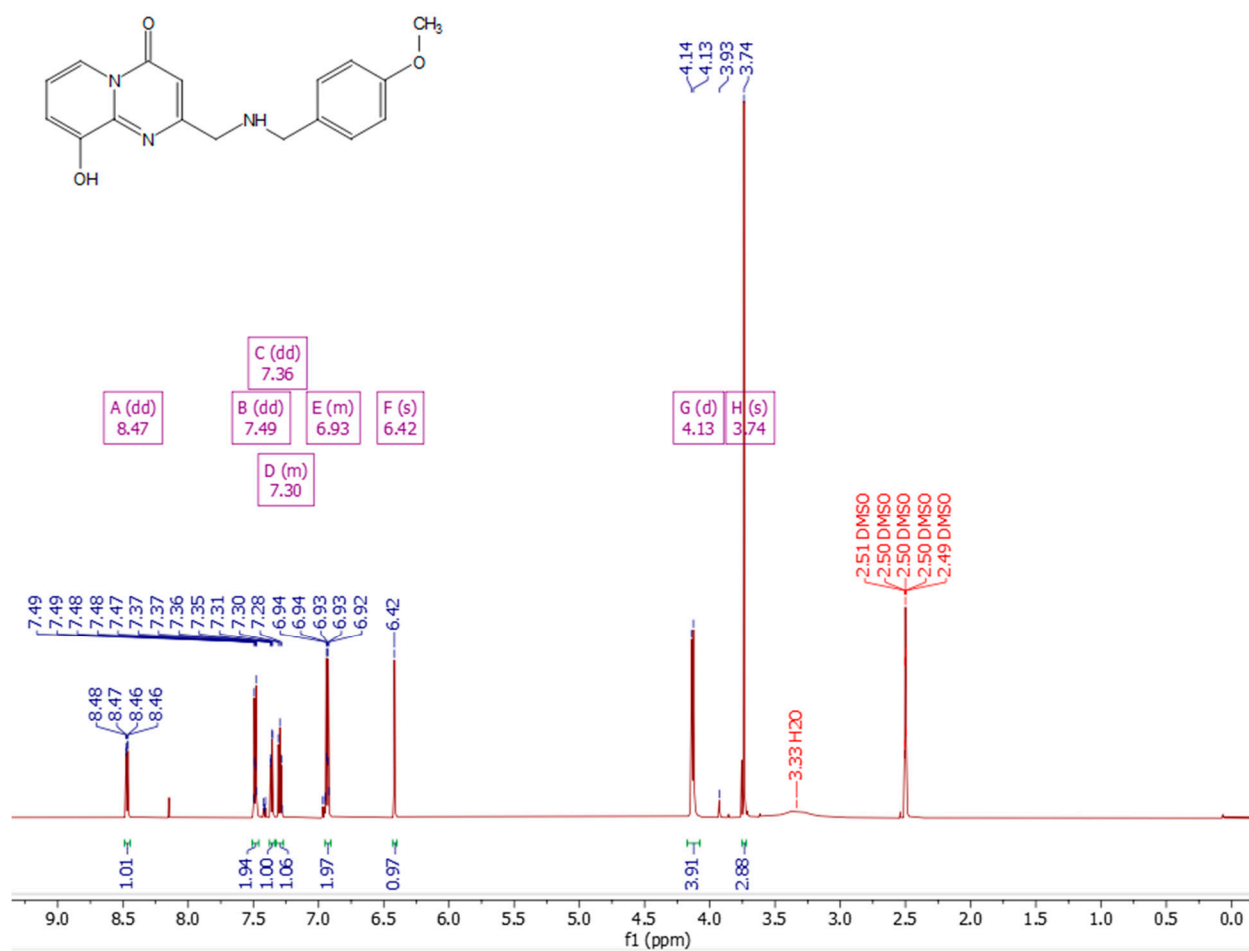


¹H NMR of **20**

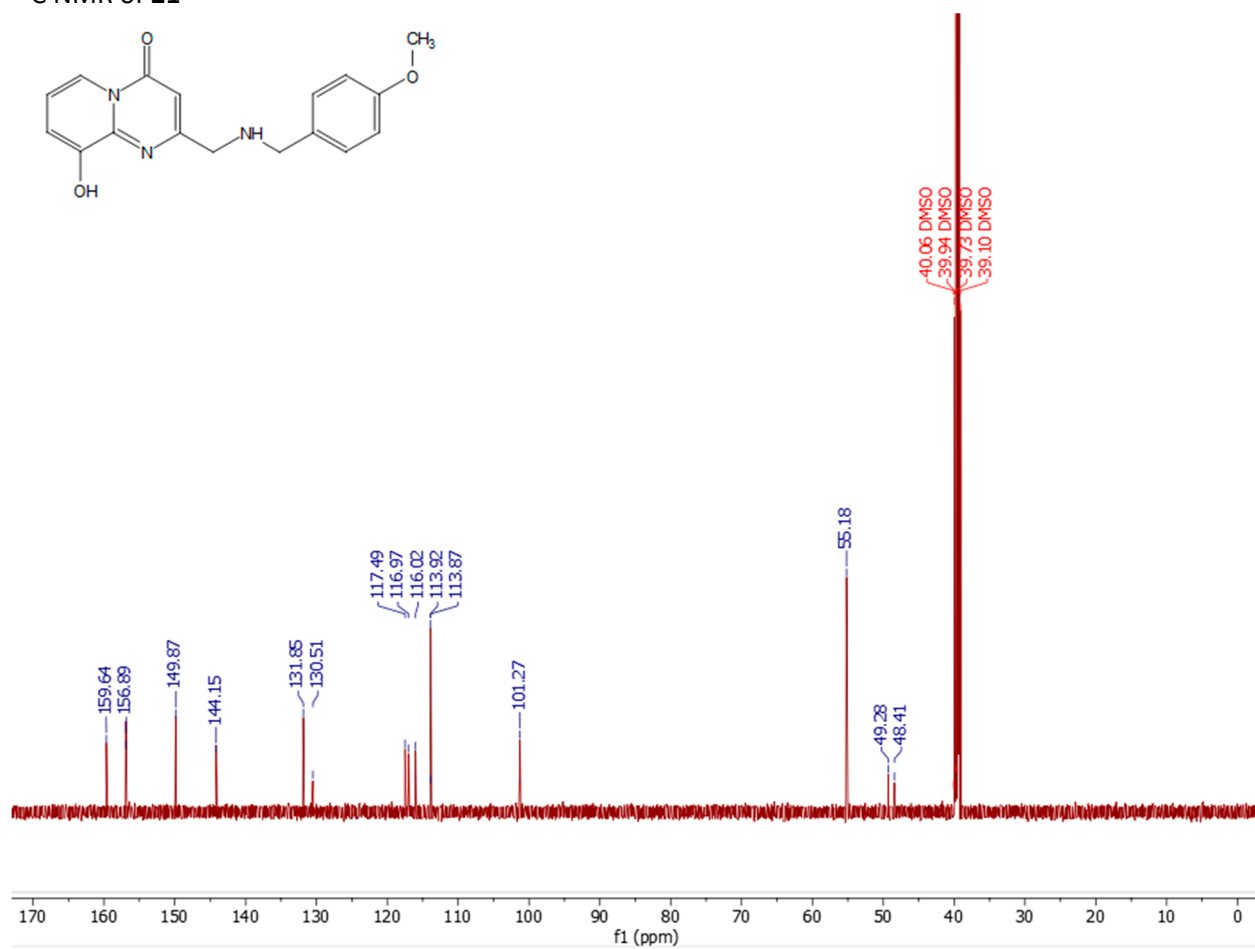
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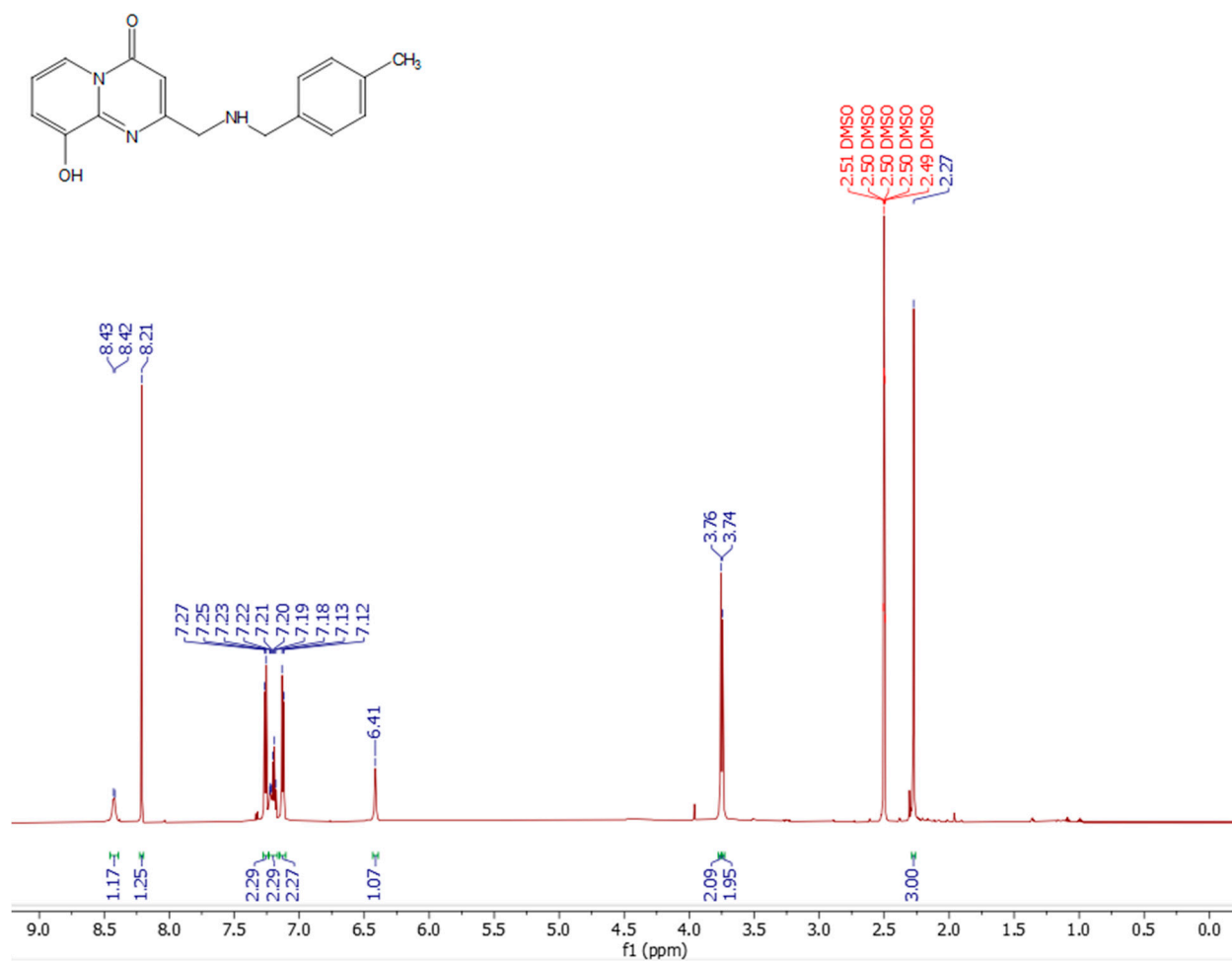
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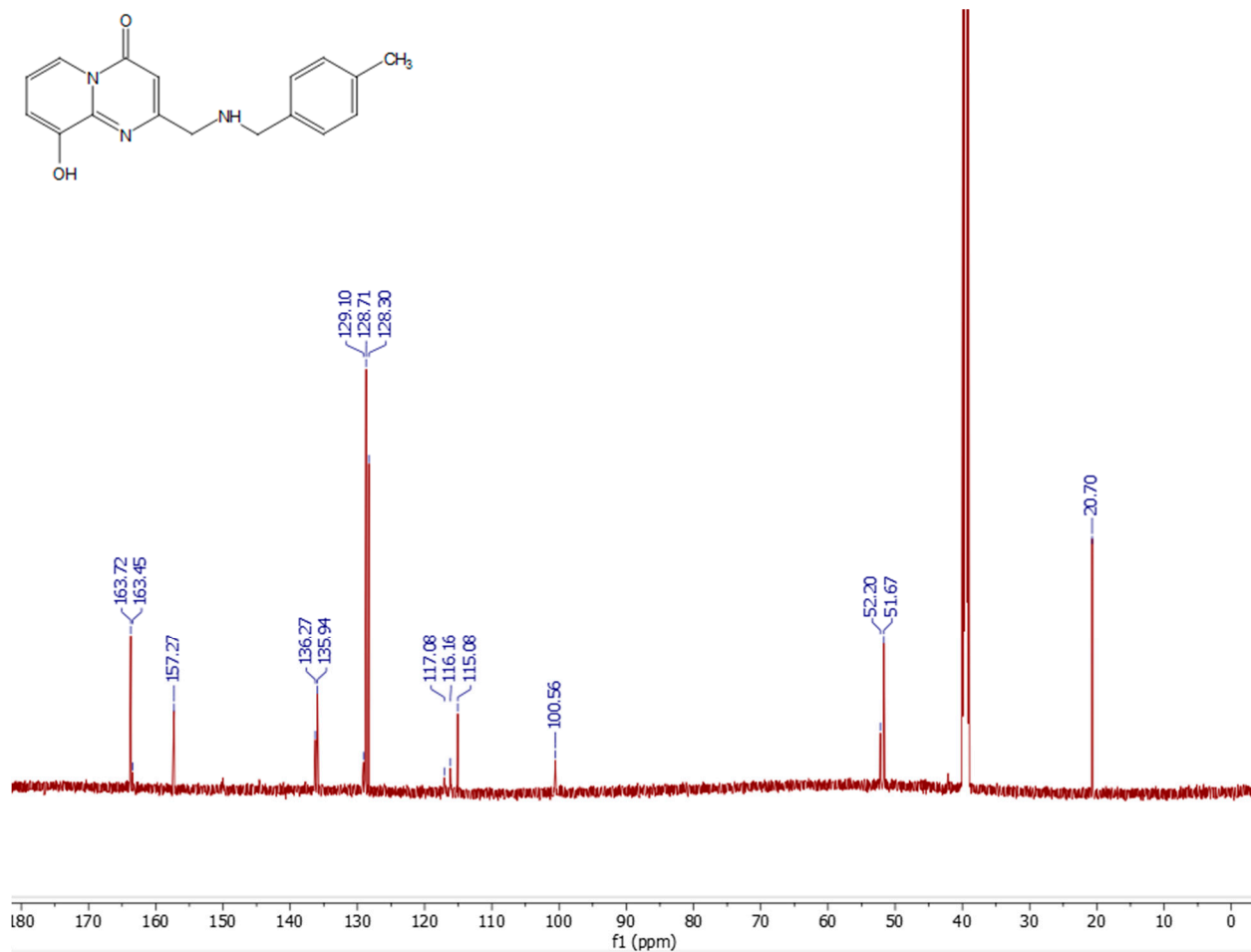
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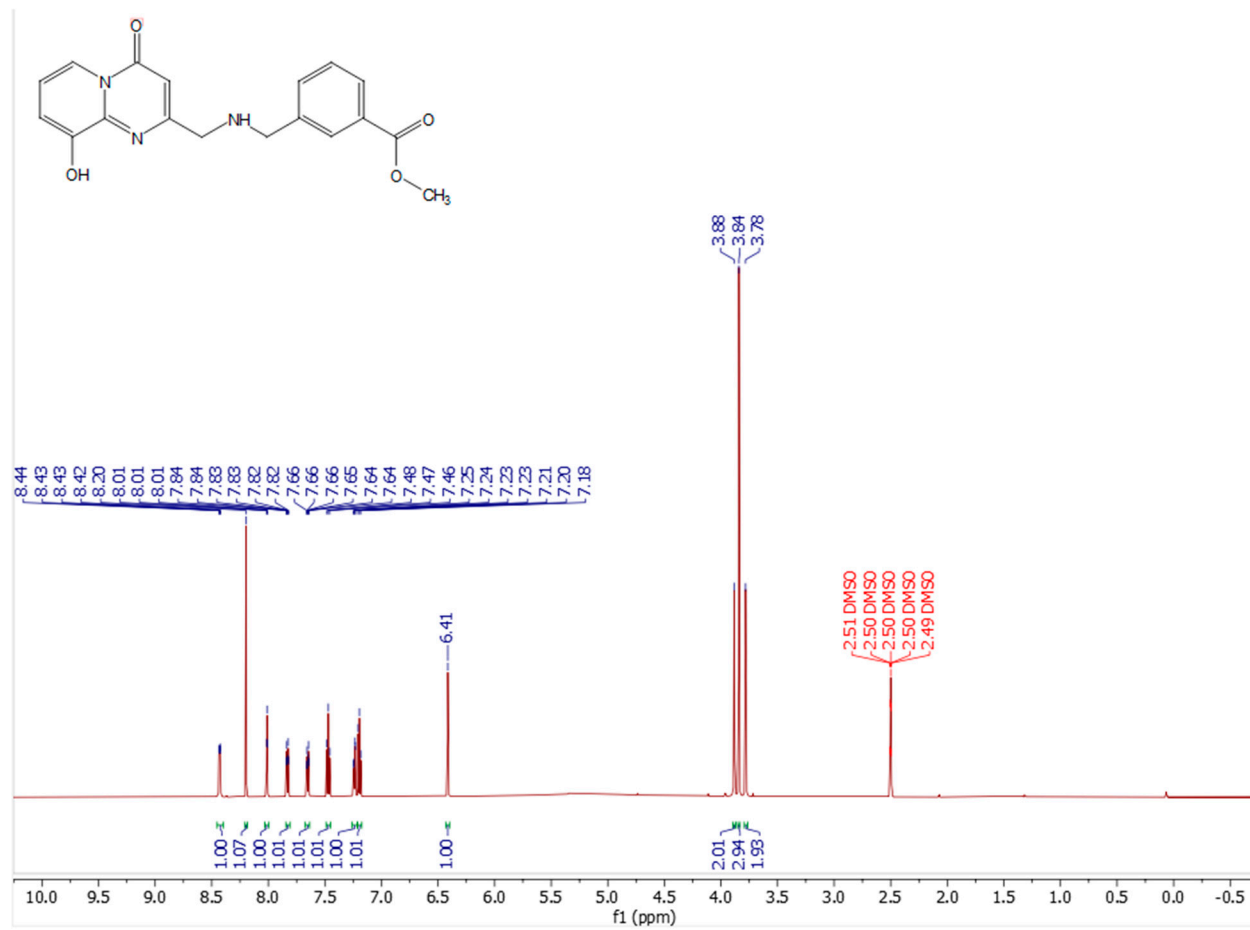
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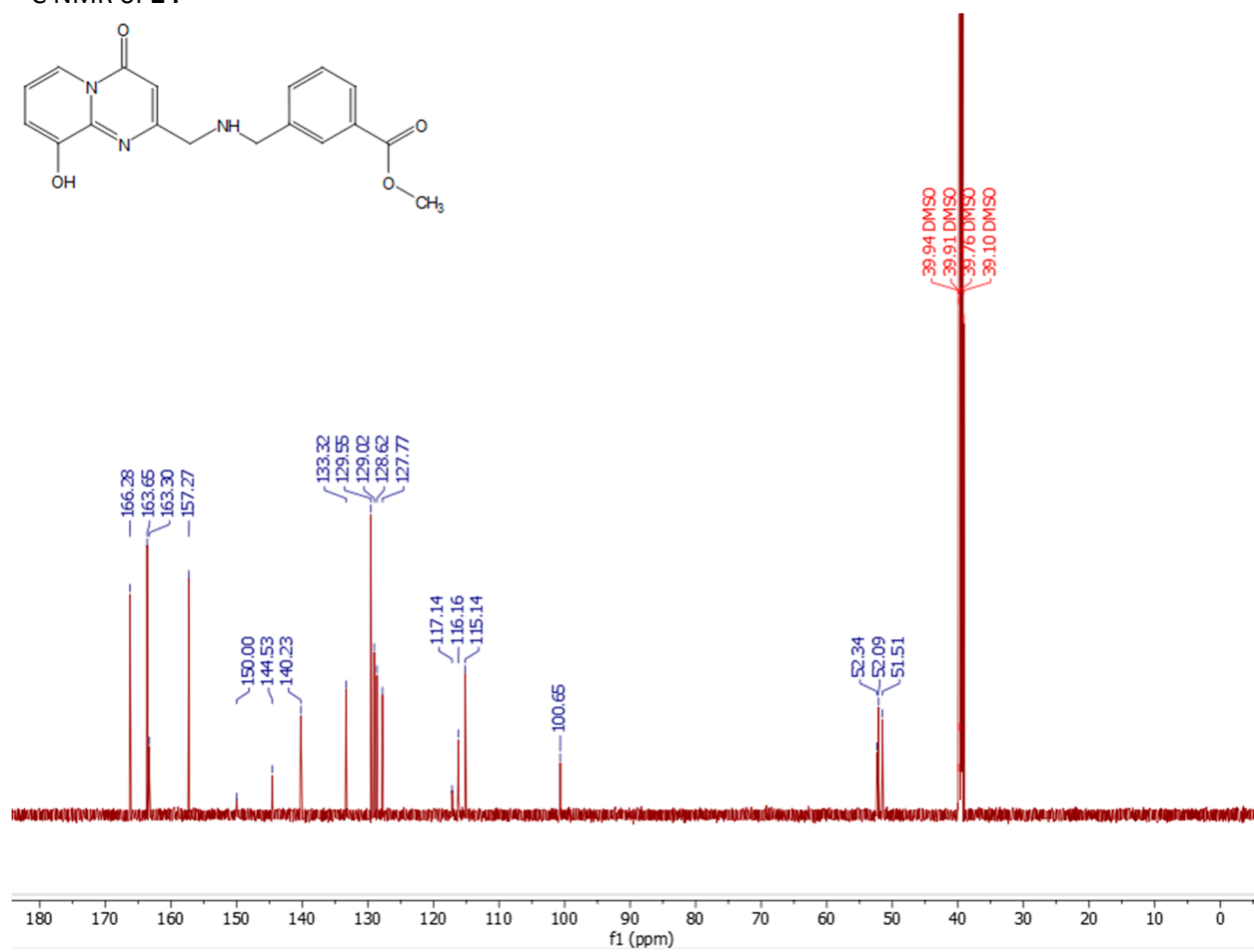
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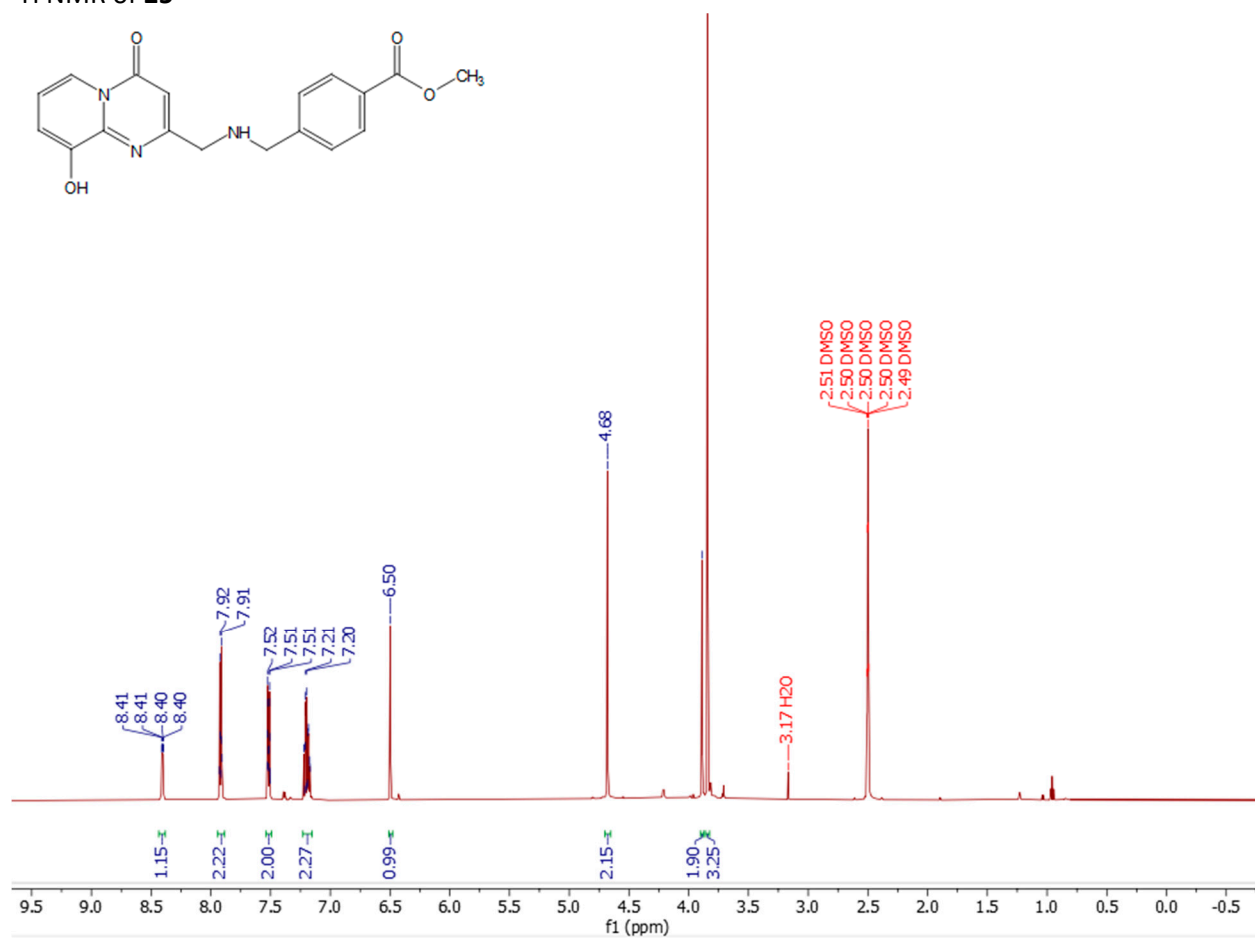
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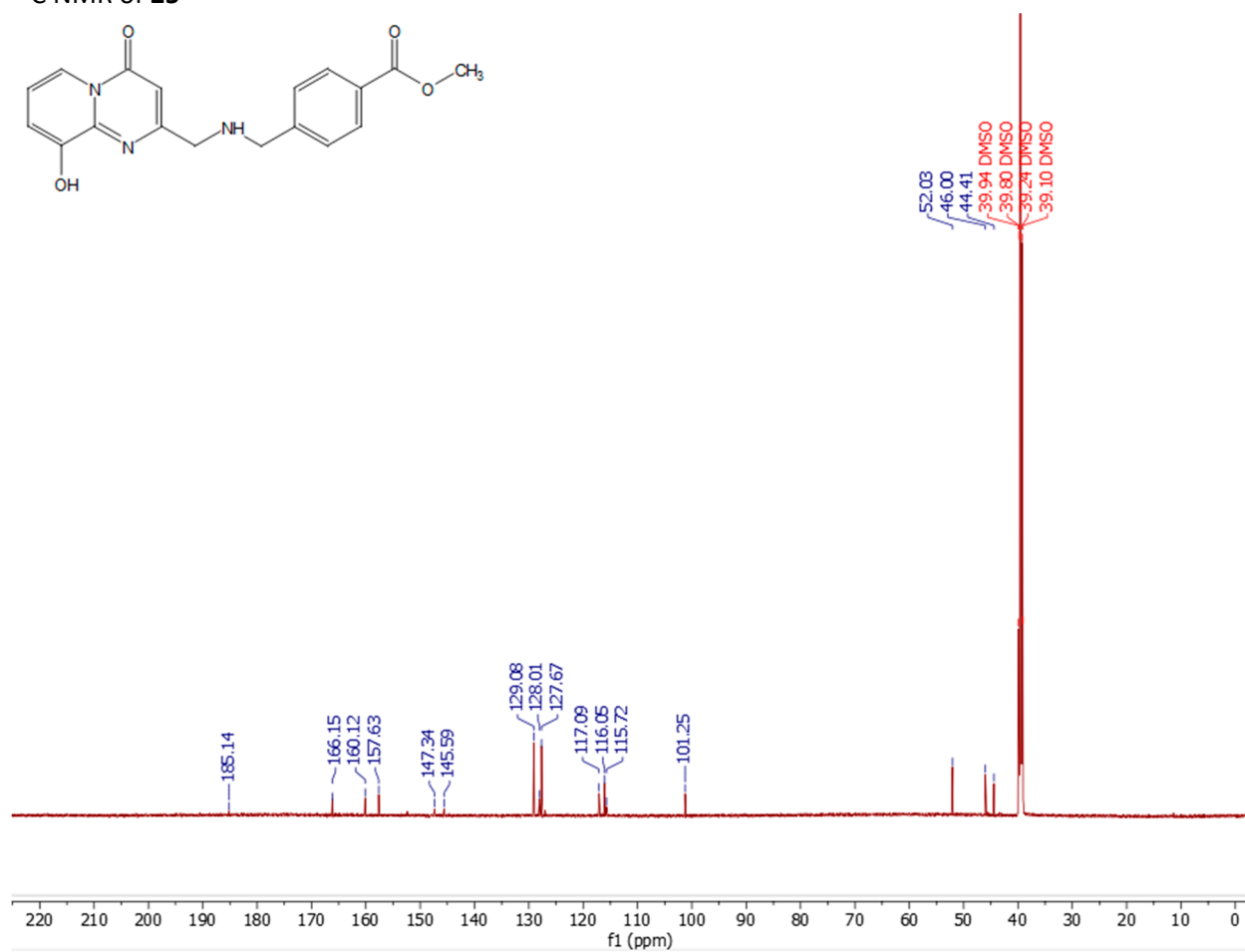
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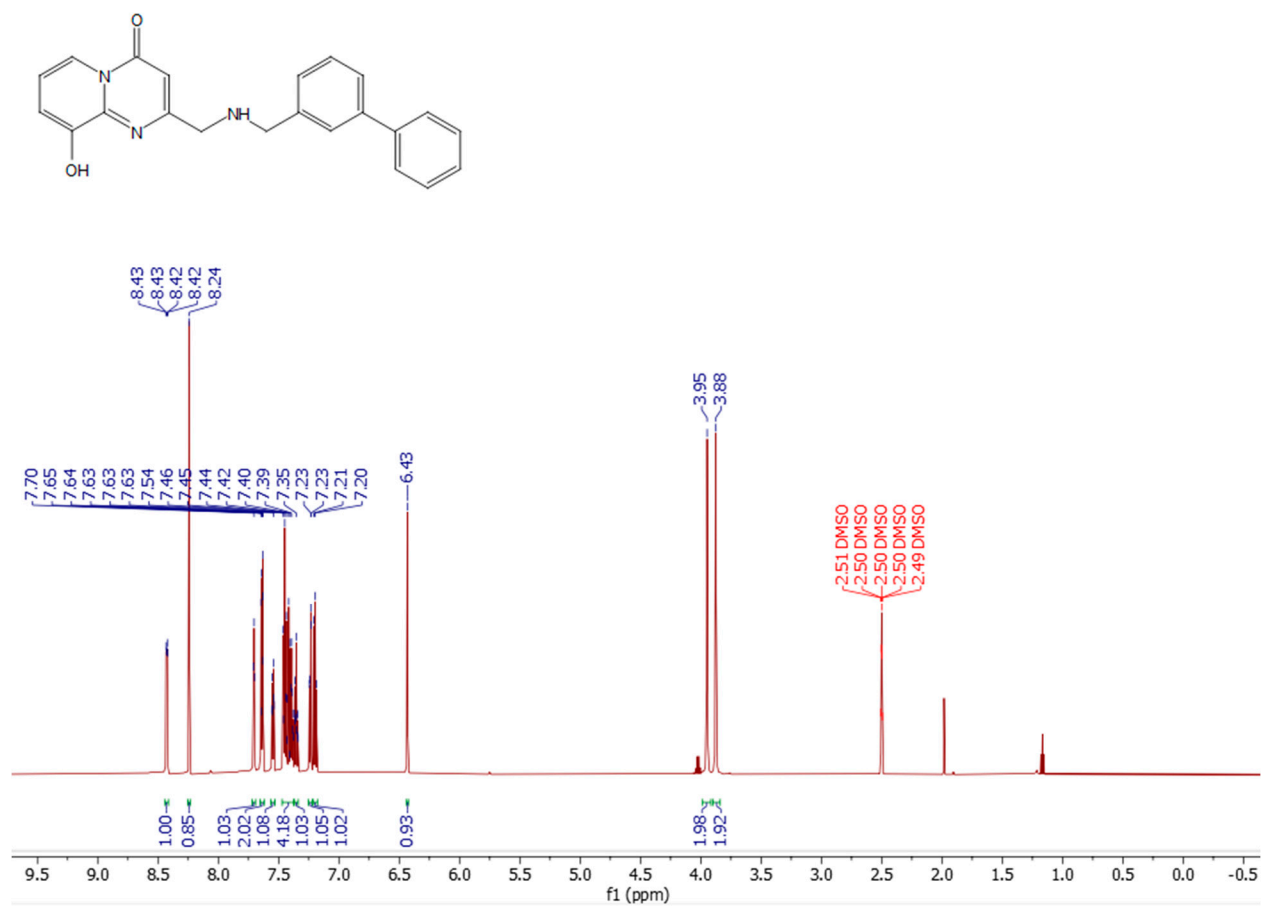
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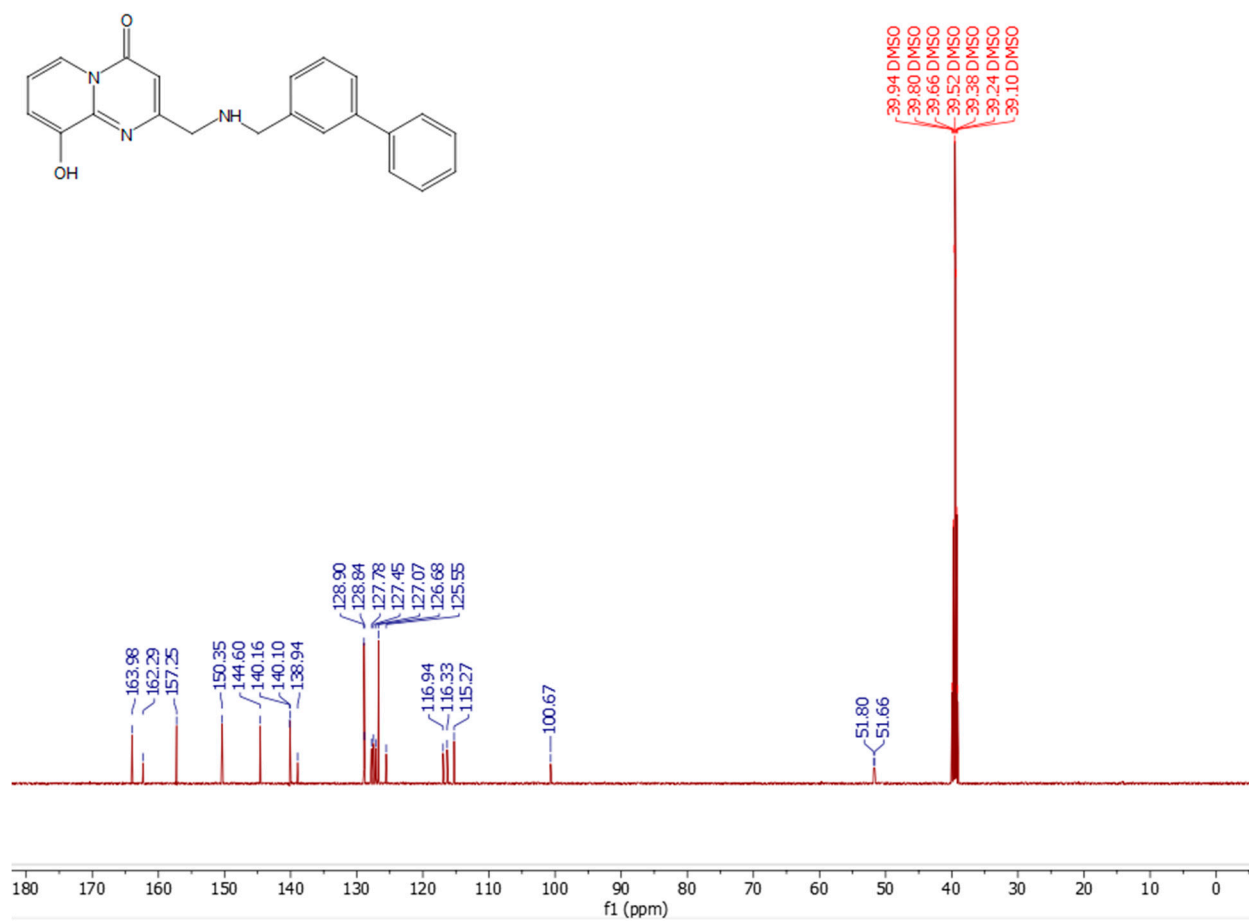
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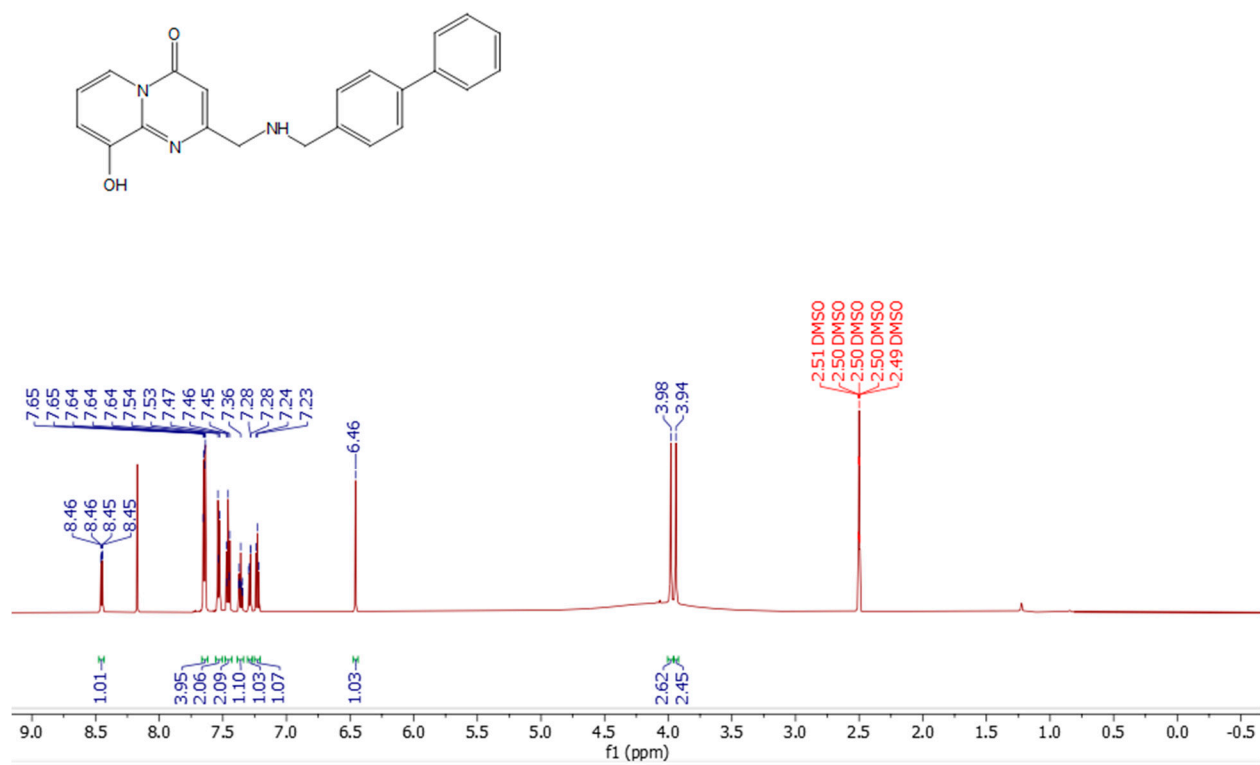
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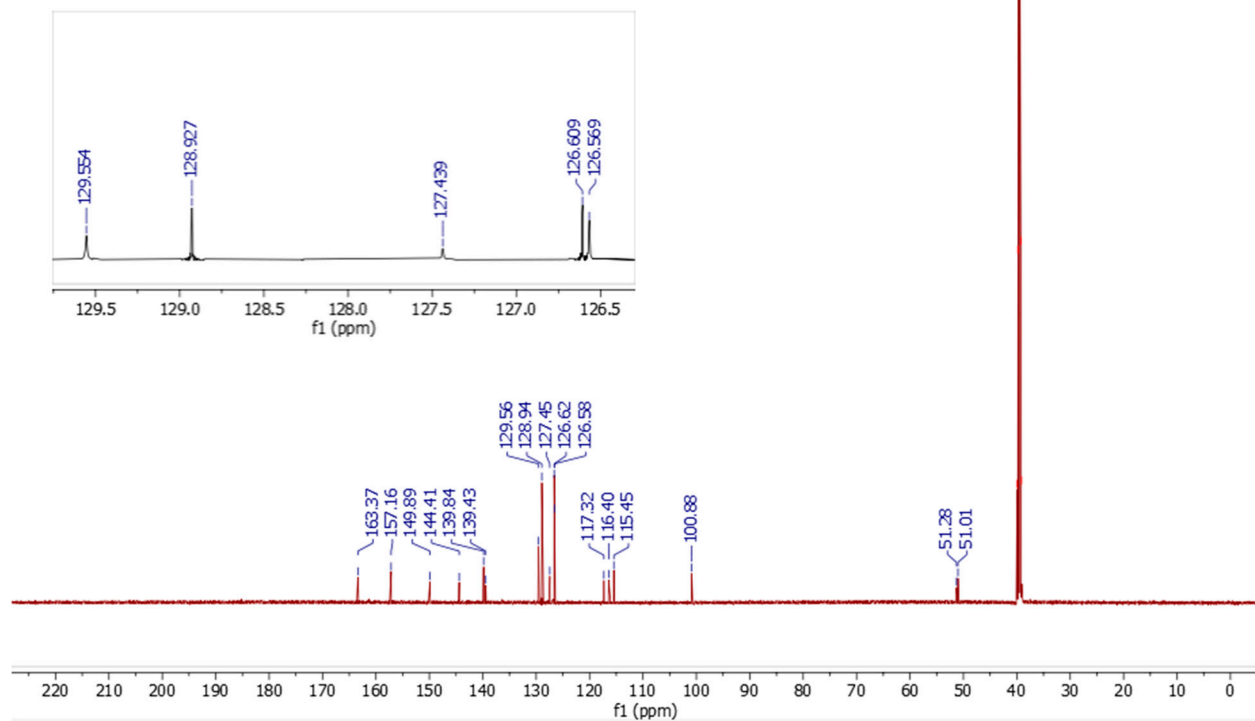
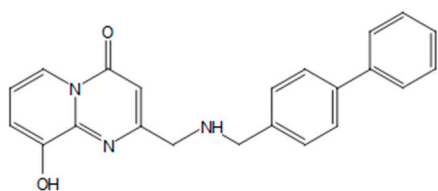
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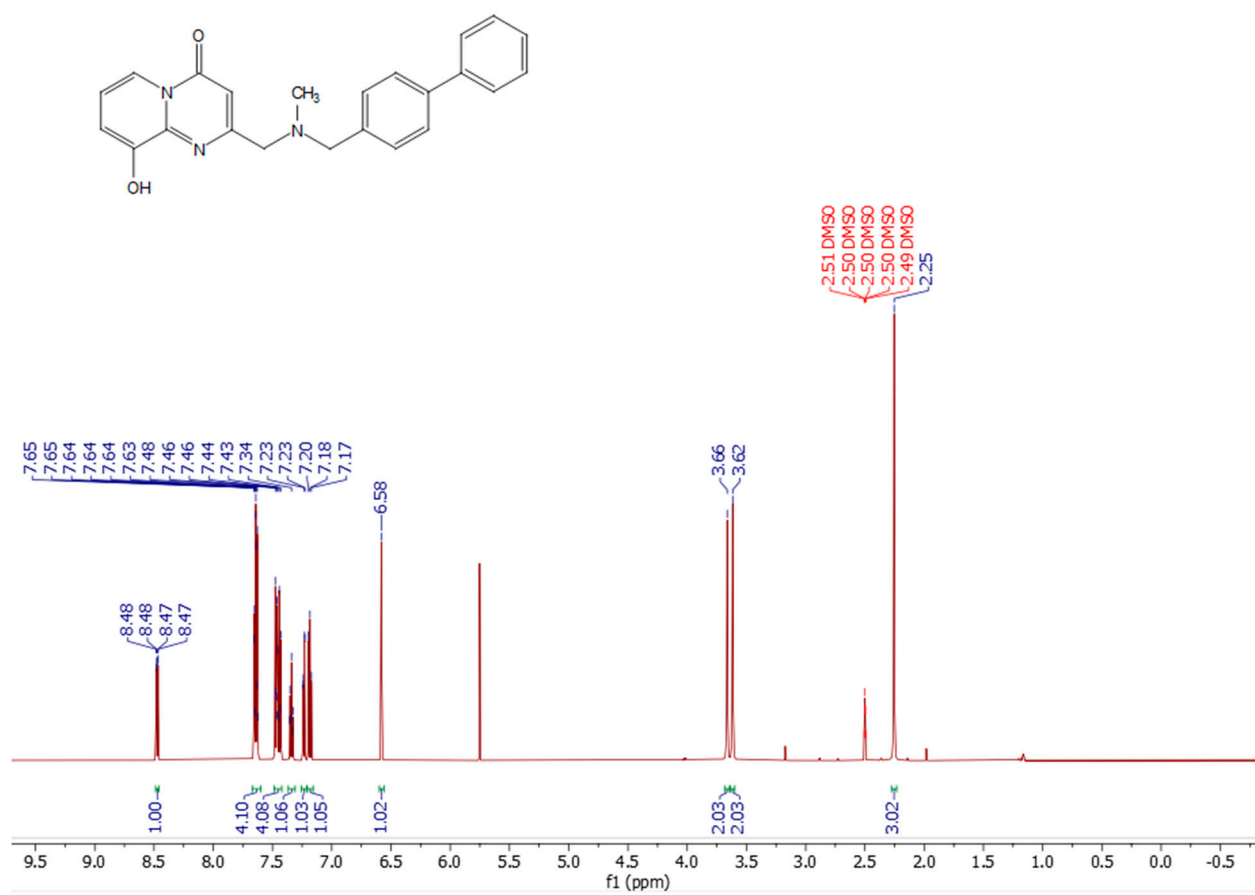
¹H NMR of **27**



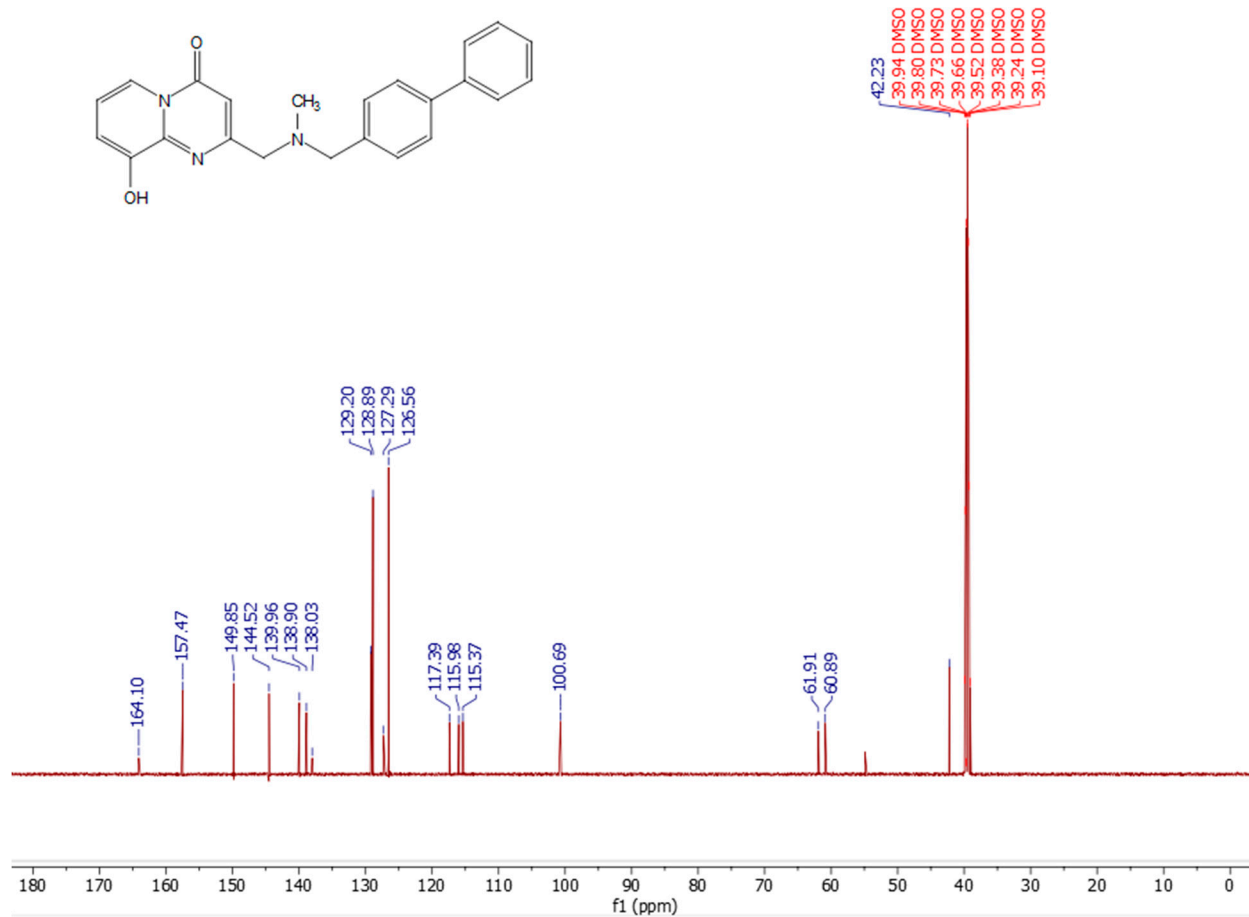
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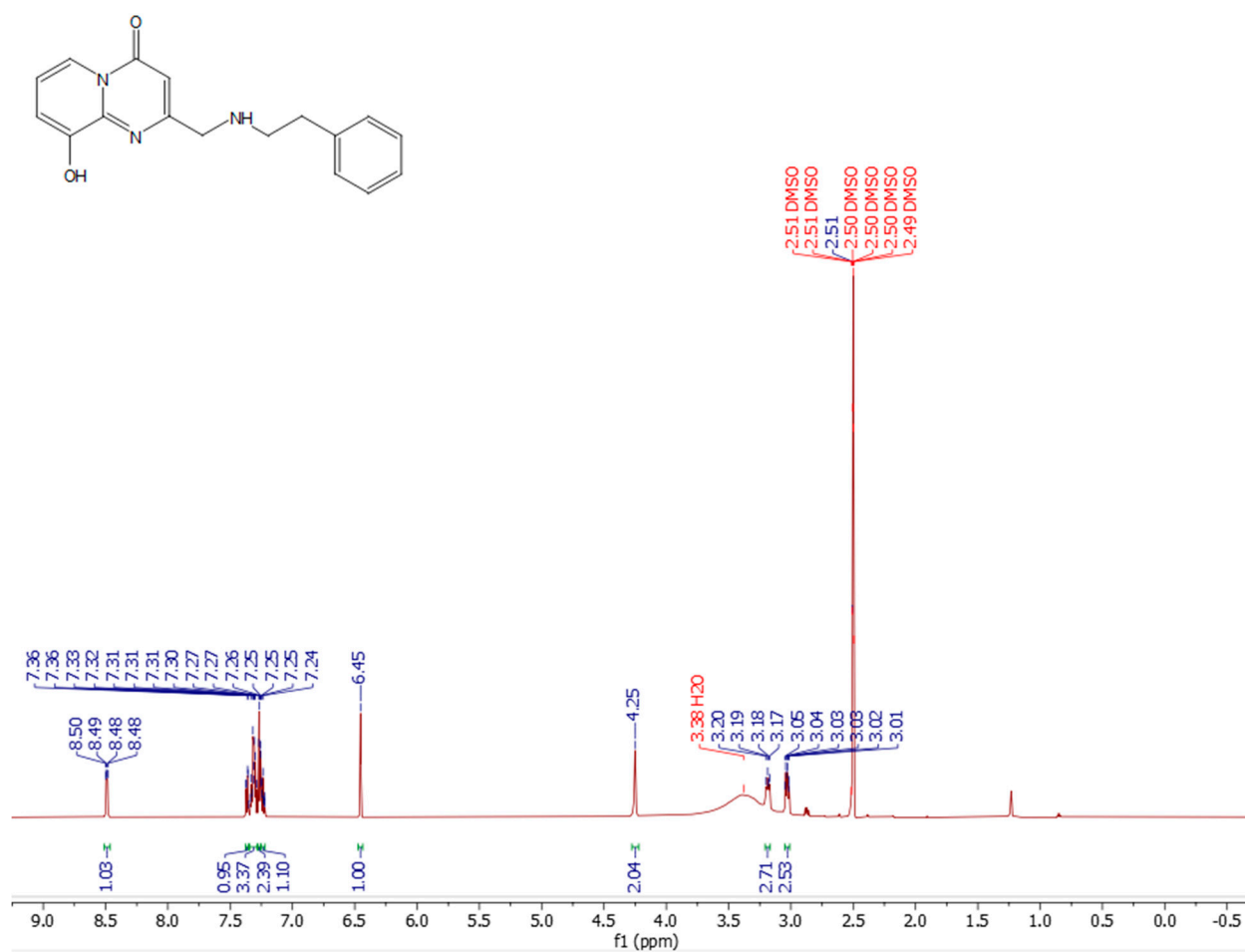
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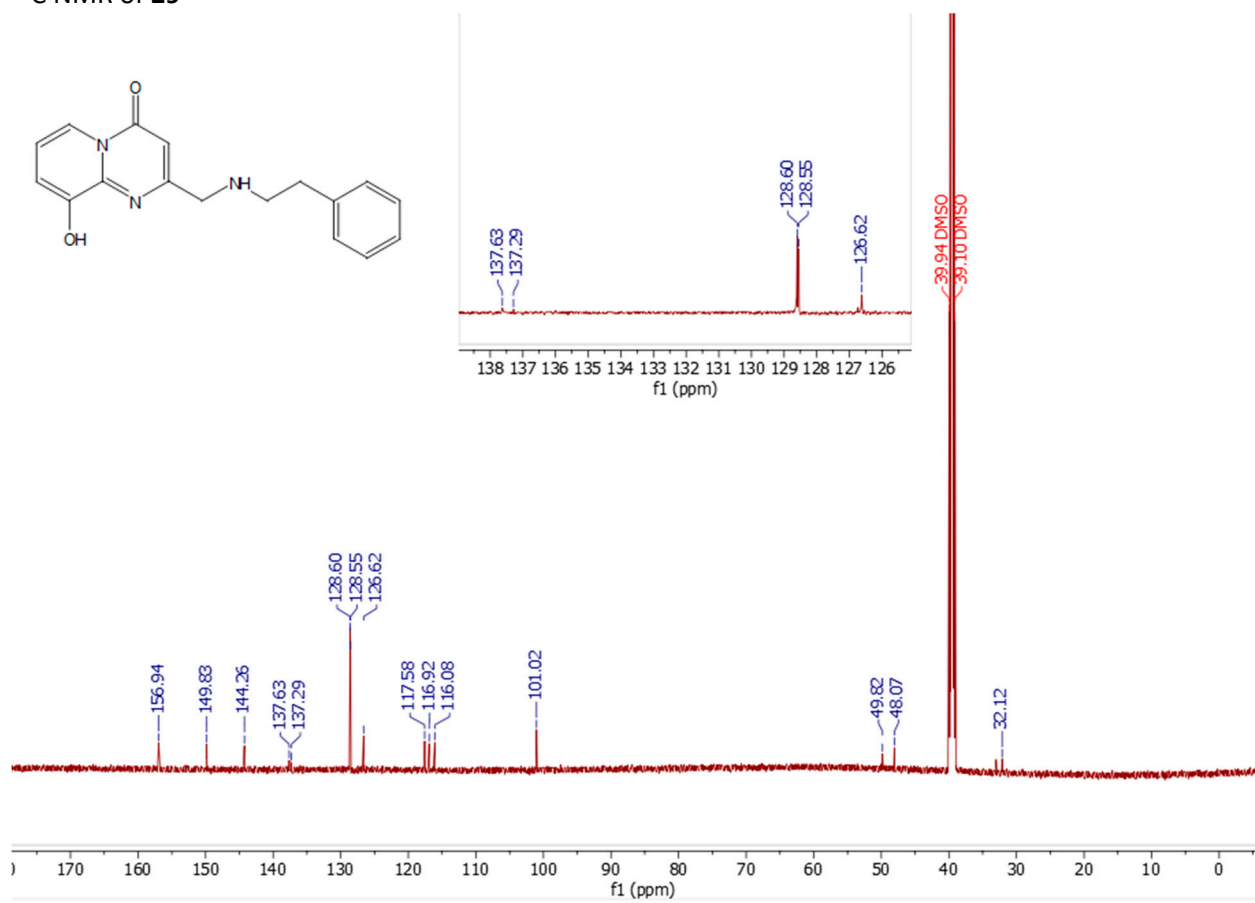
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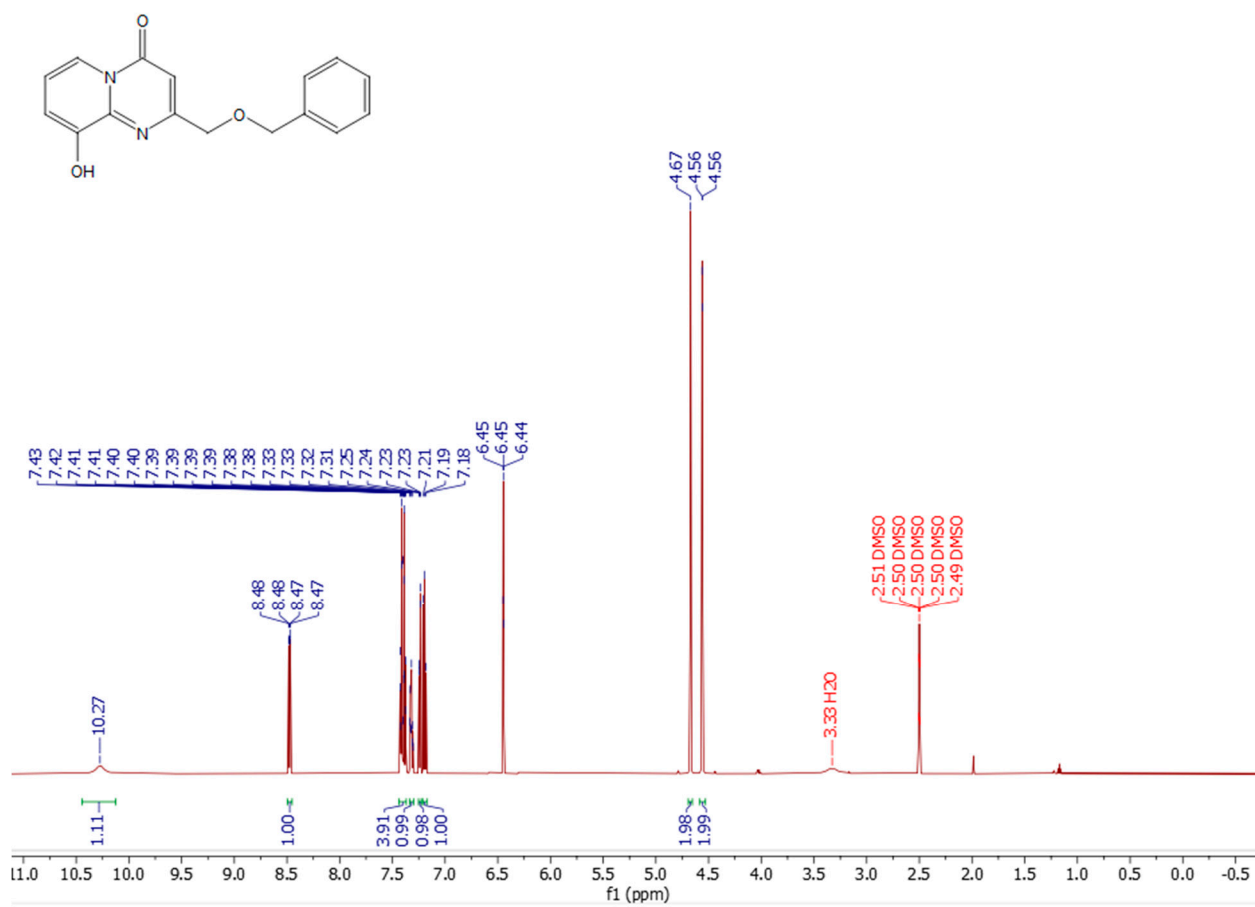
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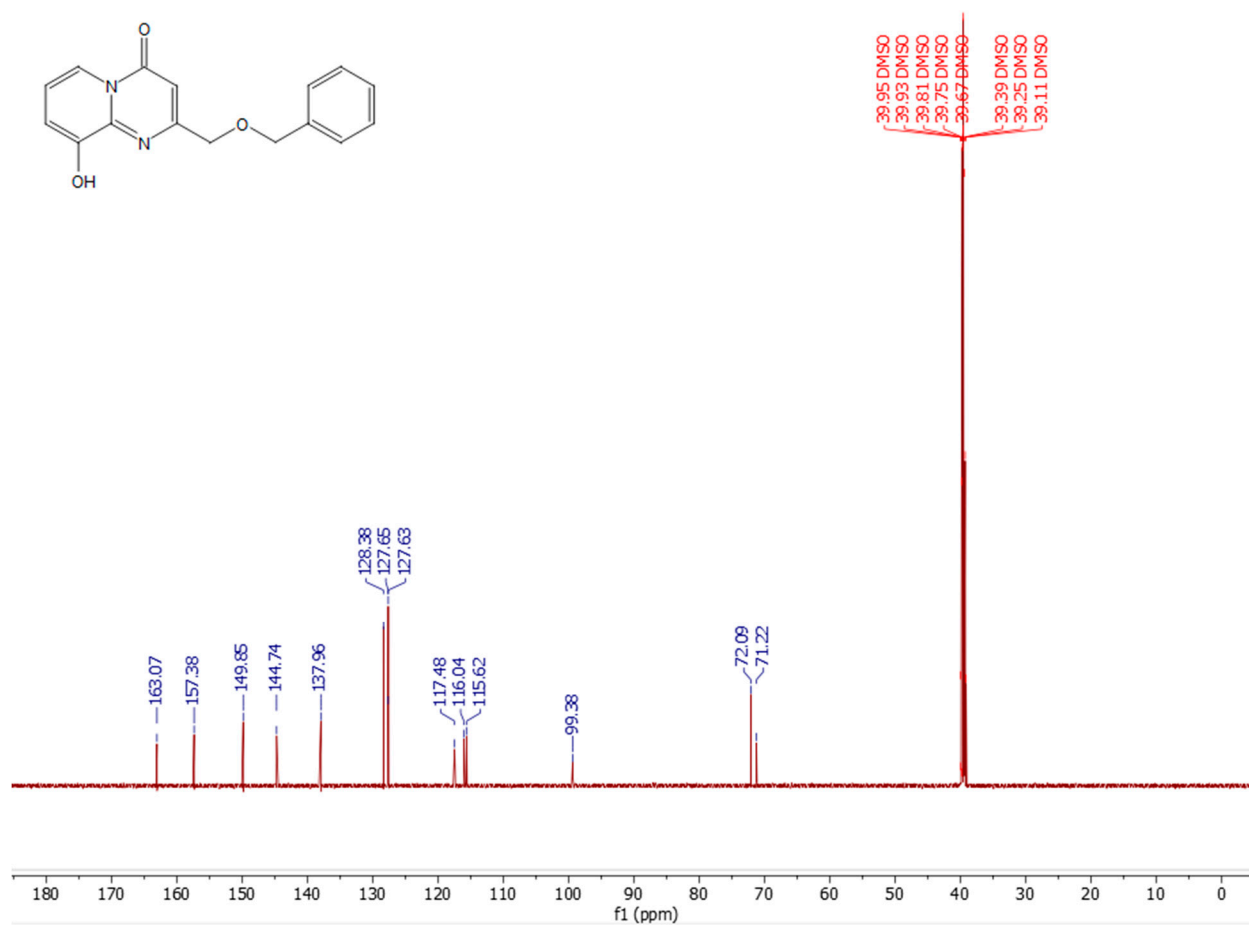
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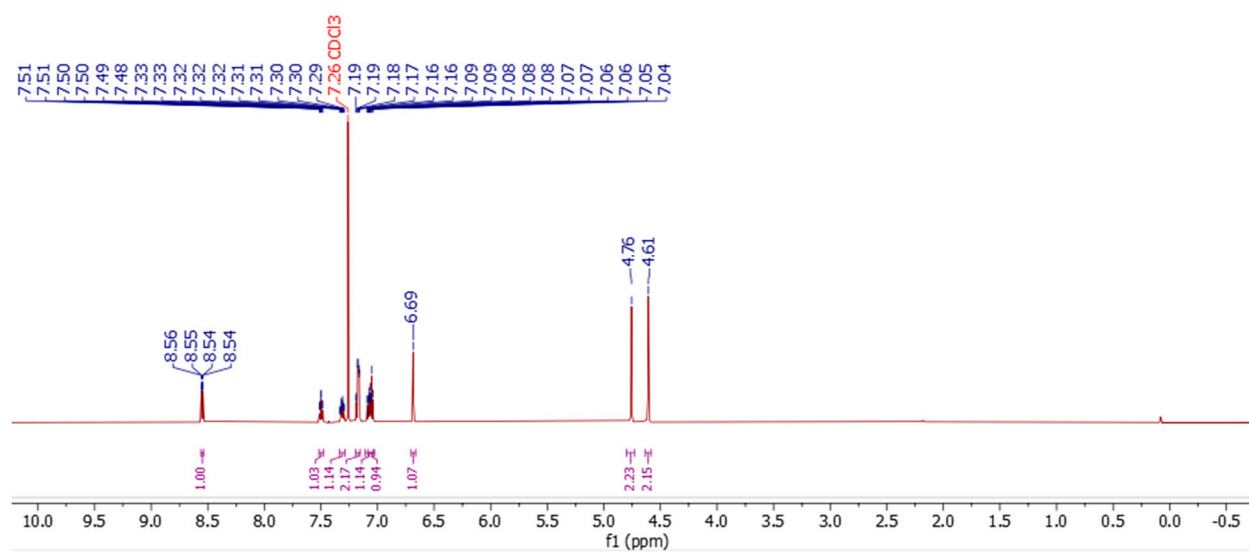
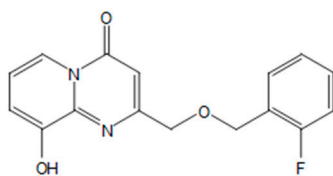
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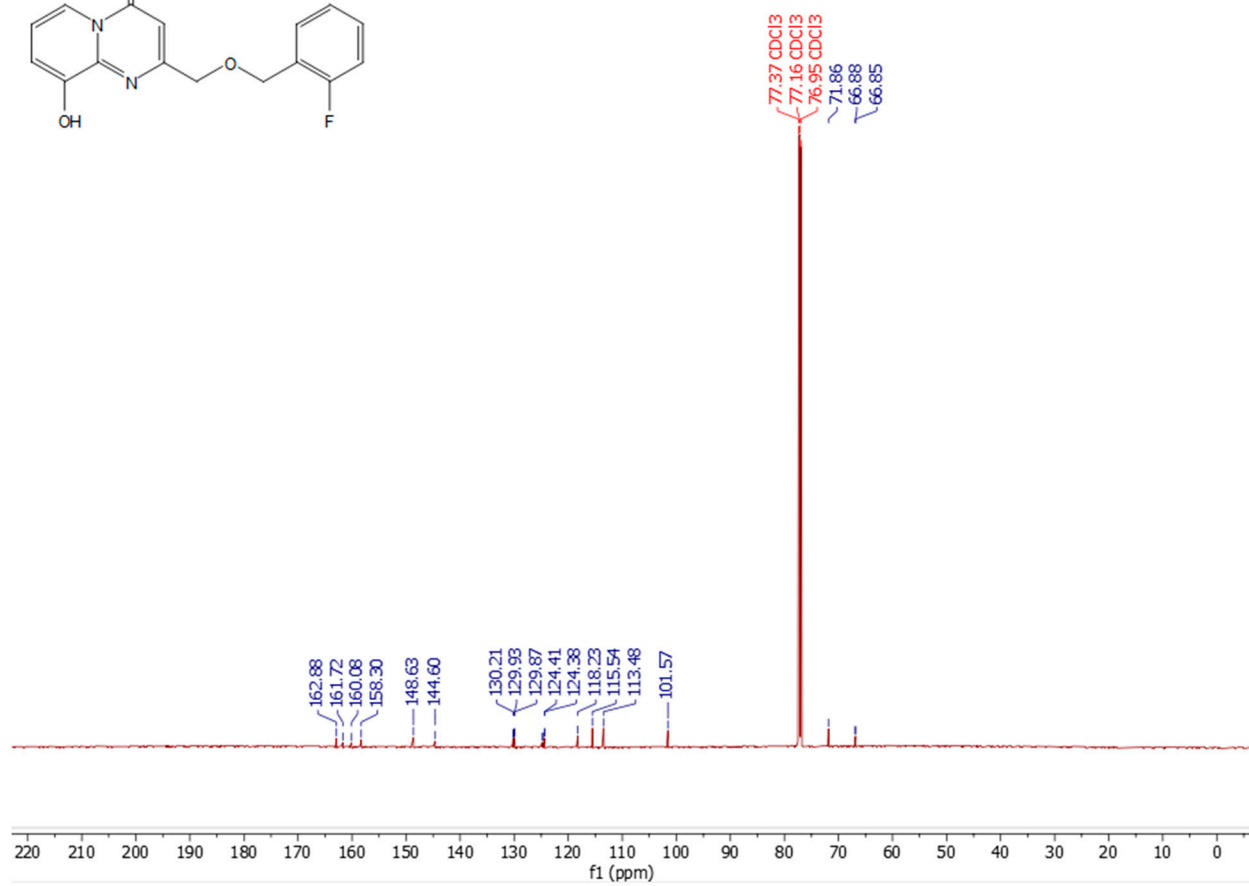
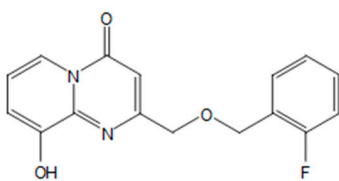
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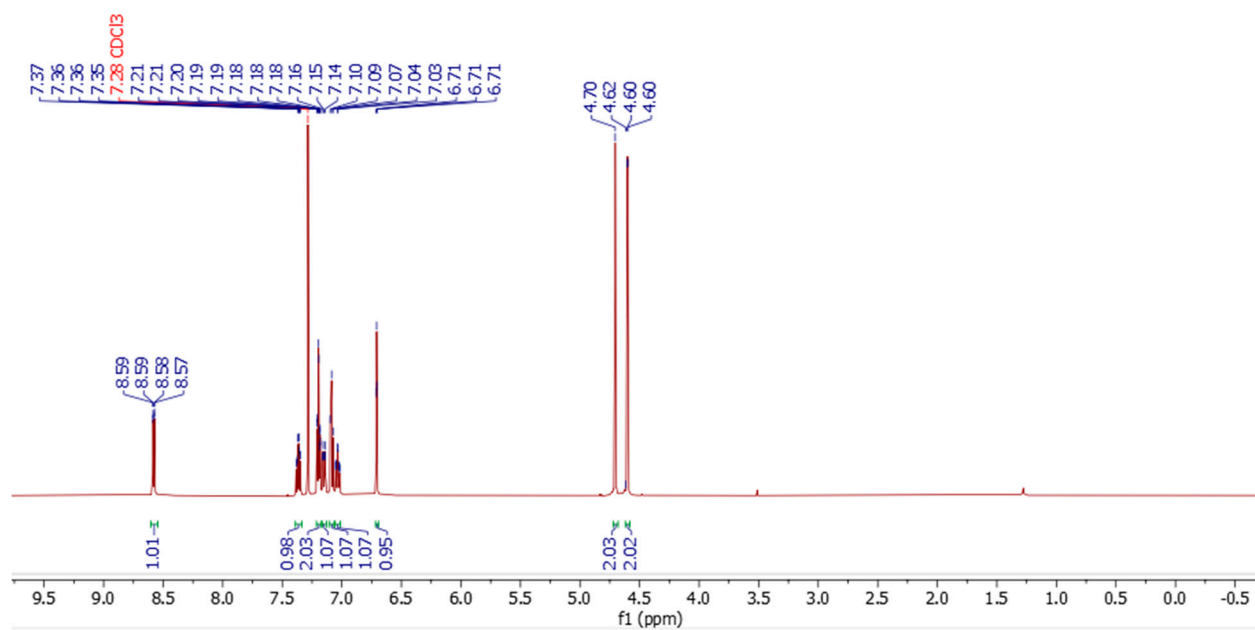
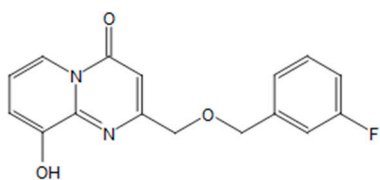
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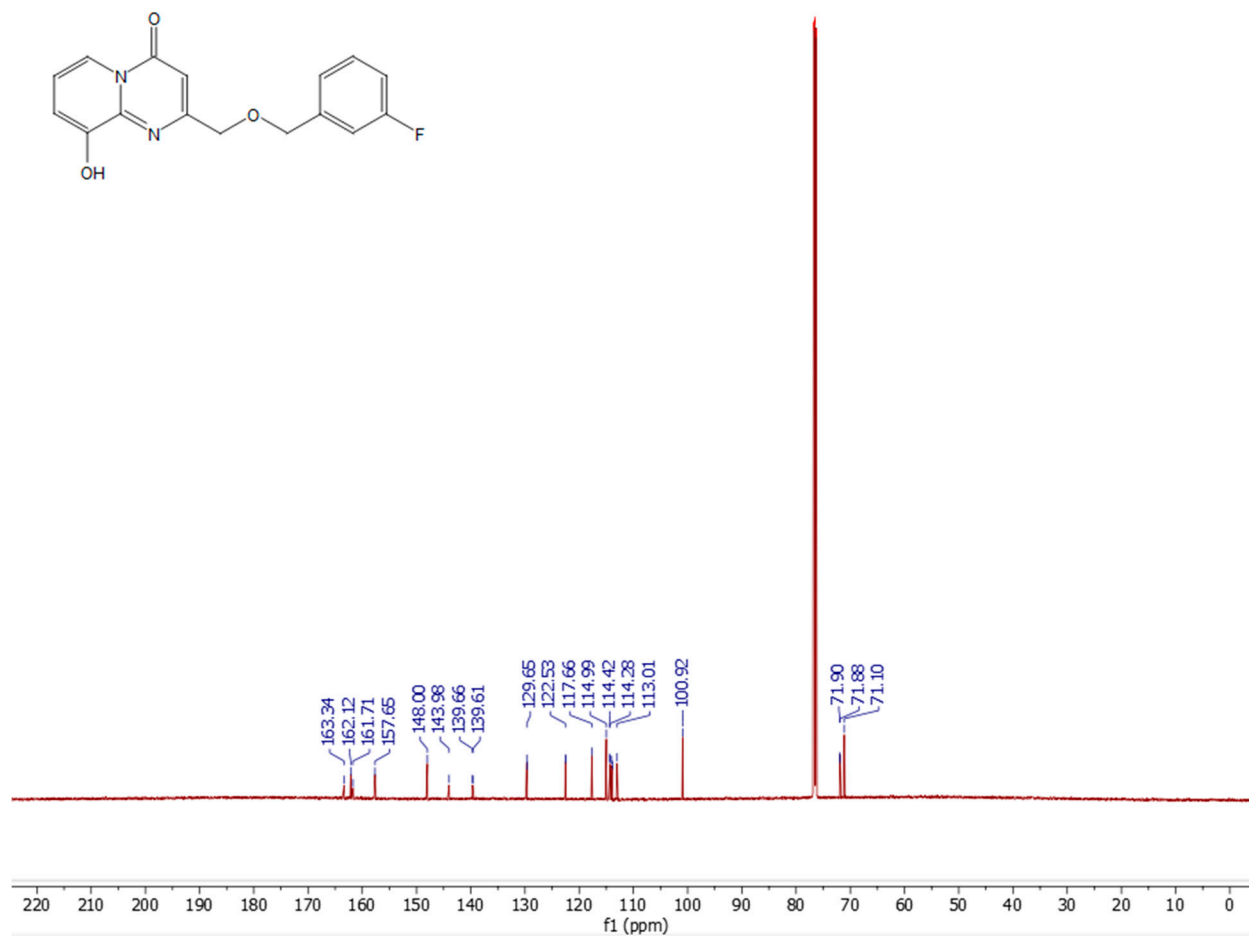
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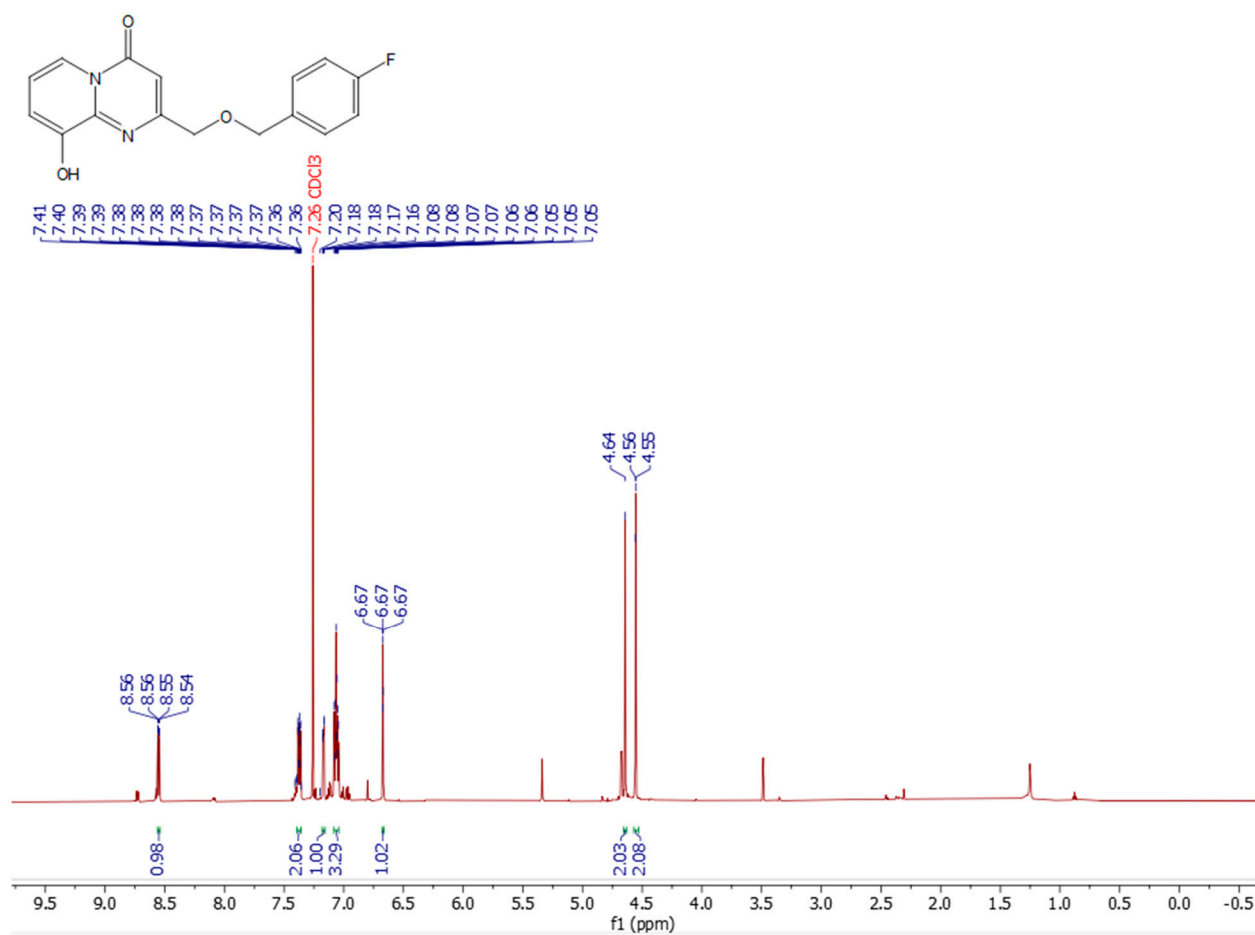
¹H NMR of **32**



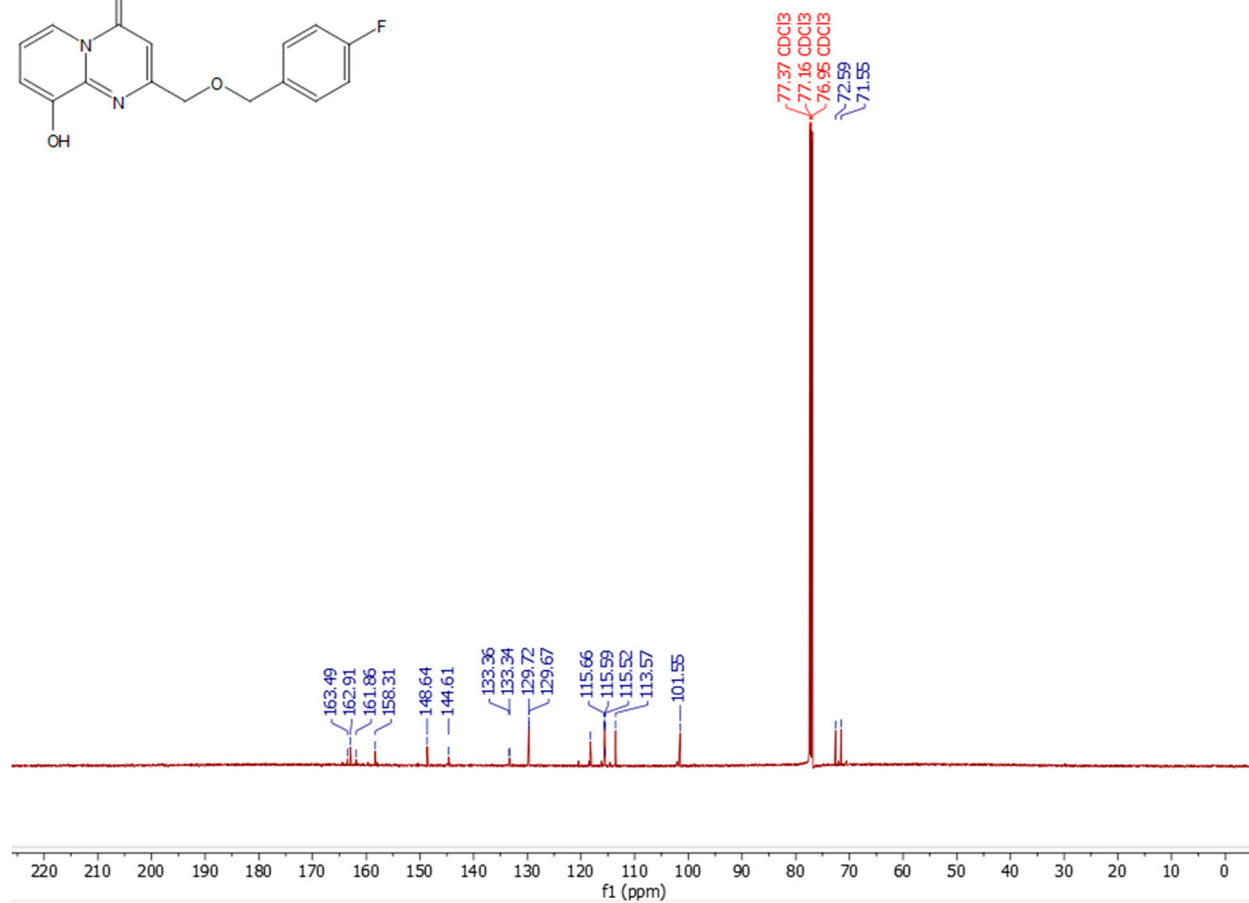
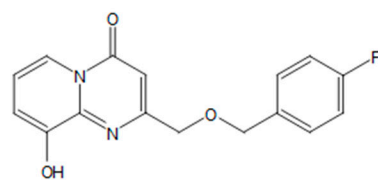
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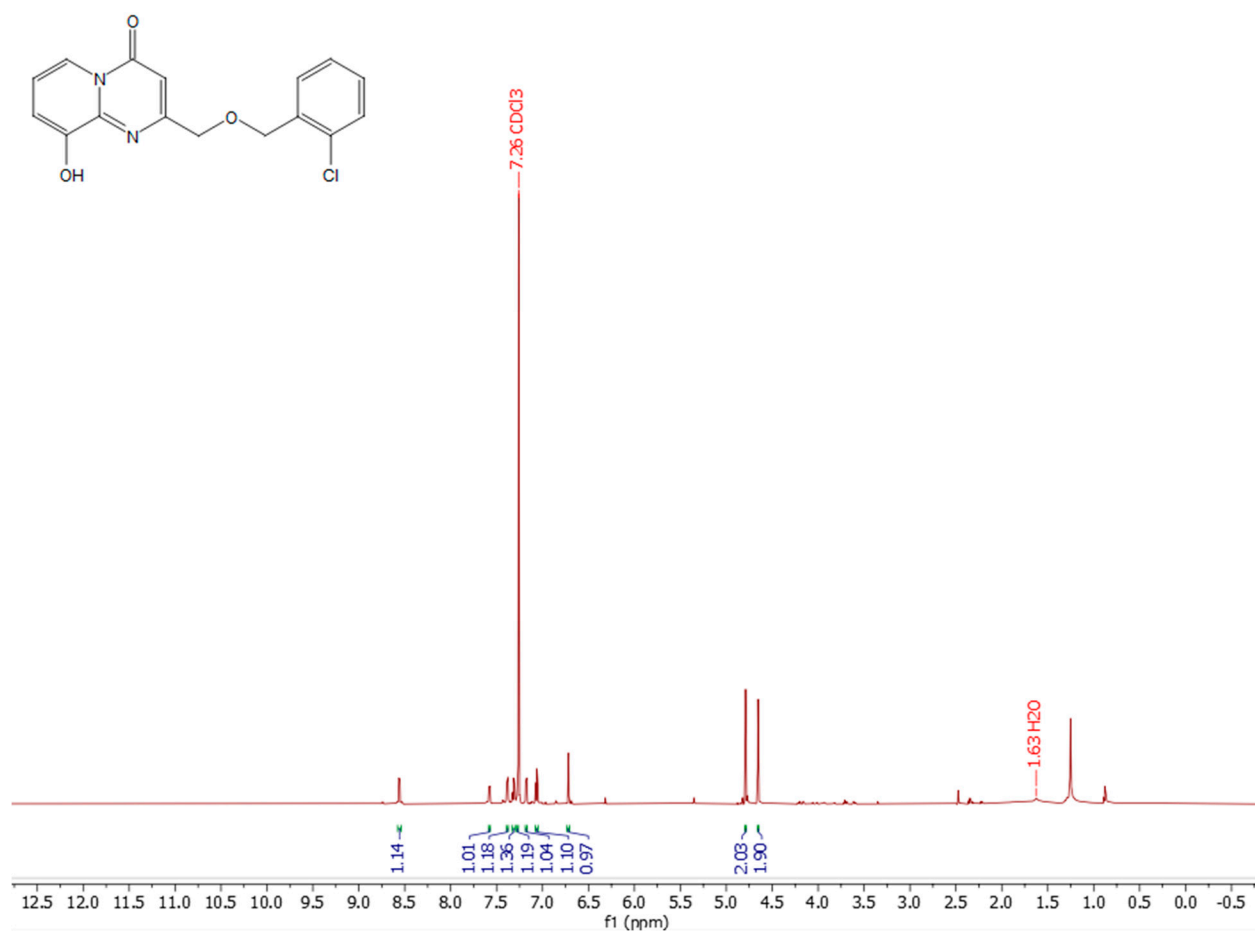
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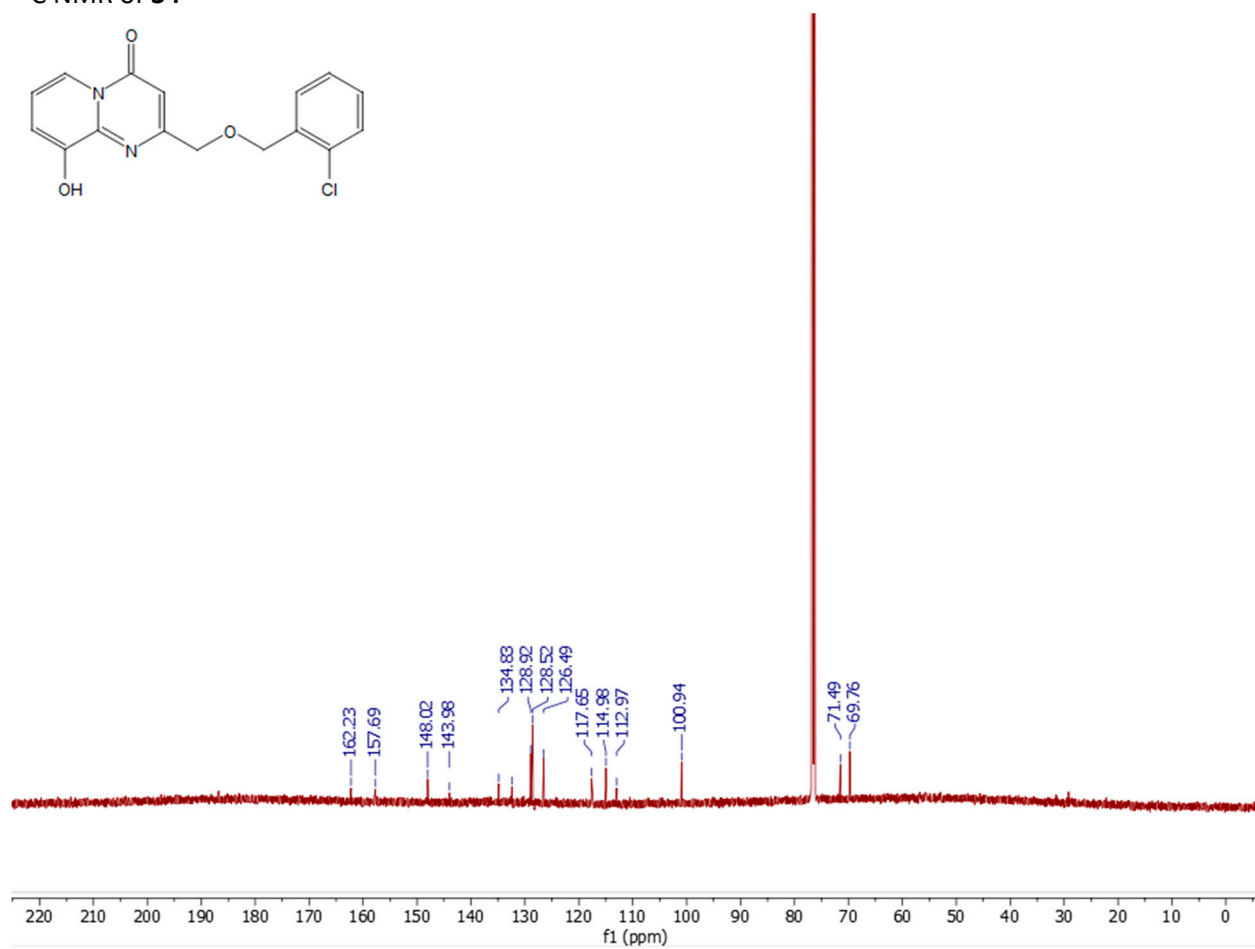
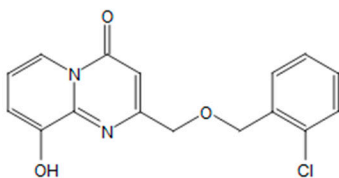
¹³C NMR of **33**



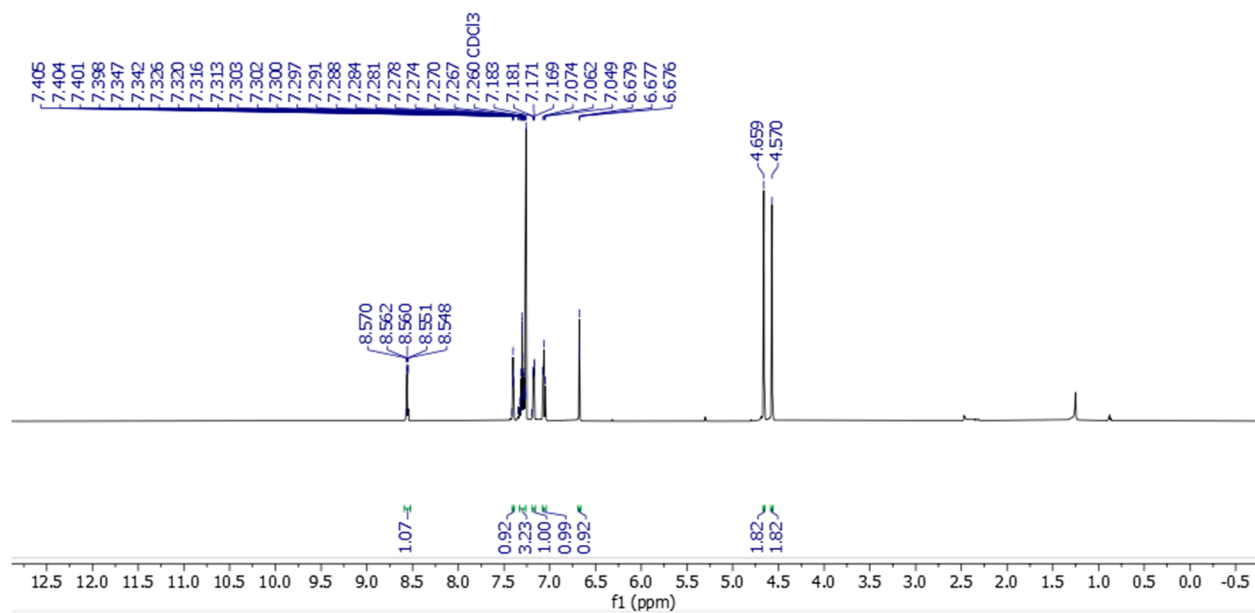
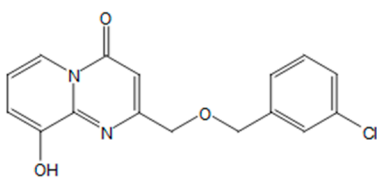
¹H NMR of **34**



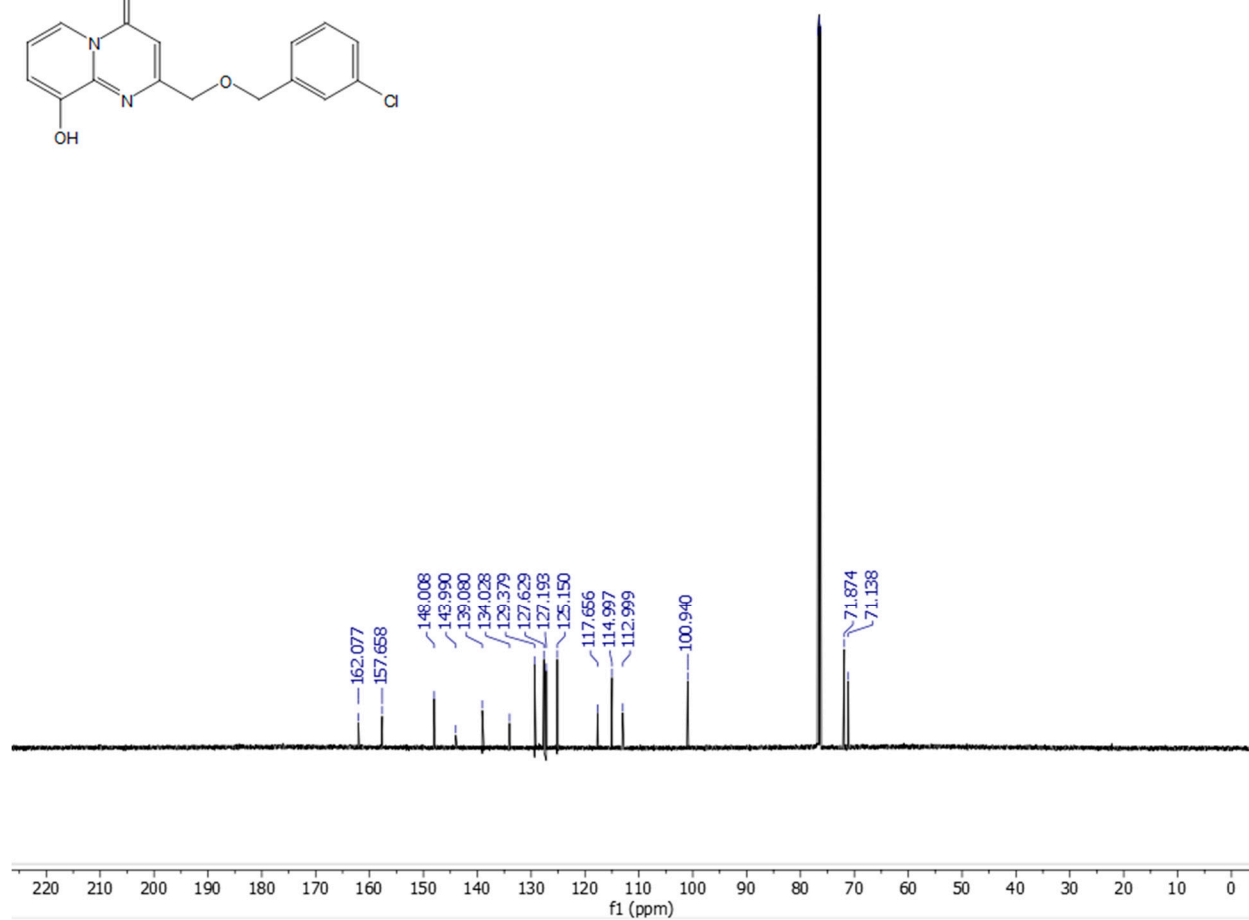
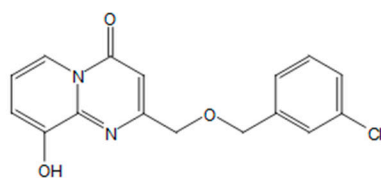
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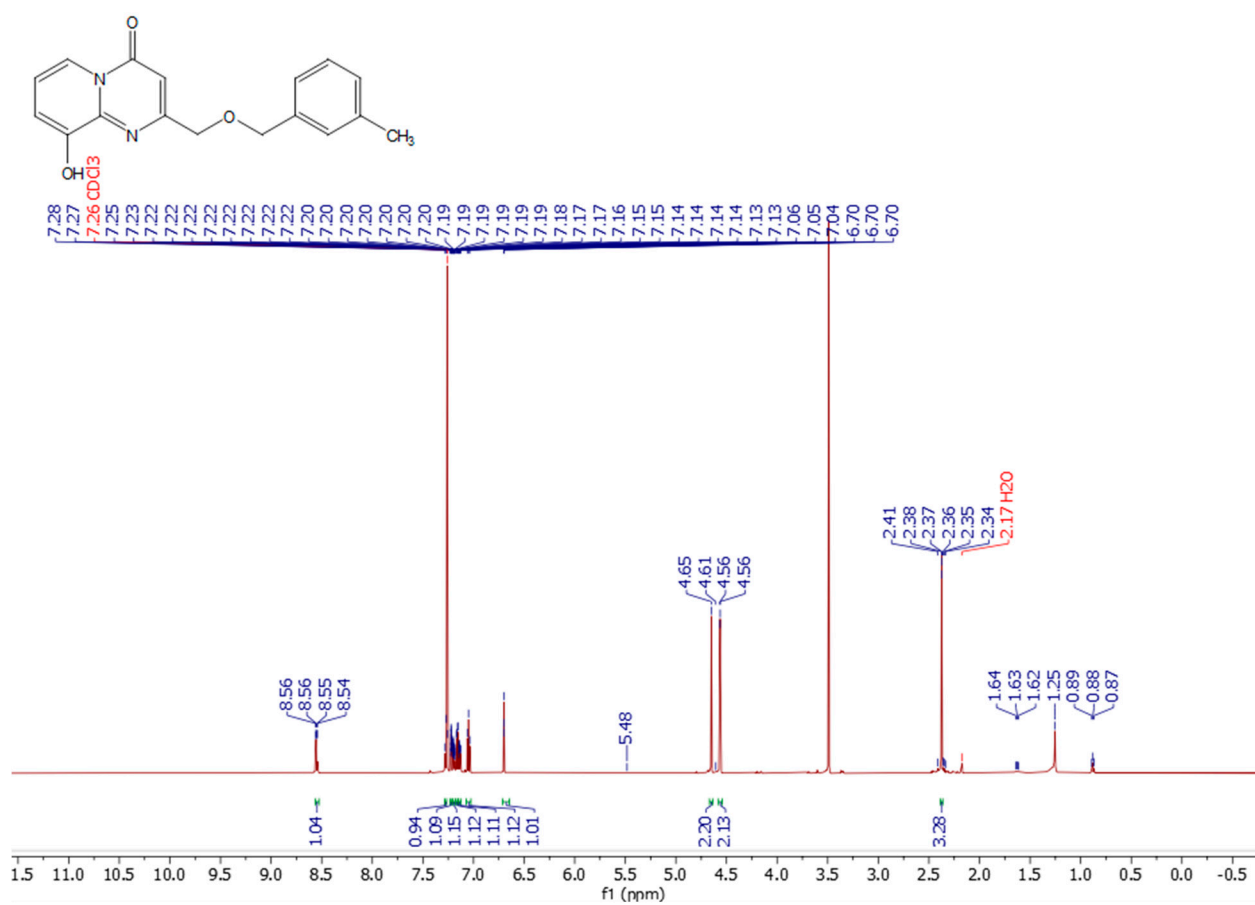
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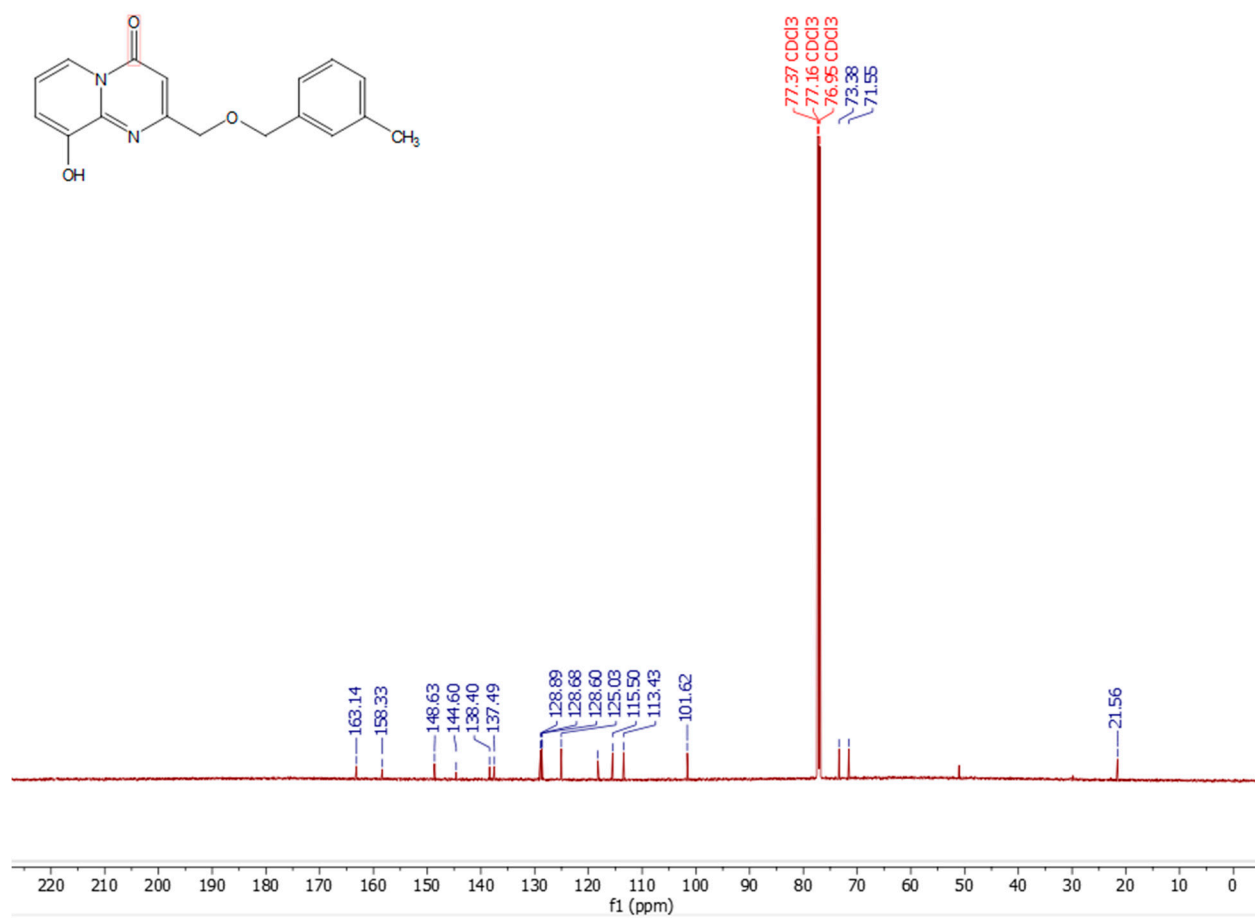
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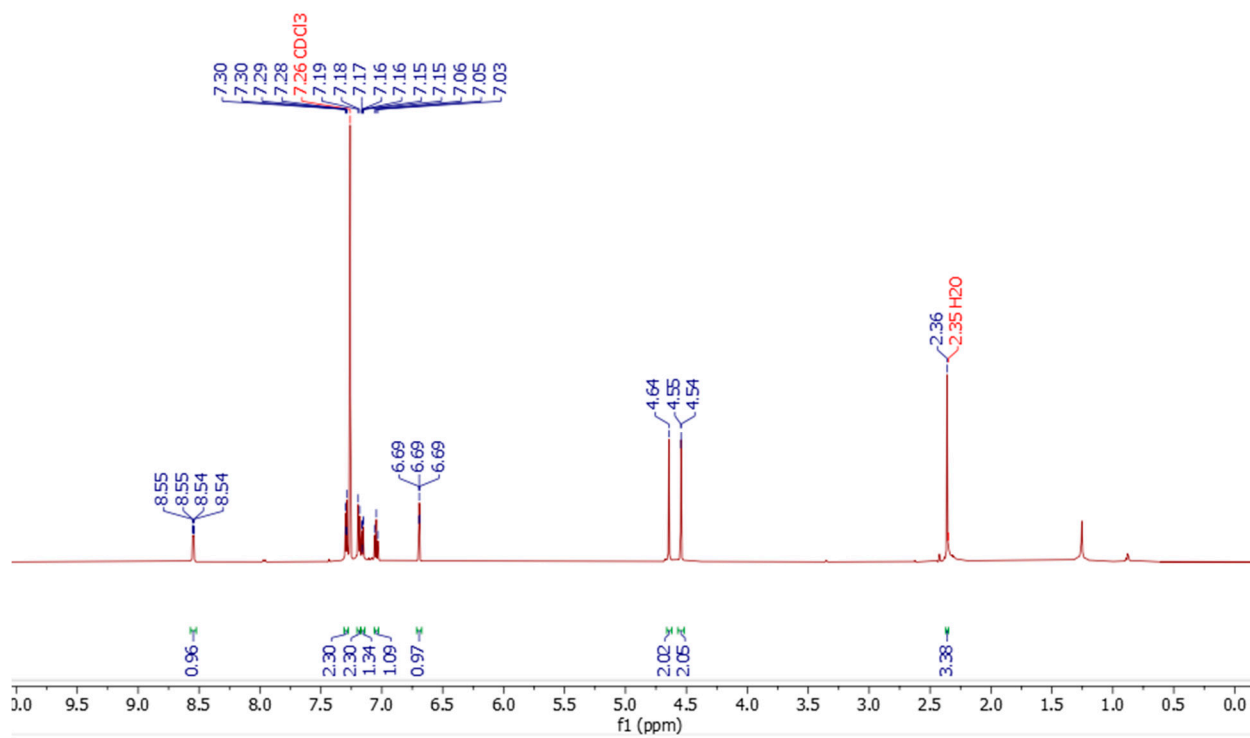
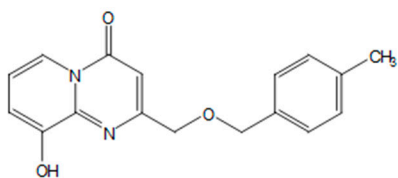
¹H NMR of **38**



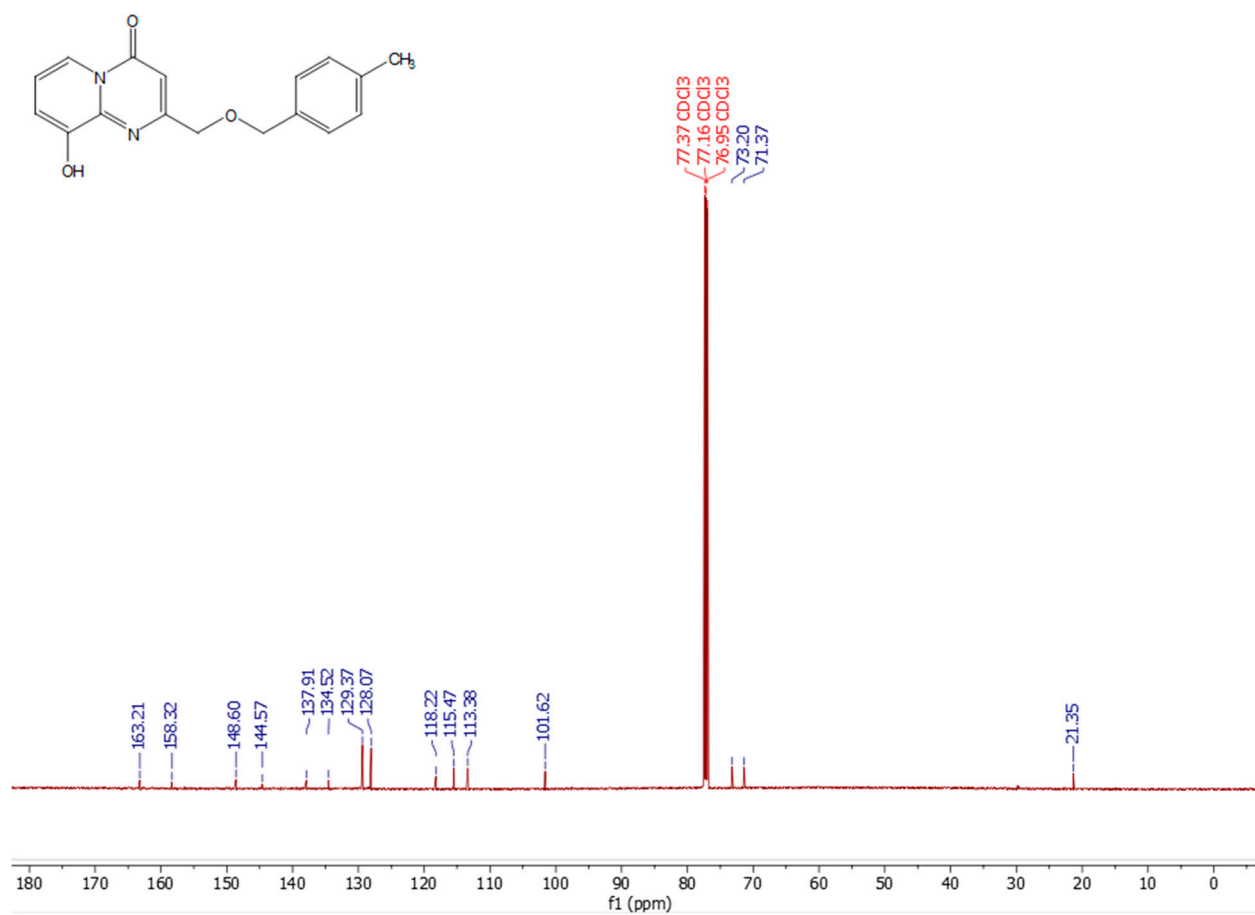
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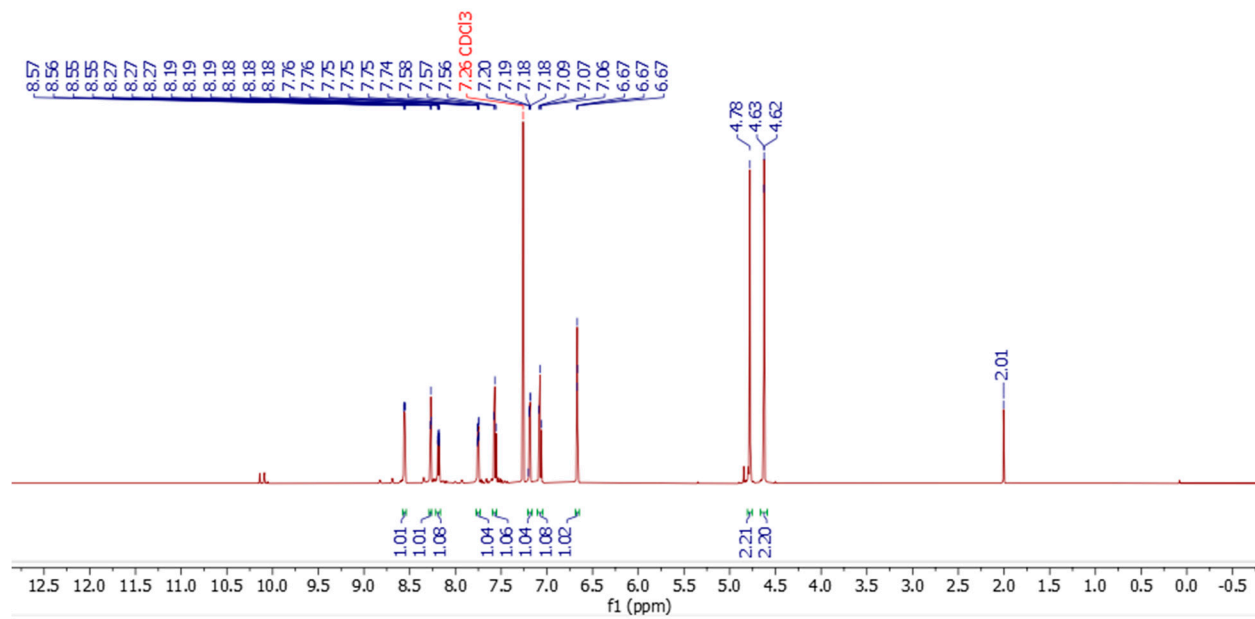
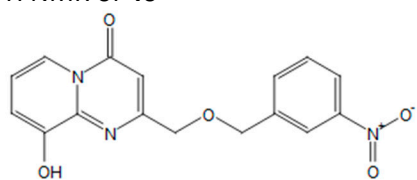
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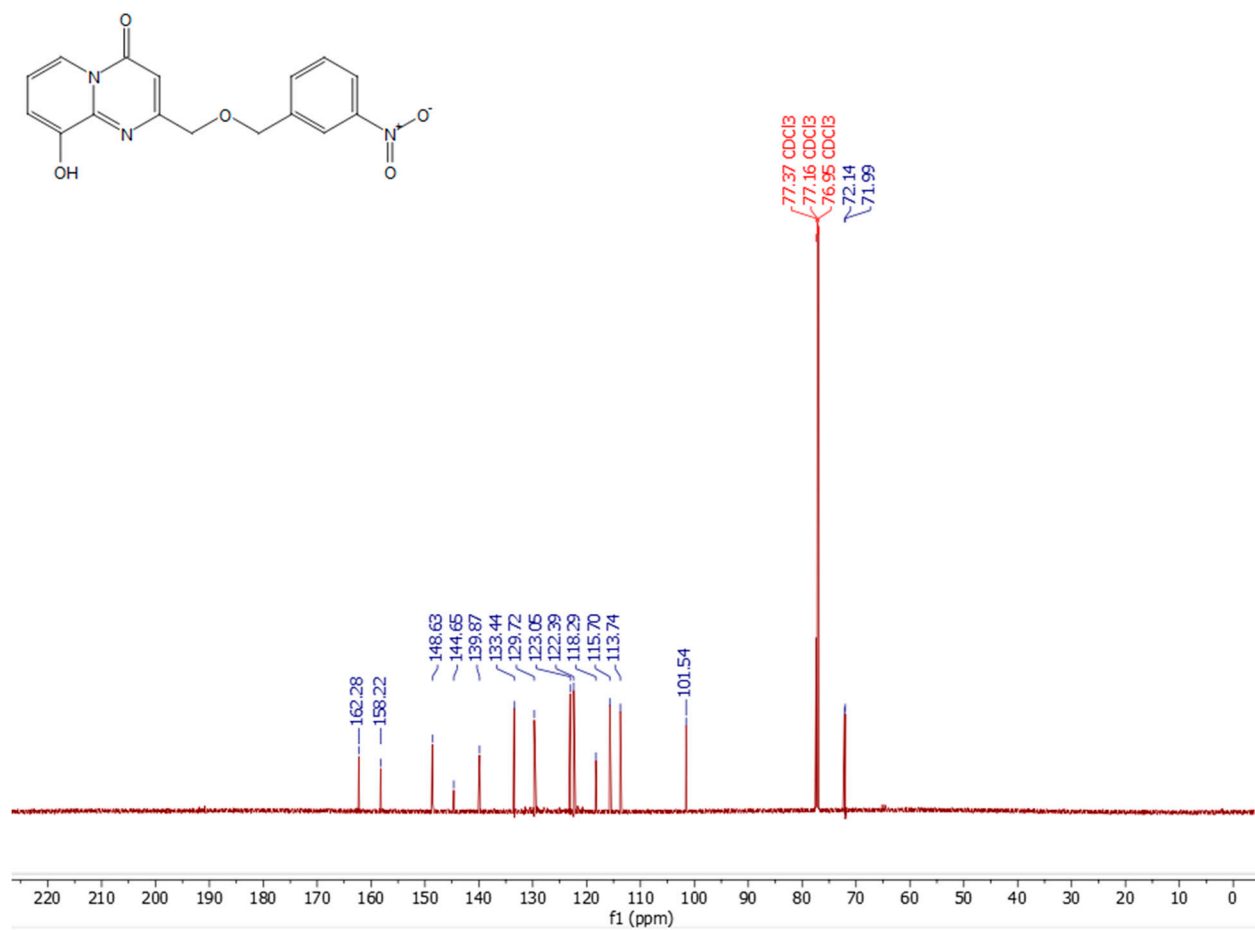
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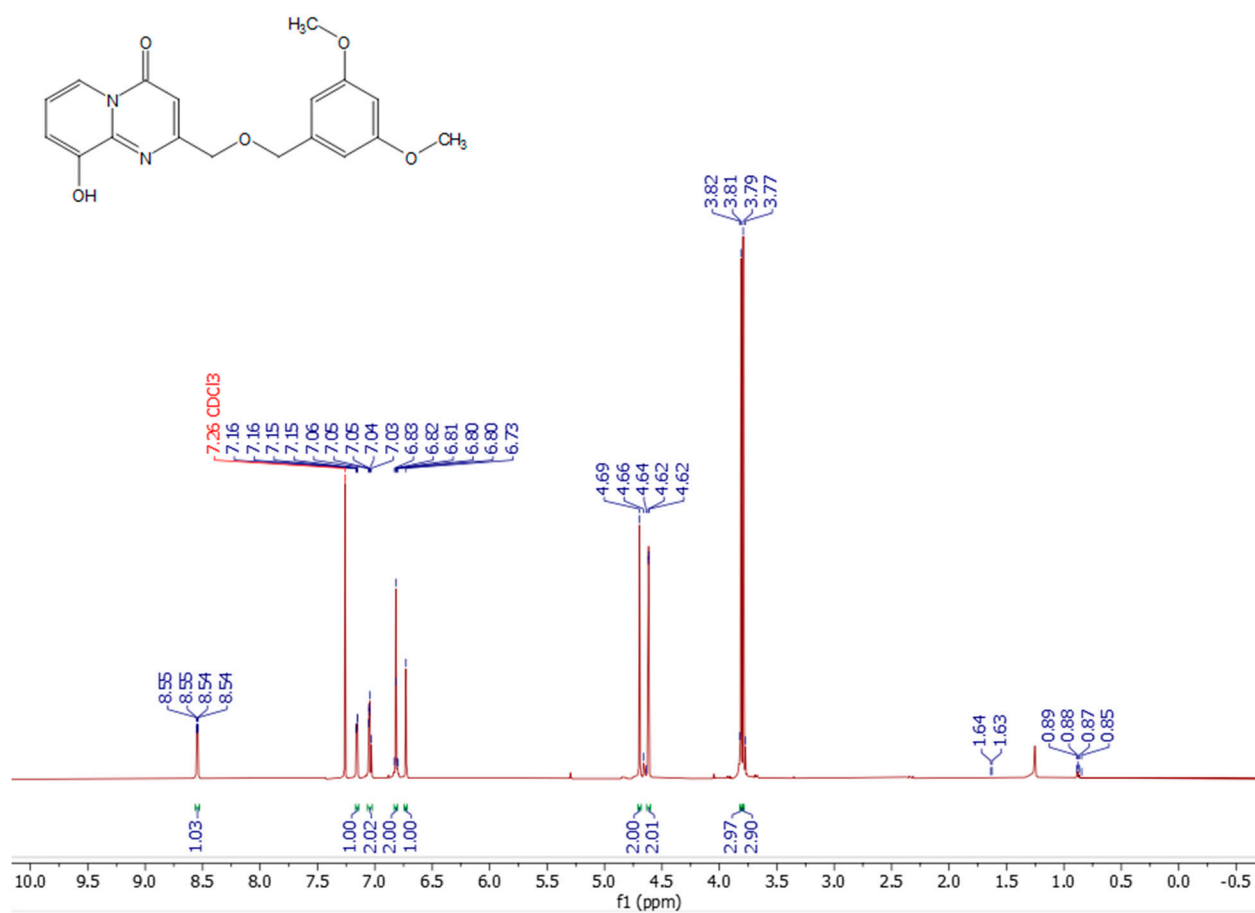
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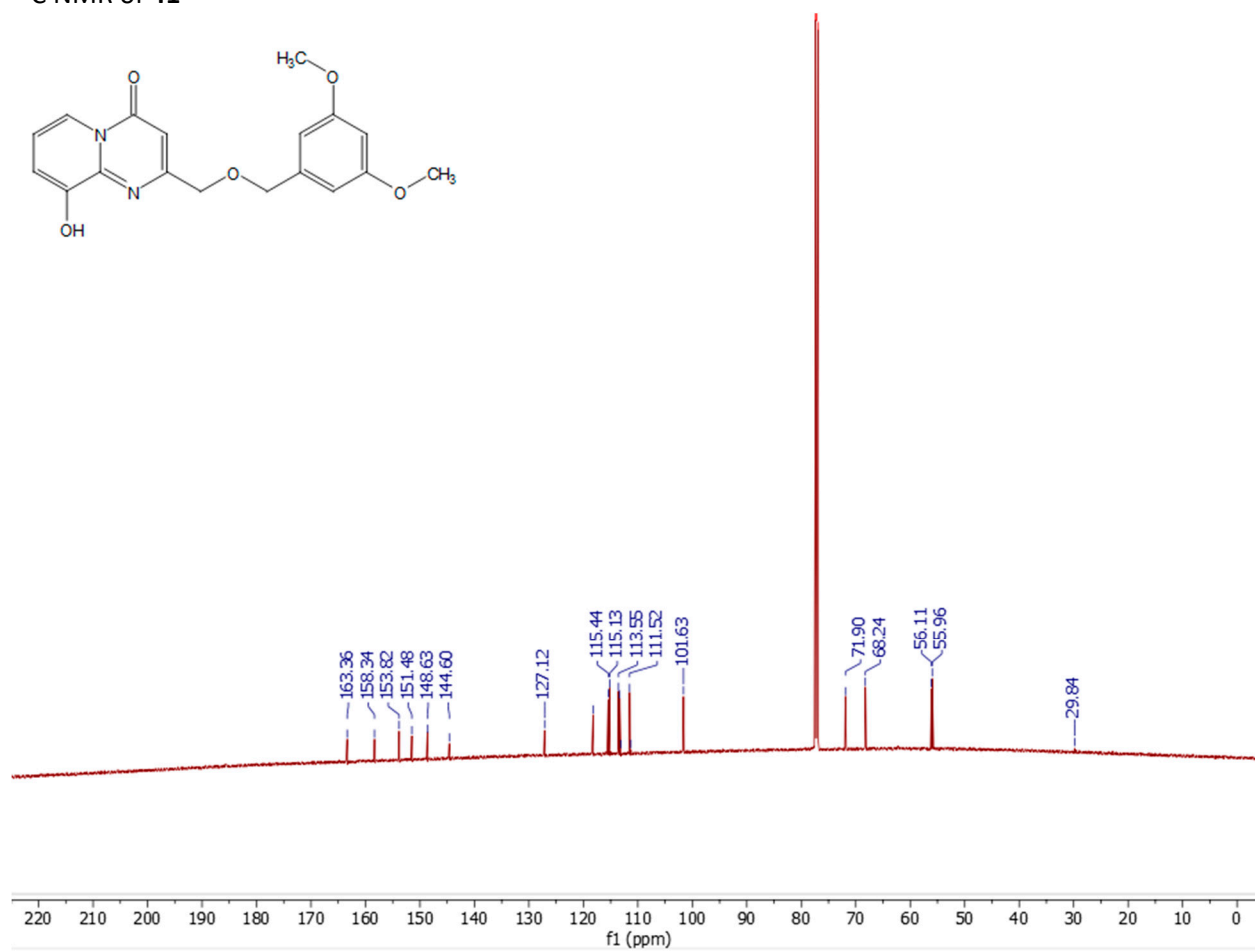
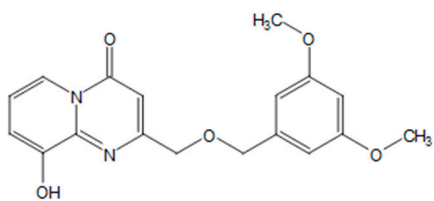
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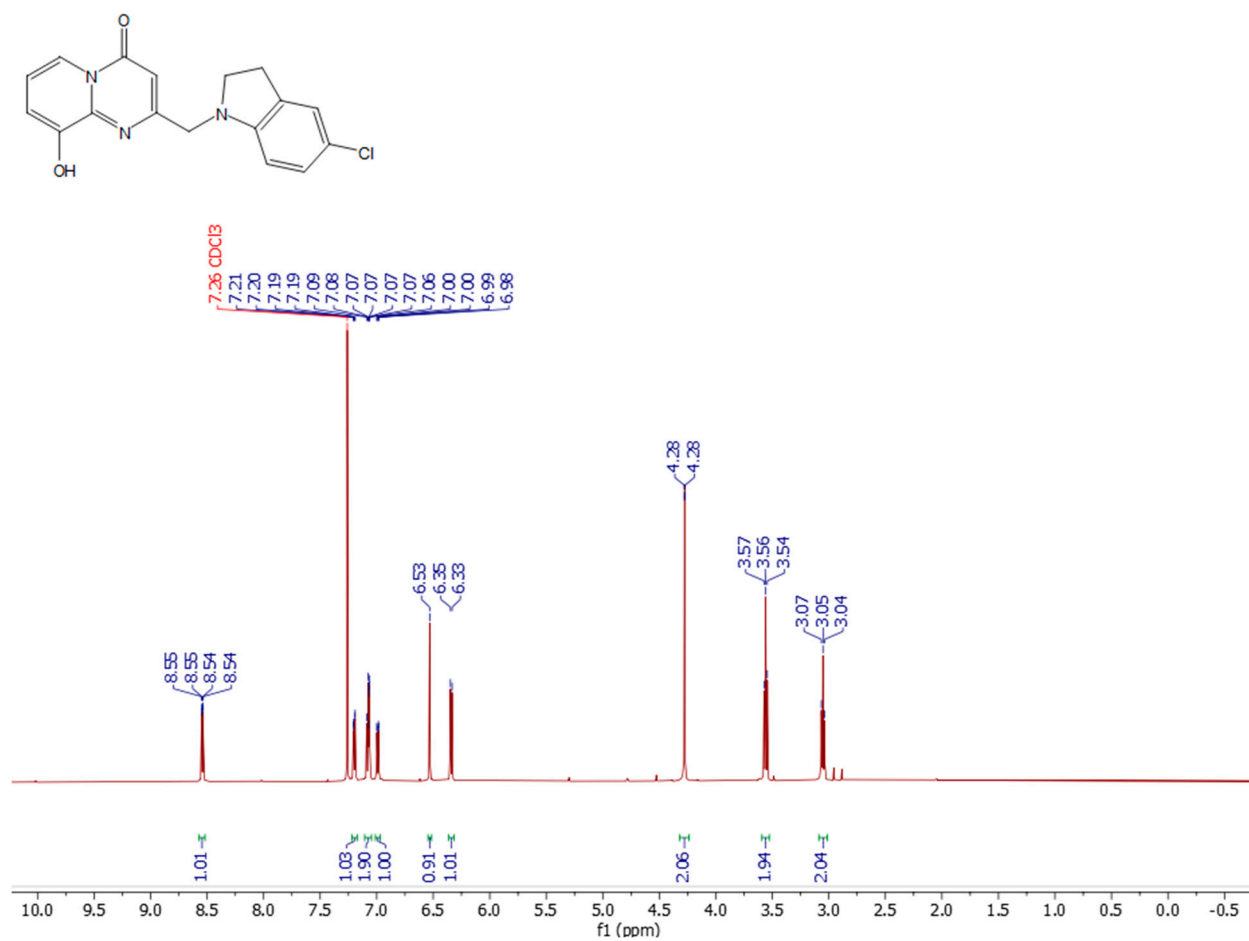
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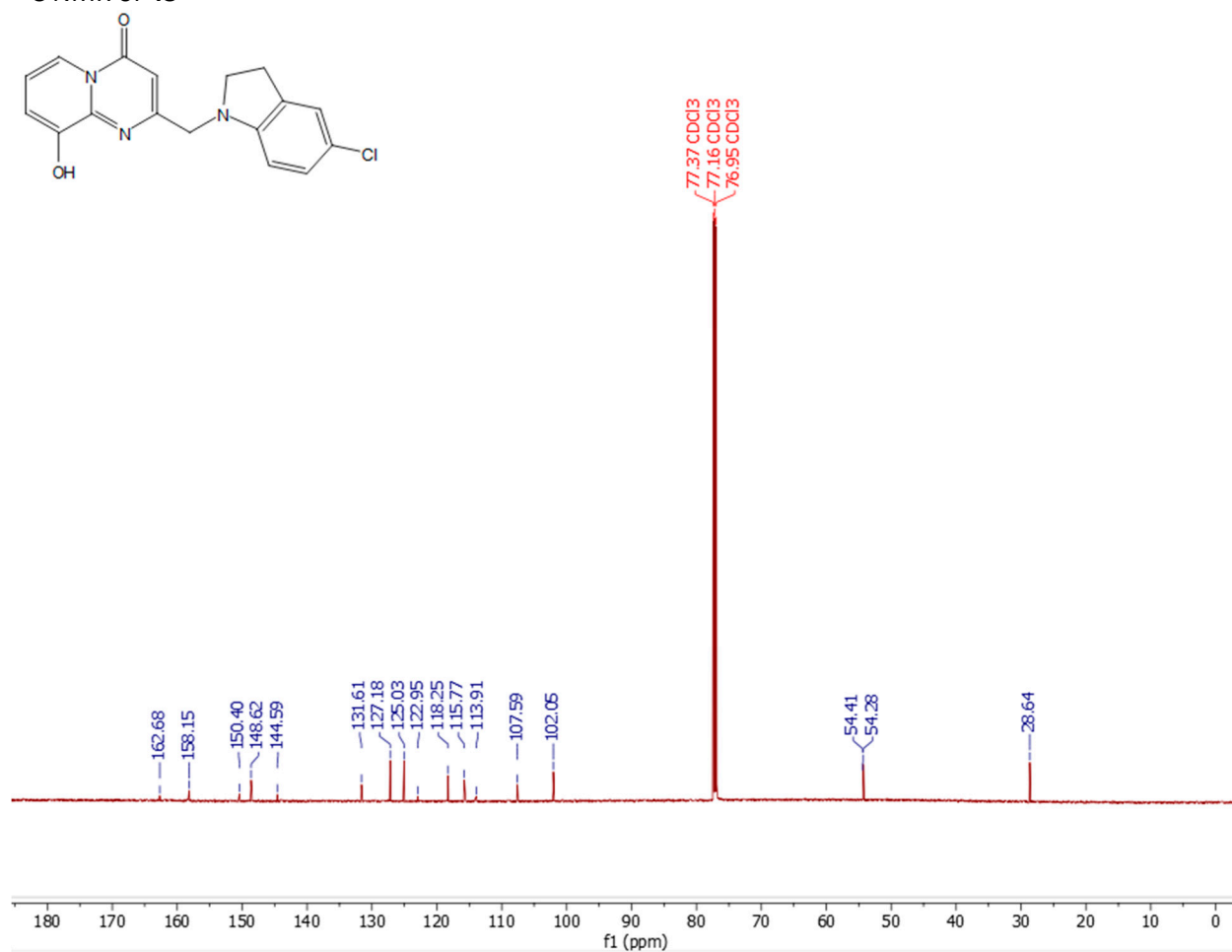
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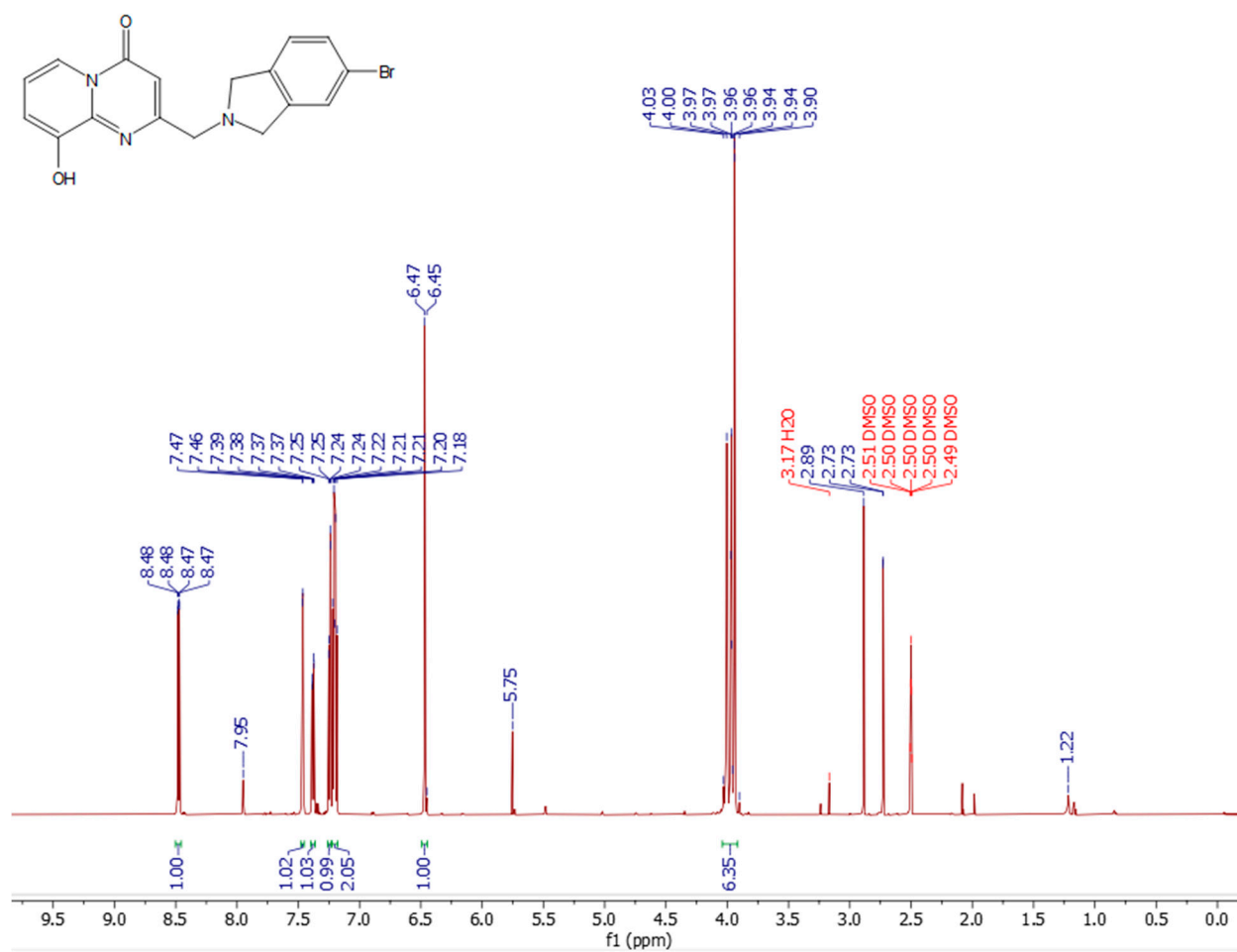
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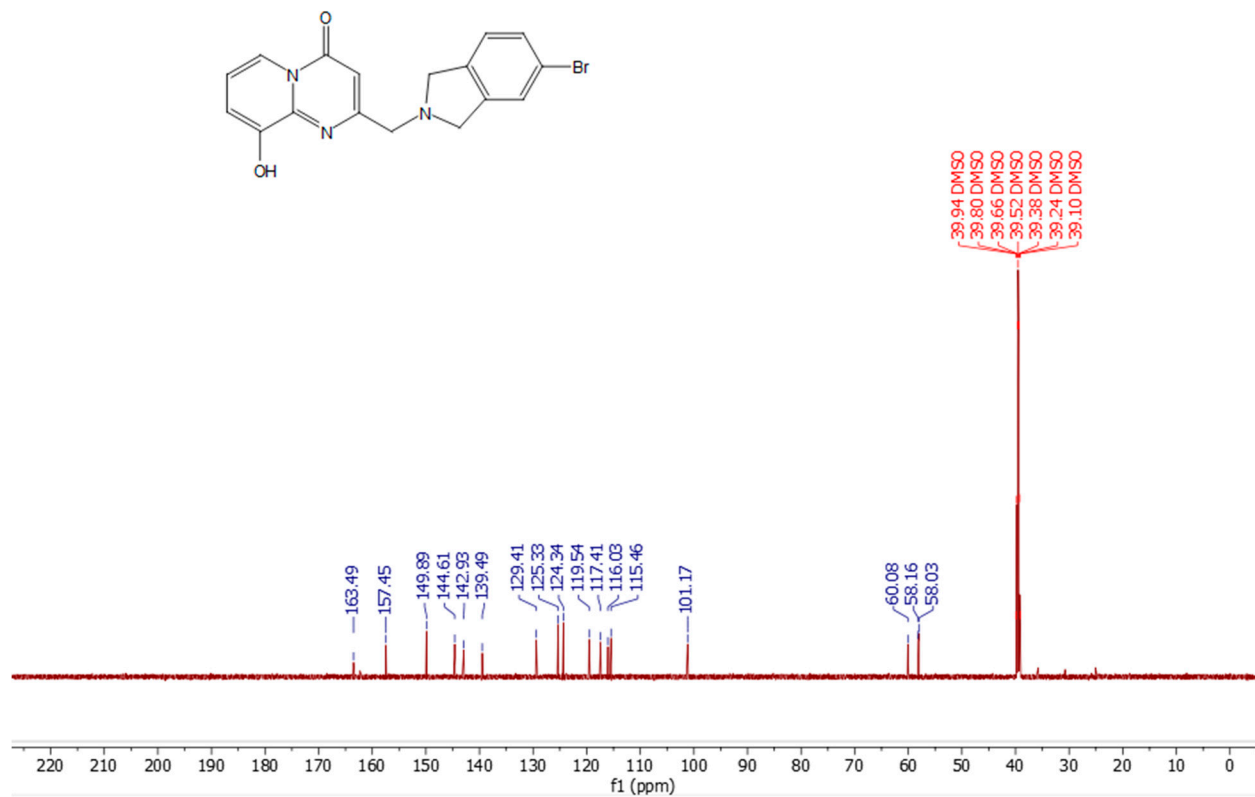
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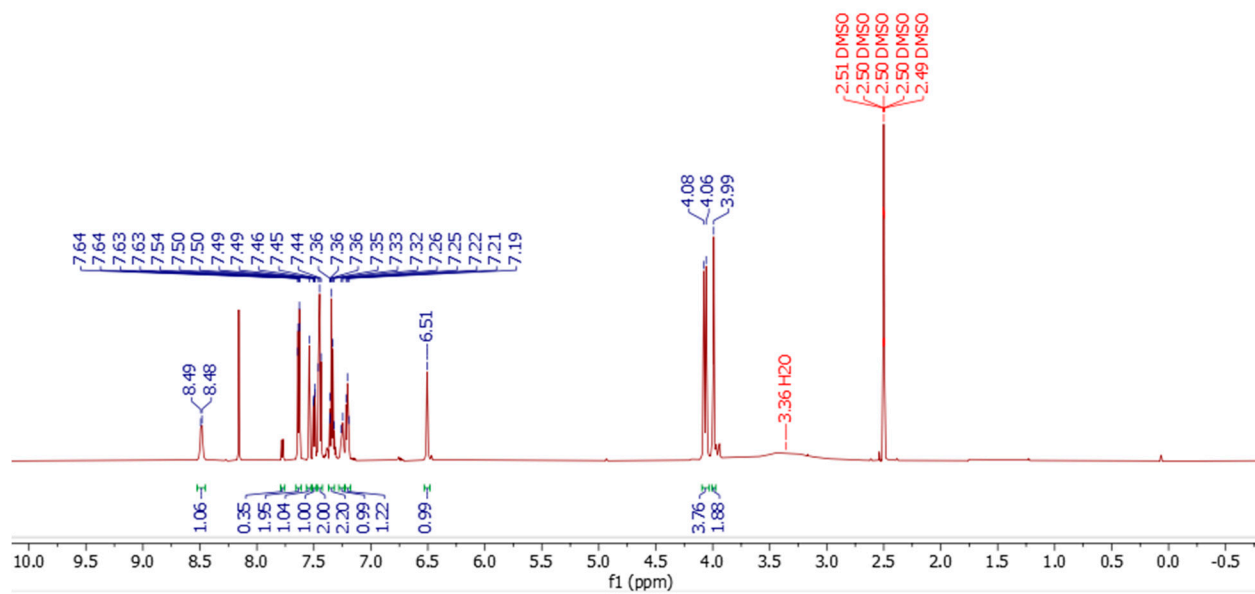
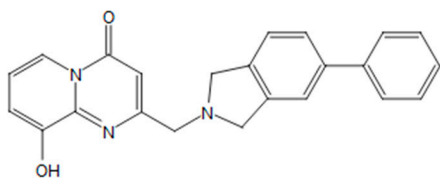
¹H NMR of **44**



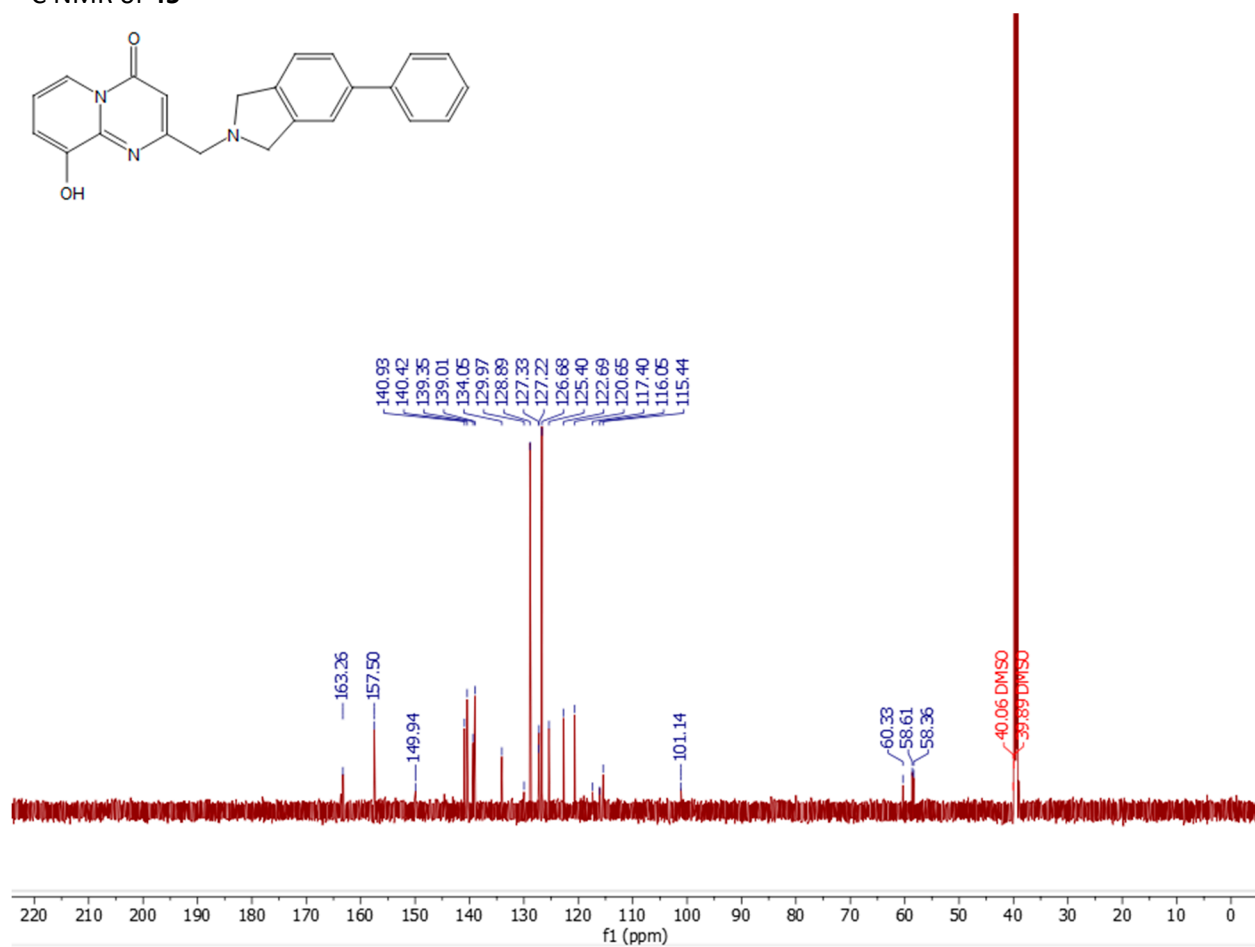
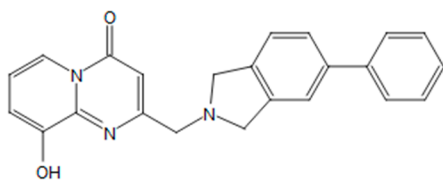
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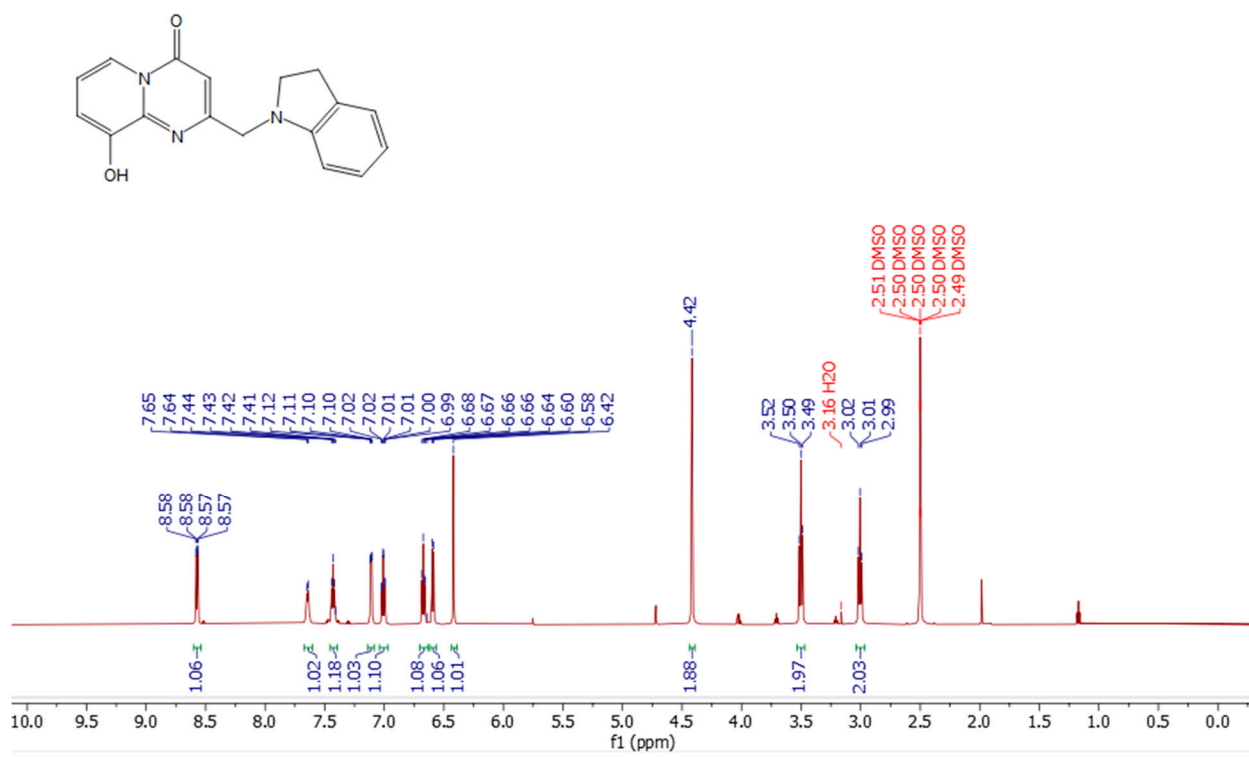
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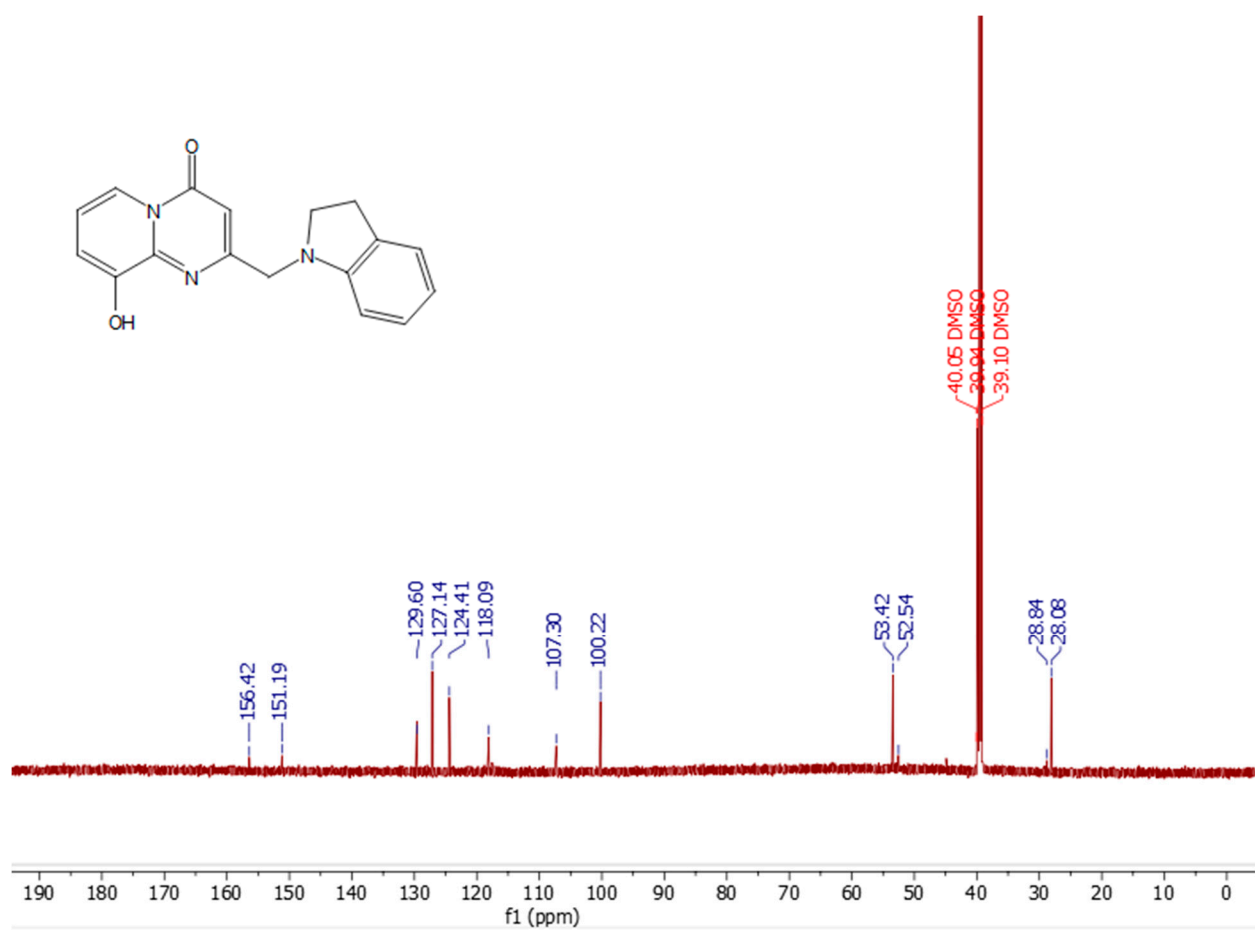
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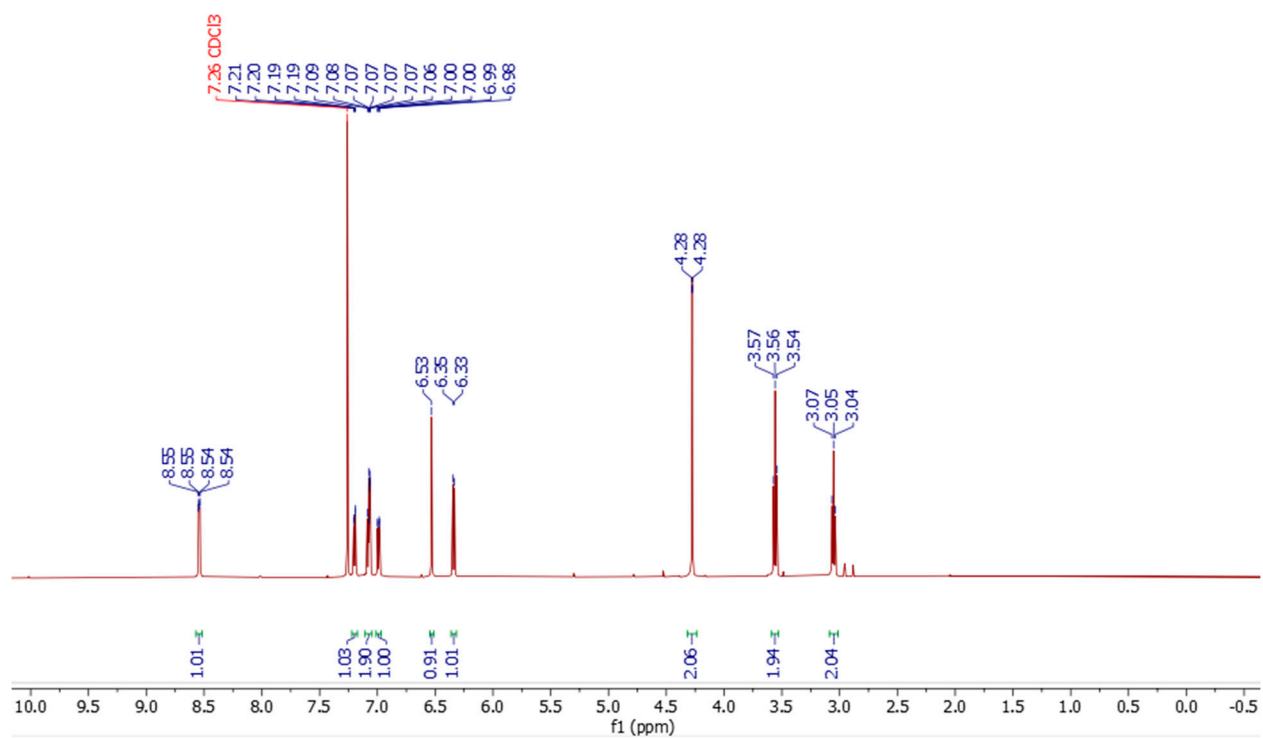
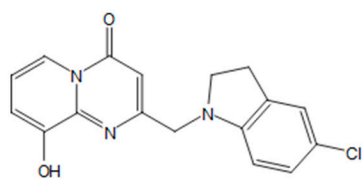
¹H NMR of 46



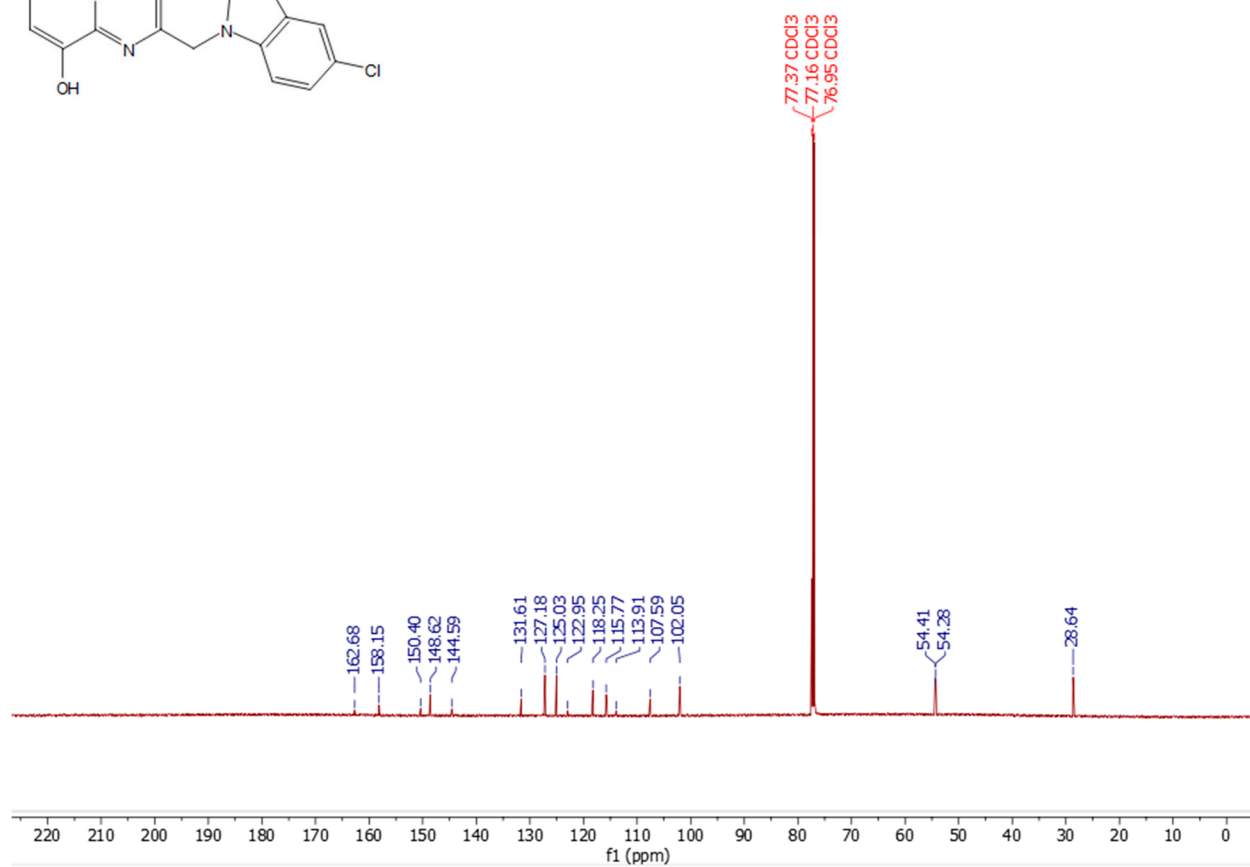
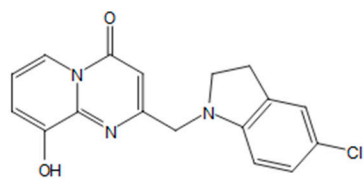
^{13}C NMR of **46**



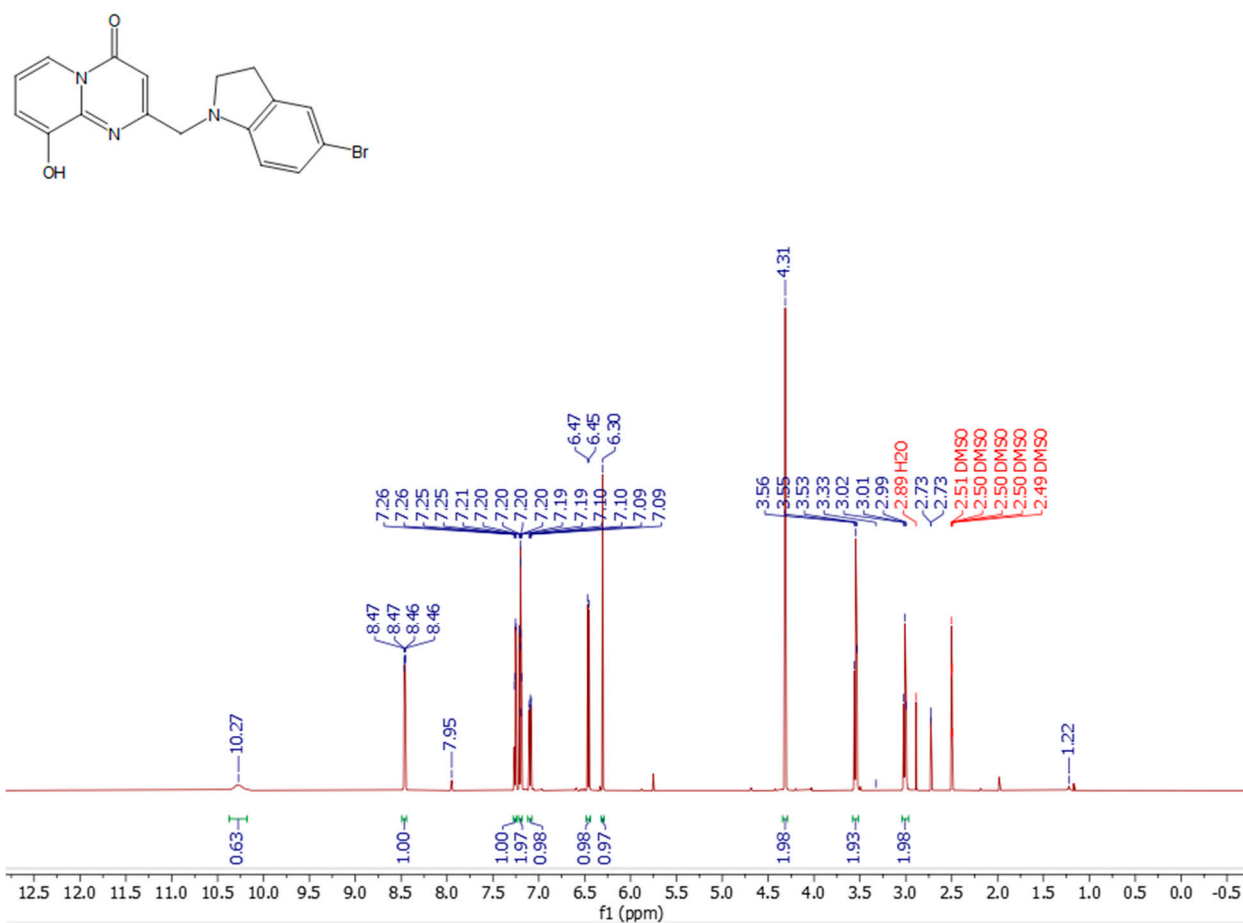
¹H NMR of **47**



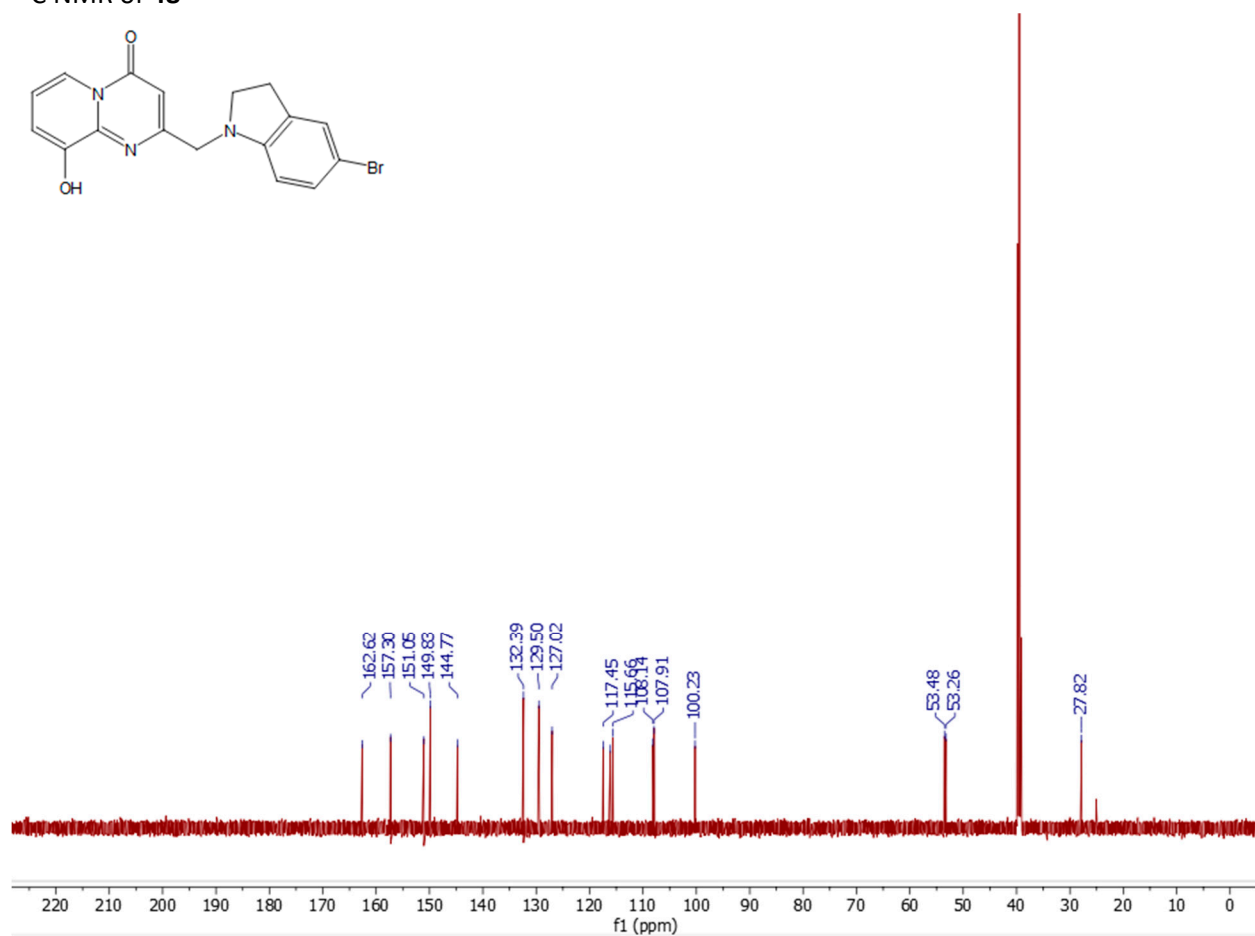
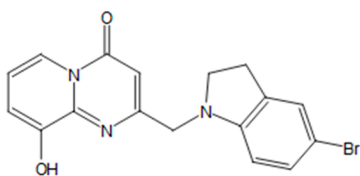
¹³C NMR of **47**



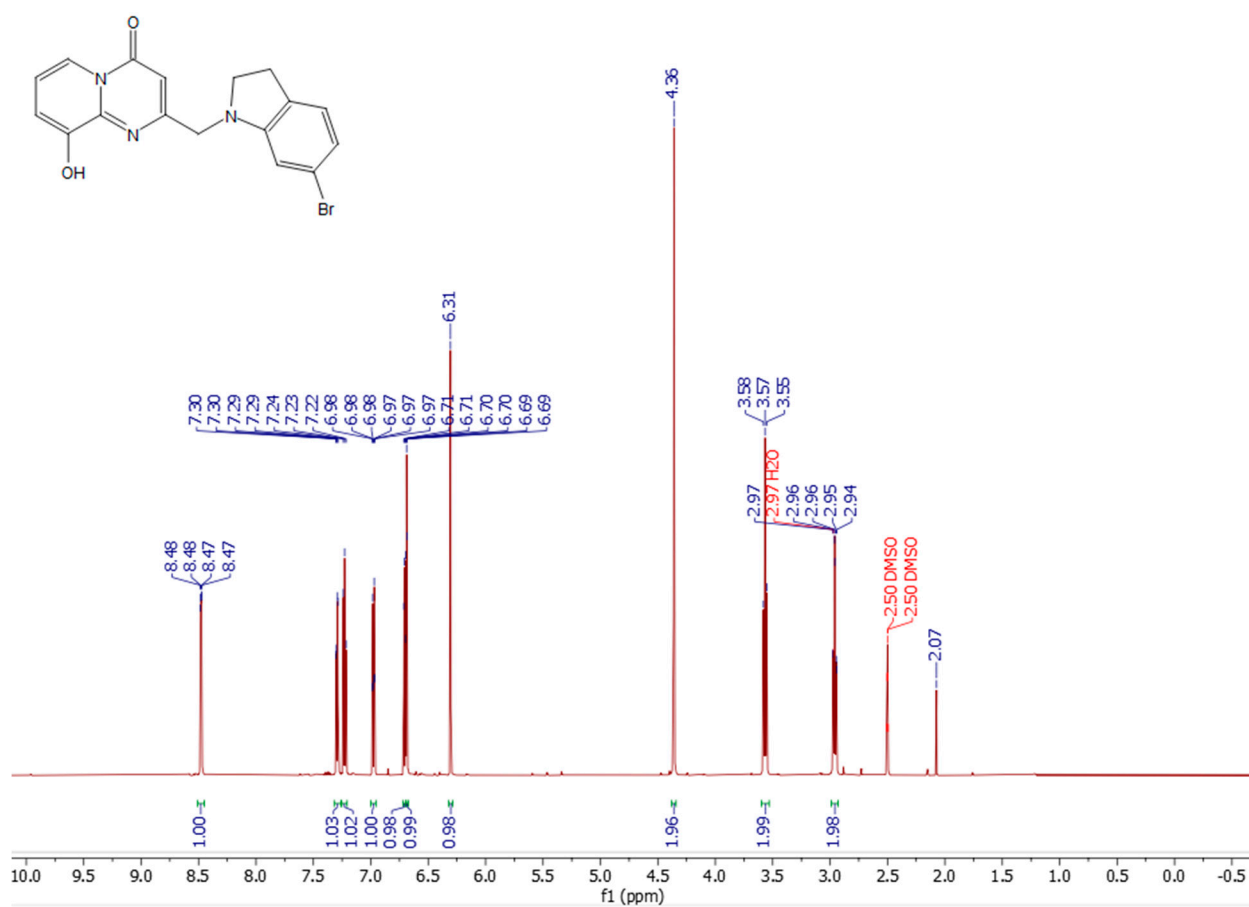
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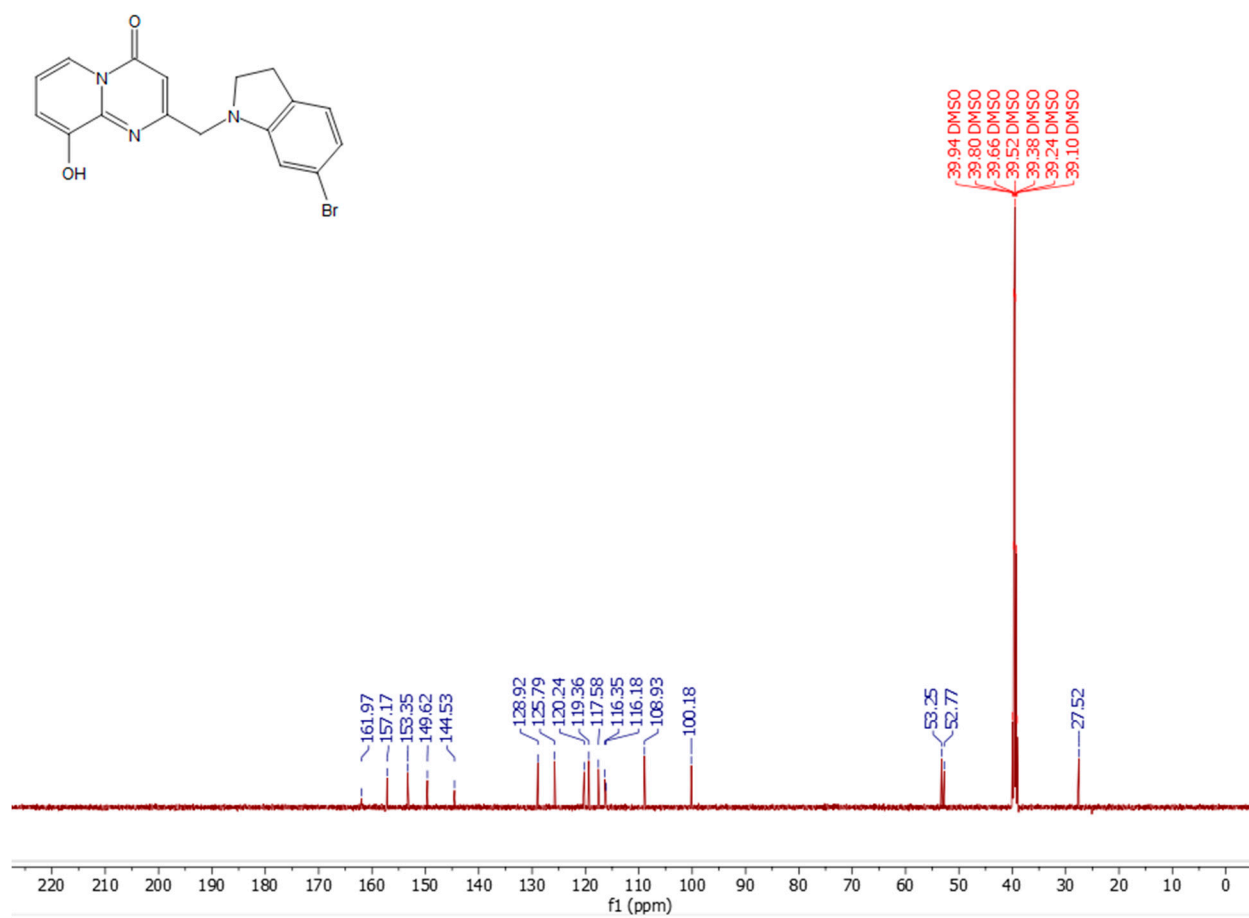
¹³C NMR of **48**



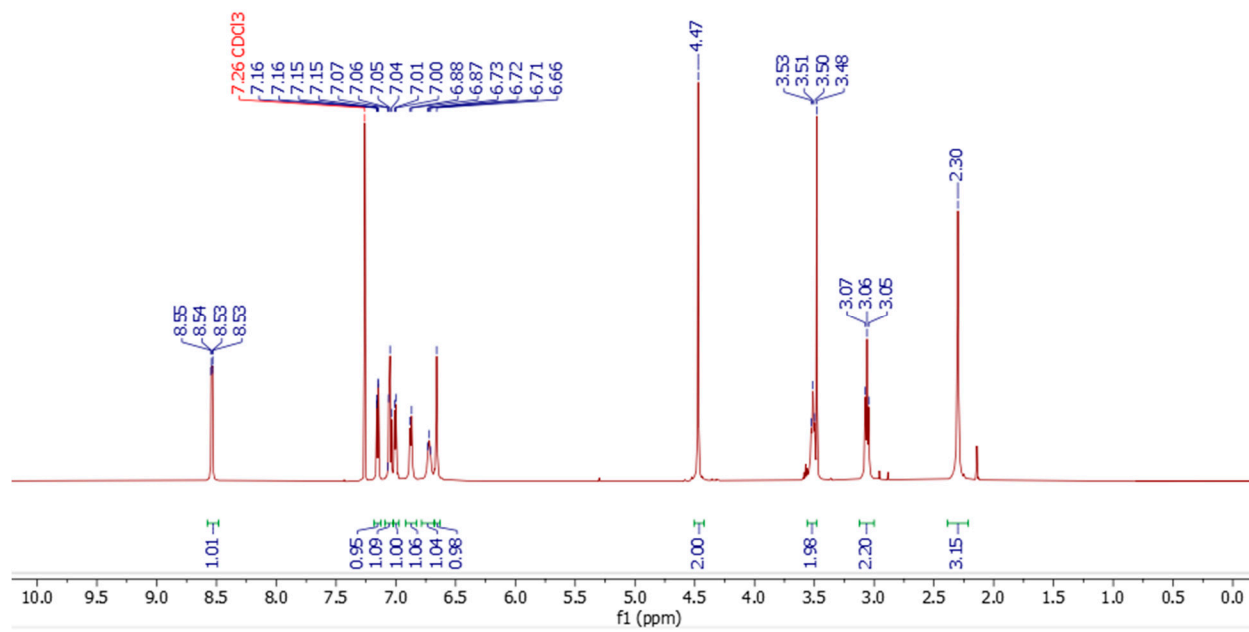
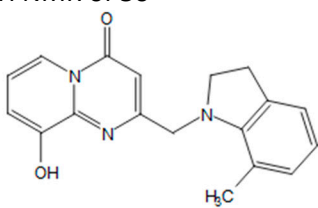
¹H NMR of **49**



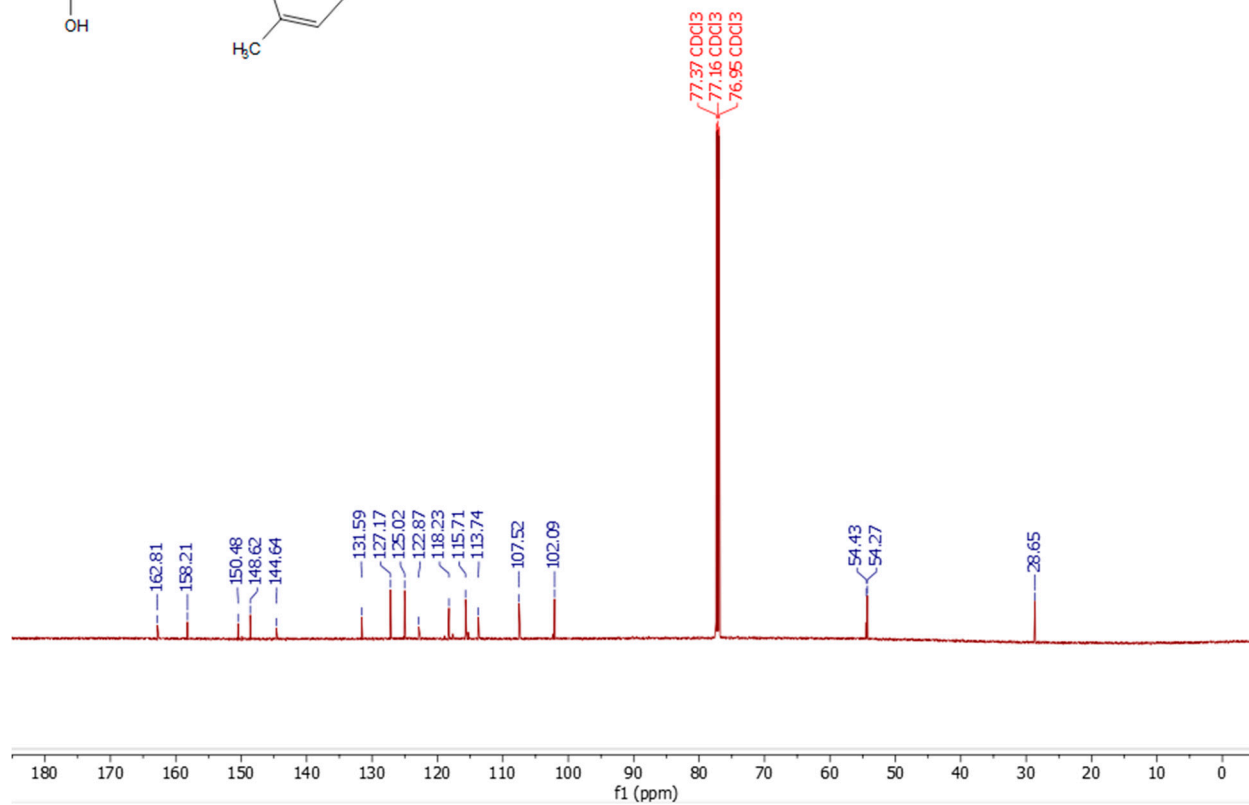
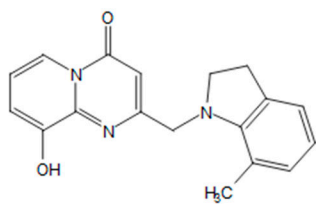
¹³C NMR of **49**



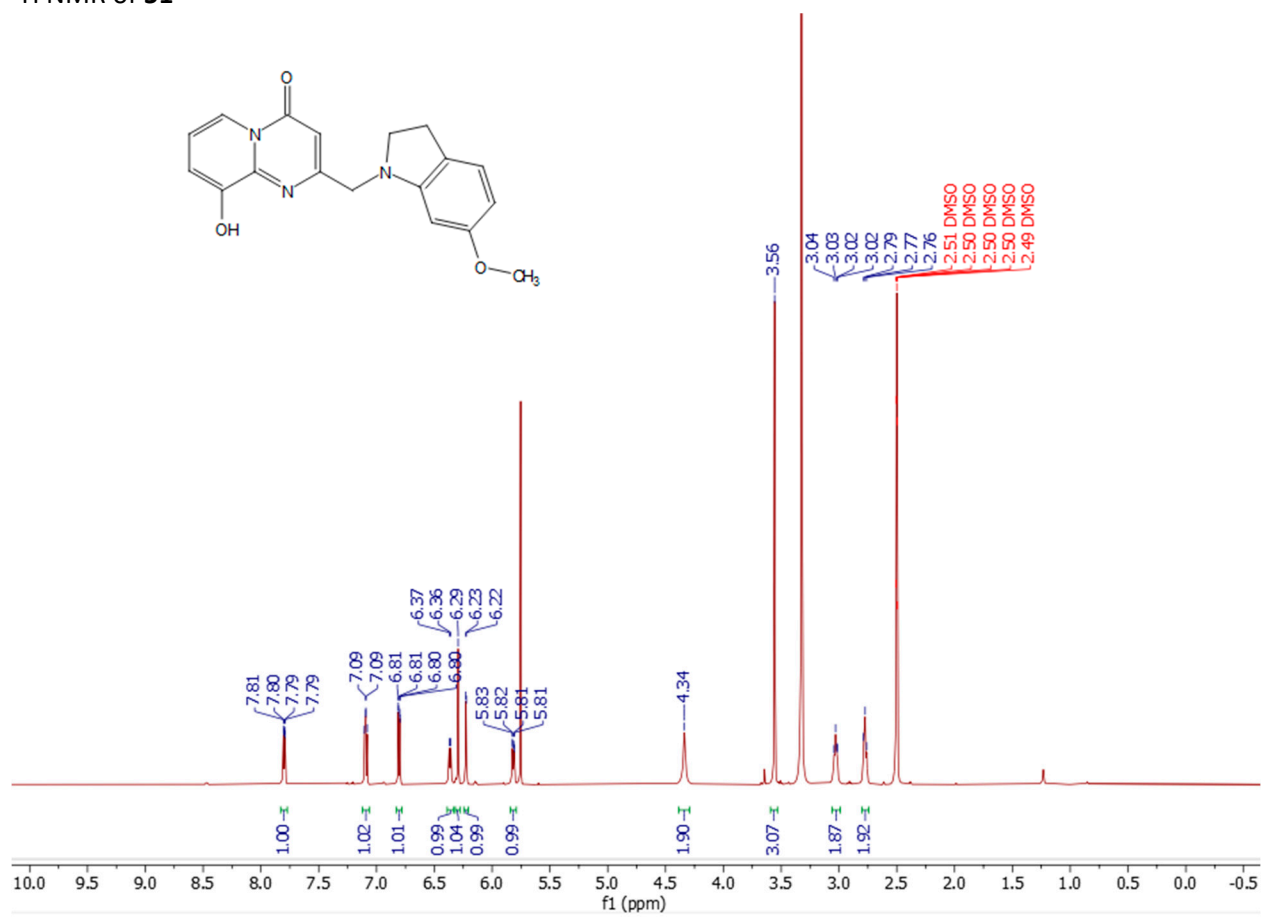
¹H NMR of **50**



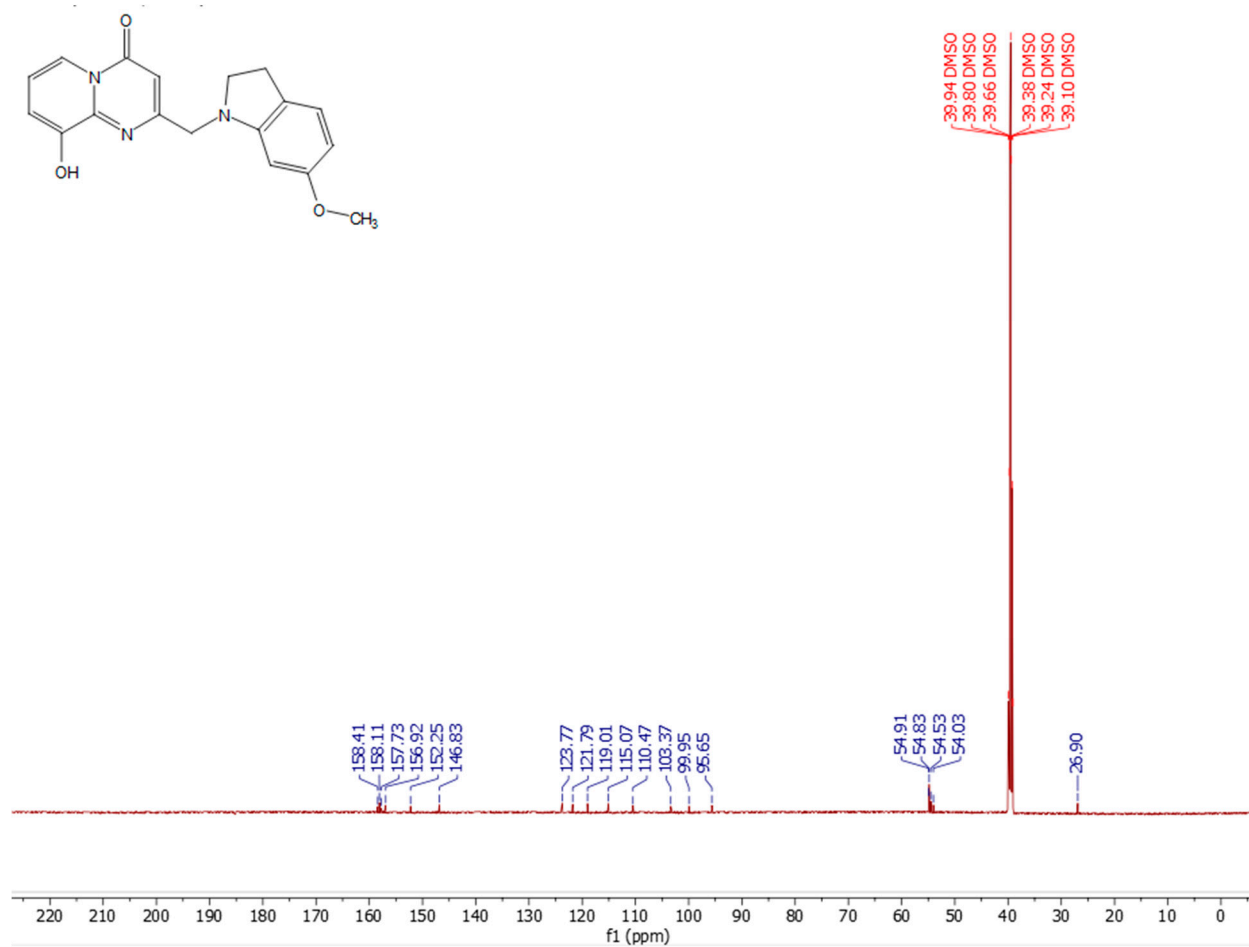
¹³C NMR of **50**



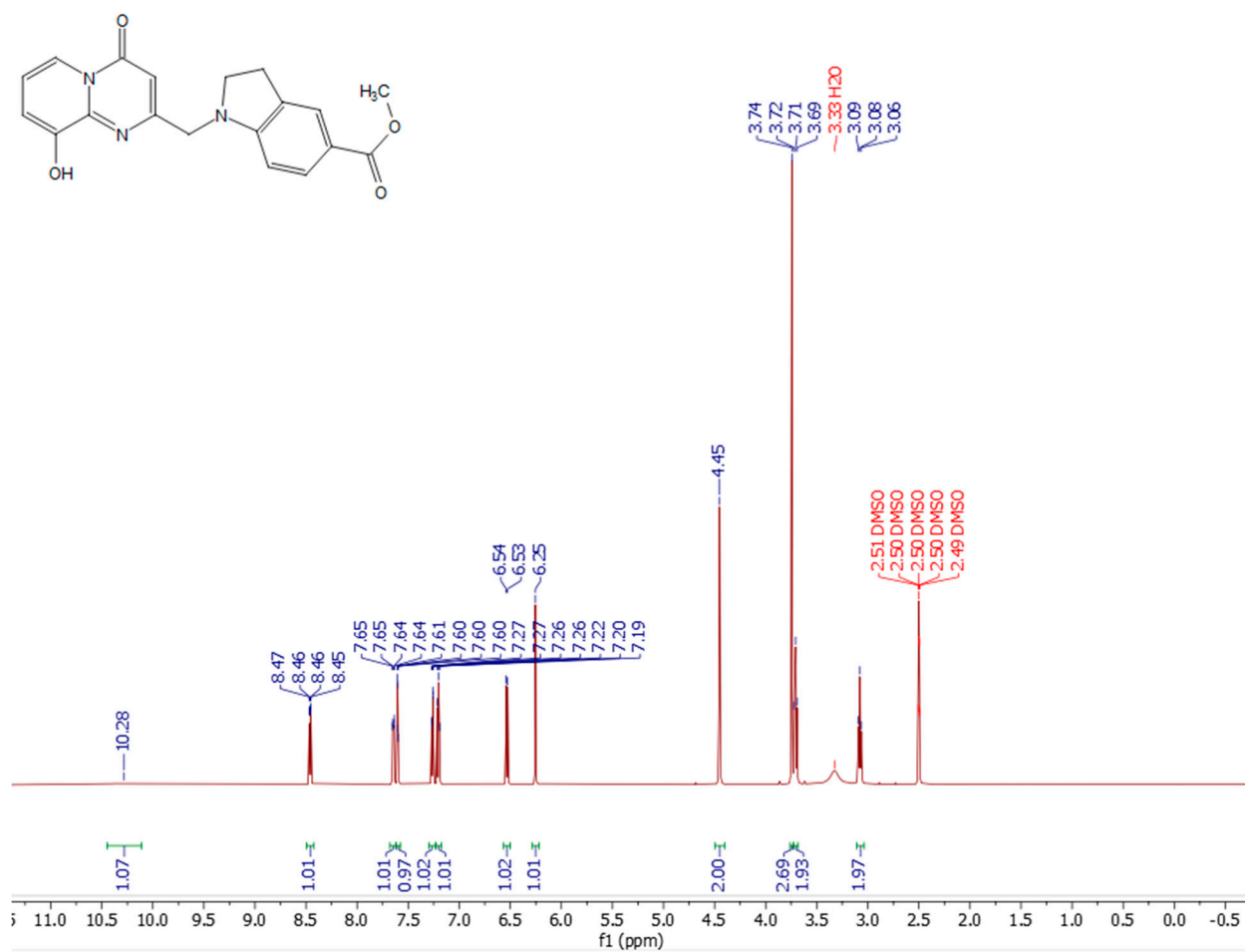
¹H NMR of **51**



¹³C NMR of **51**



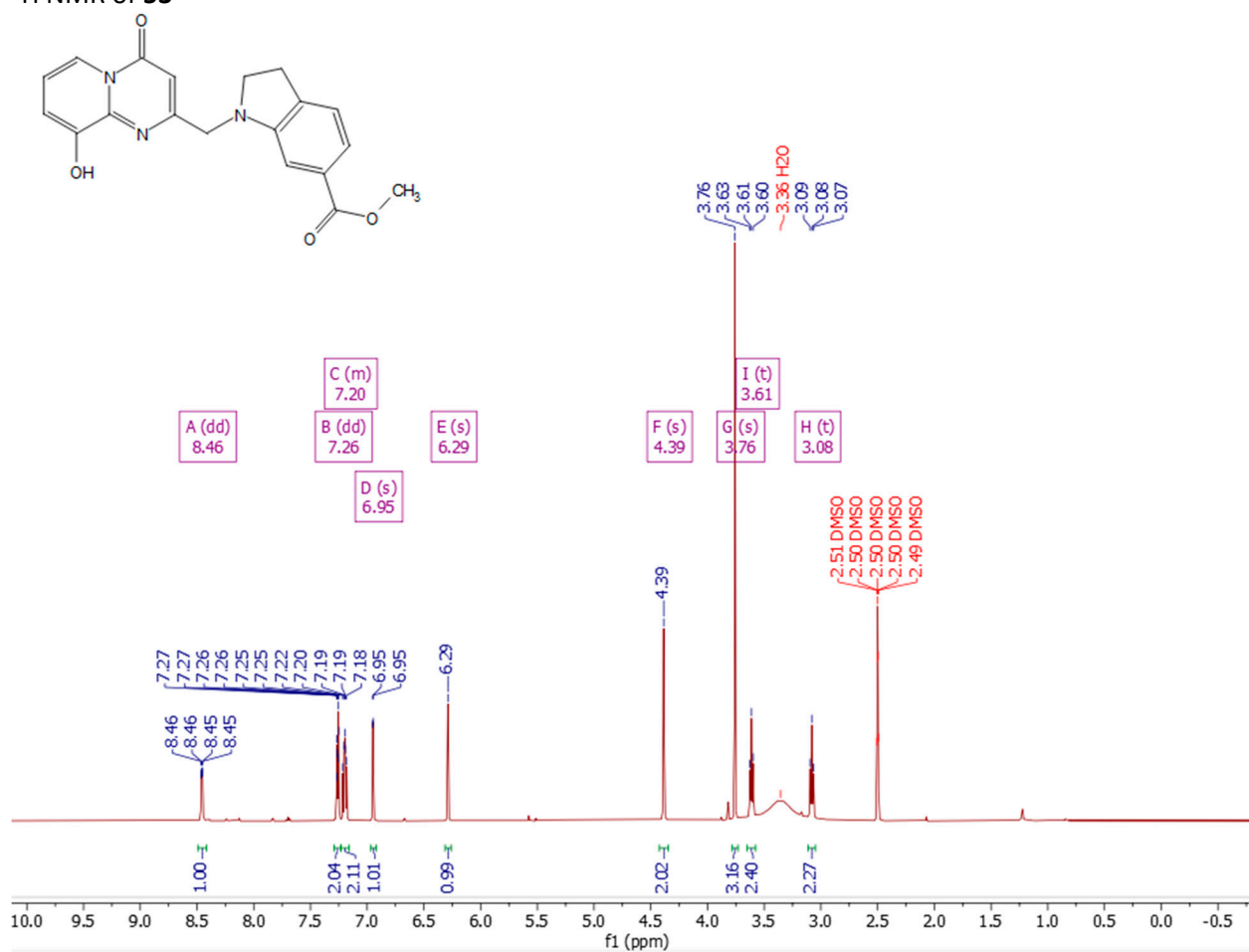
¹H NMR of **52**



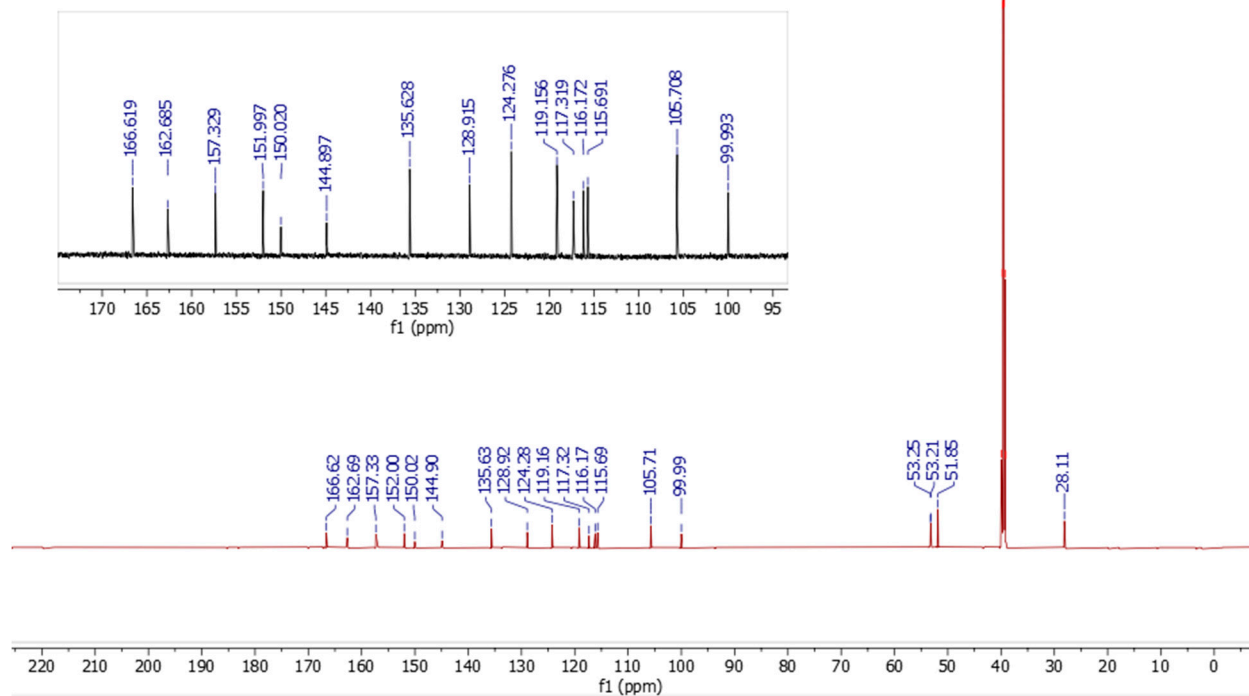
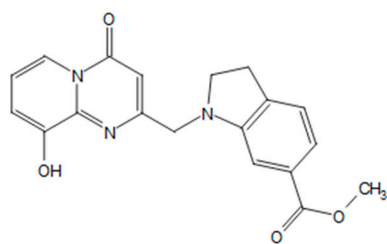
¹³C NMR of **52**



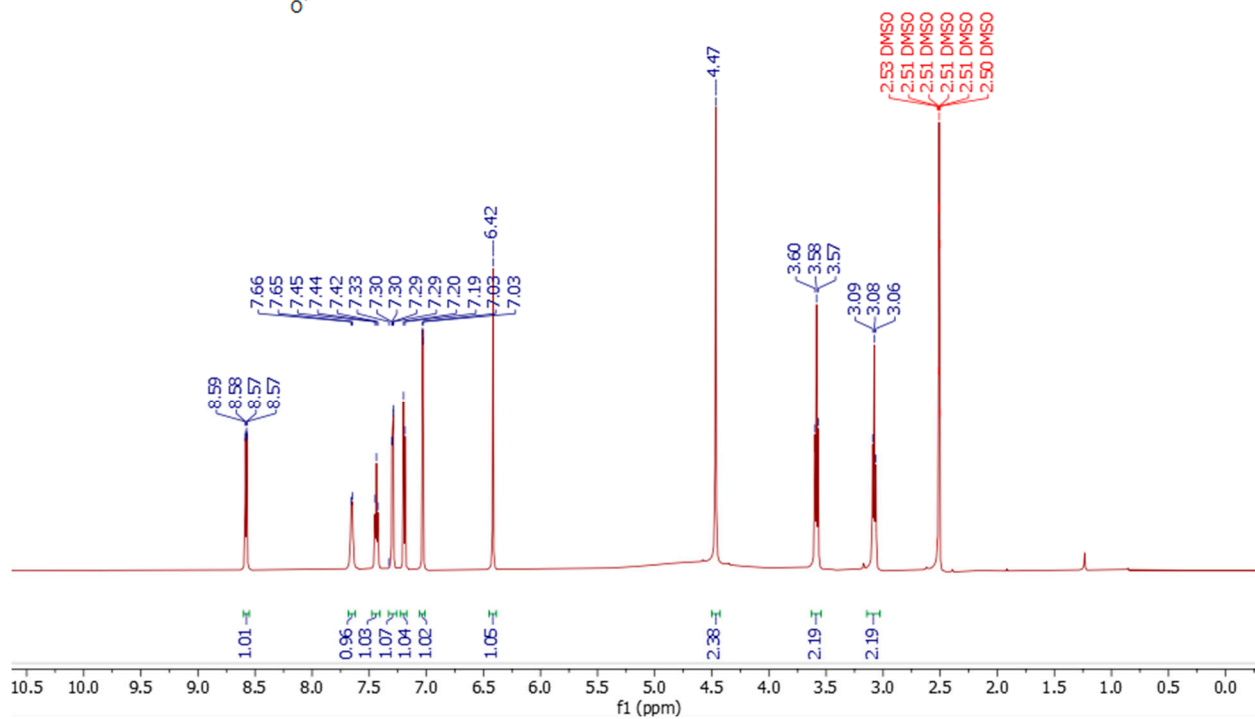
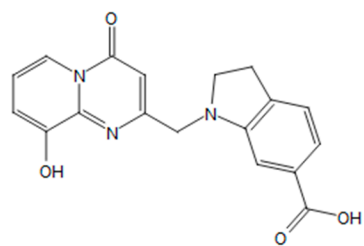
¹H NMR of **53**



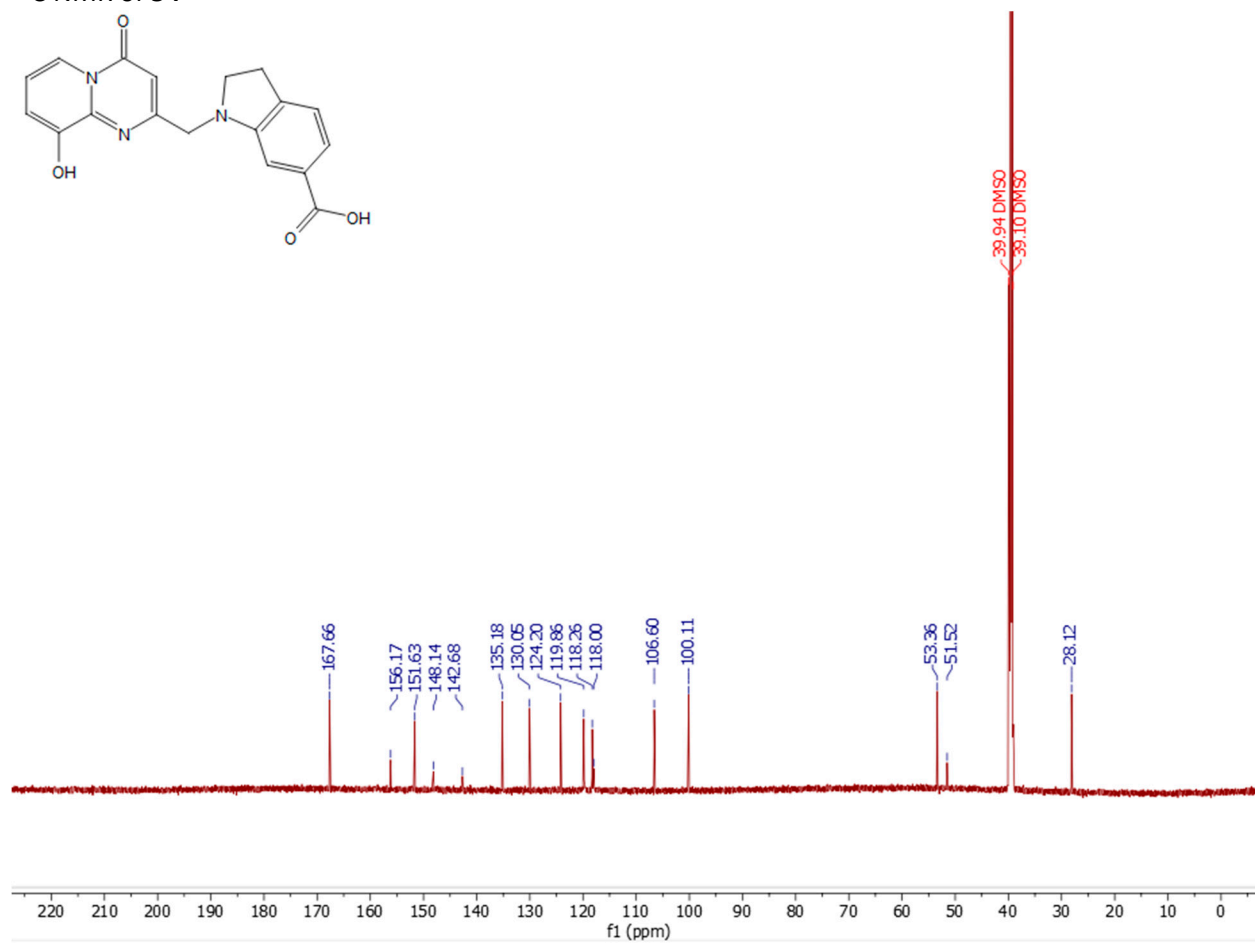
¹³C NMR of **53**



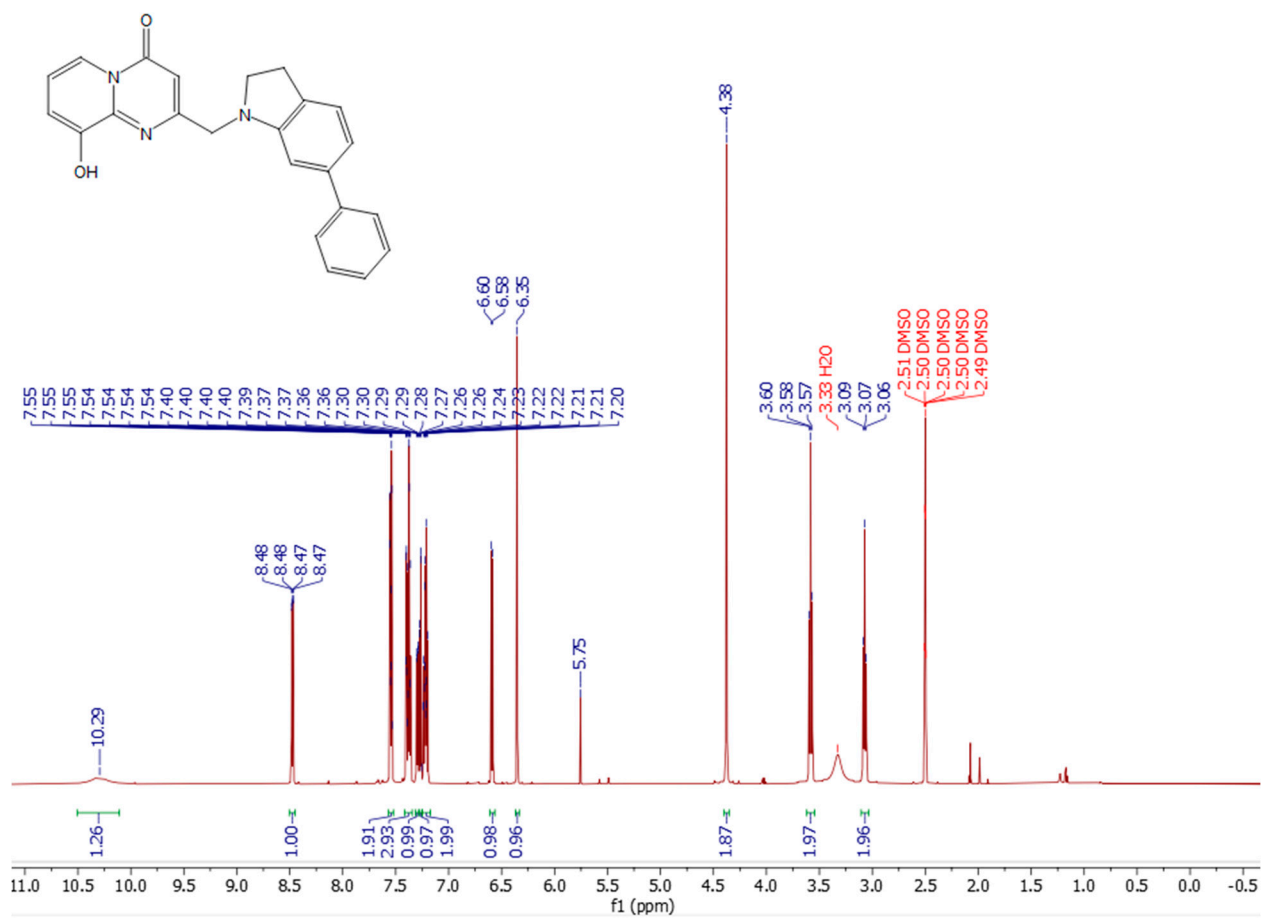
¹H NMR of **54**



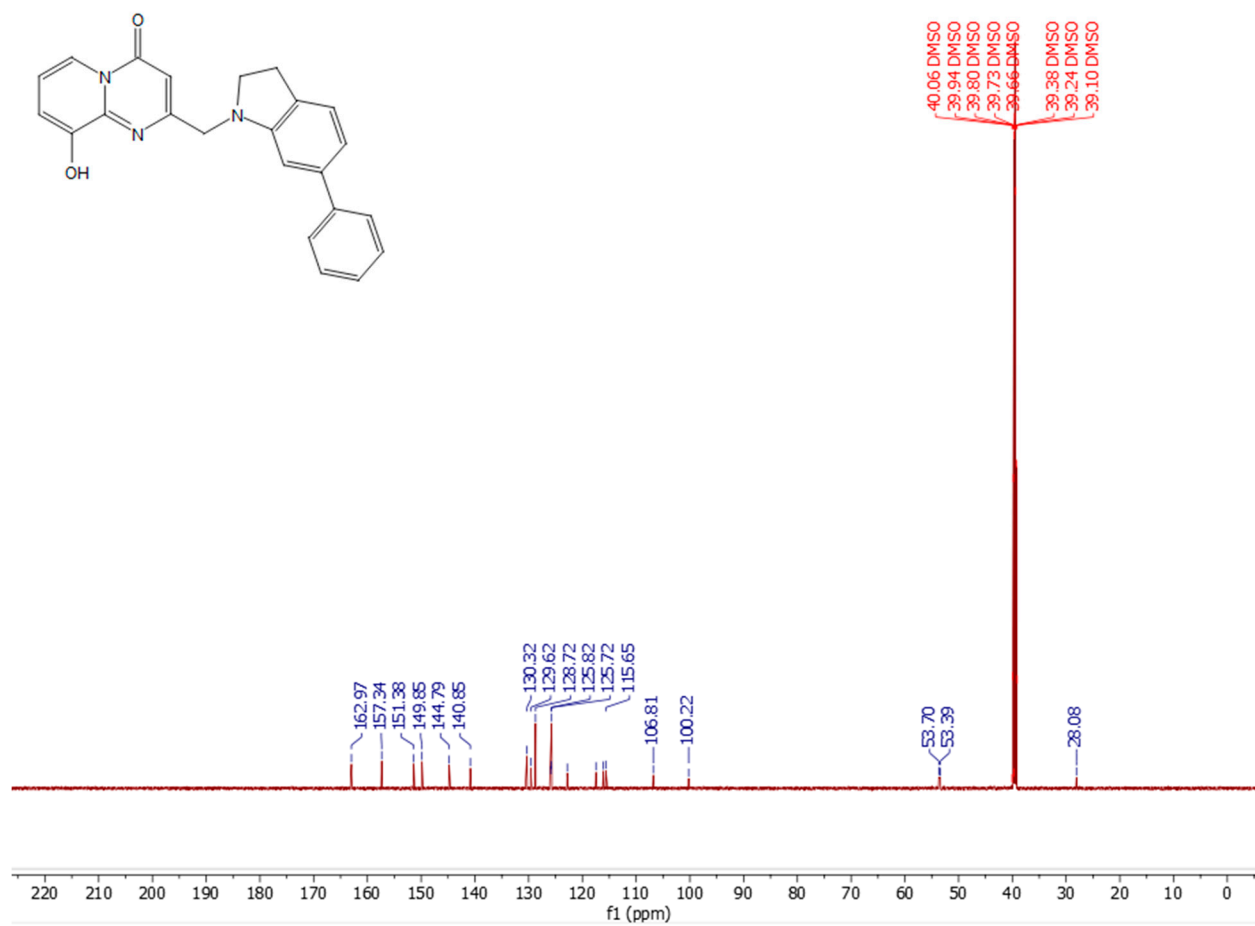
¹³C NMR of **54**



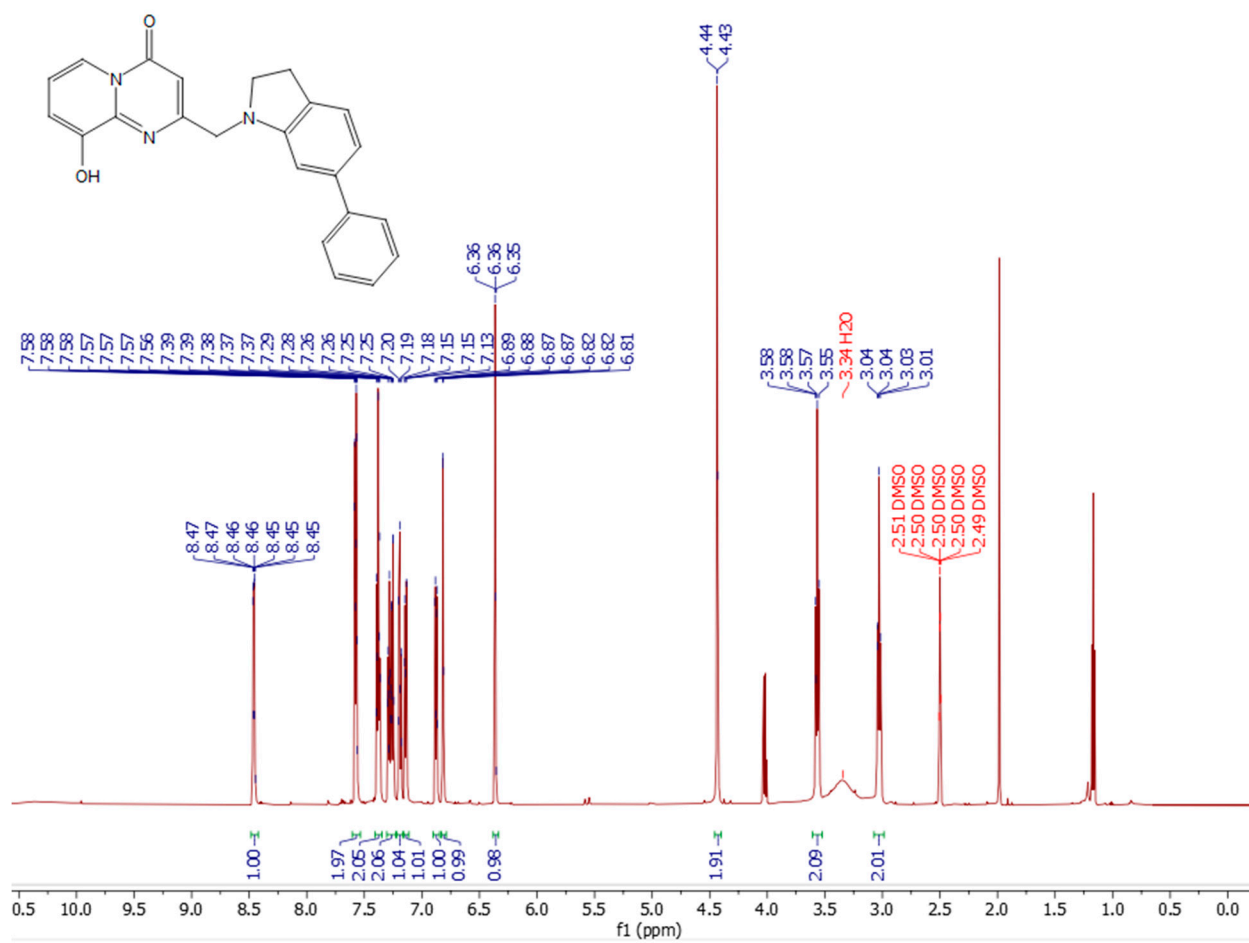
¹H NMR of **55**



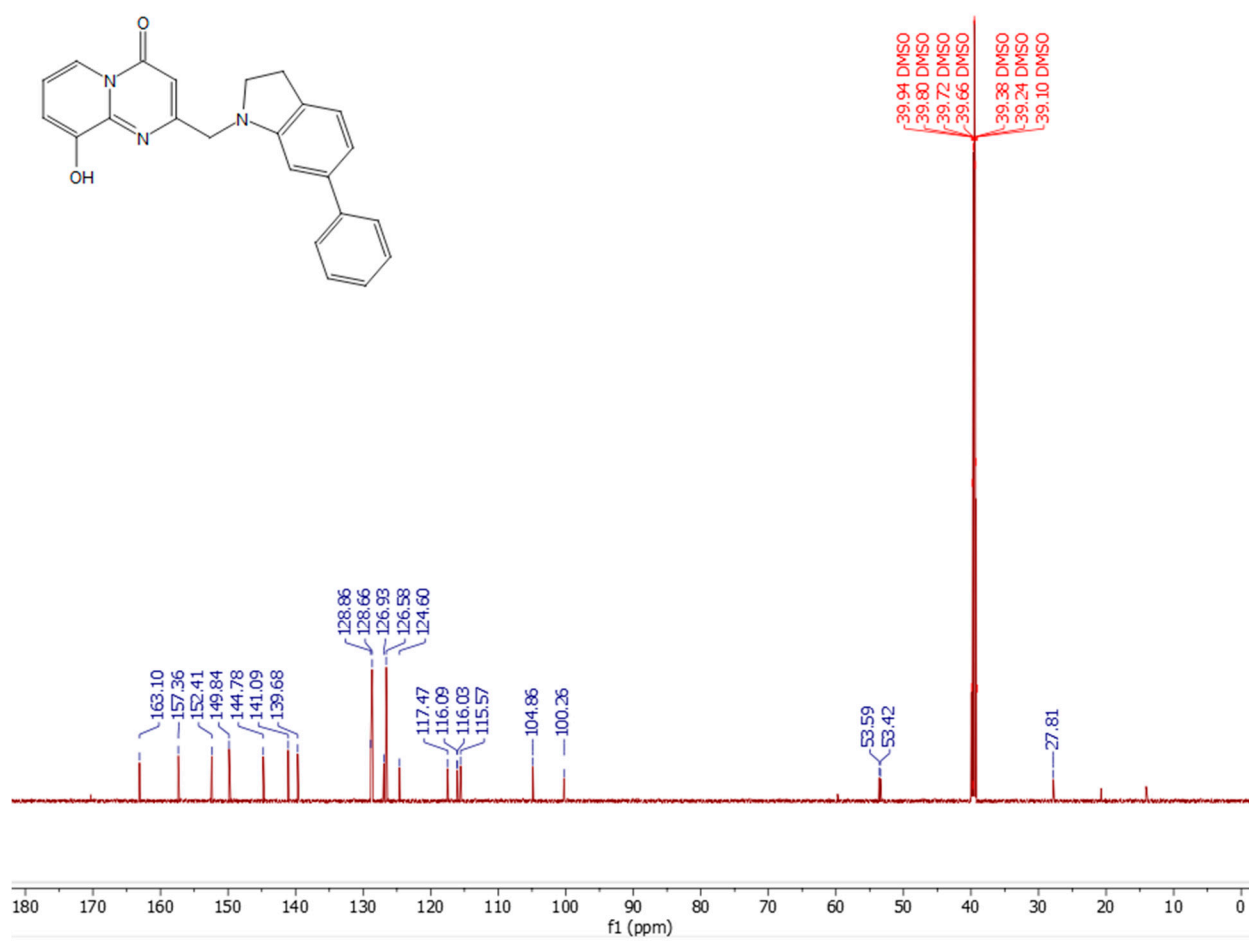
¹³C NMR of **55**



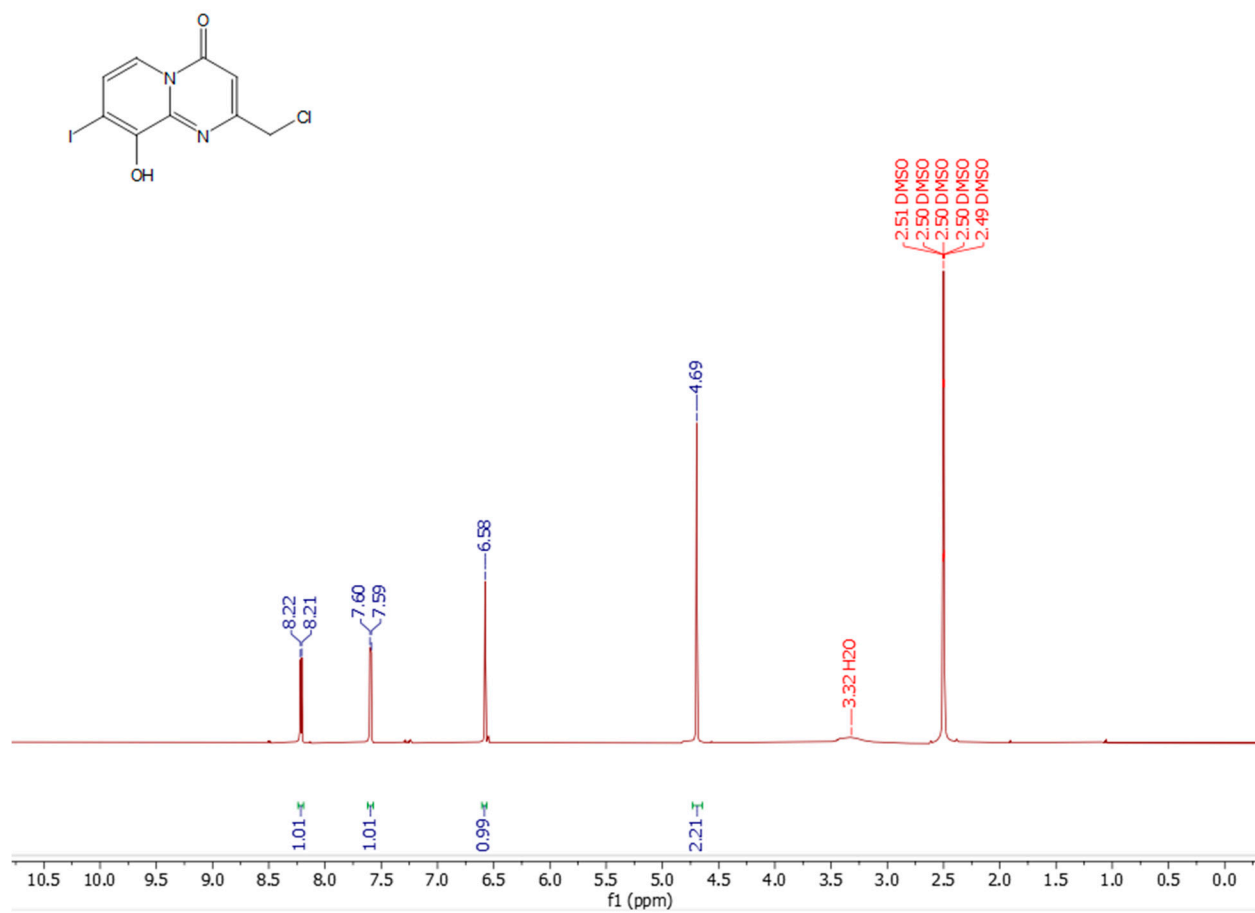
¹H NMR of 56



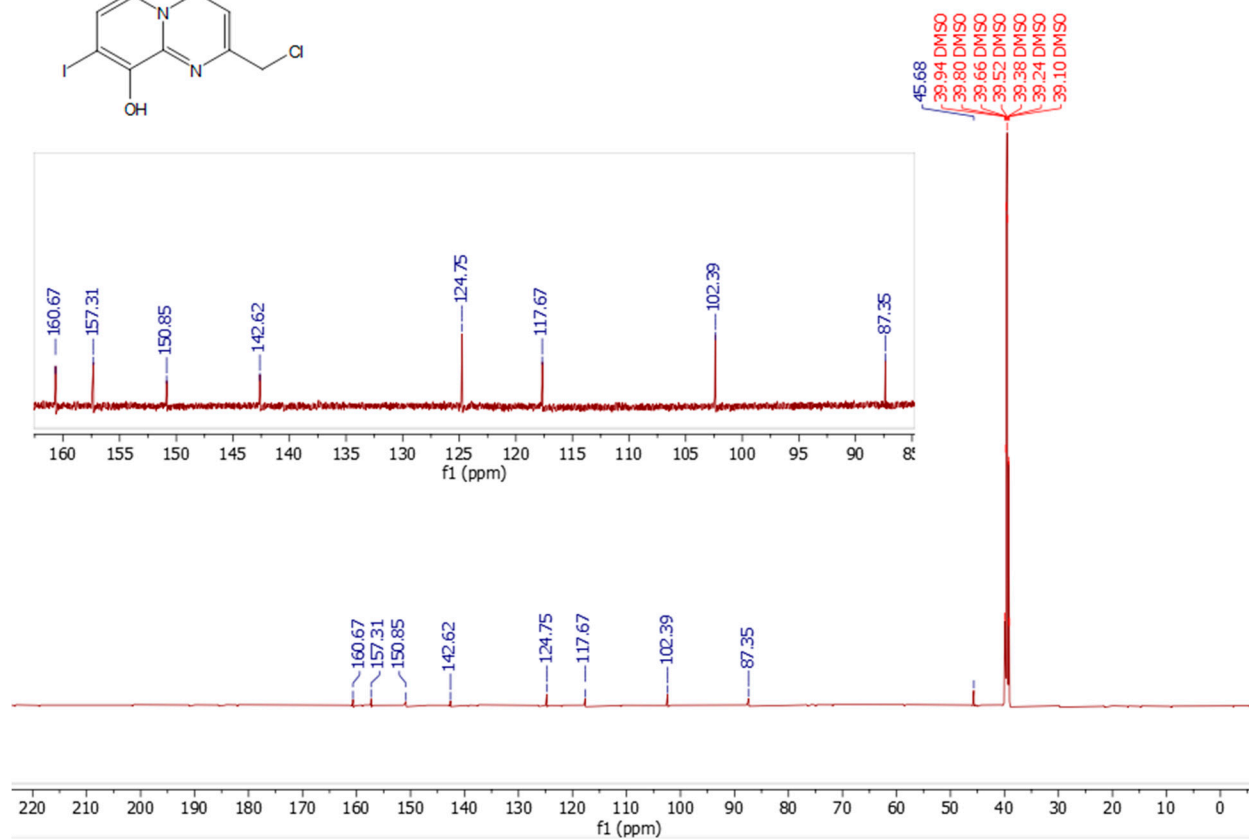
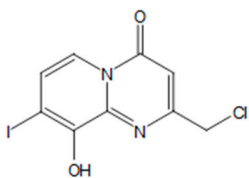
¹³C NMR of **56**



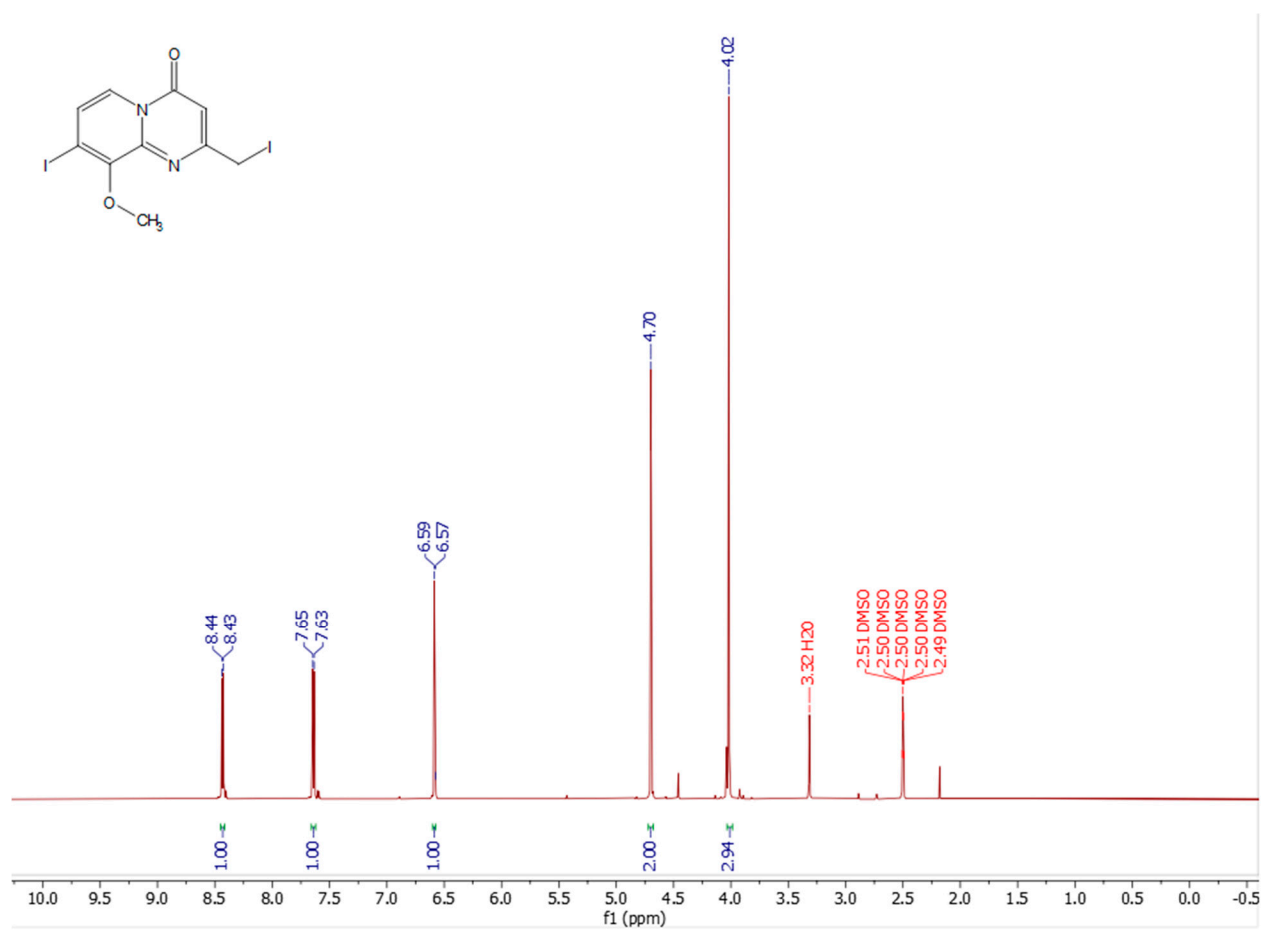
¹H NMR of **57**



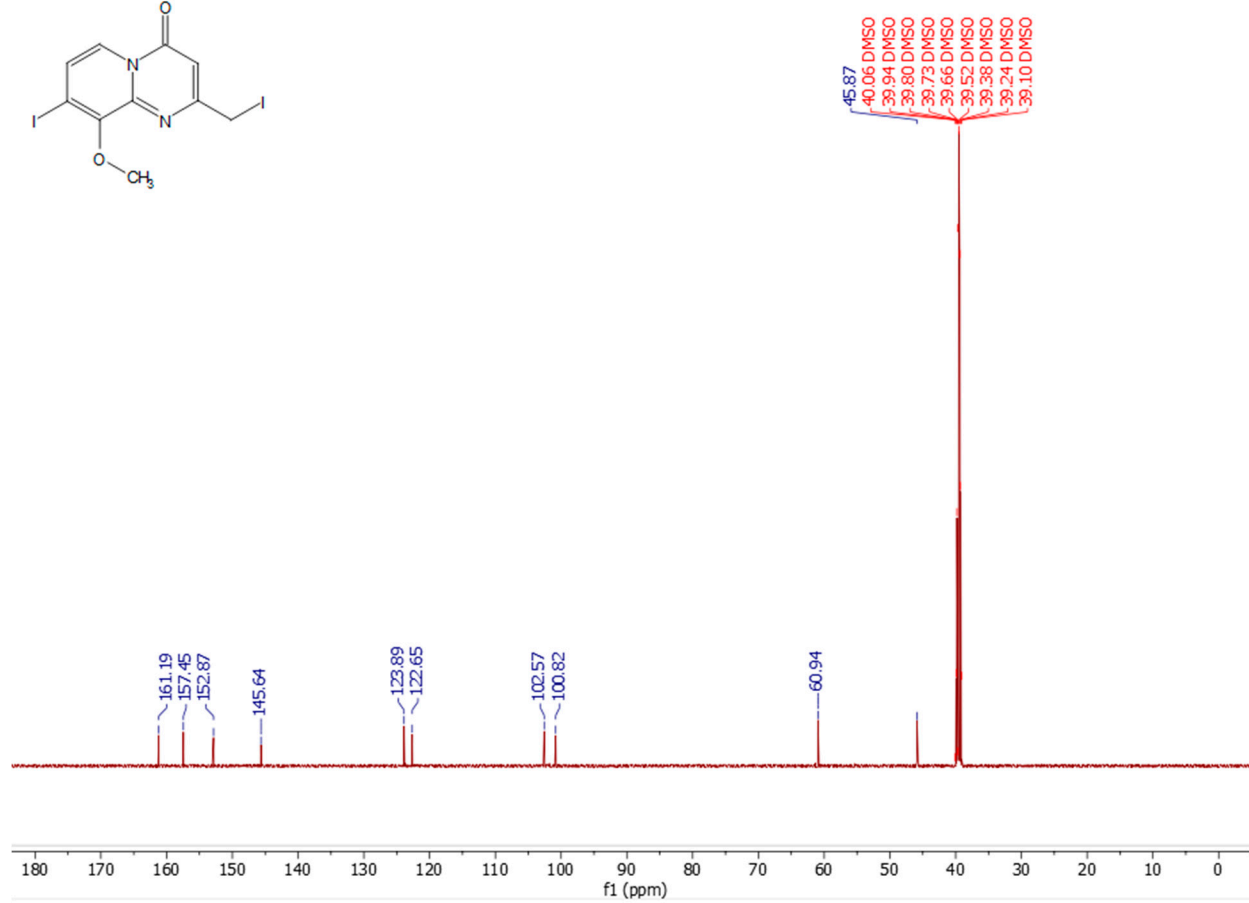
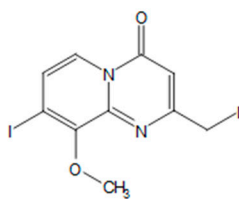
¹³C NMR of **57**



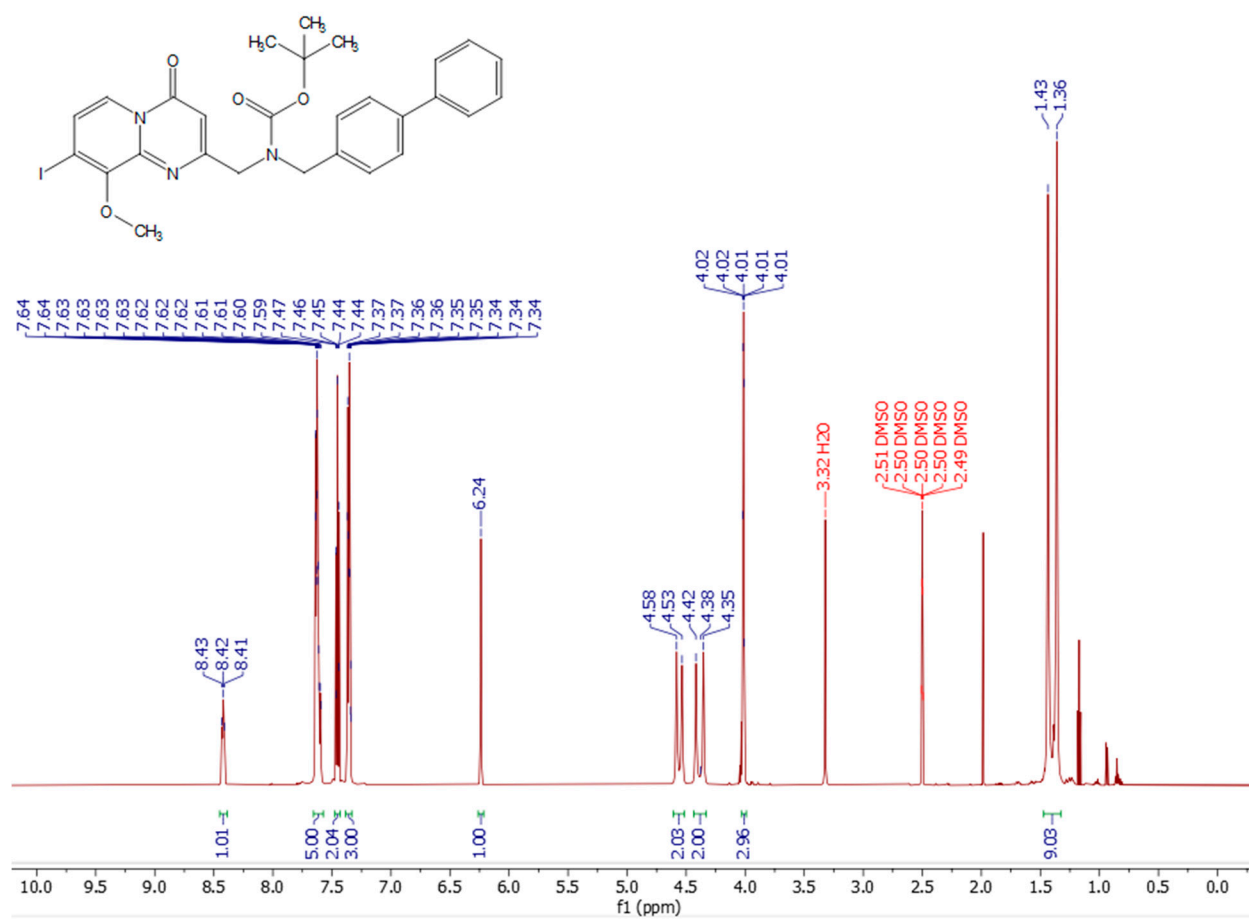
¹H NMR of **58**



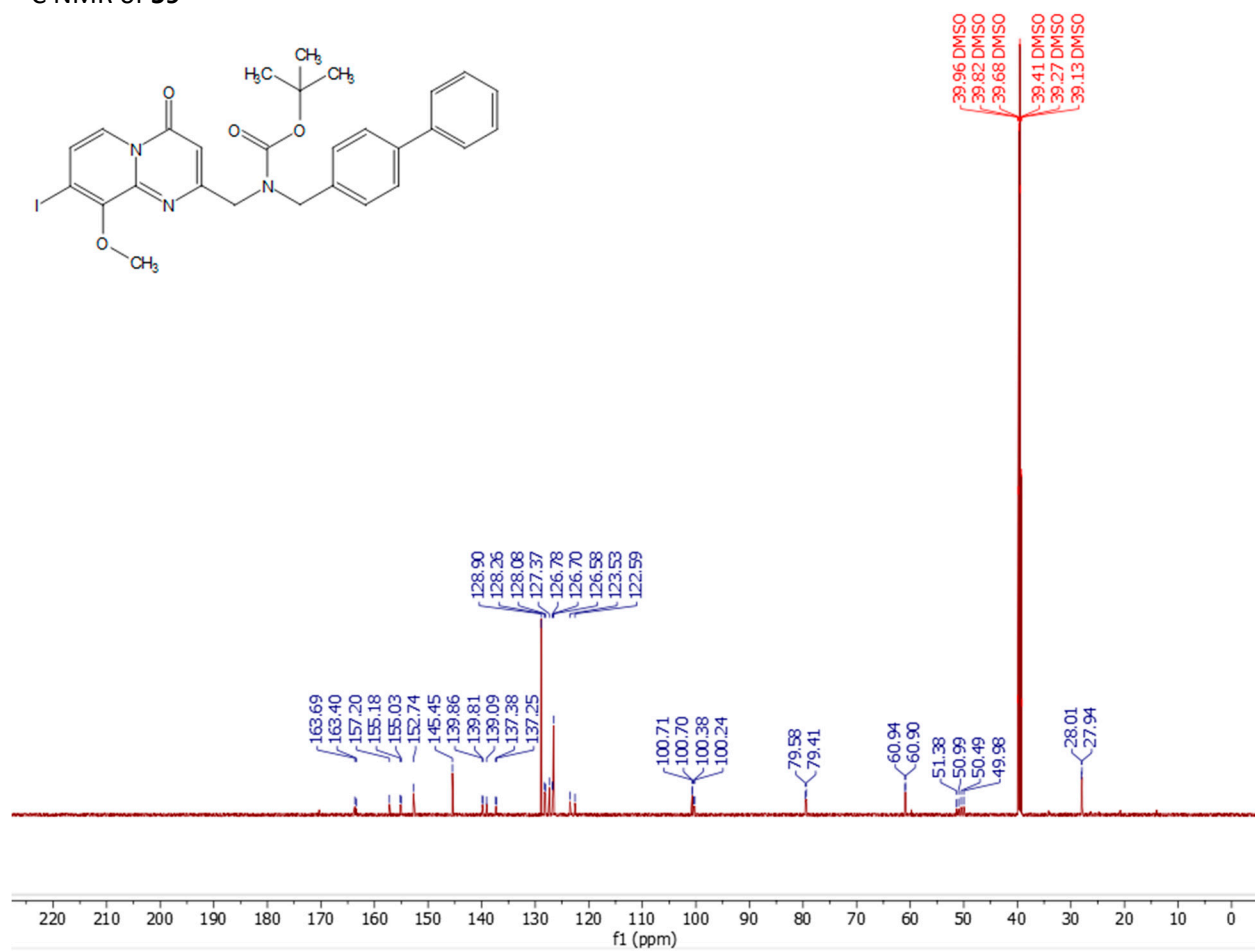
¹³C NMR of **58**



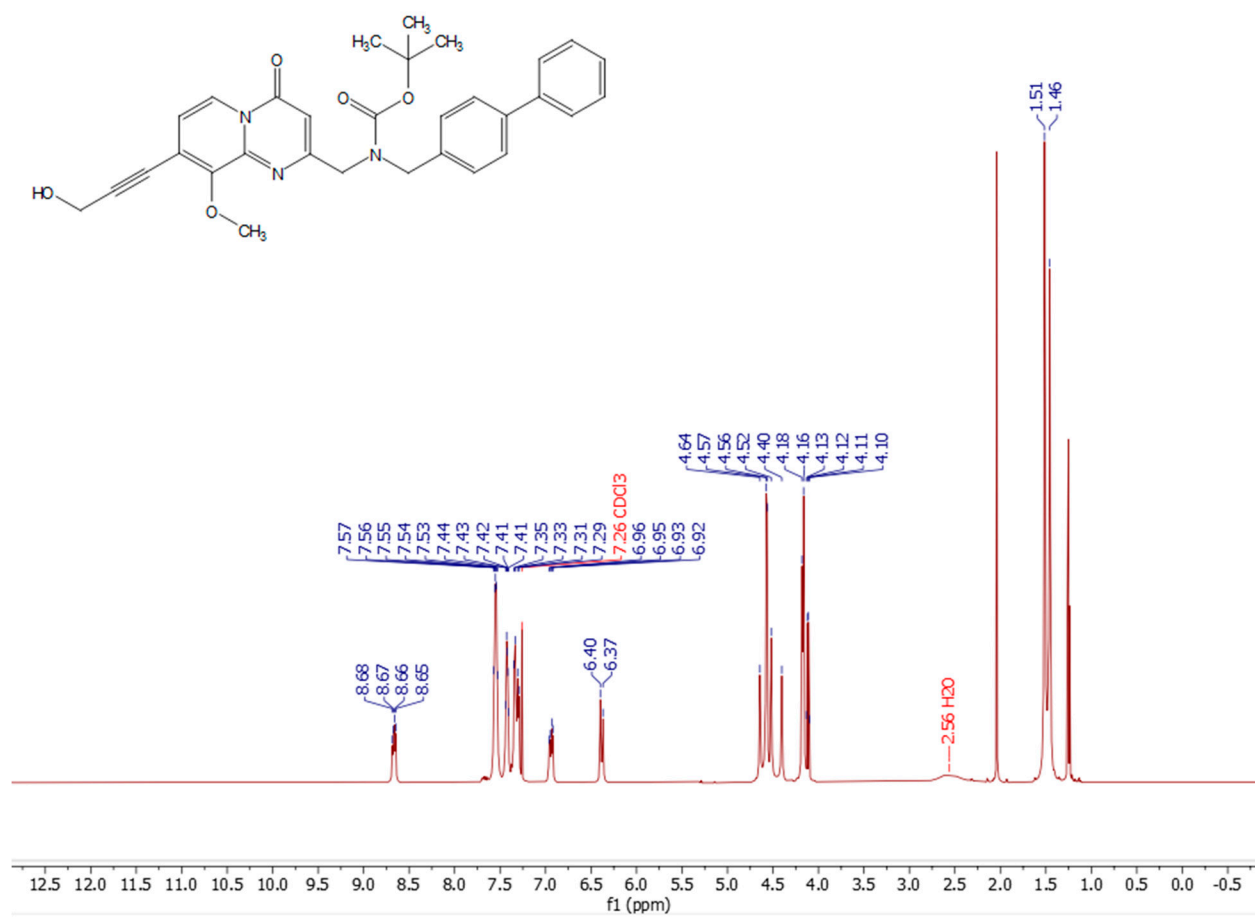
¹H NMR of **59**



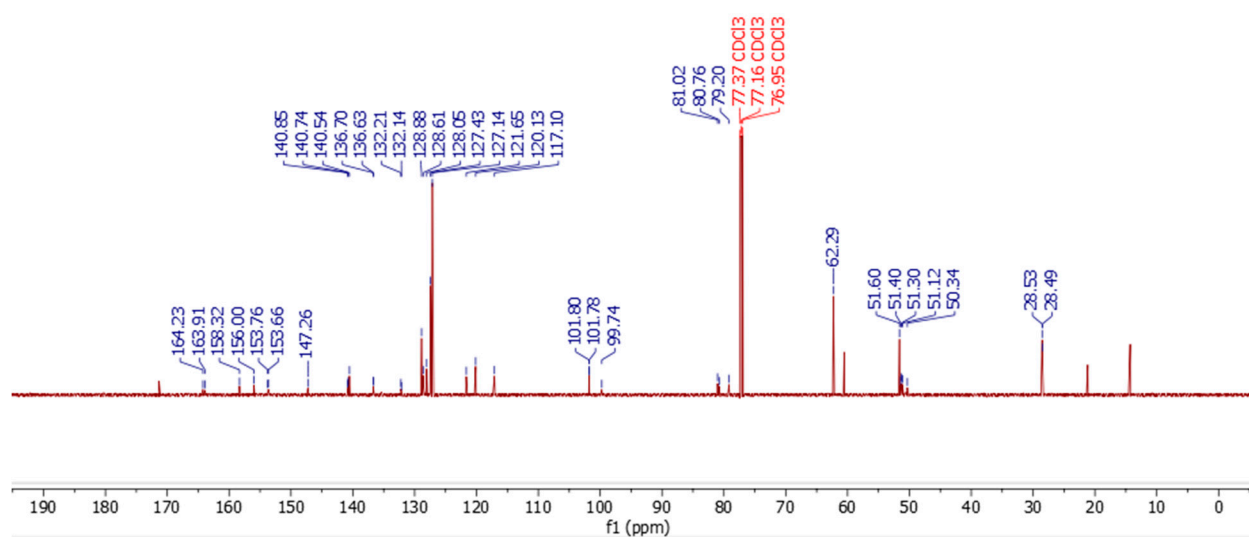
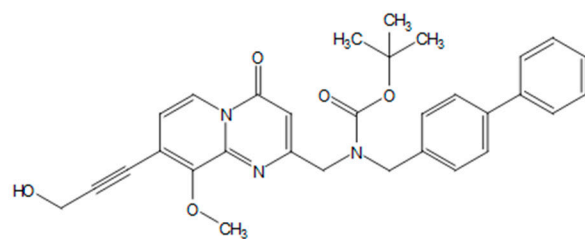
¹³C NMR of **59**



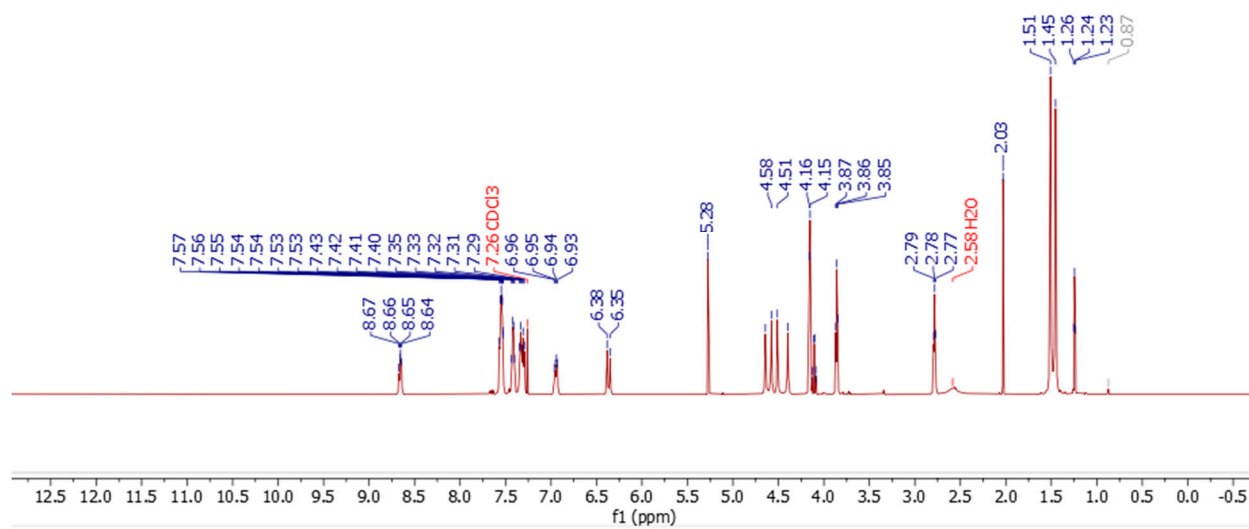
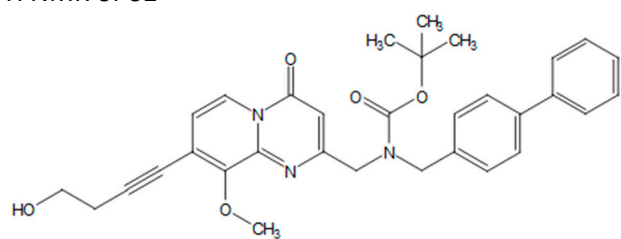
¹H NMR of **60**



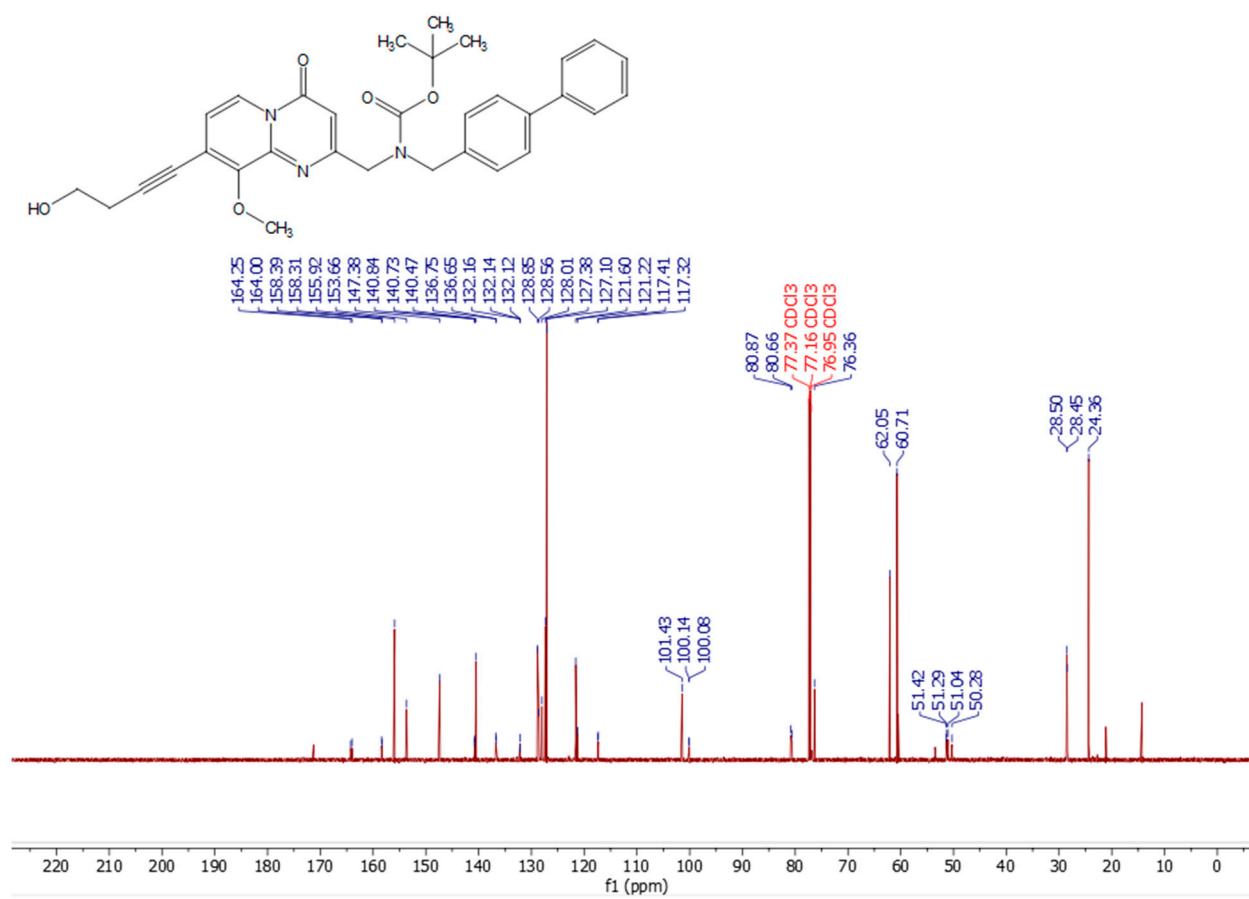
¹³C NMR of **60**



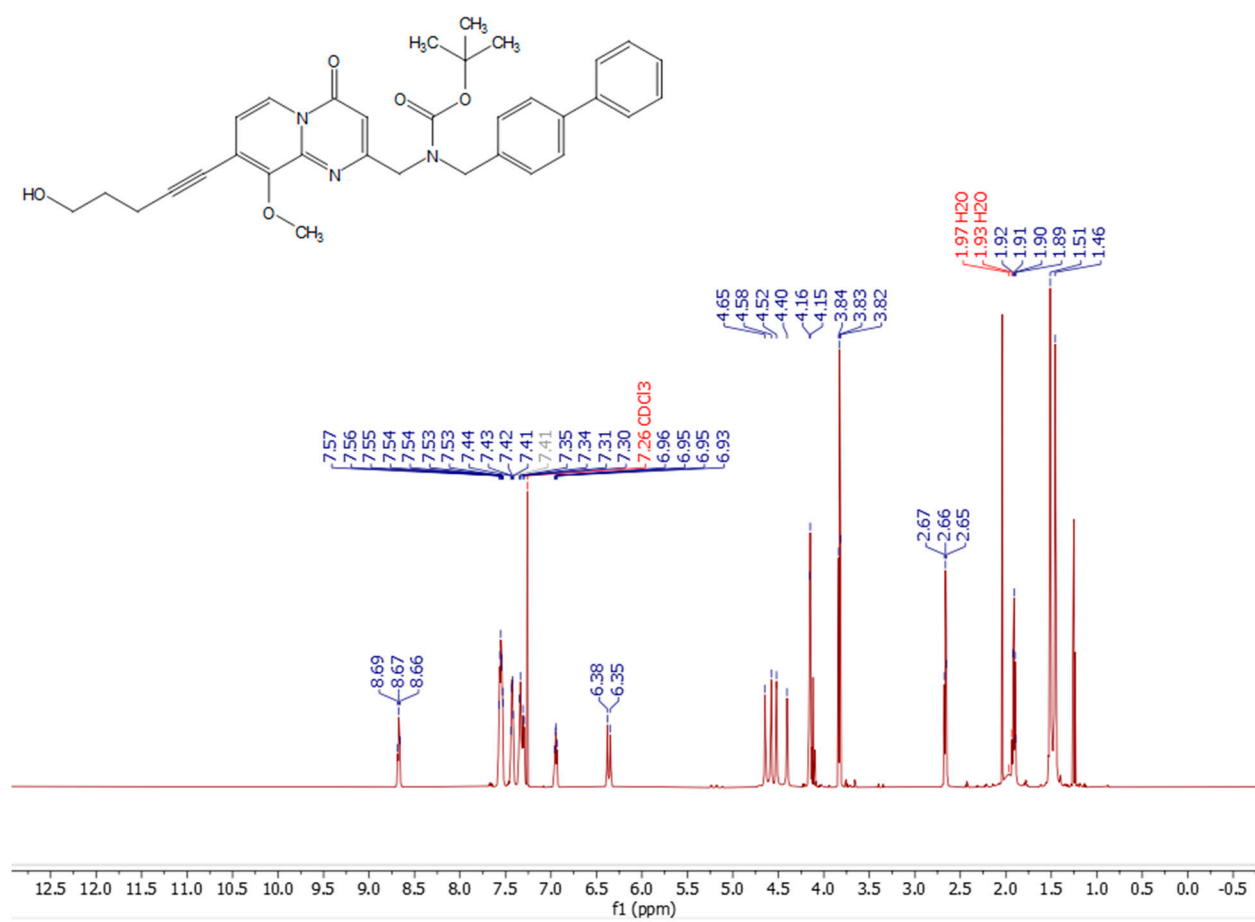
¹H NMR of **61**



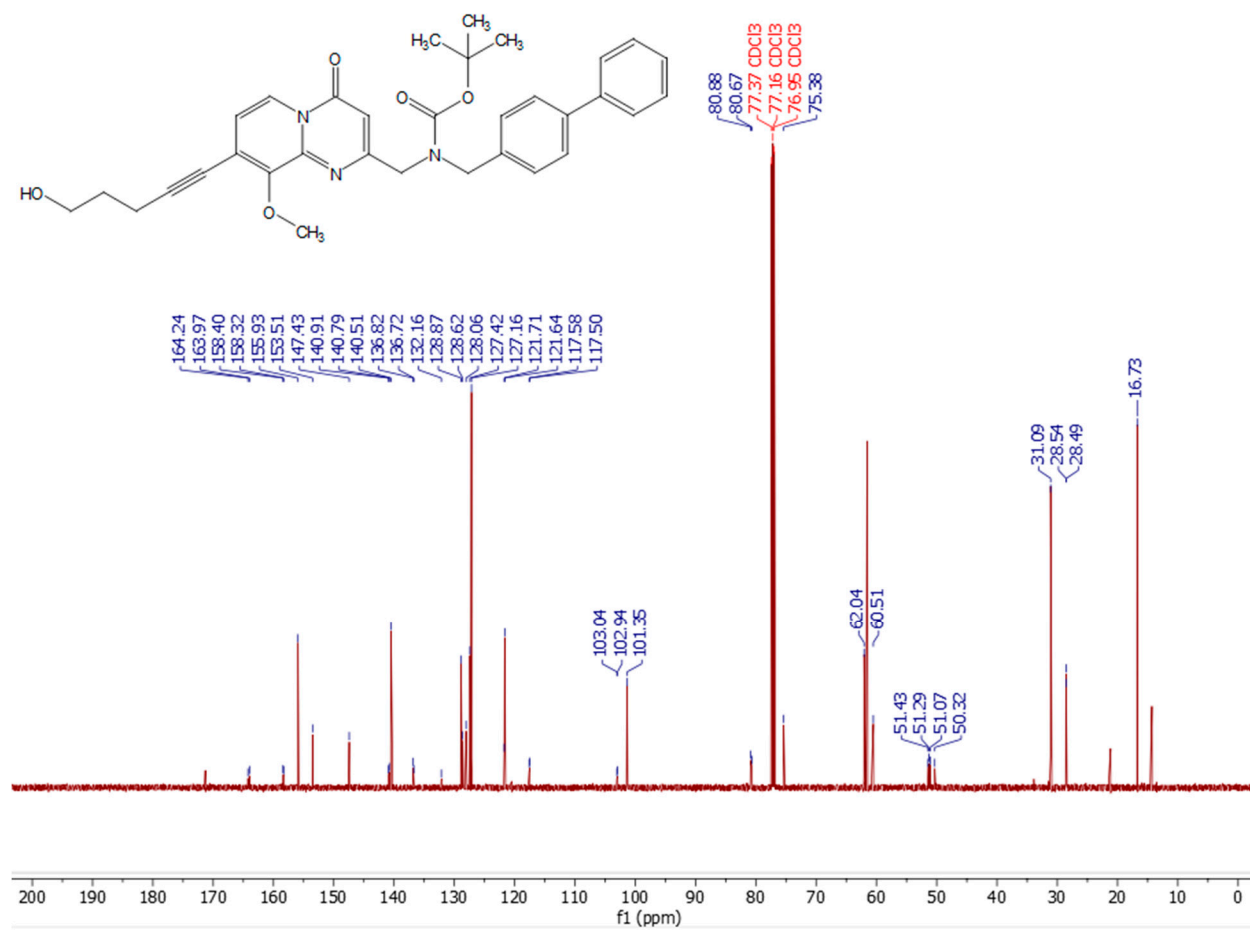
¹³C NMR of **61**



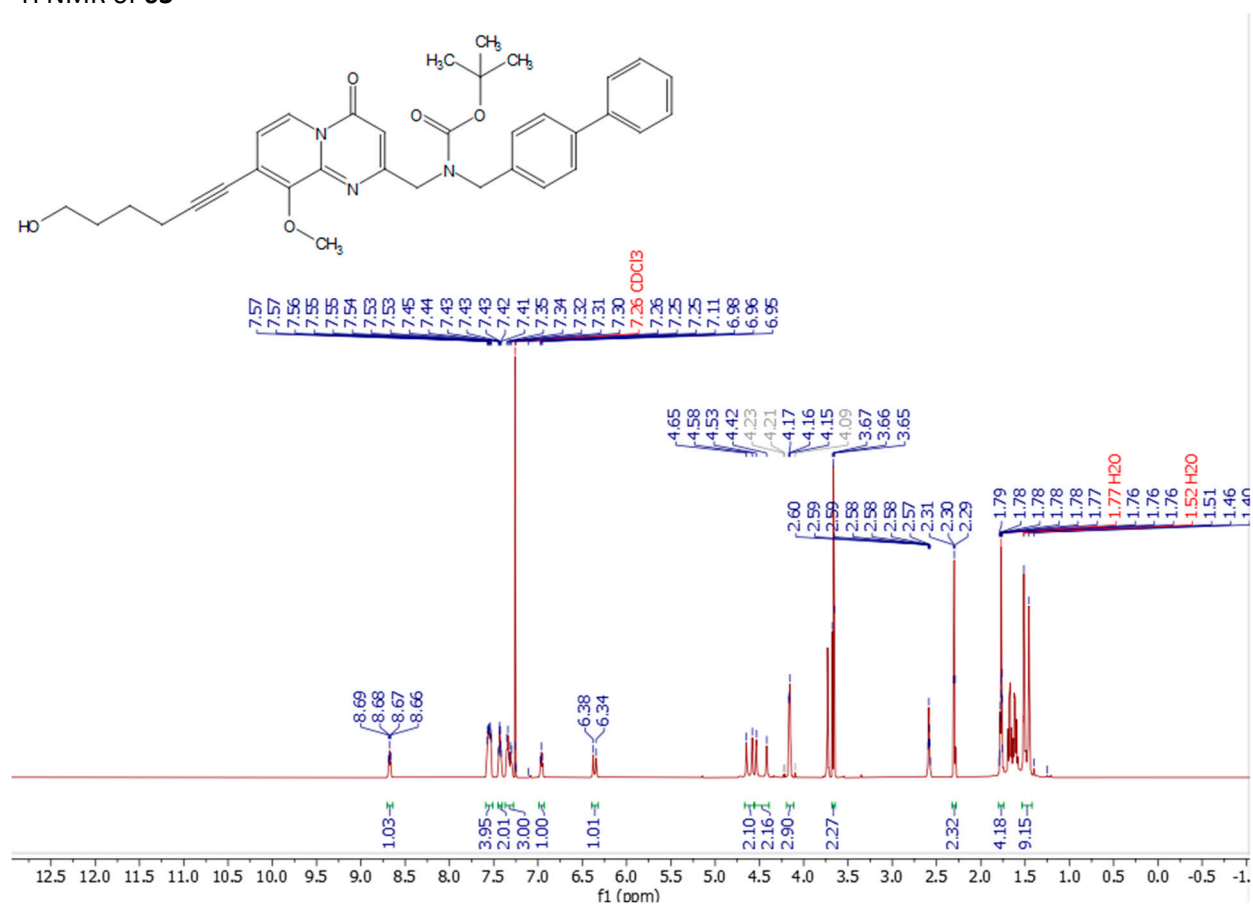
¹H NMR of **62**



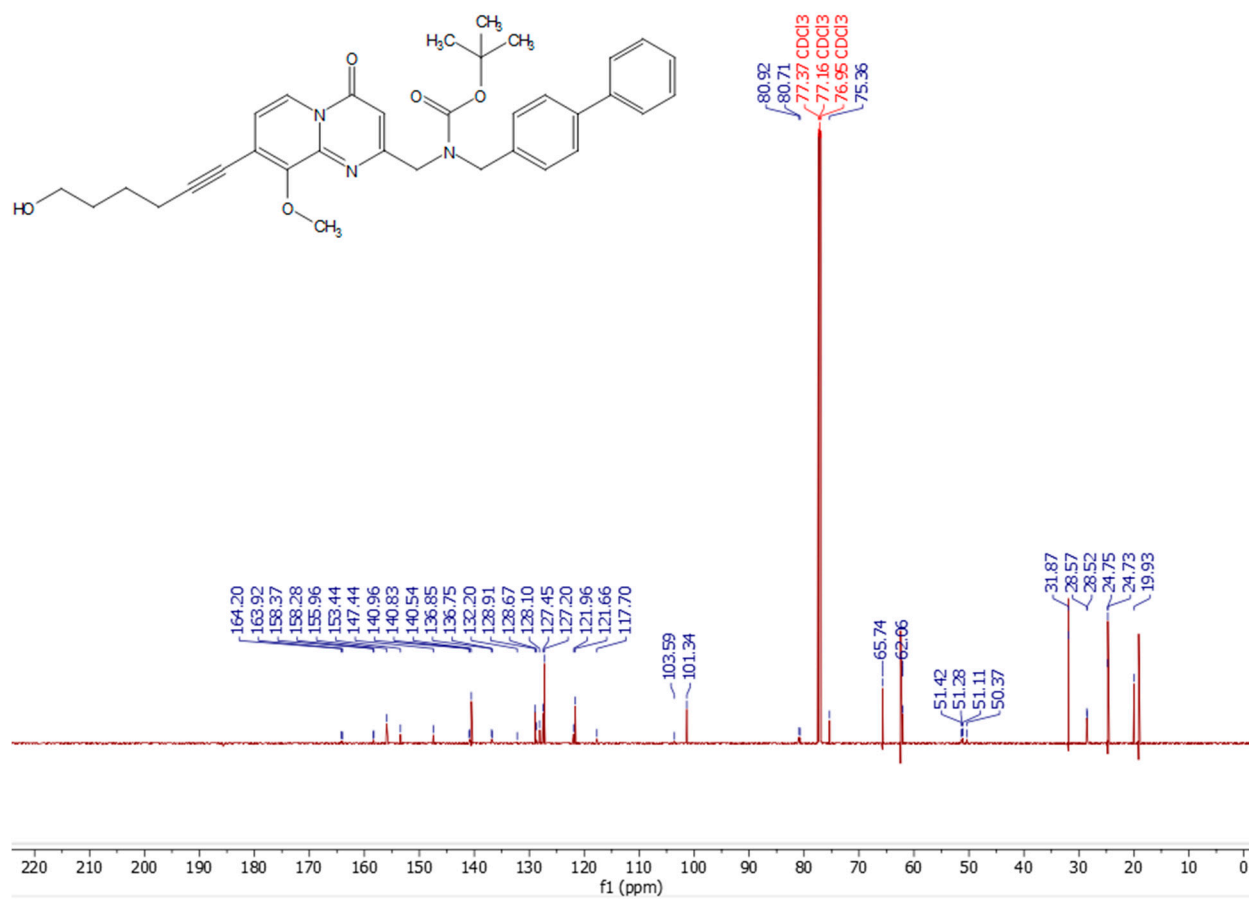
¹³C NMR of **62**



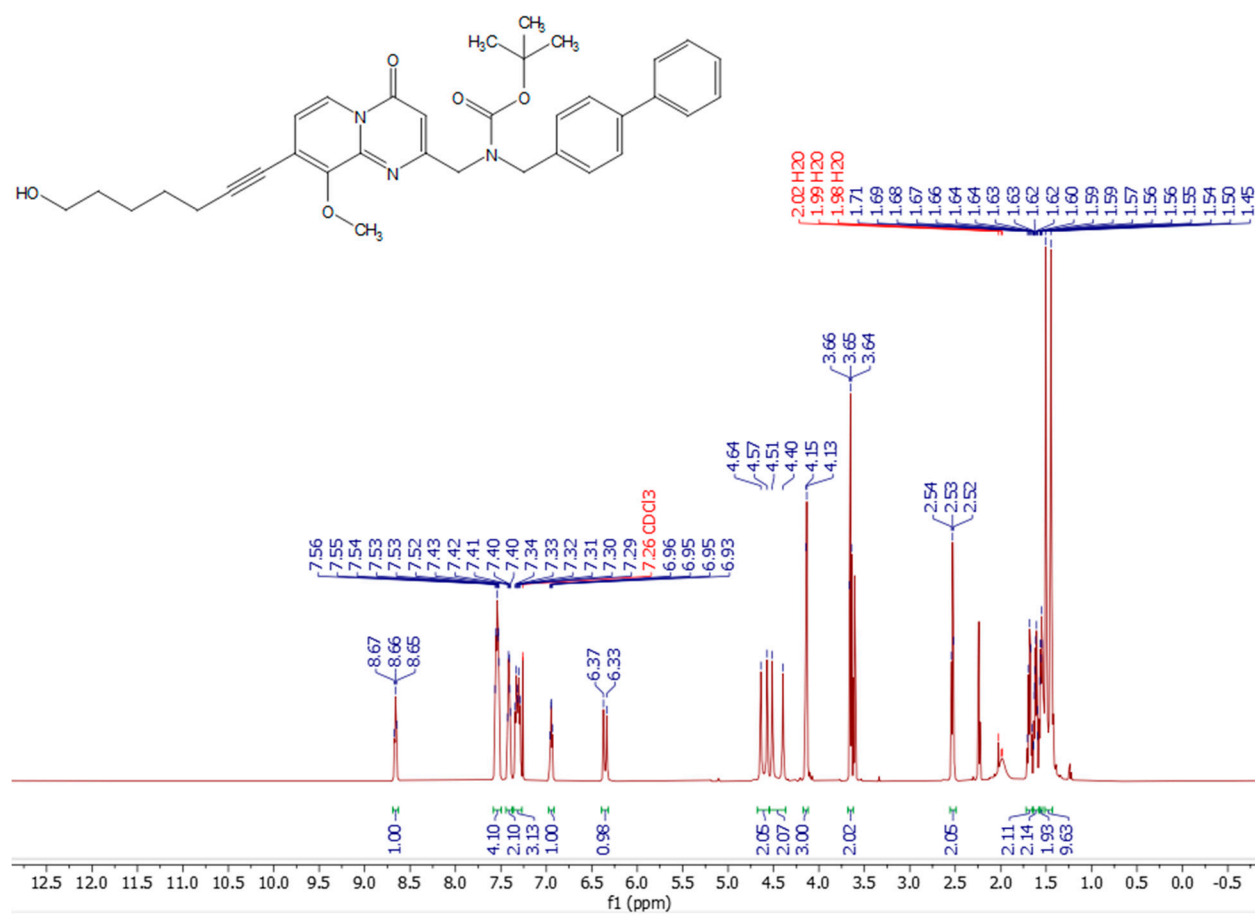
¹H NMR of **63**



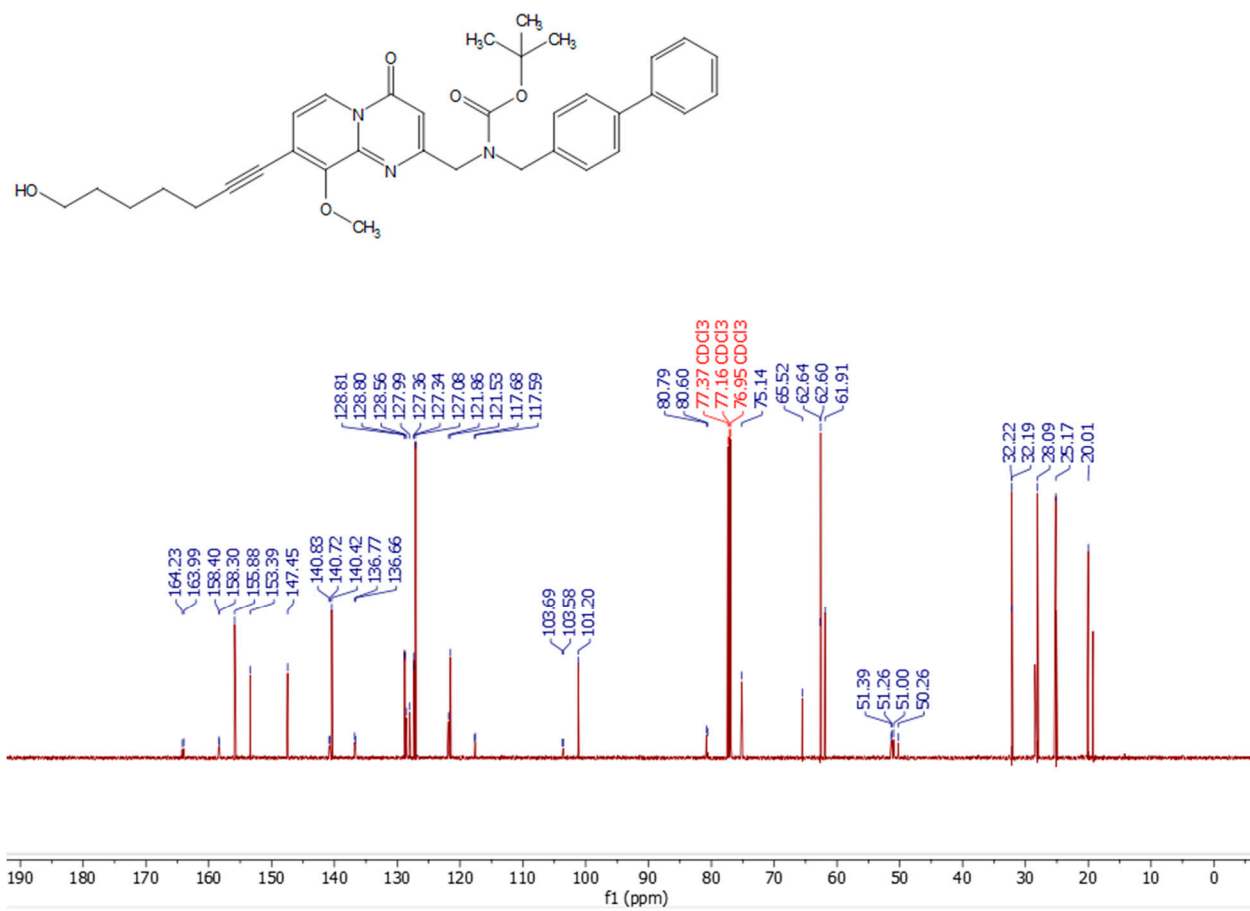
¹³C NMR of **63**



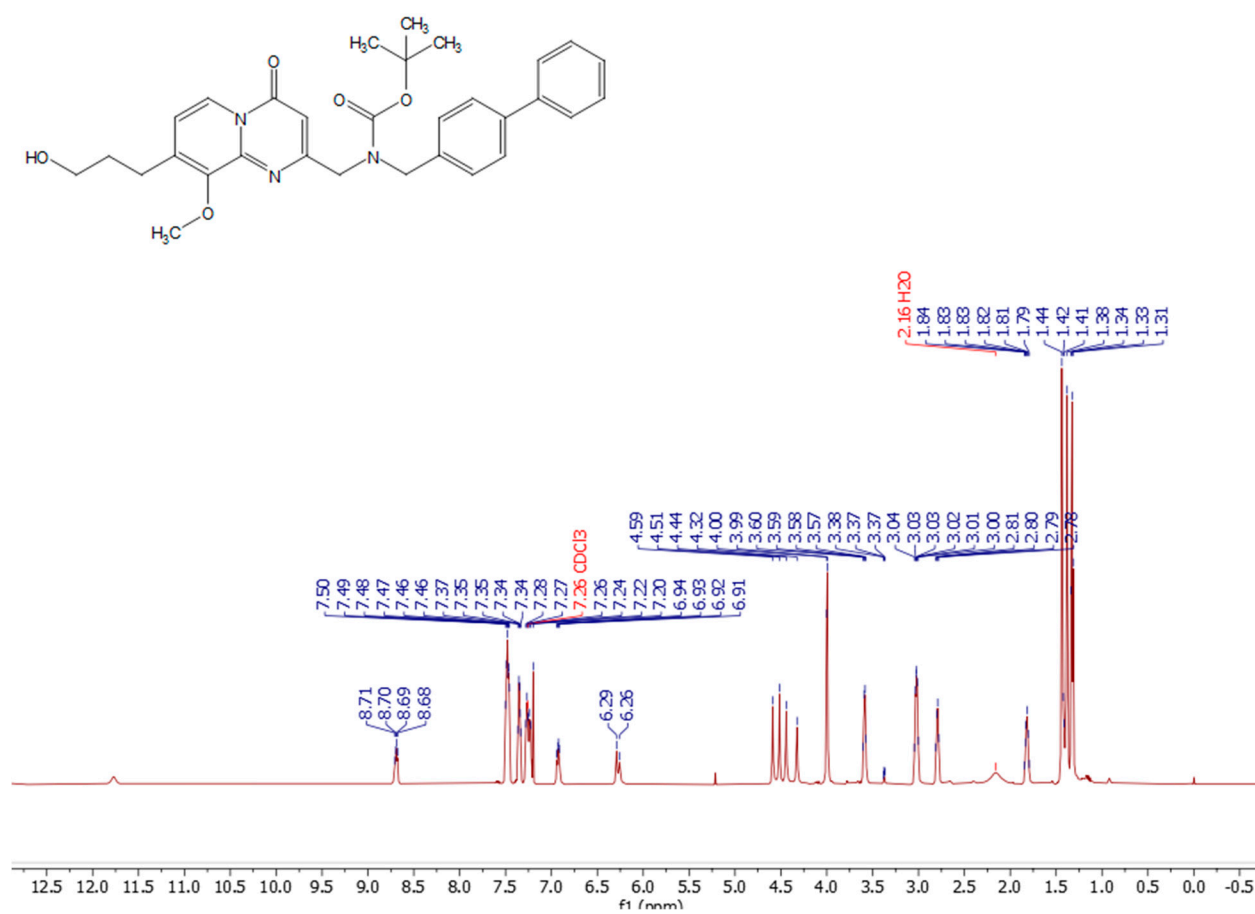
¹H NMR of **64**



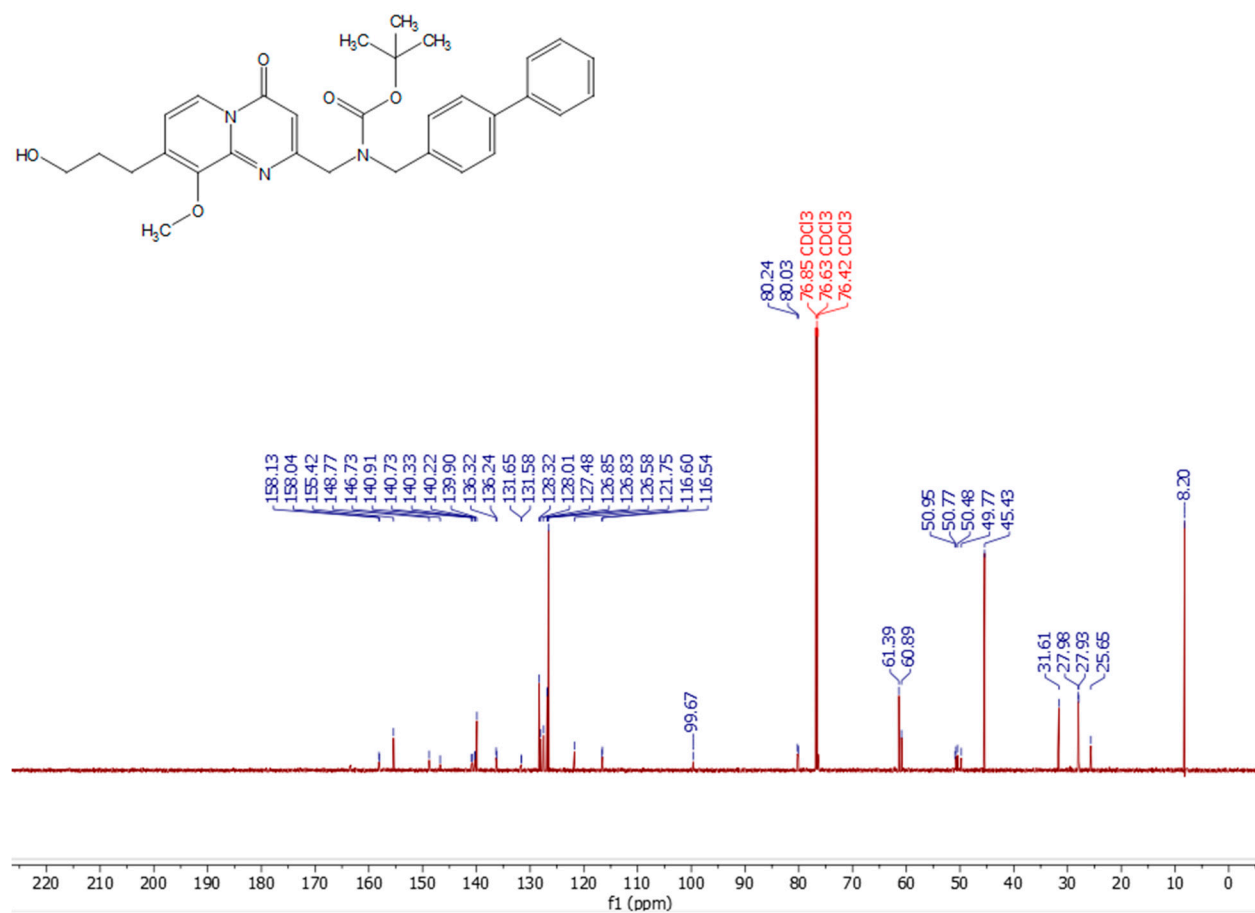
¹³C NMR of **64**



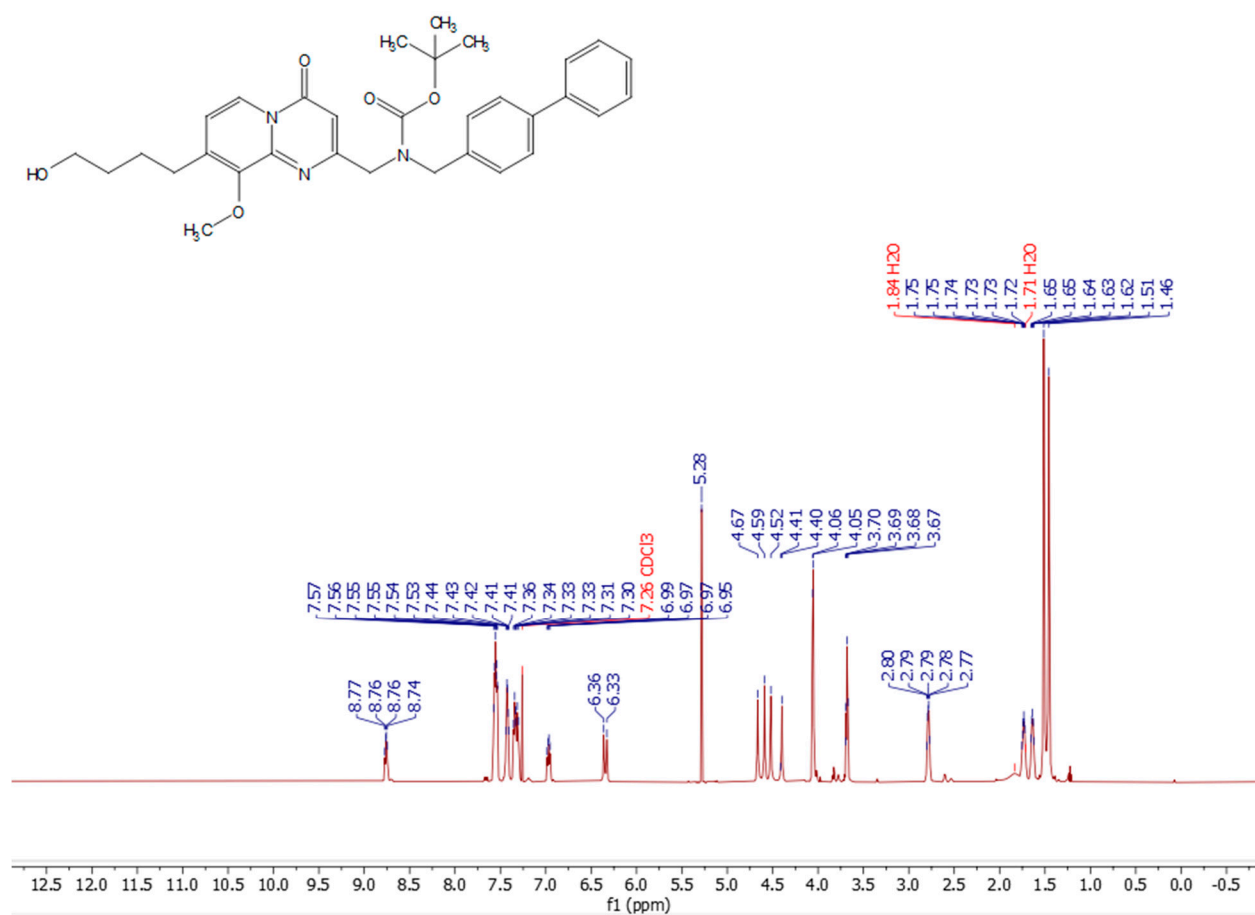
¹H NMR of **65**



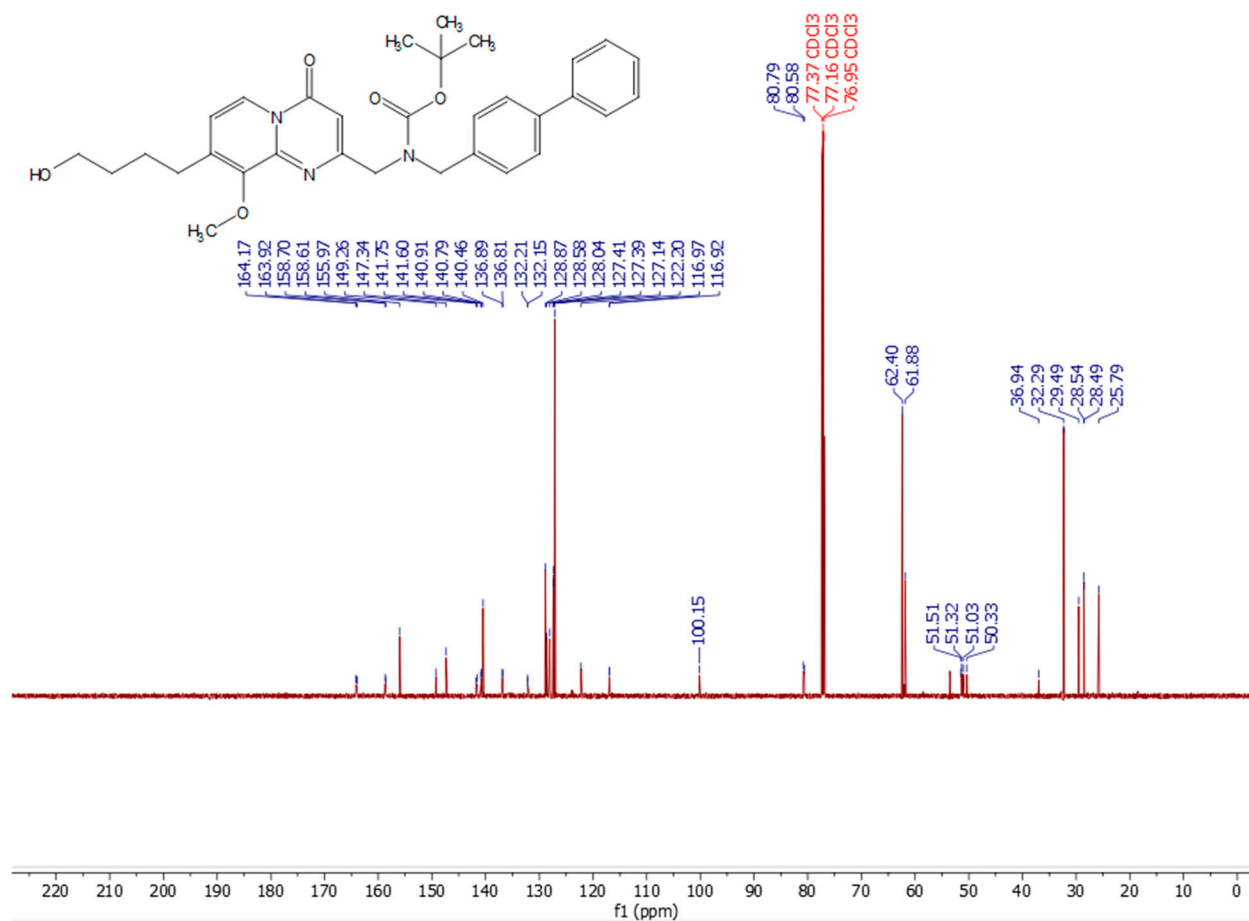
¹³C NMR of **65**



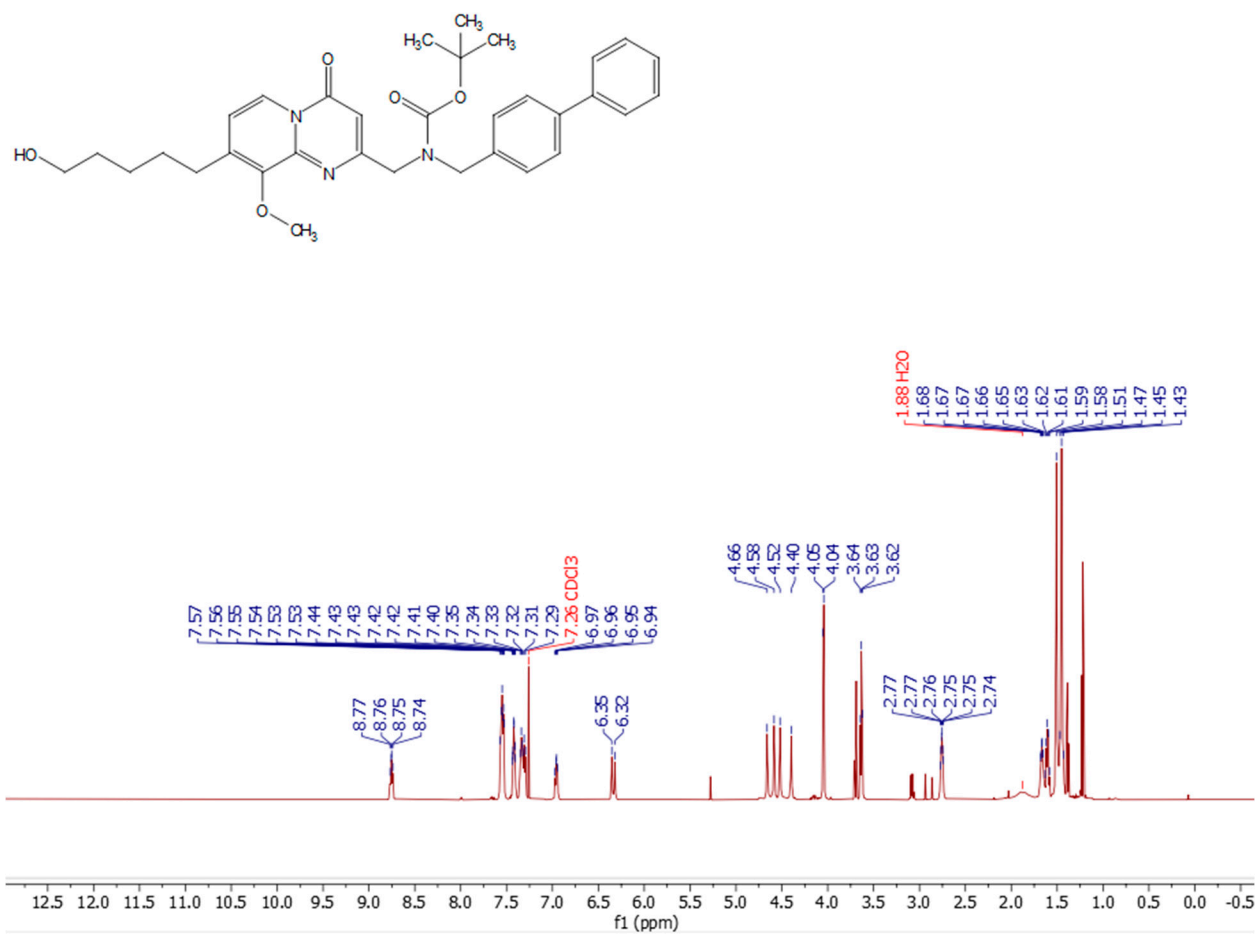
¹H NMR of 66



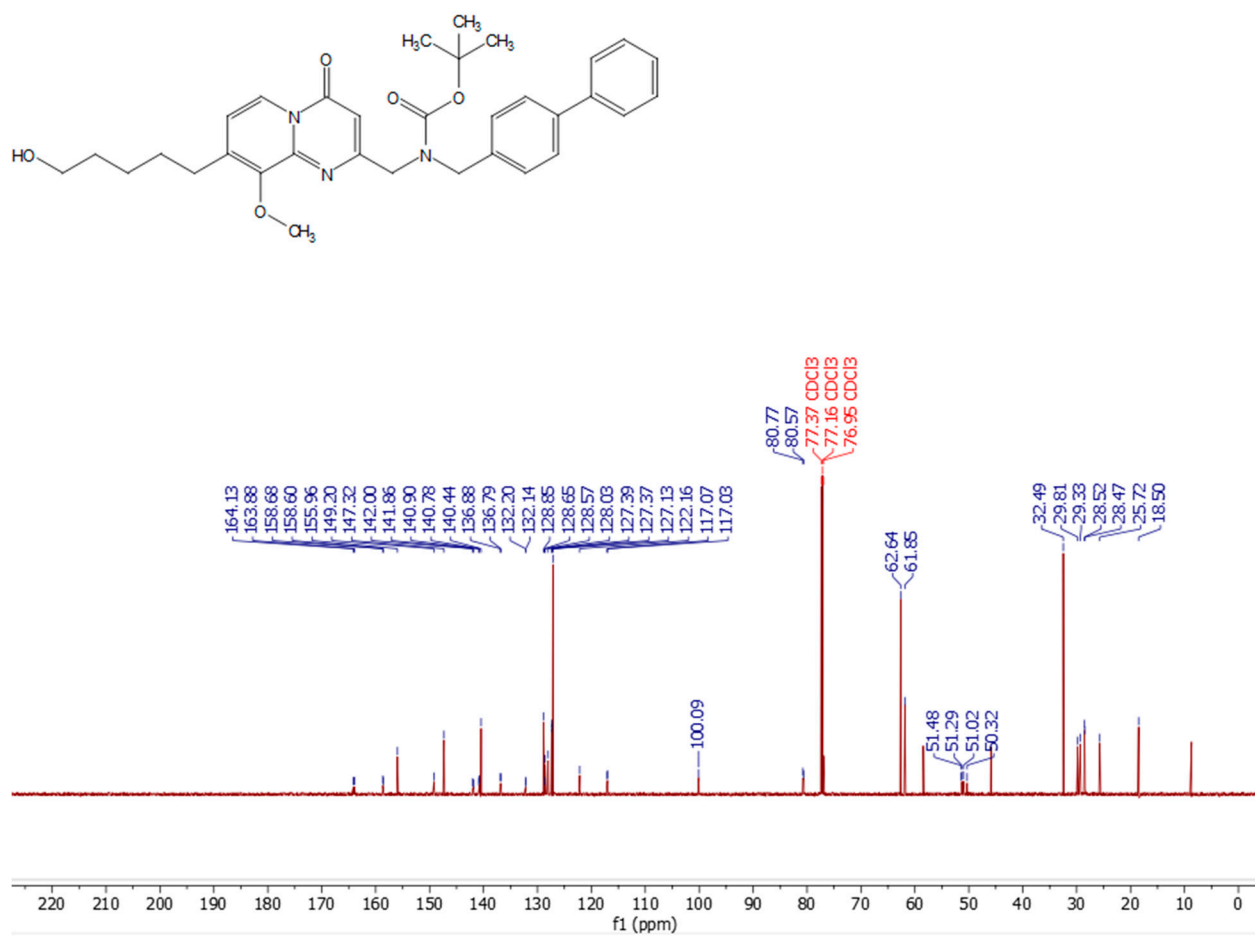
¹³C NMR of **66**



¹H NMR of **67**

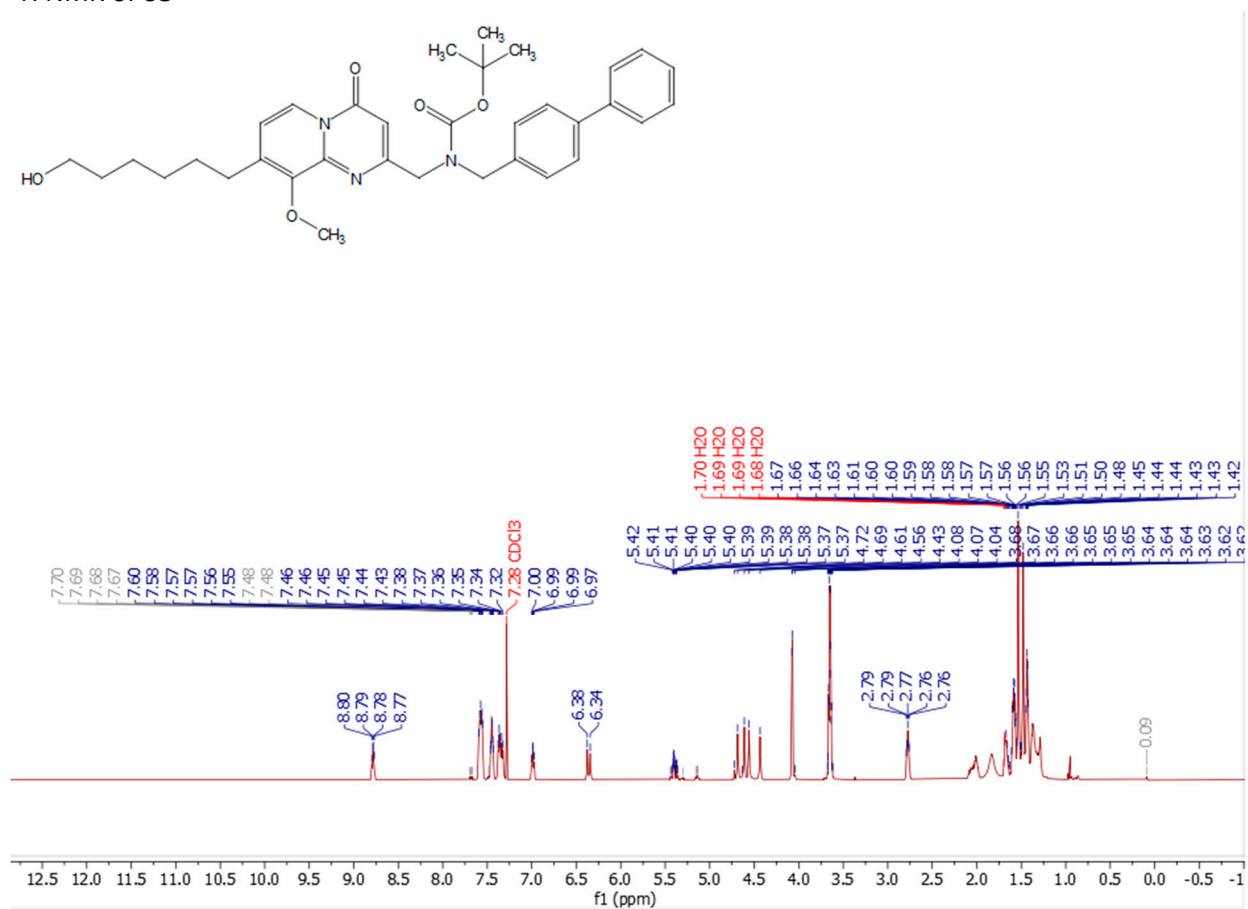


¹³C NMR of **67**

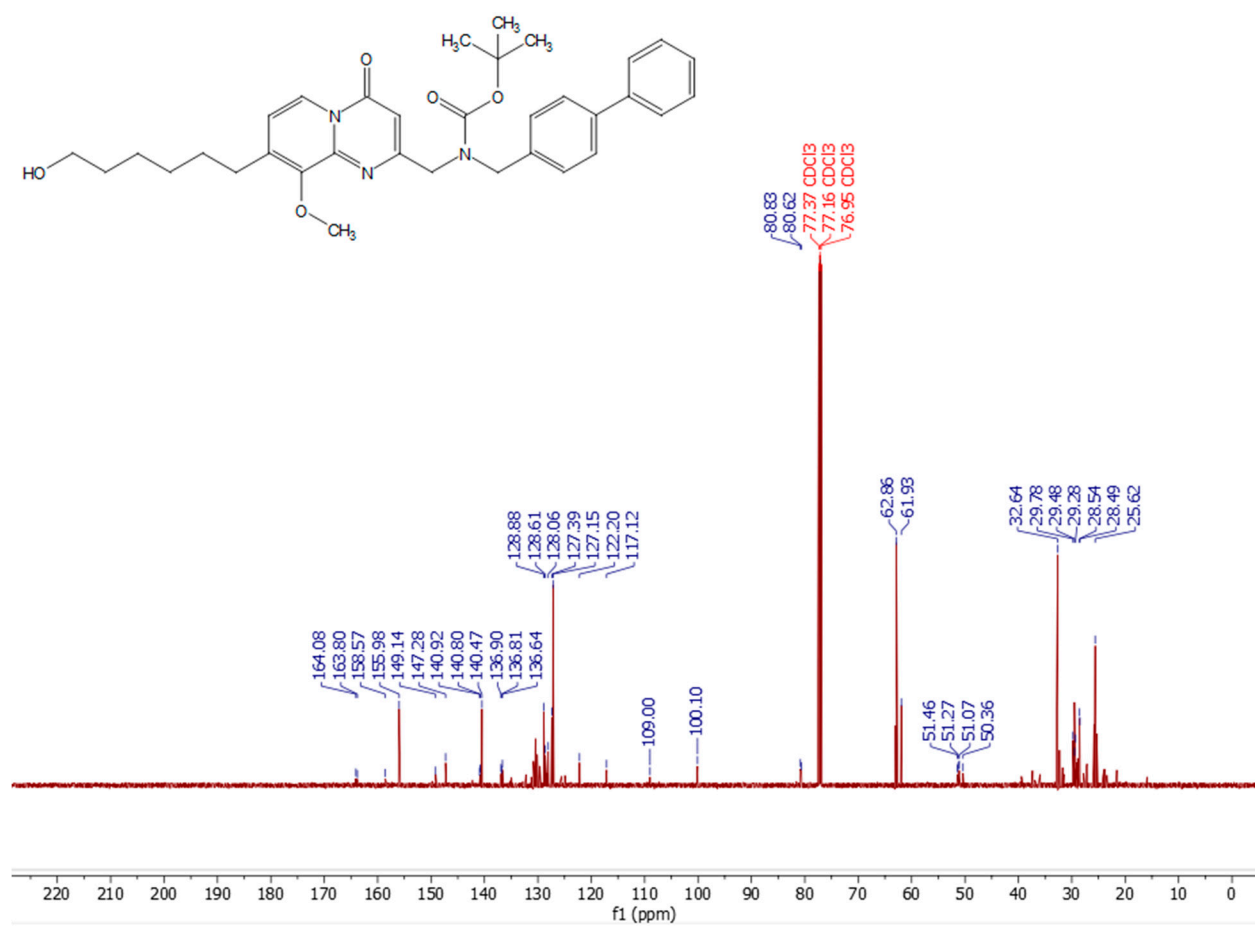


CCCCCCCCc1cc(OC)c2nc(CN(Cc3ccc(cc3)C(=O)OC(C)(C)C)c4ccccc4)c(=O)n2

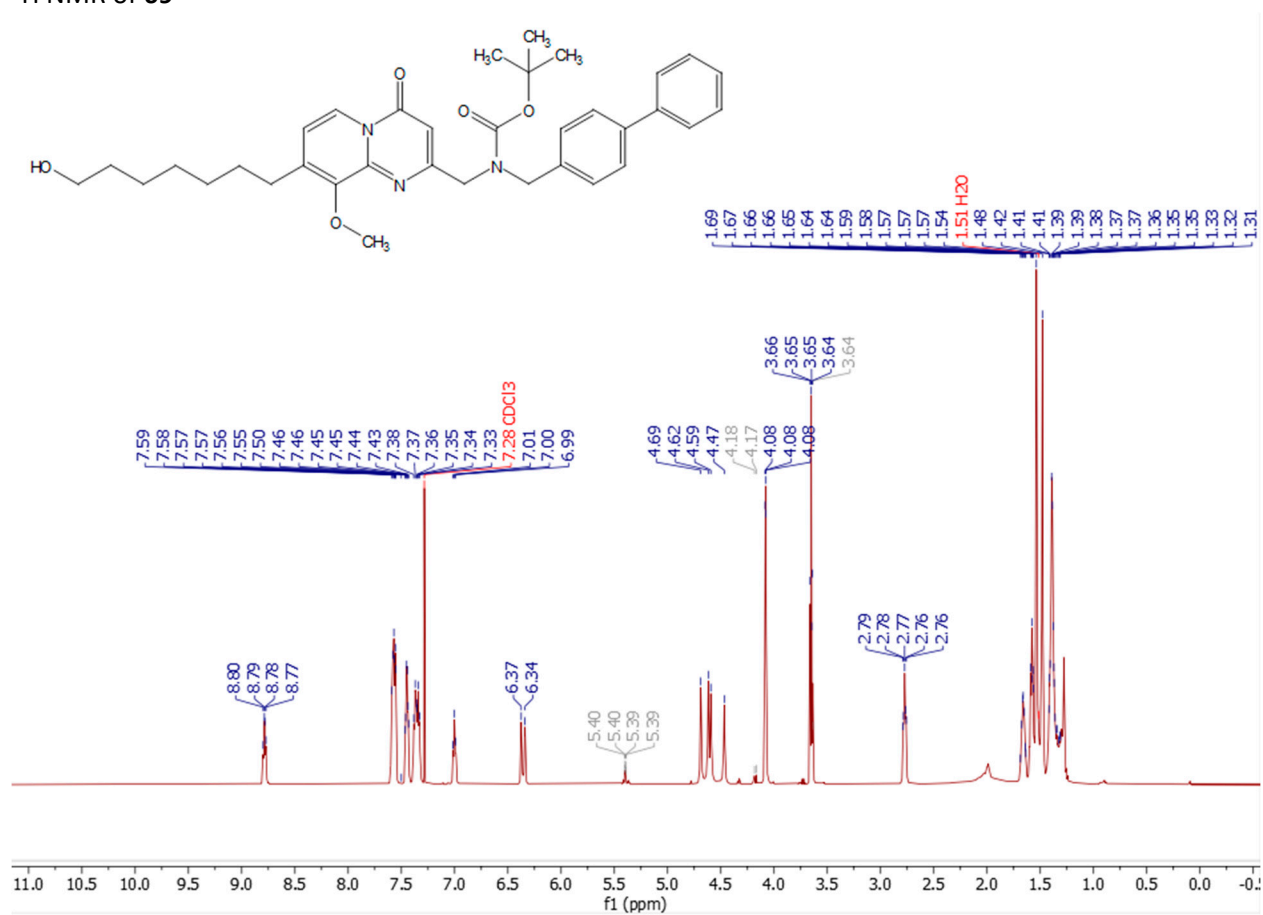
¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks from 1.42 to 7.70 ppm. Key features include a triplet at 7.32 ppm (7.28 CDCl₃), a multiplet at 7.40-7.60 ppm, a doublet at 8.78 ppm (8.80, 8.77), a doublet at 6.34 ppm (6.38), a multiplet at 3.60-3.70 ppm, a multiplet at 1.60-1.70 ppm (1.68 H₂O), and a multiplet at 1.40-1.50 ppm (1.69 H₂O). Integration values are shown below the peaks.



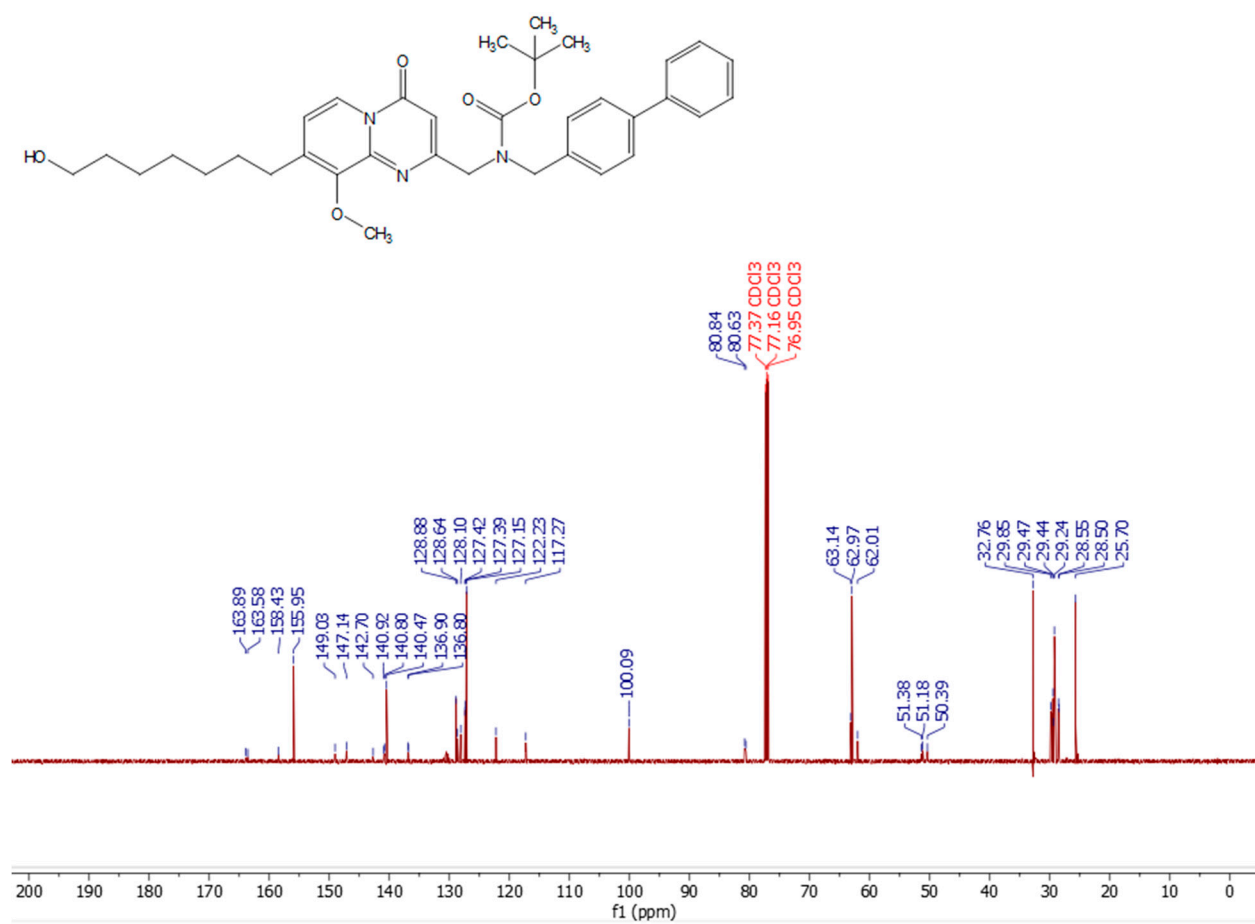
¹³C NMR of **68**



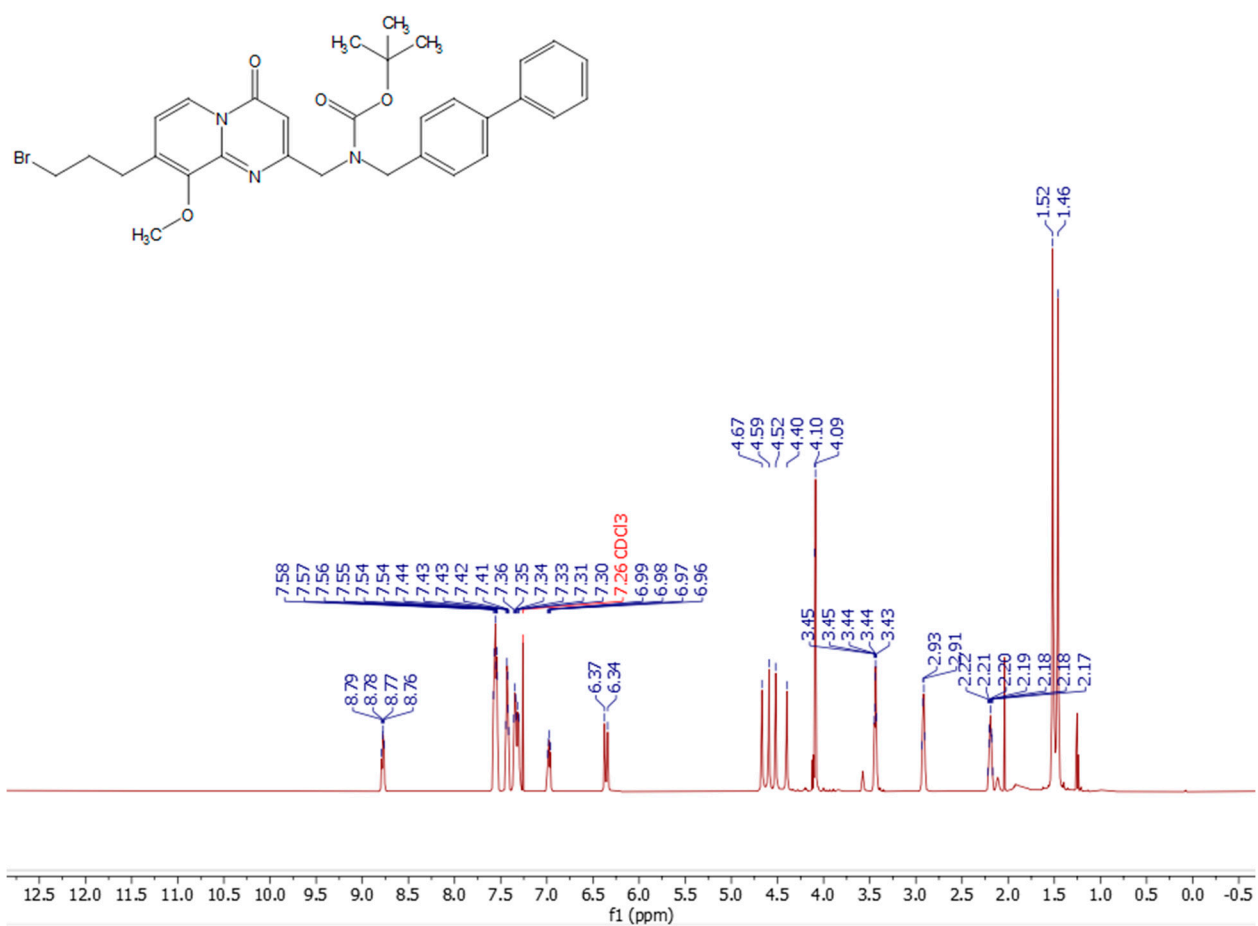
¹H NMR of 69



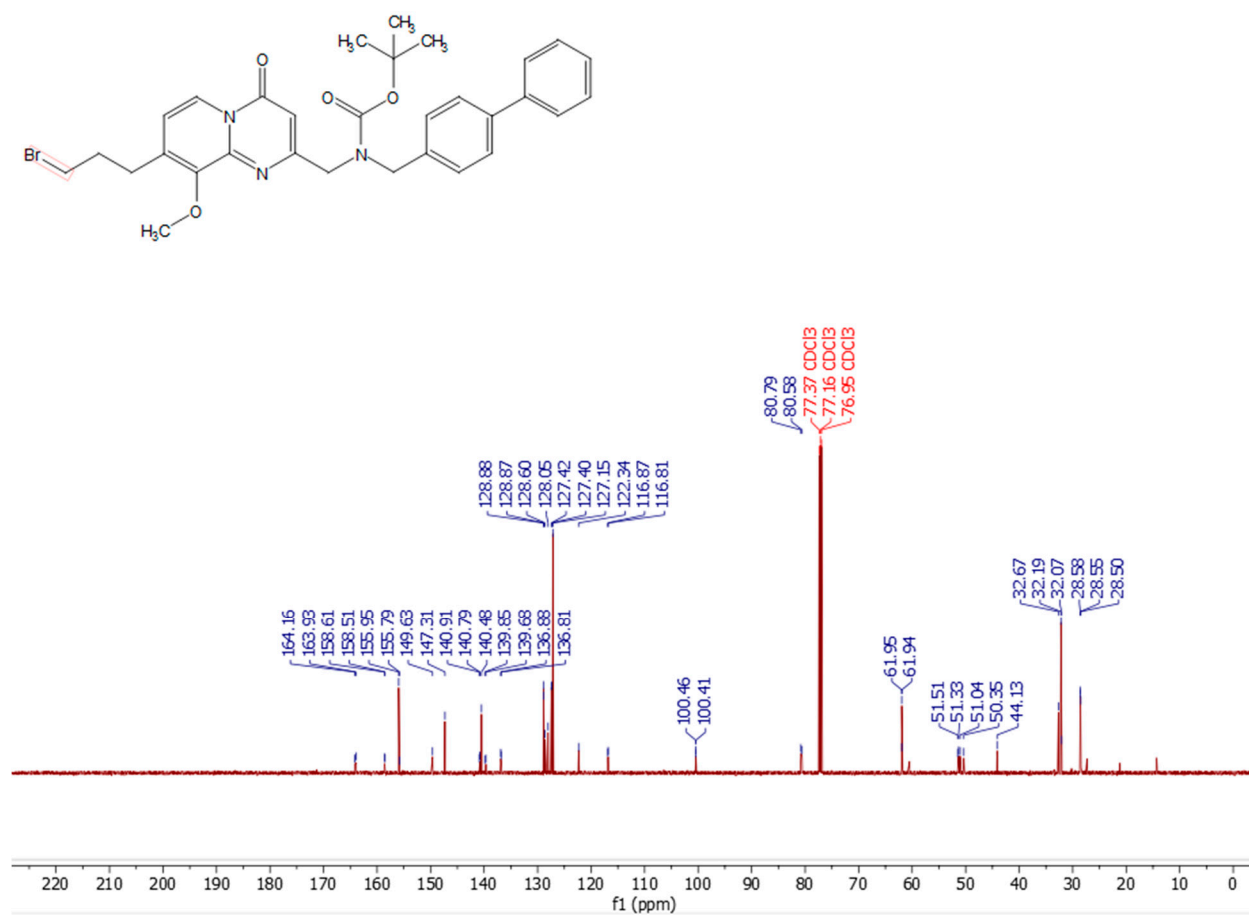
¹³C NMR of **69**



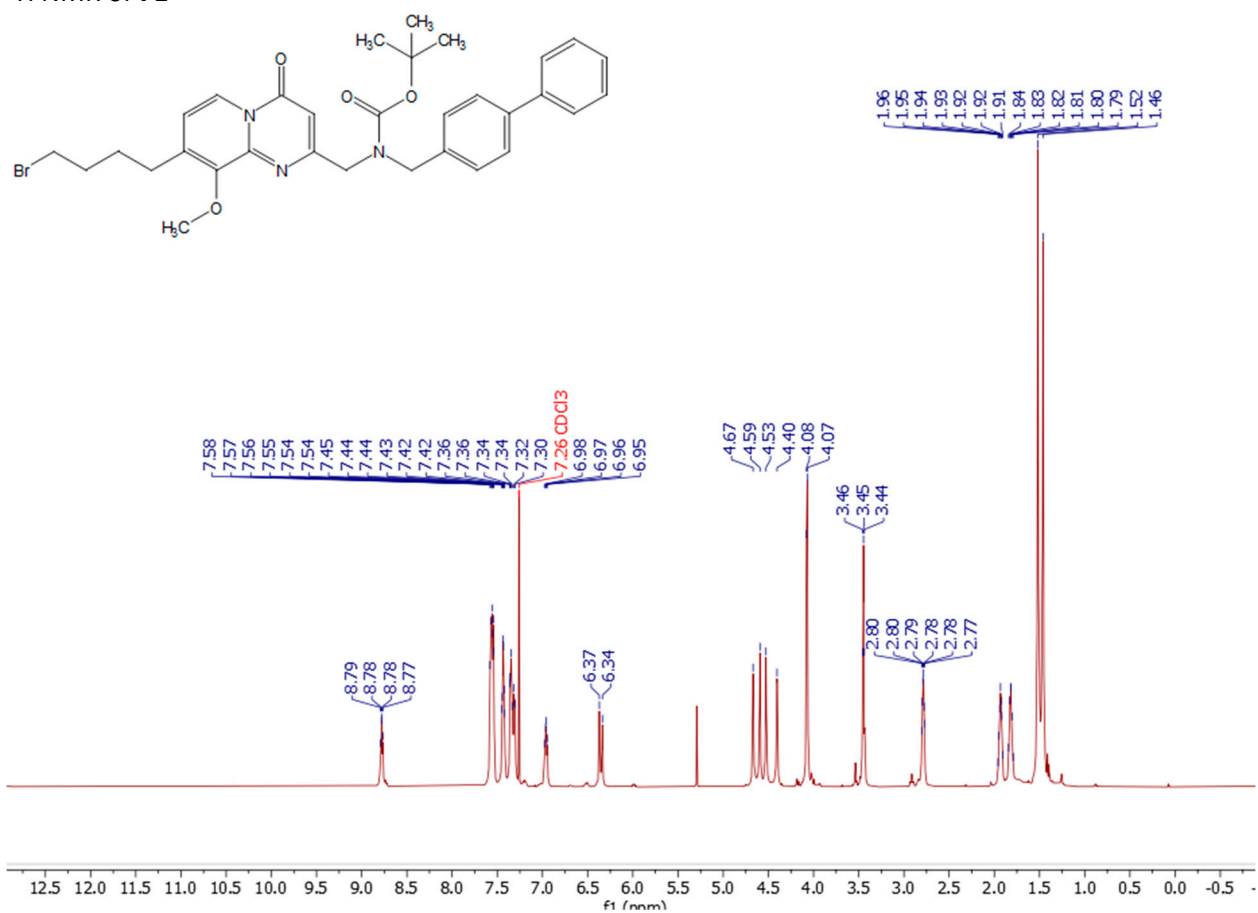
¹H NMR of **70**



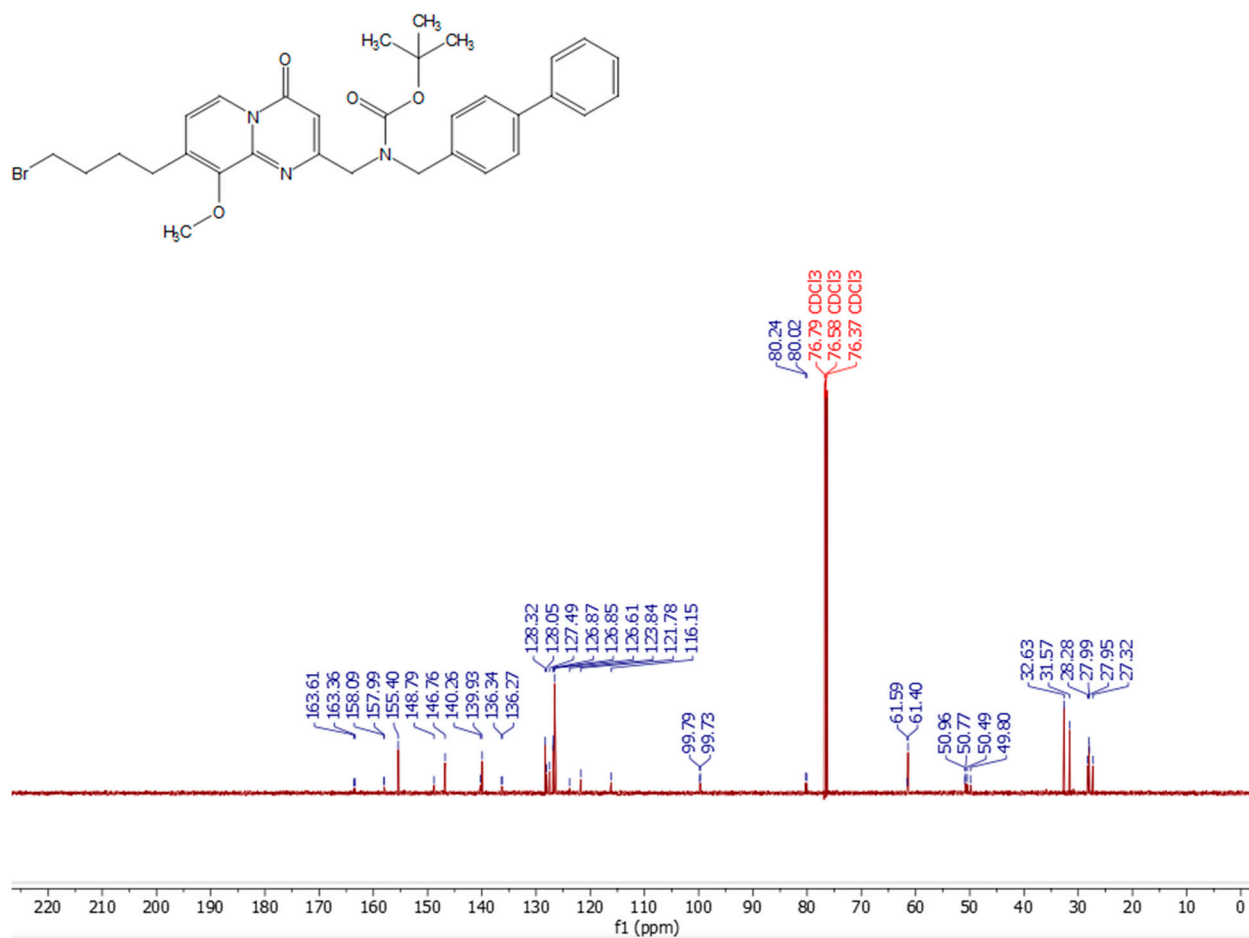
¹³C NMR of **70**



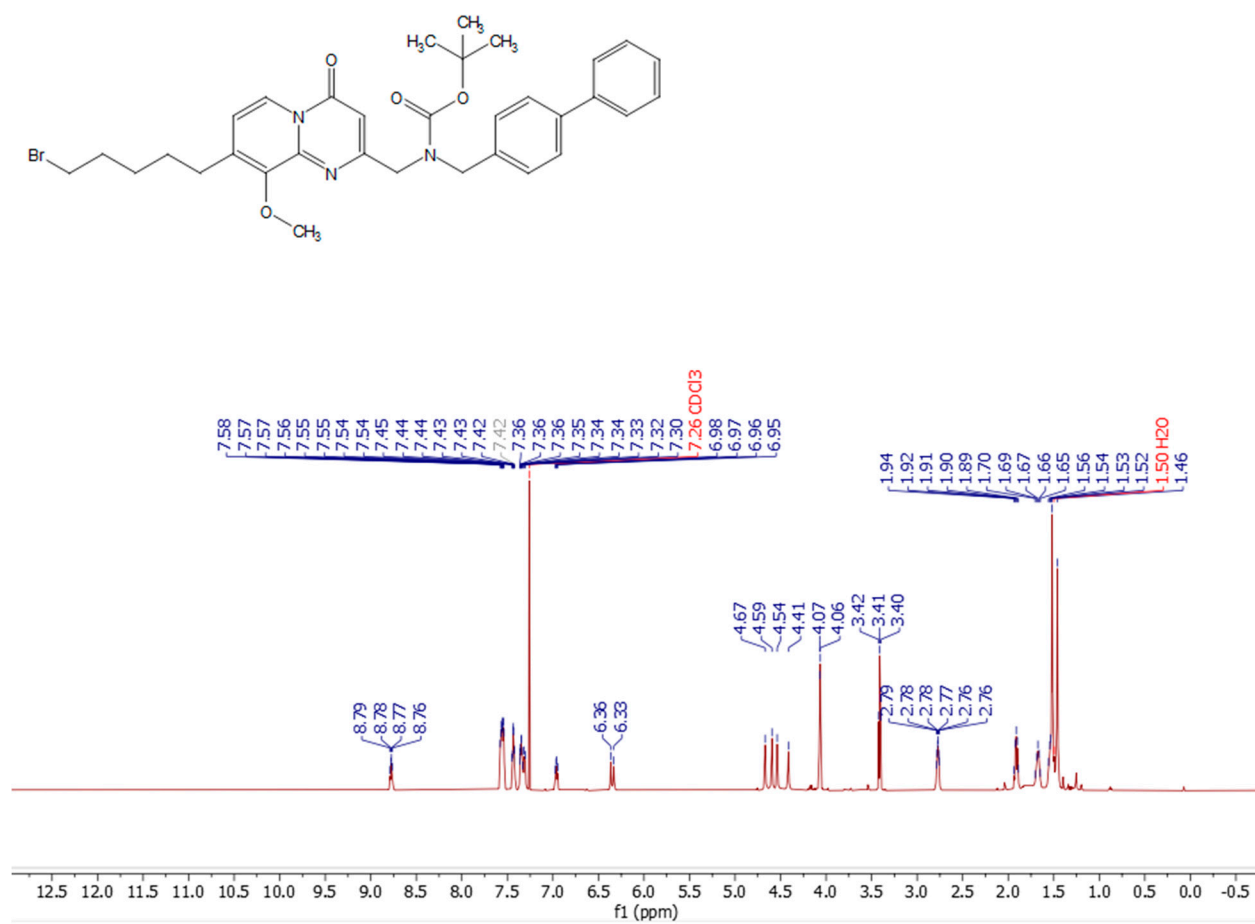
¹H NMR of **71**



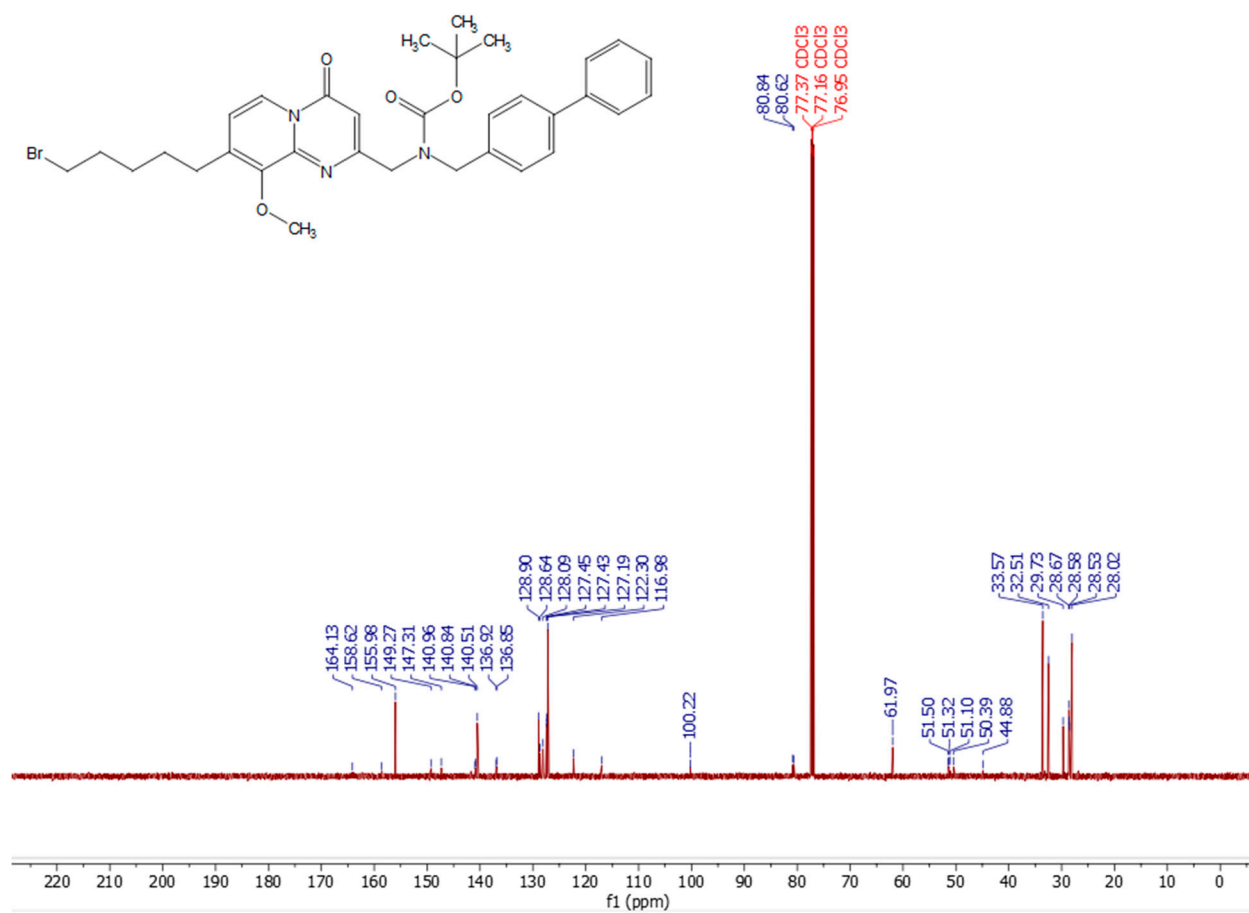
¹³C NMR of **71**



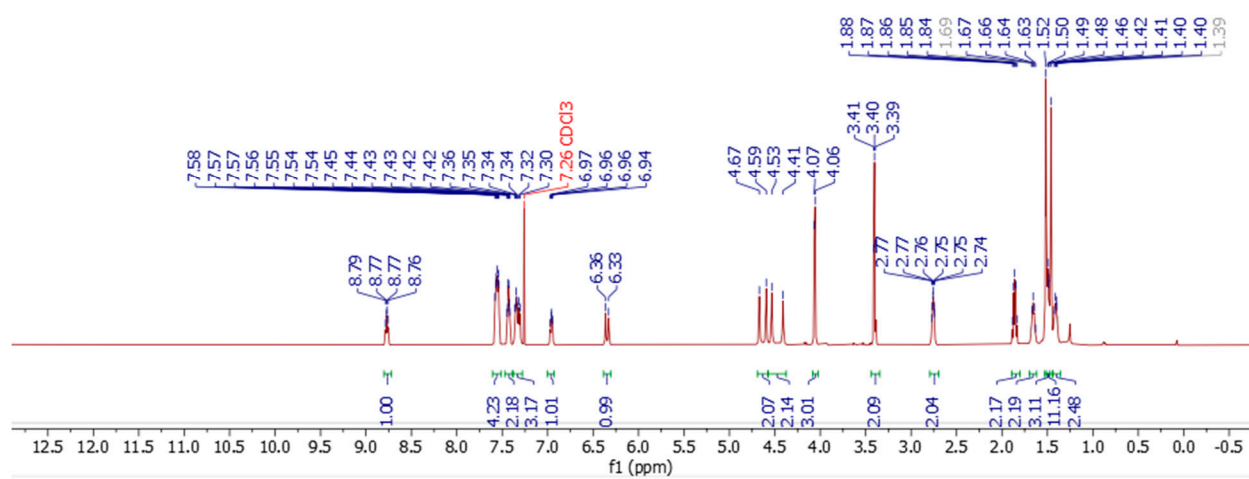
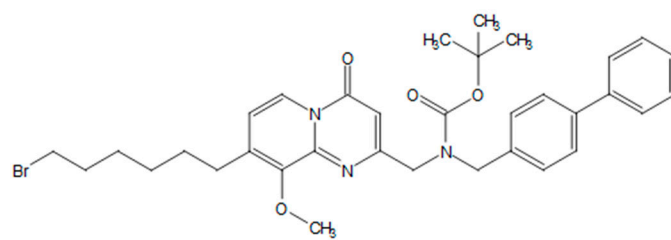
¹H NMR of **72**



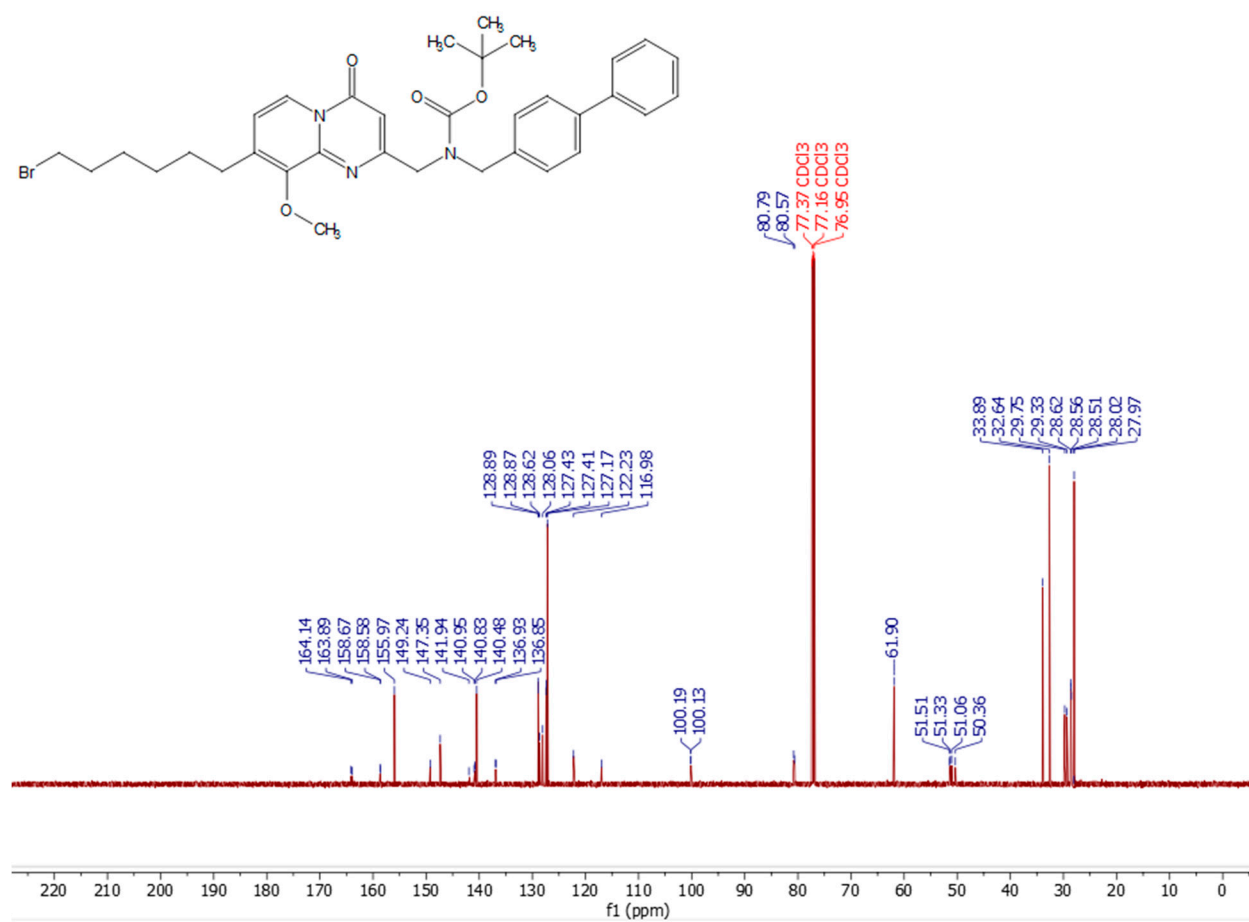
^{13}C NMR of **72**



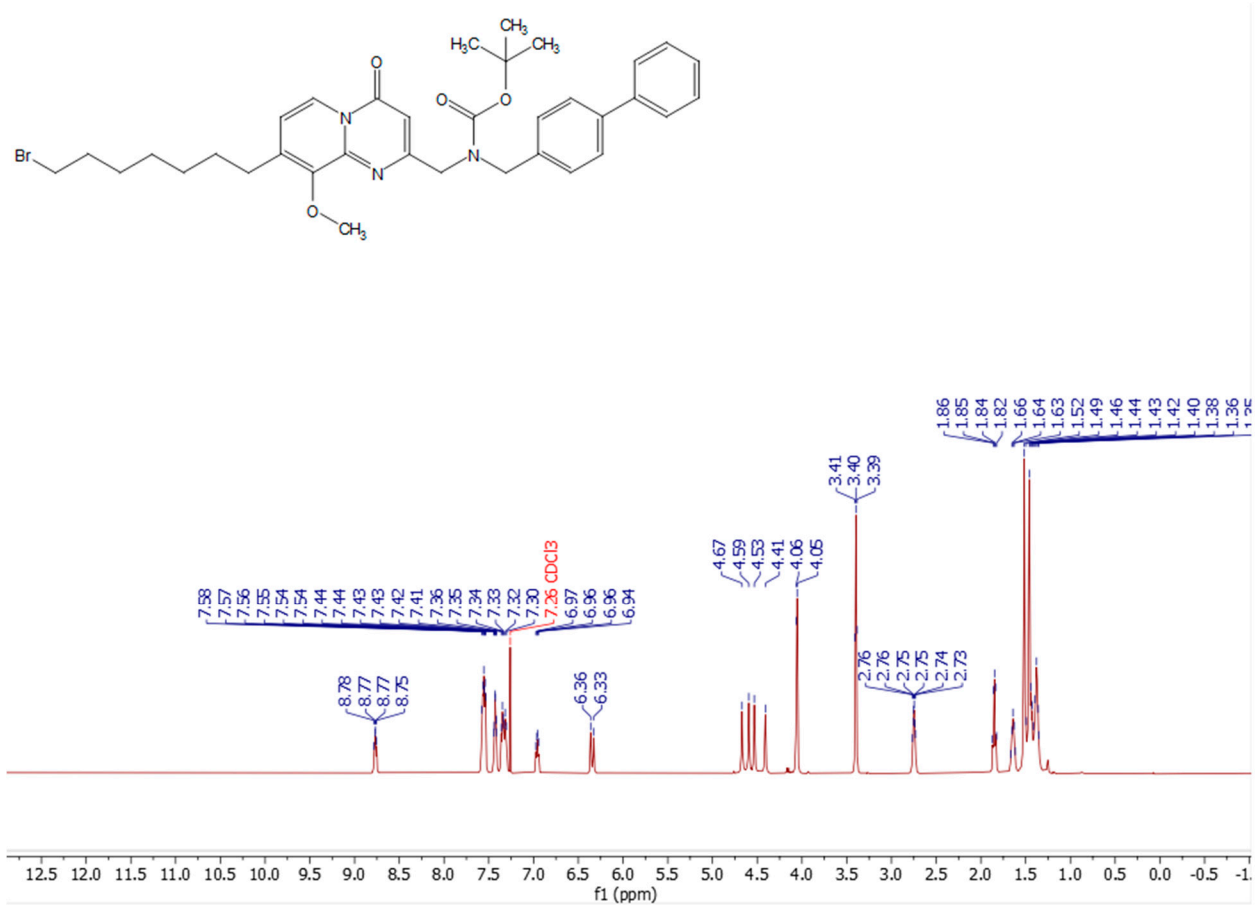
¹H NMR of **73**



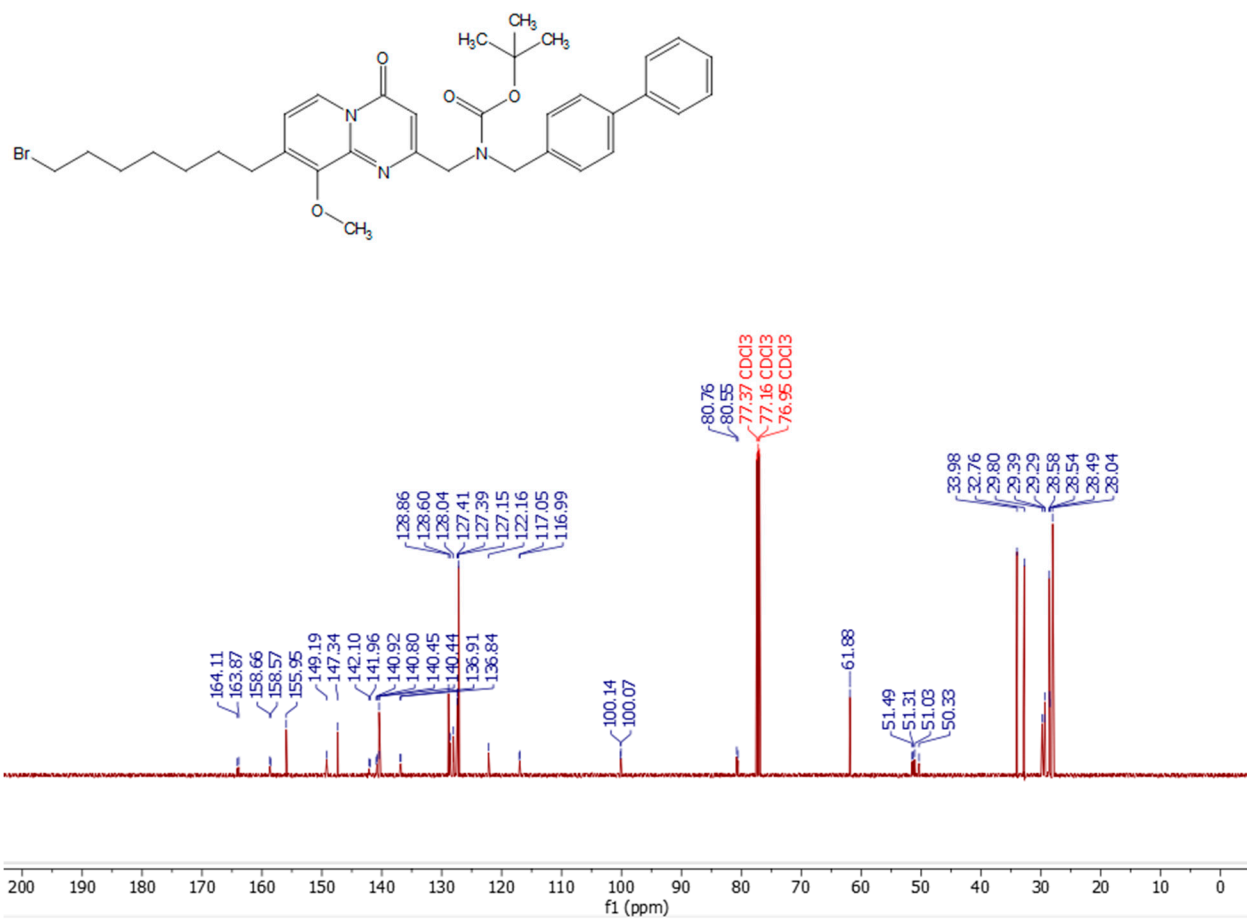
¹³C NMR of **73**

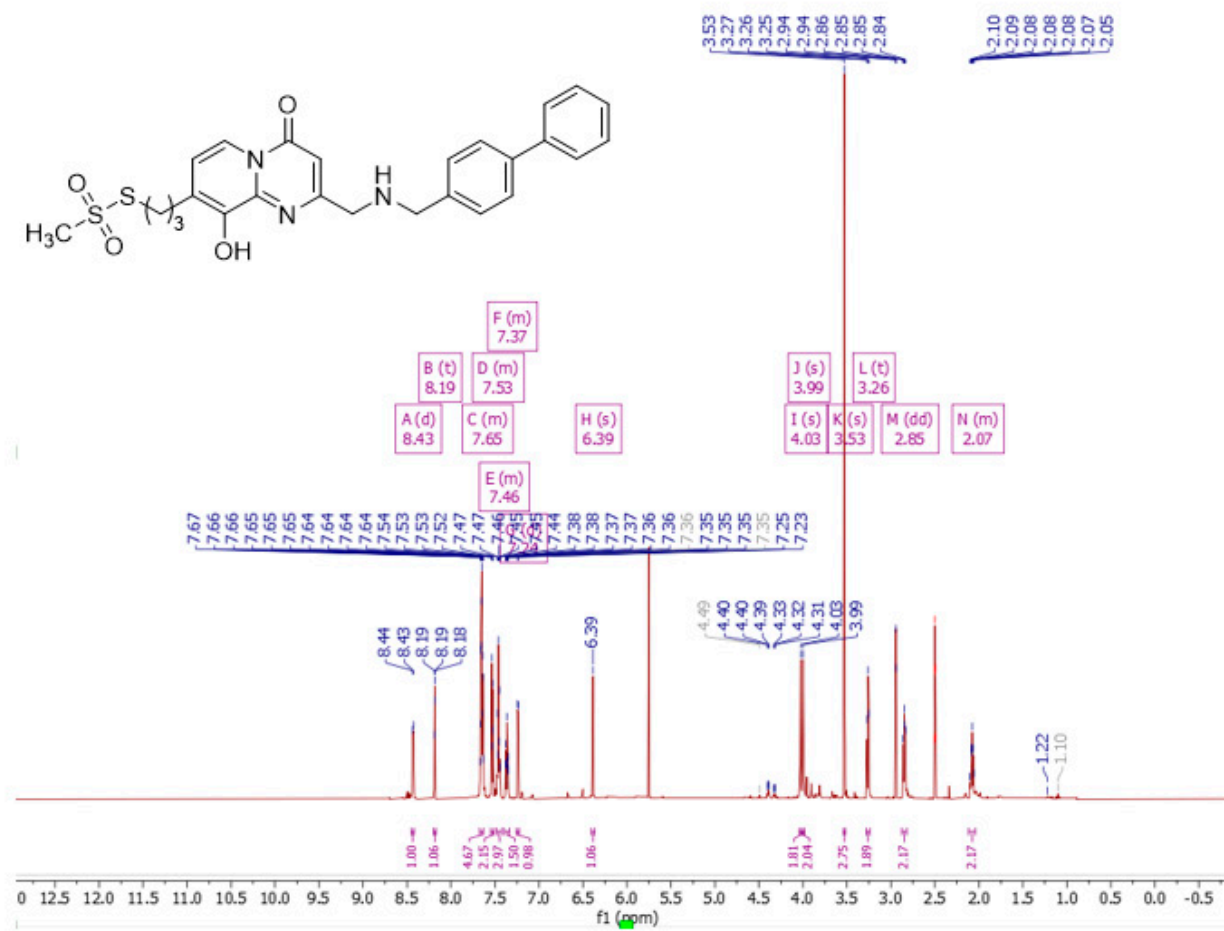


¹H NMR of **74**

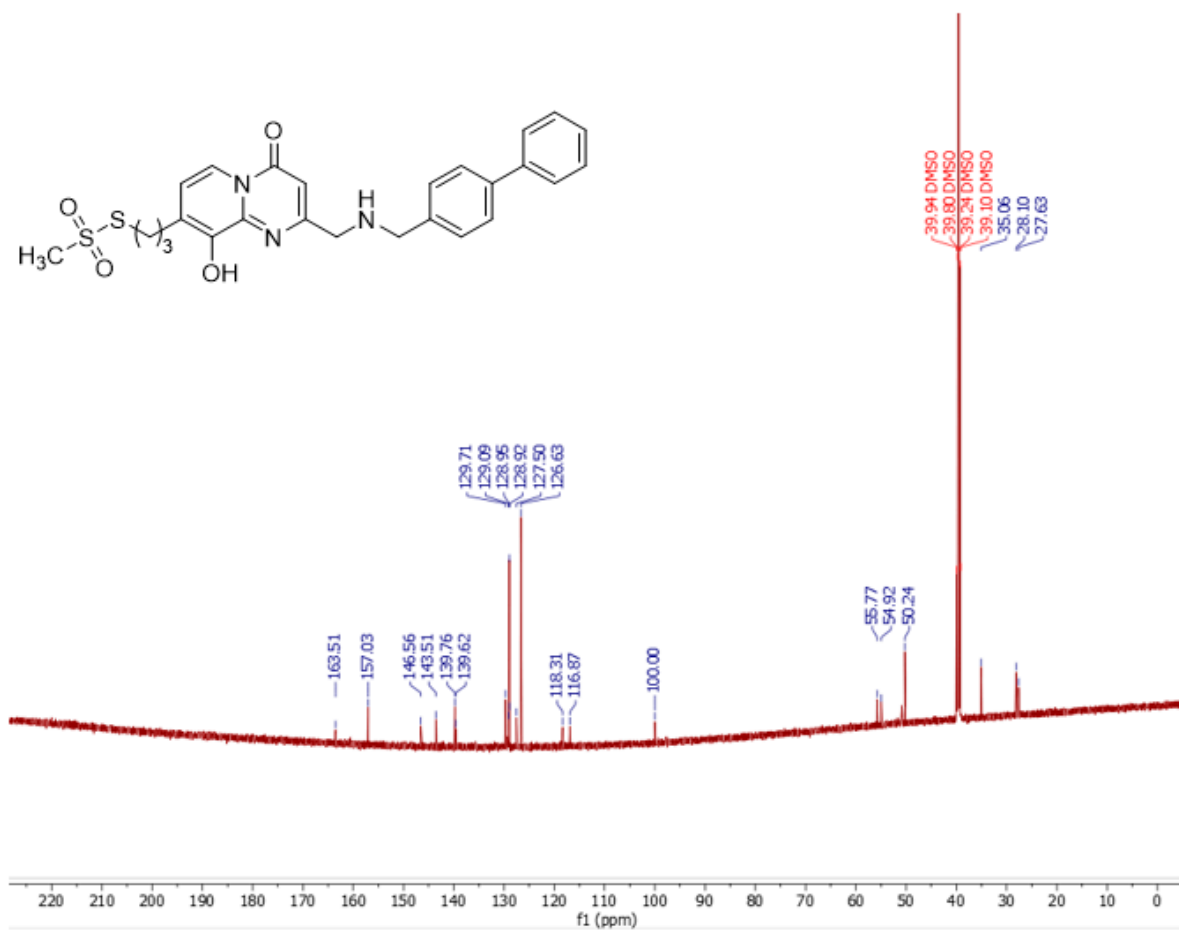


¹³C NMR of **74**

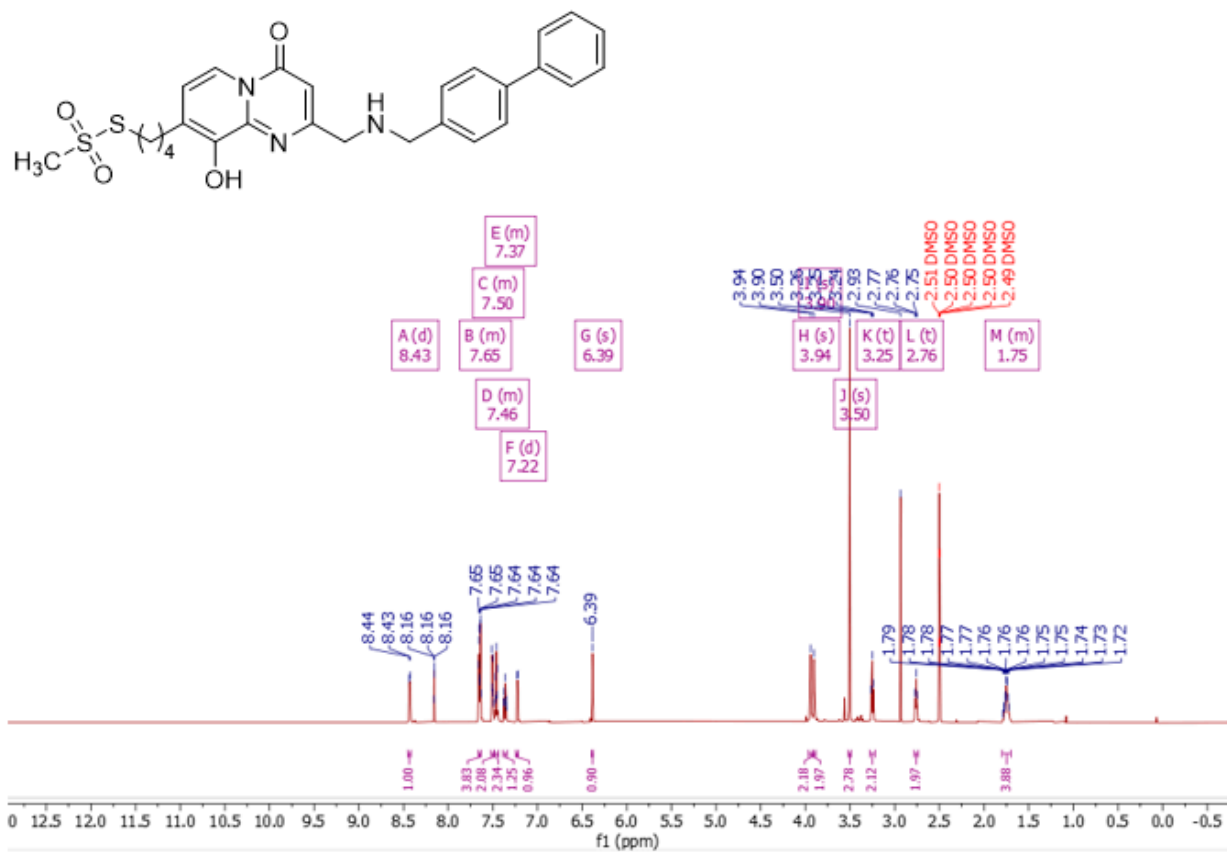


¹H NMR of **80**

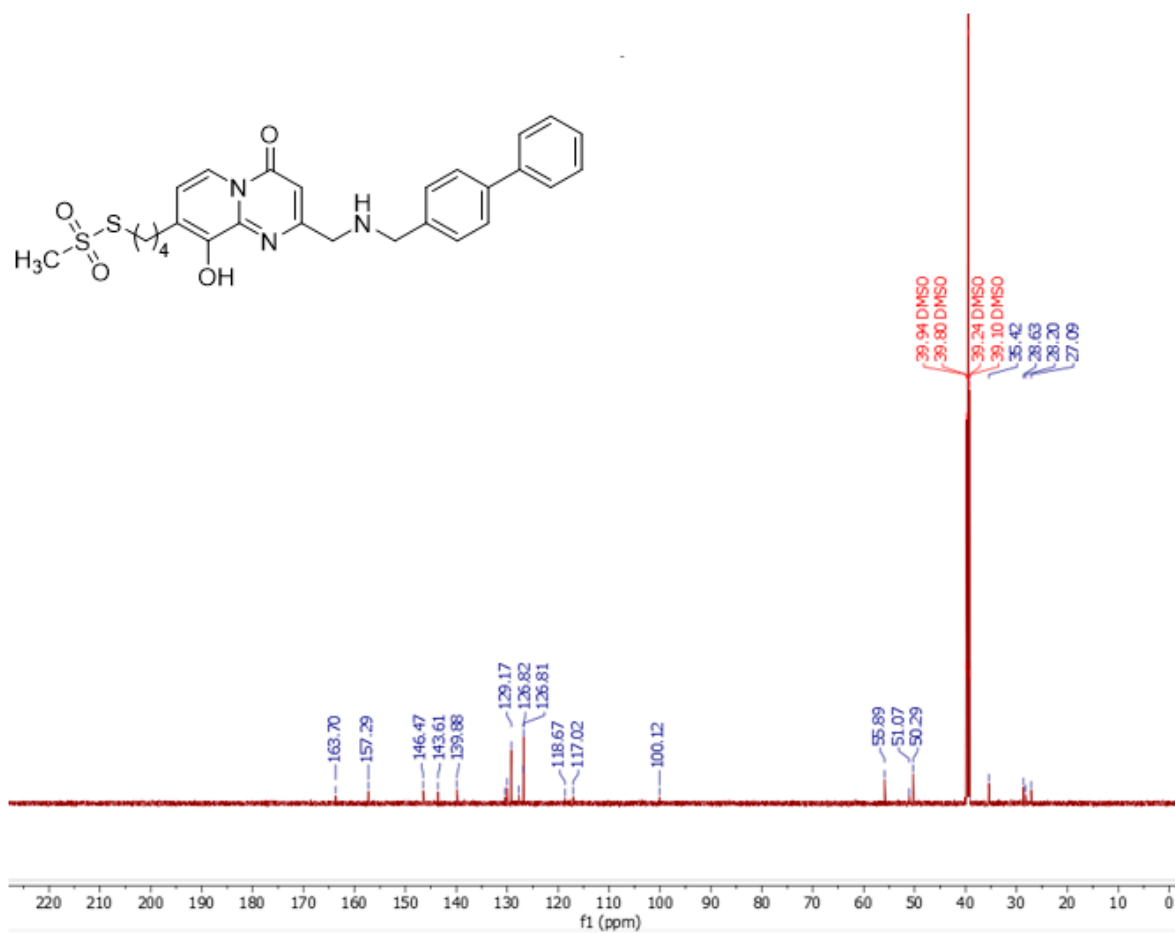
¹³C NMR of **80**



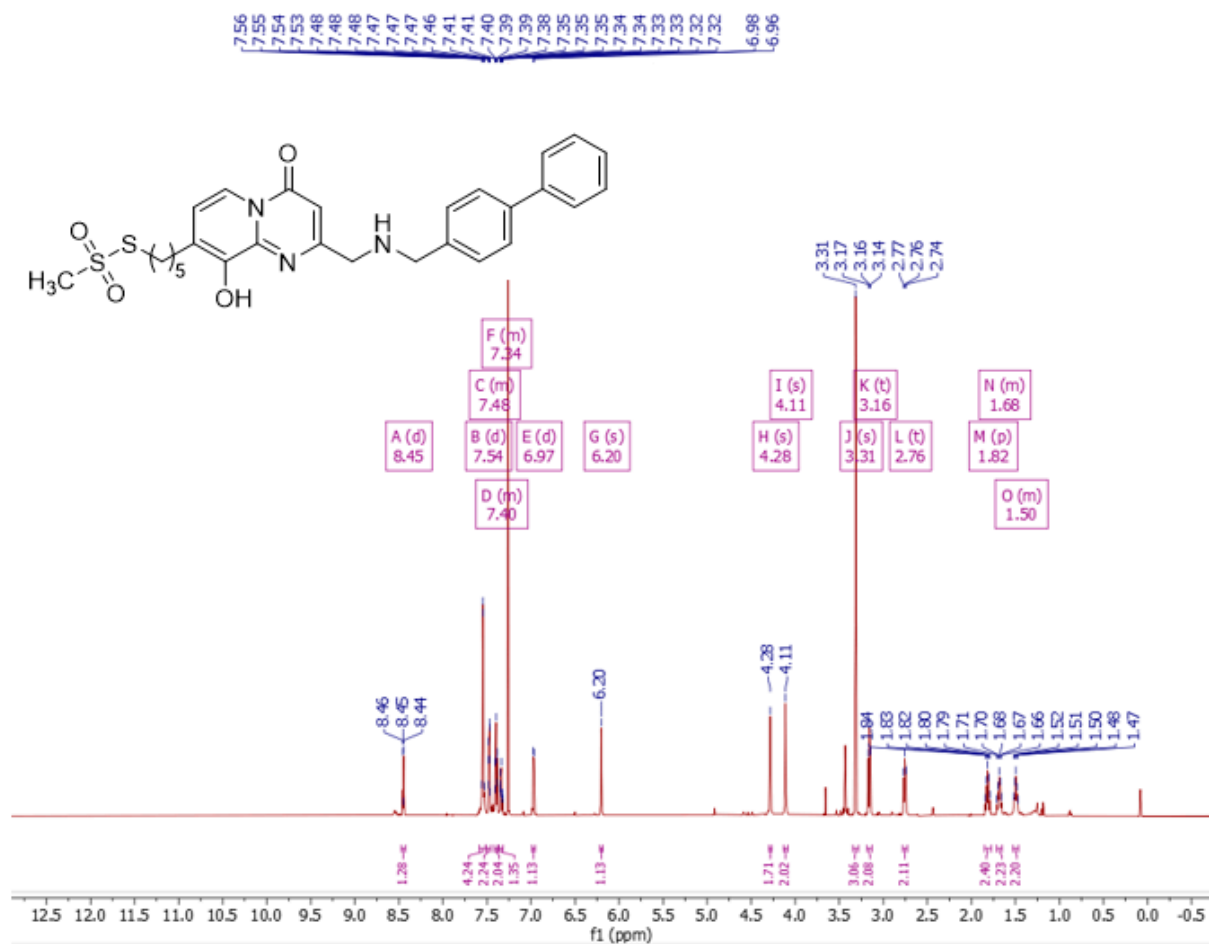
¹H NMR of **81**



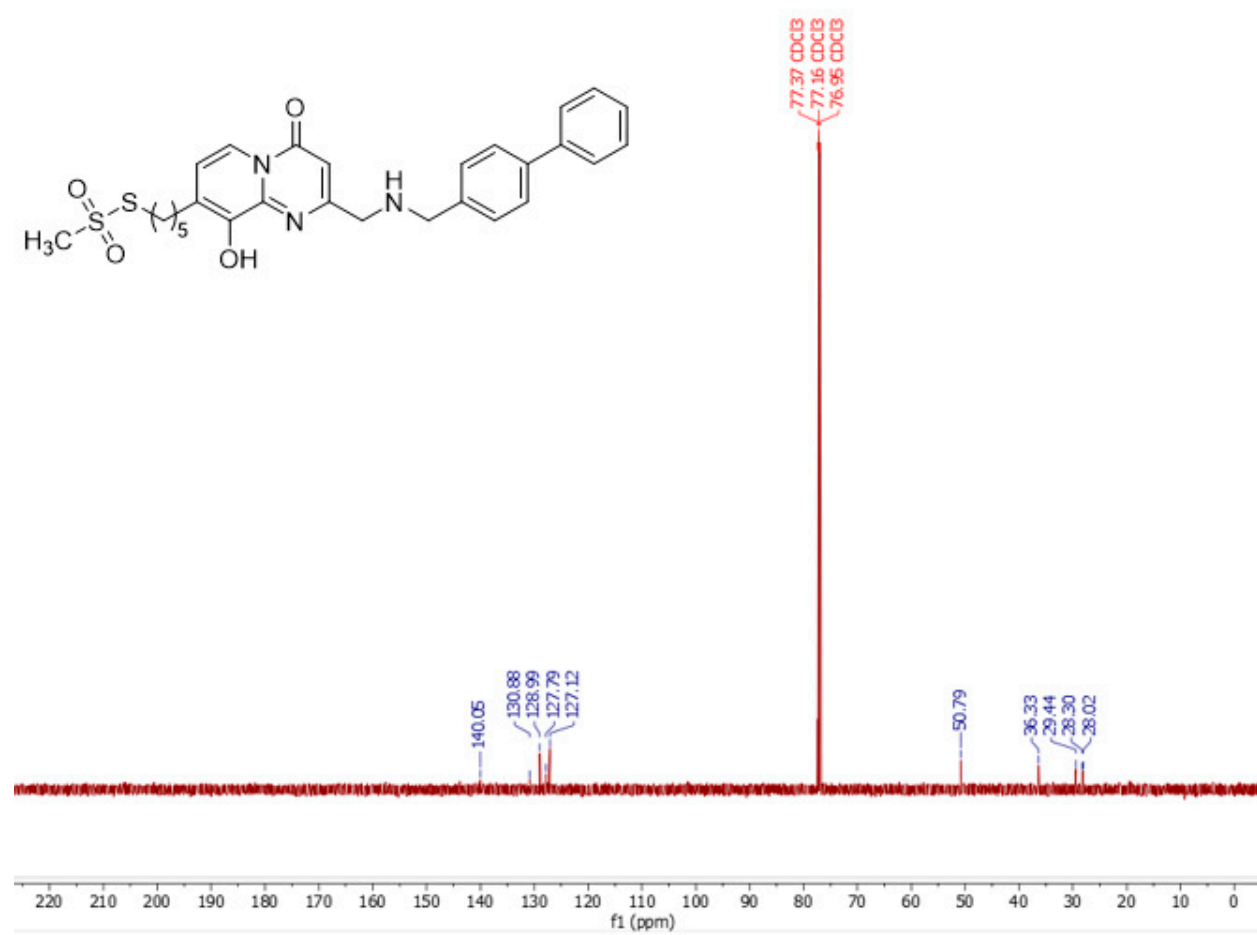
¹³C NMR of **81**



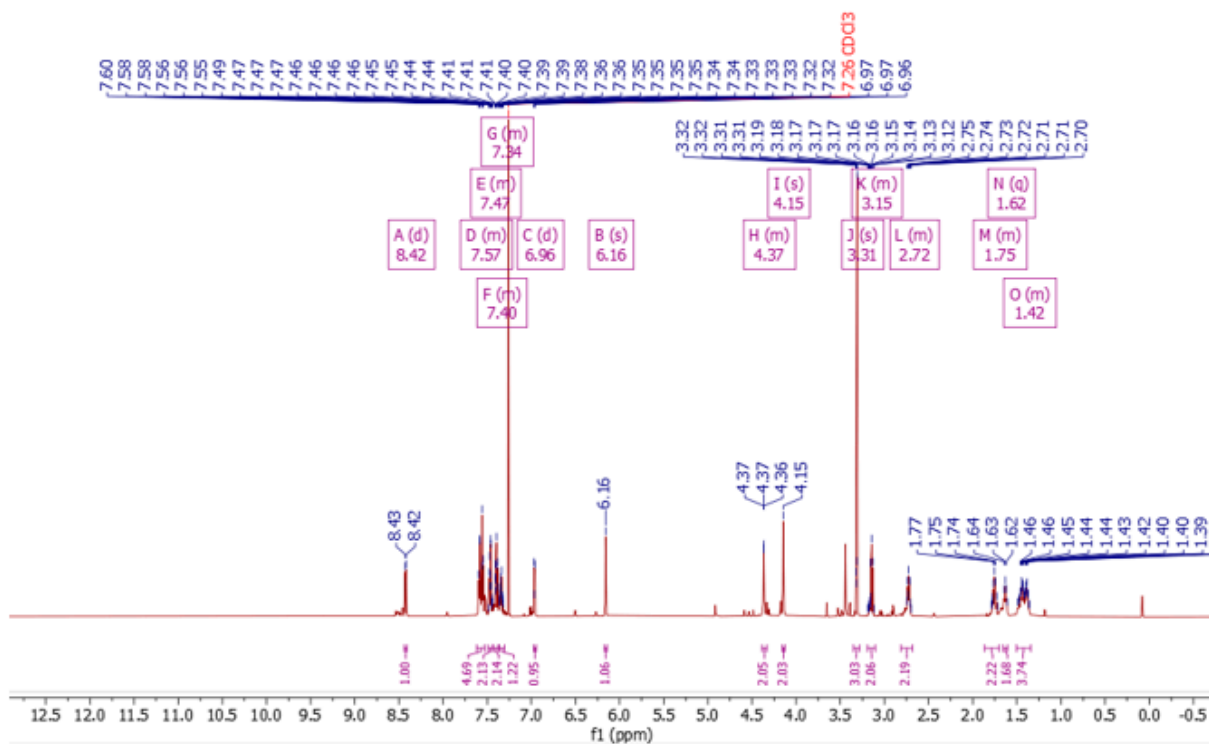
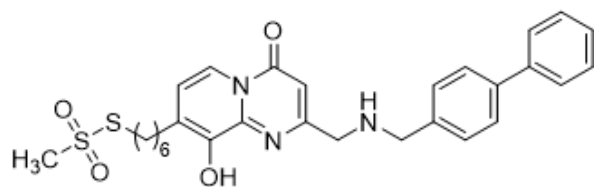
¹H NMR of **82**



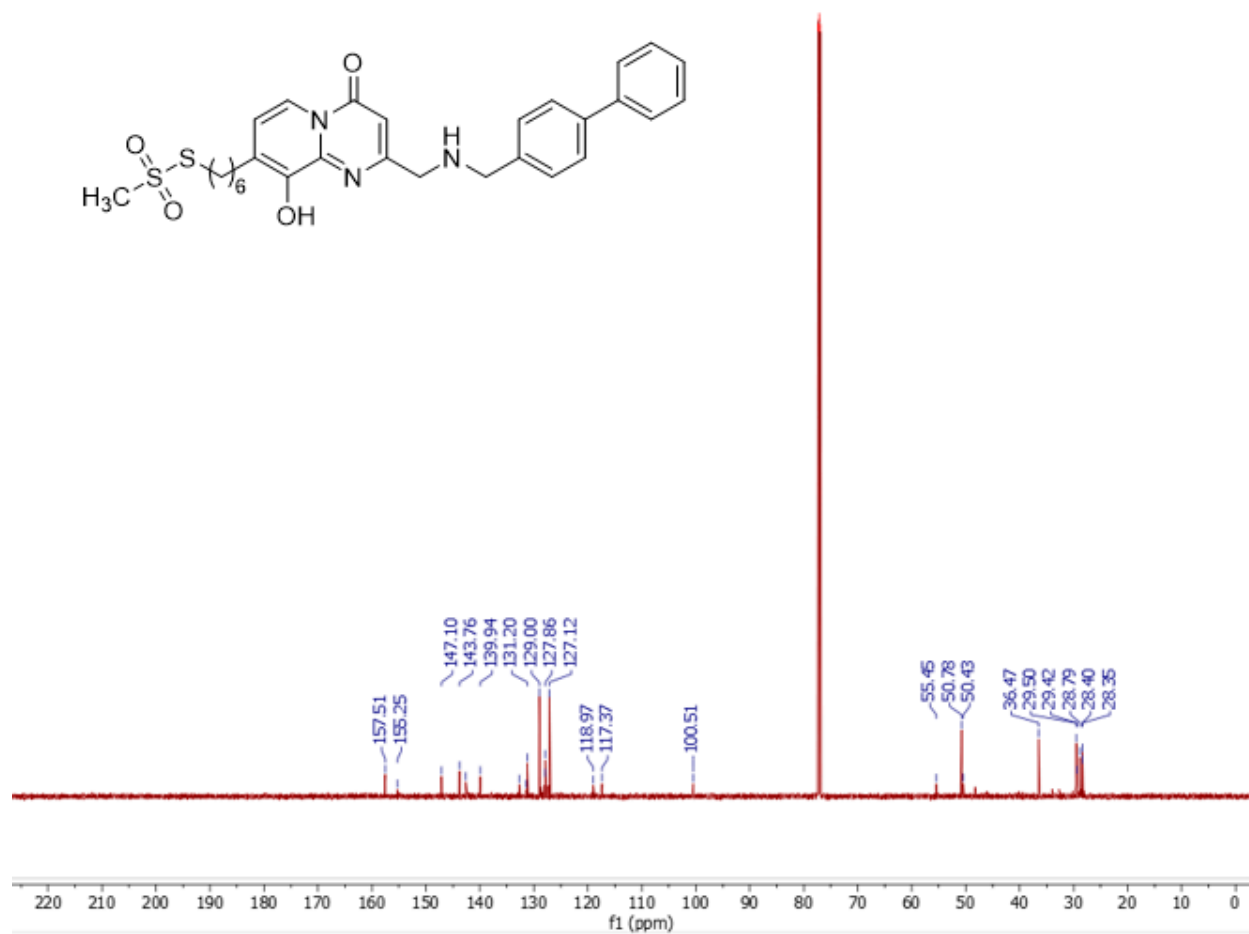
^{13}C NMR of **82**



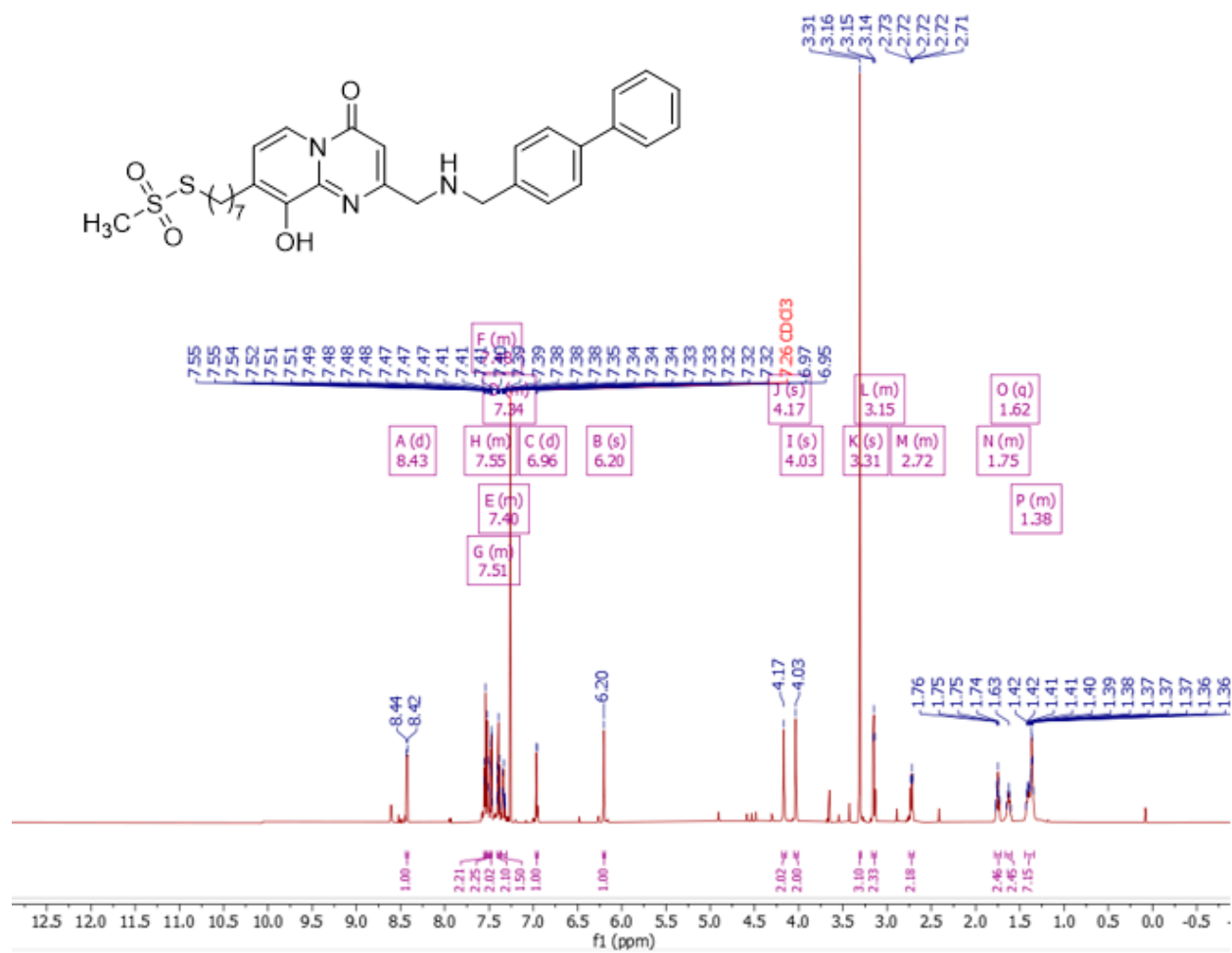
¹H NMR of **83**



¹³C NMR of **83**



¹H NMR of **84**



¹³C NMR of **84**

