

Electronic Supplementary Information

Rh-catalyzed C-H activation/intramolecular condensation for construction of benzo[*f*]pyrazolo[1,5-*a*][1,3]diazepines

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Li, Yongjia Shang*

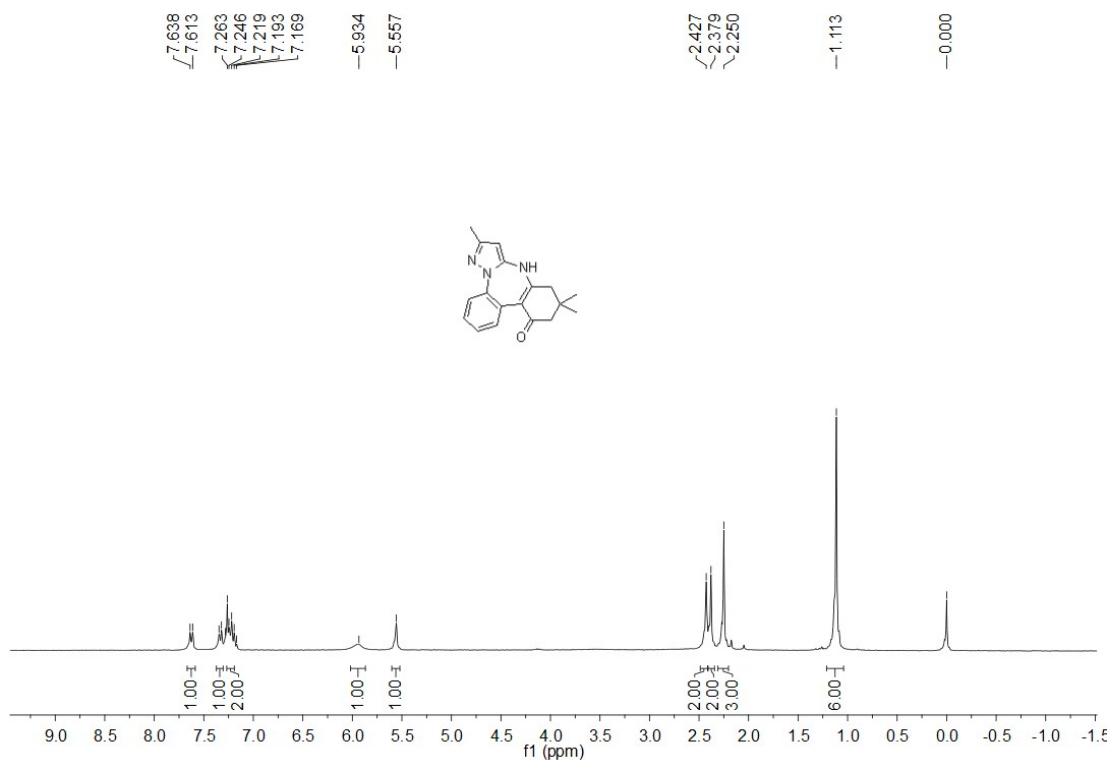
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P.R. China*

Copies of ¹H, and ¹³C NMR Spectra for all compounds-----S2-S27

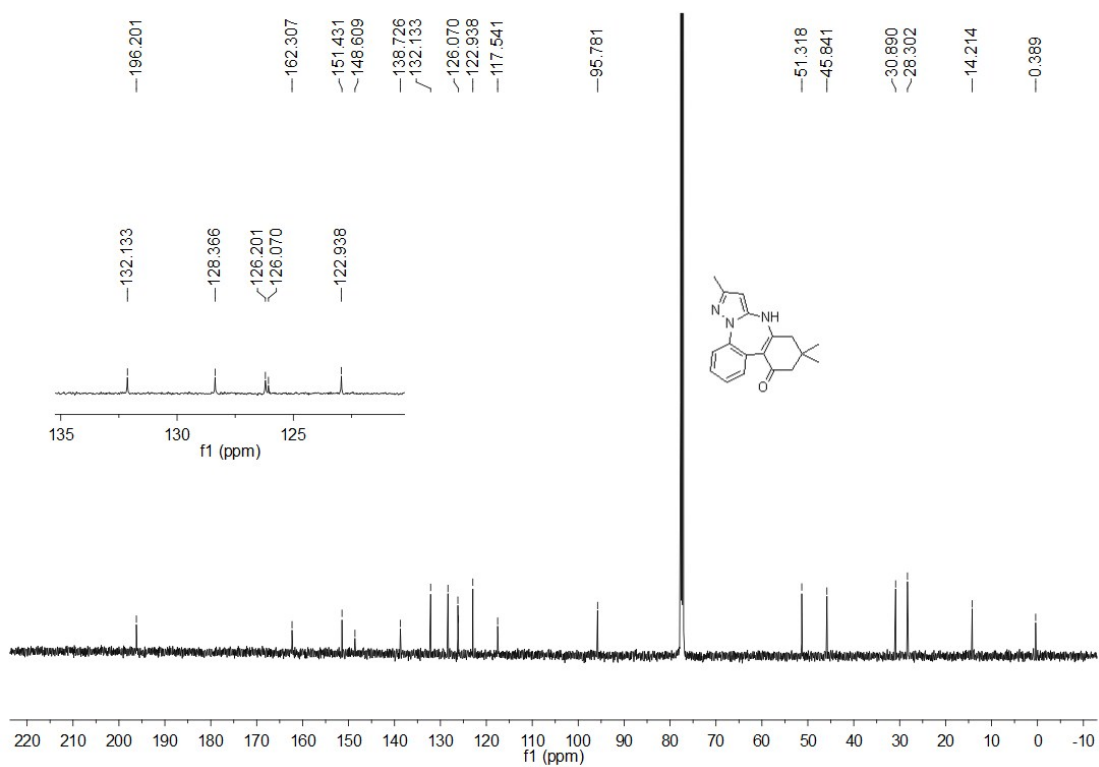
X-Ray Crystallography structures of Compounds **3a**-----S28

X-Ray Crystallography structures of Compounds **5b**-----S29

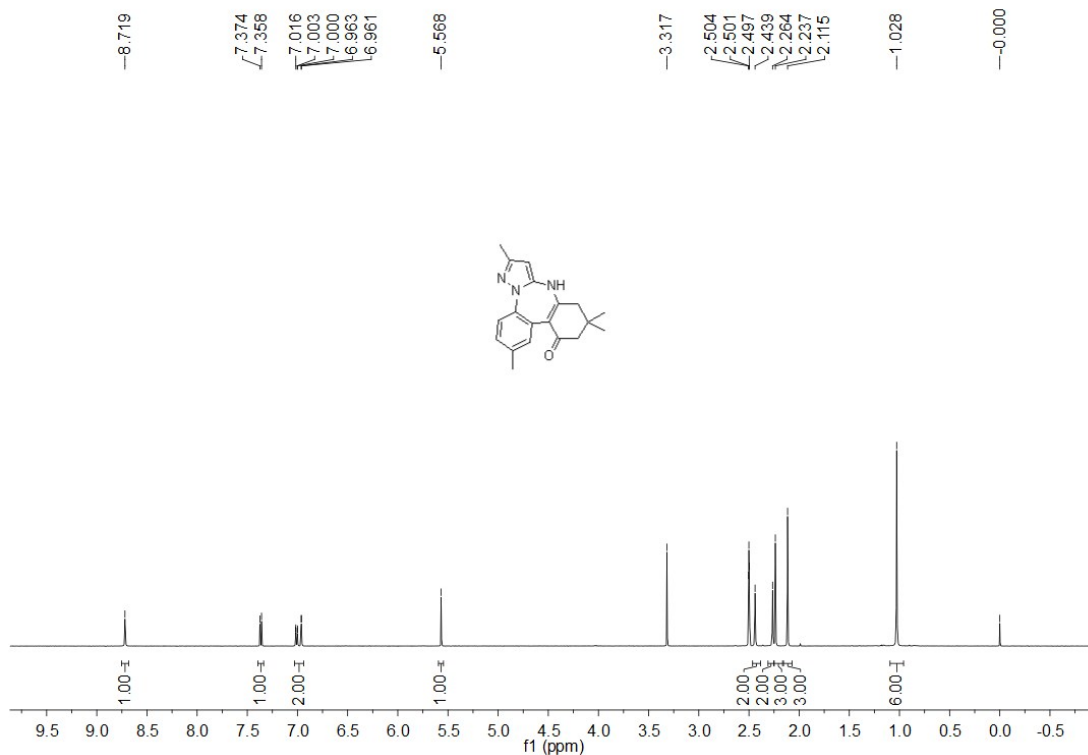
Copies of ^1H and ^{13}C NMR Spectra



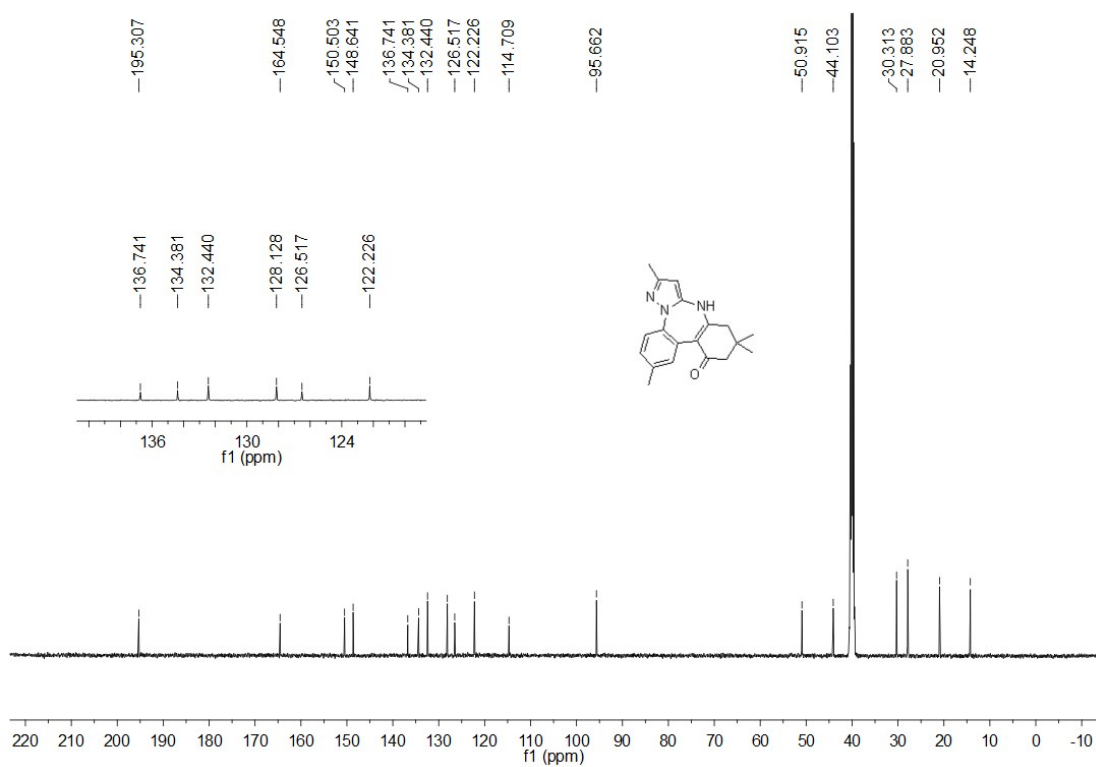
^1H NMR Spectrum of Compound 3a



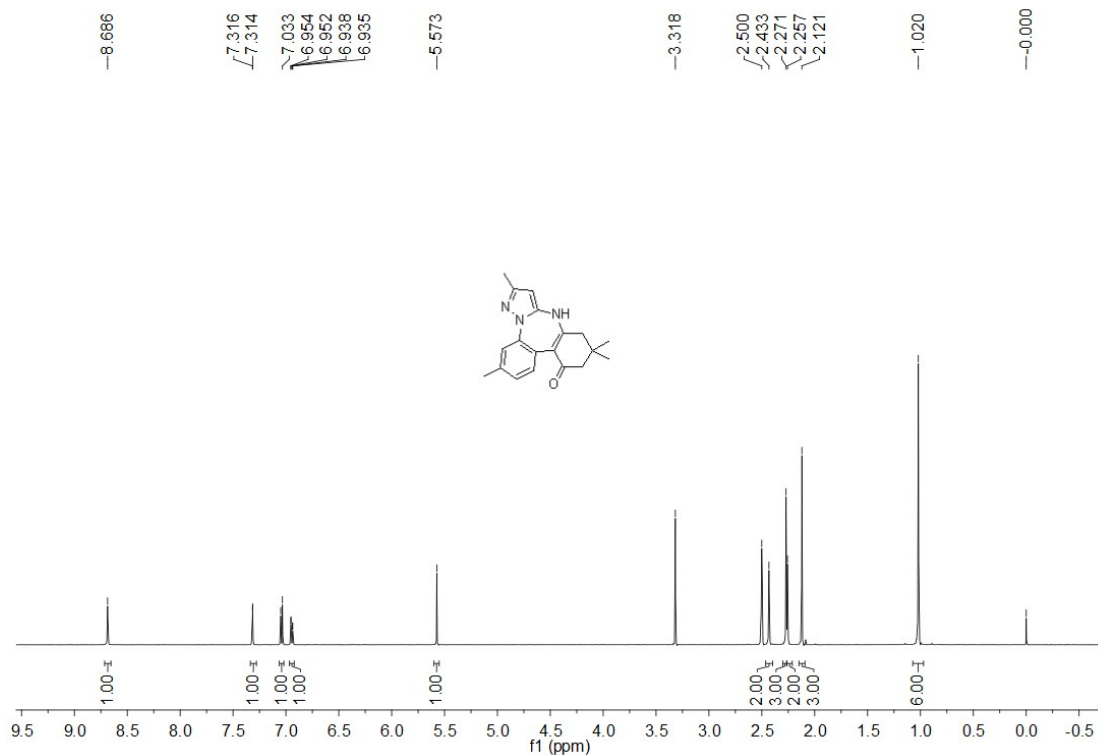
^{13}C NMR Spectrum of Compound 3a



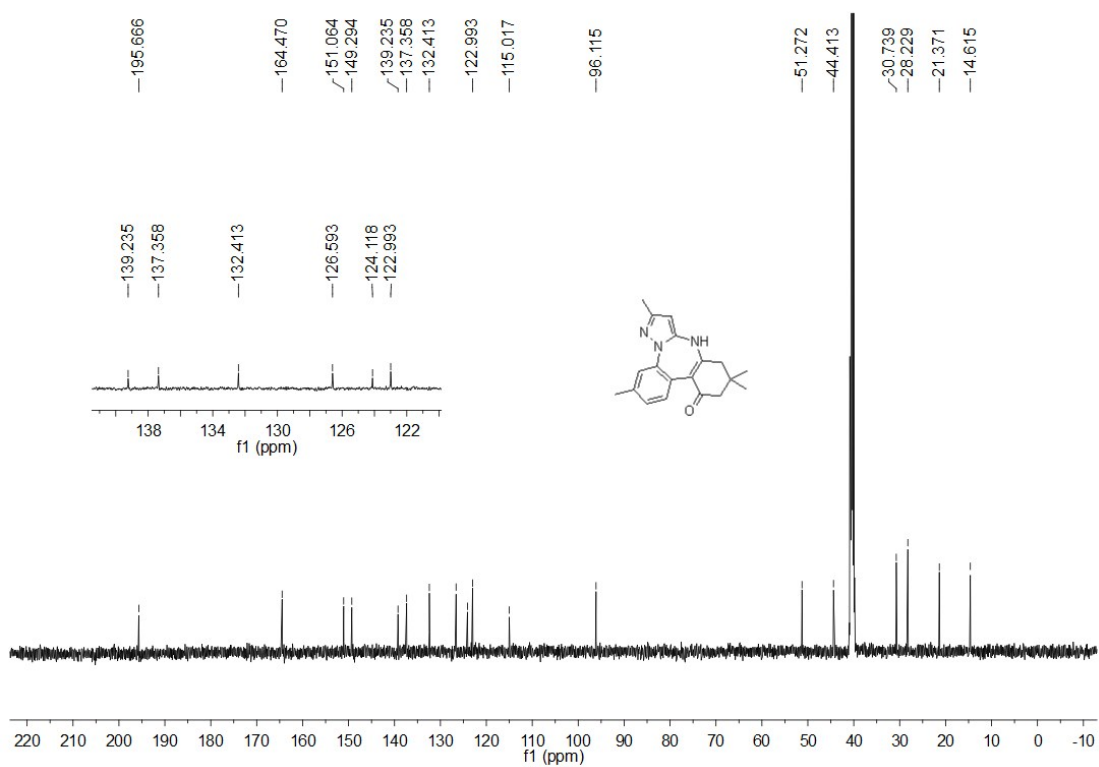
¹H NMR Spectrum of Compound 3b



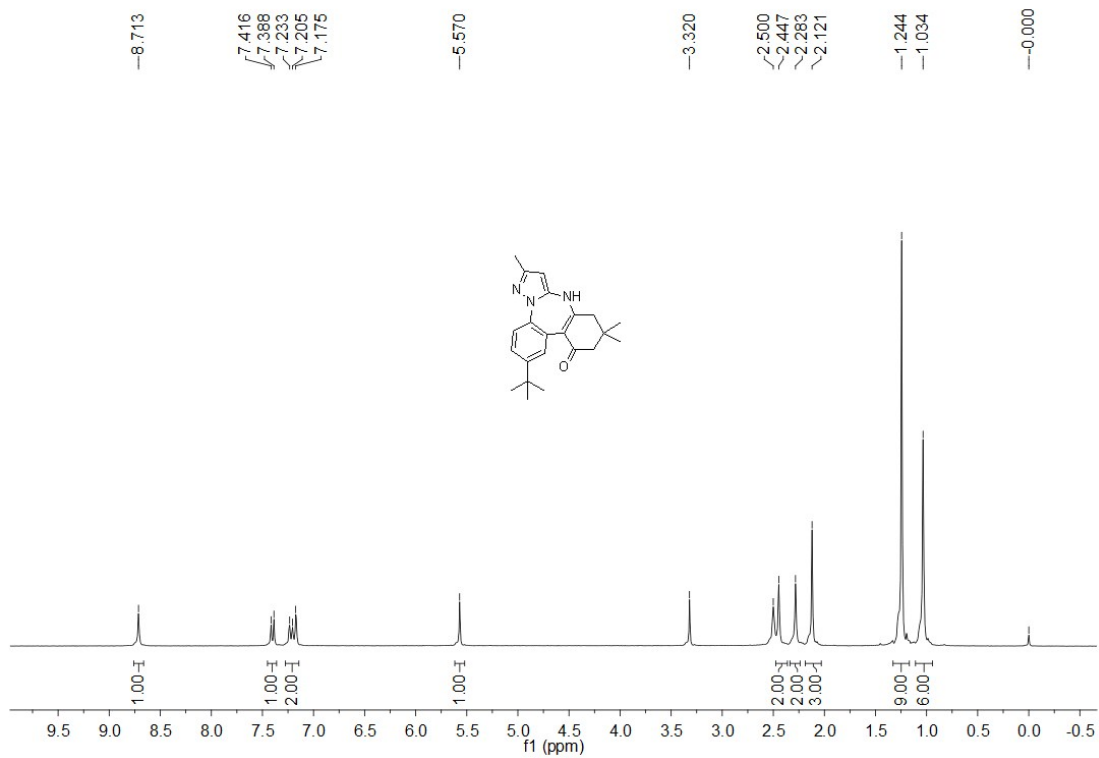
¹³C NMR Spectrum of Compound 3b



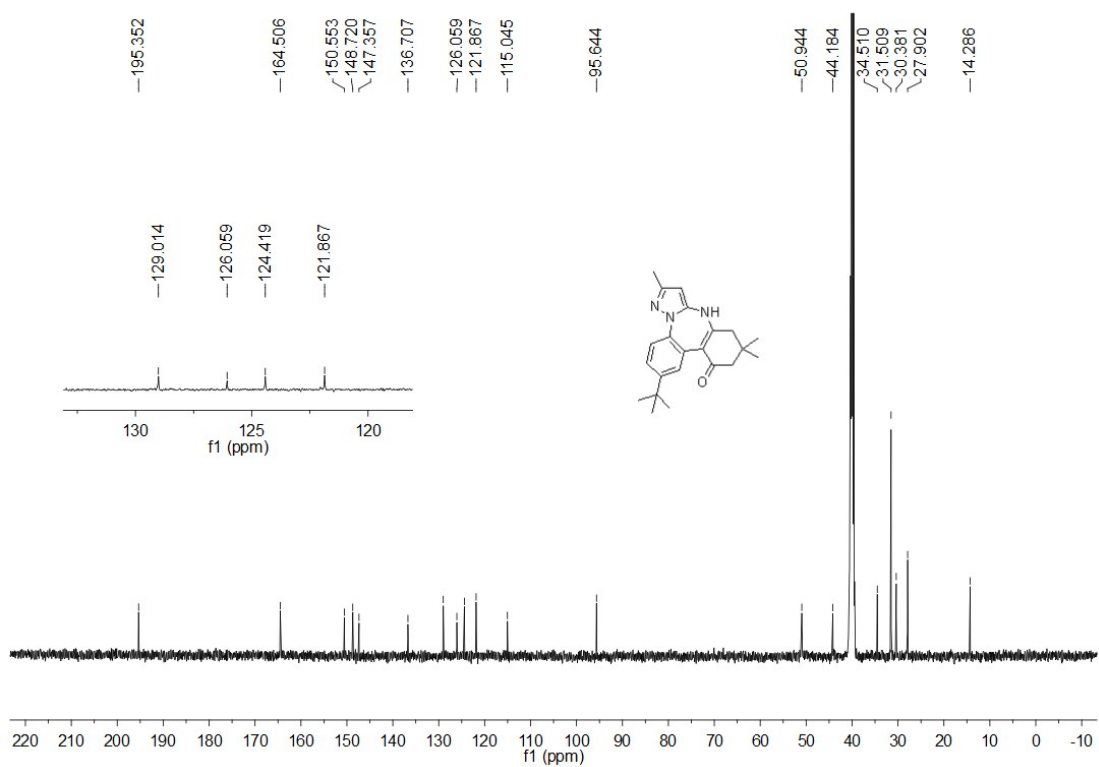
¹H NMR Spectrum of Compound 3c



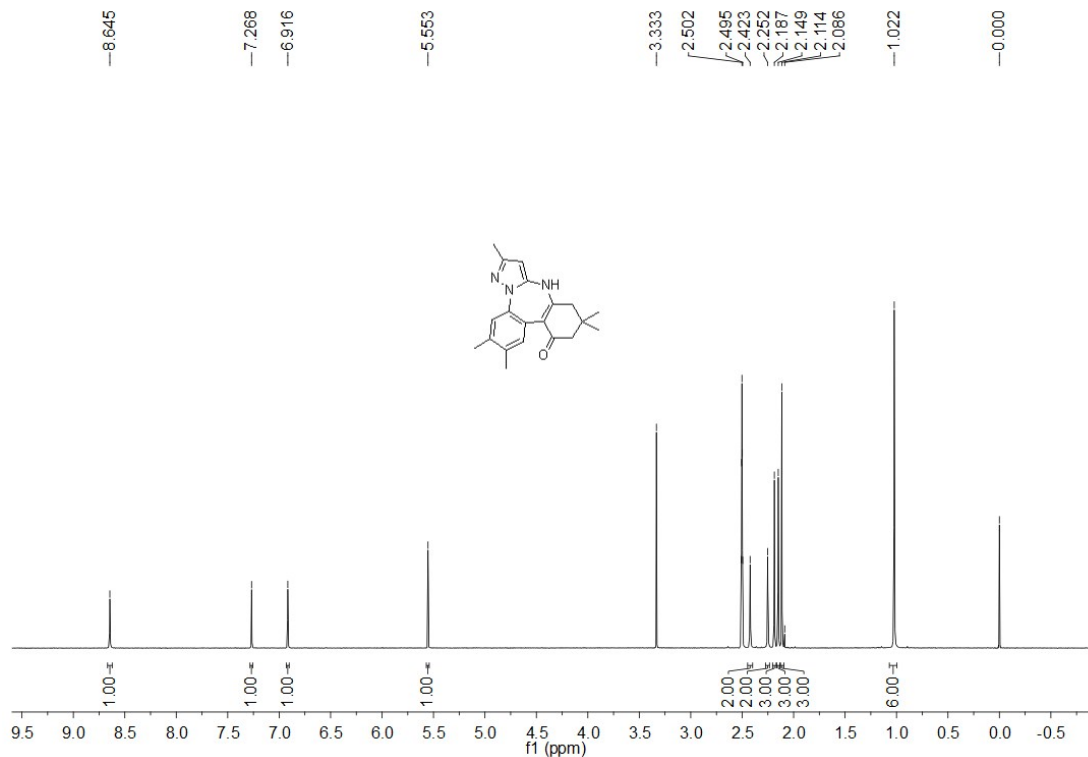
¹³C NMR Spectrum of Compound 3c



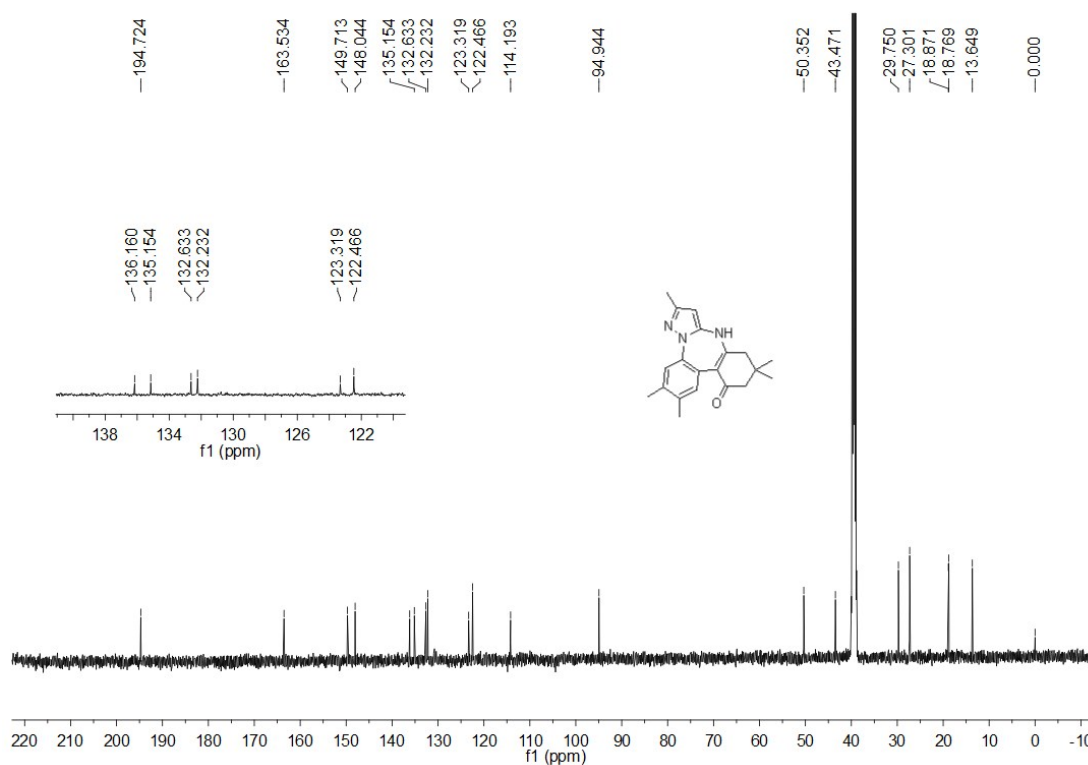
¹H NMR Spectrum of Compound 3d



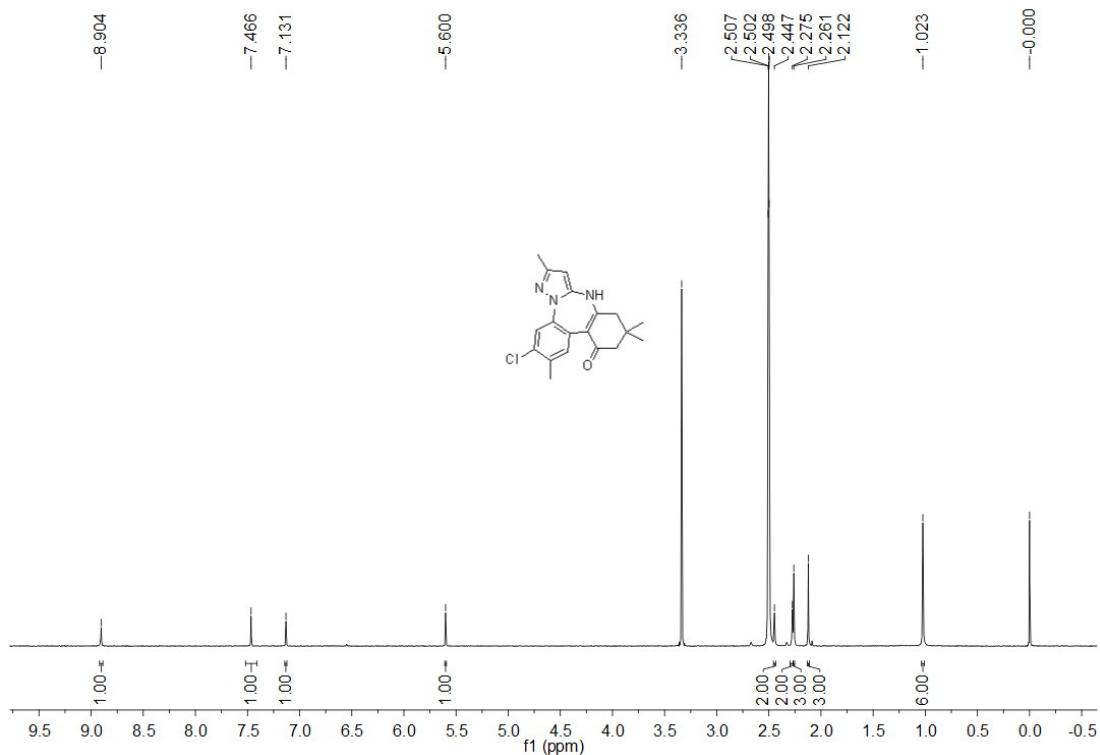
¹³C NMR Spectrum of Compound 3d



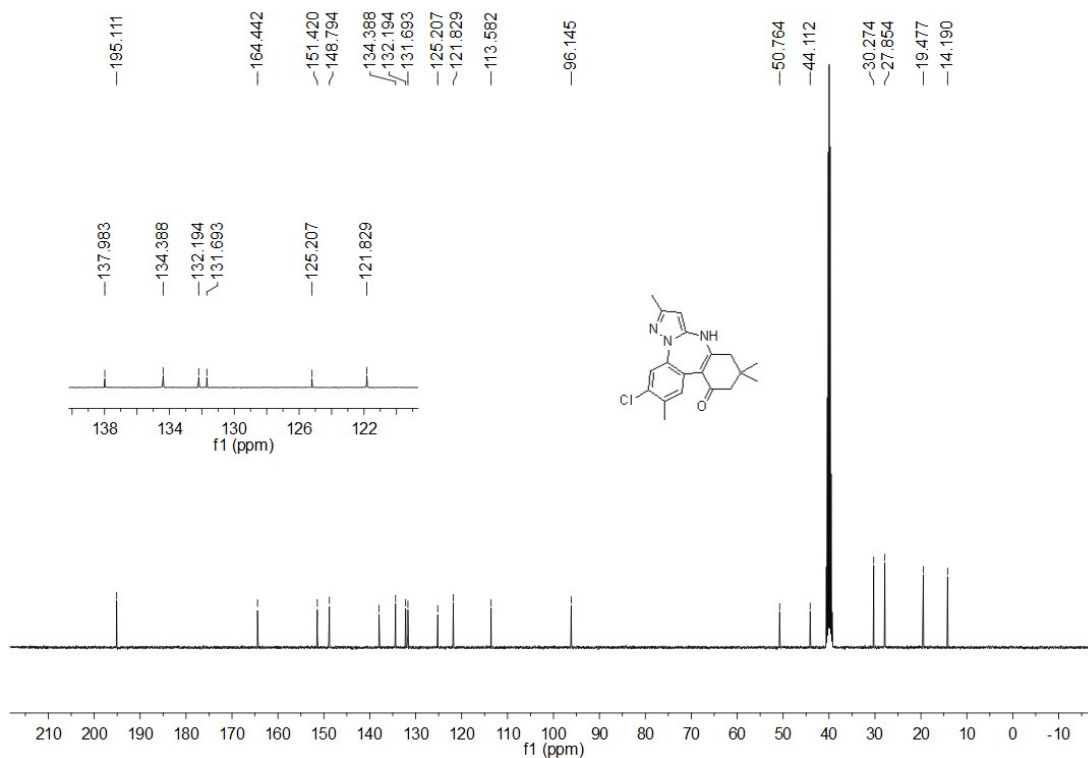
¹H NMR Spectrum of Compound 3e



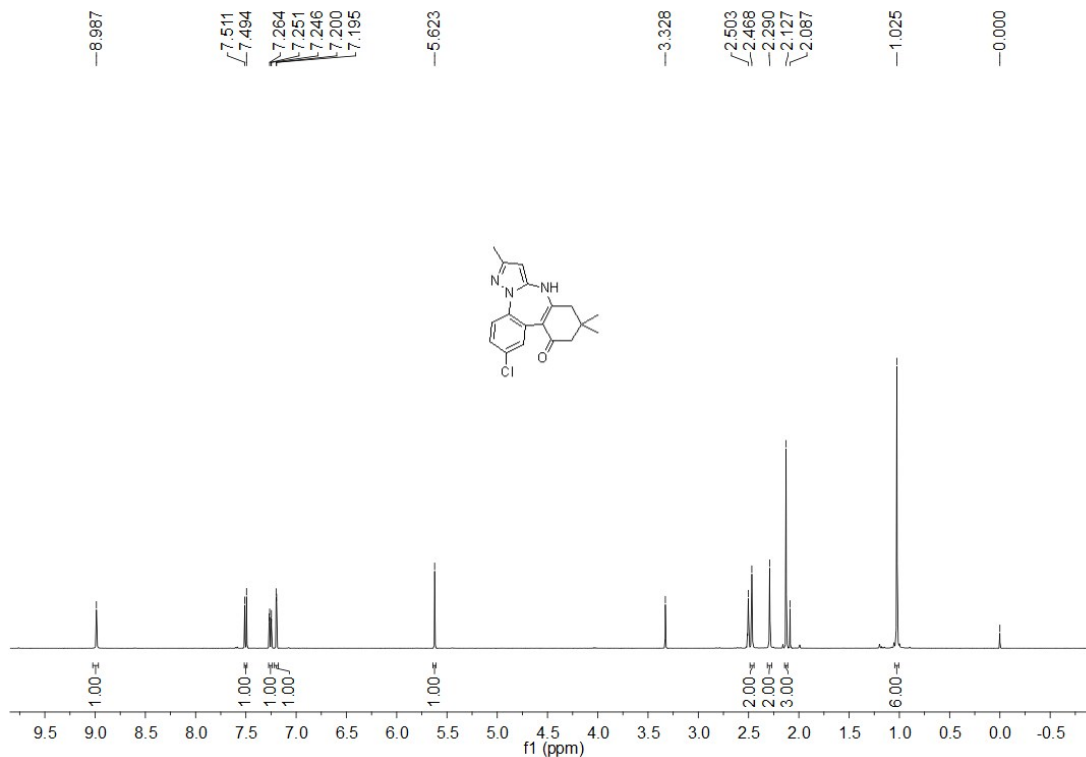
¹³C NMR Spectrum of Compound 3e



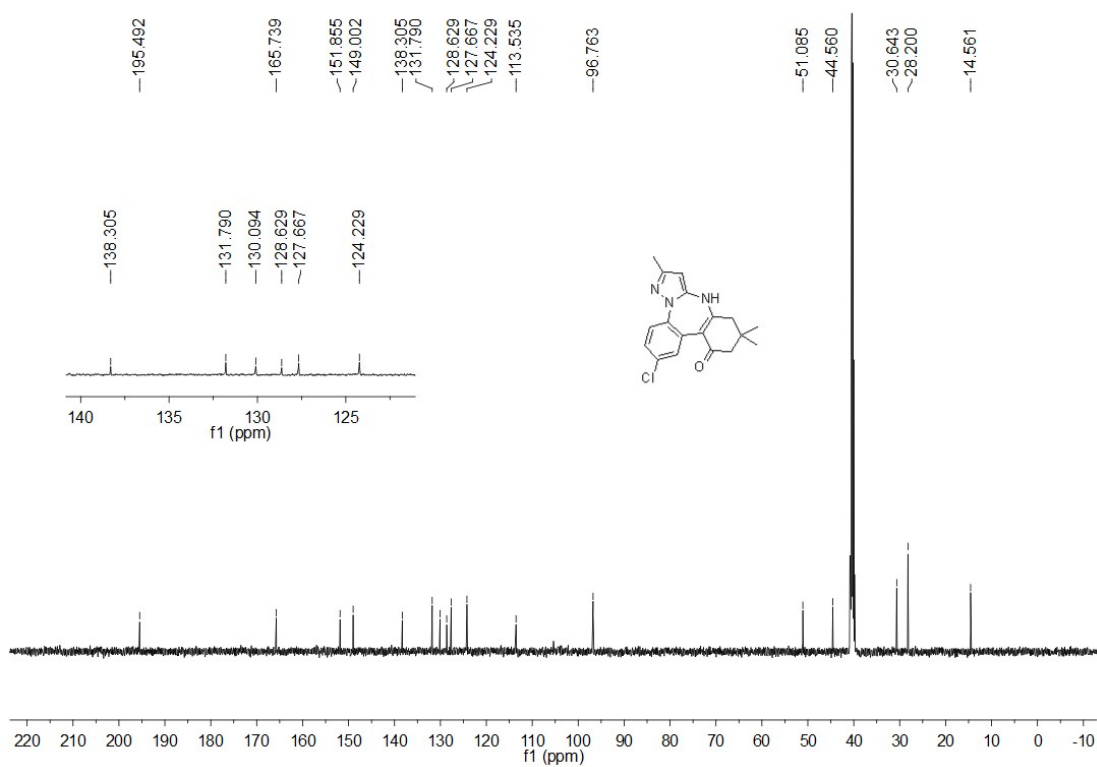
¹H NMR Spectrum of Compound 3f



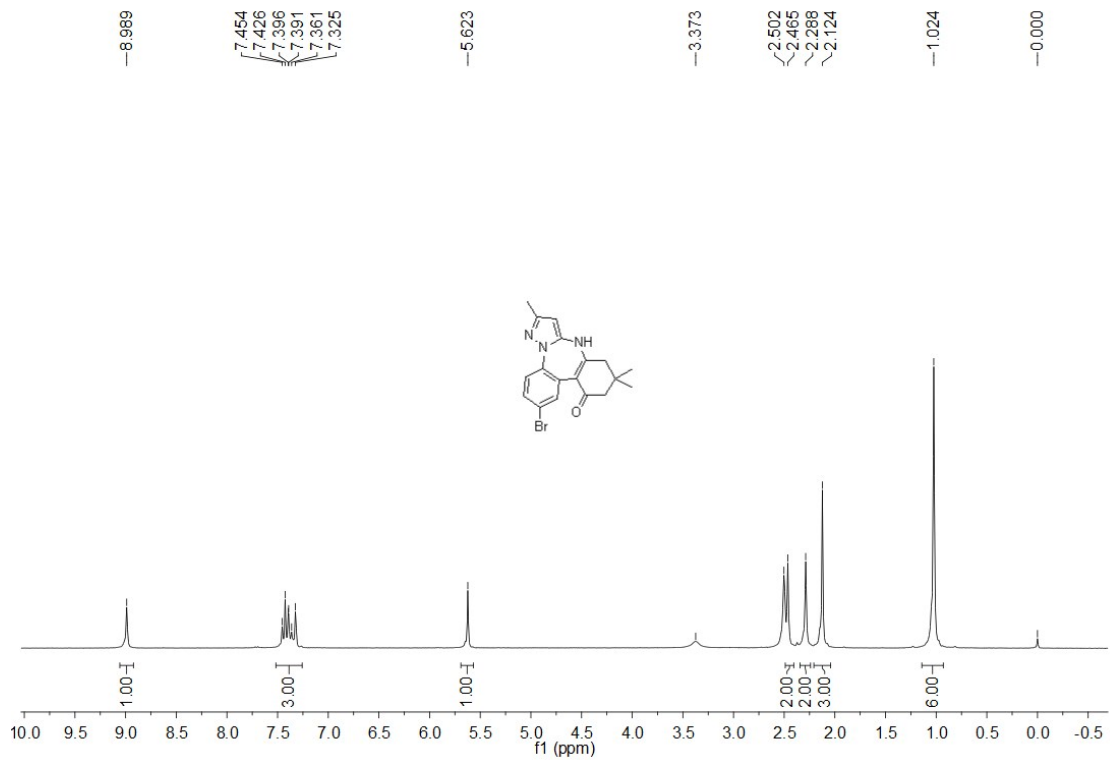
¹³C NMR Spectrum of Compound 3f



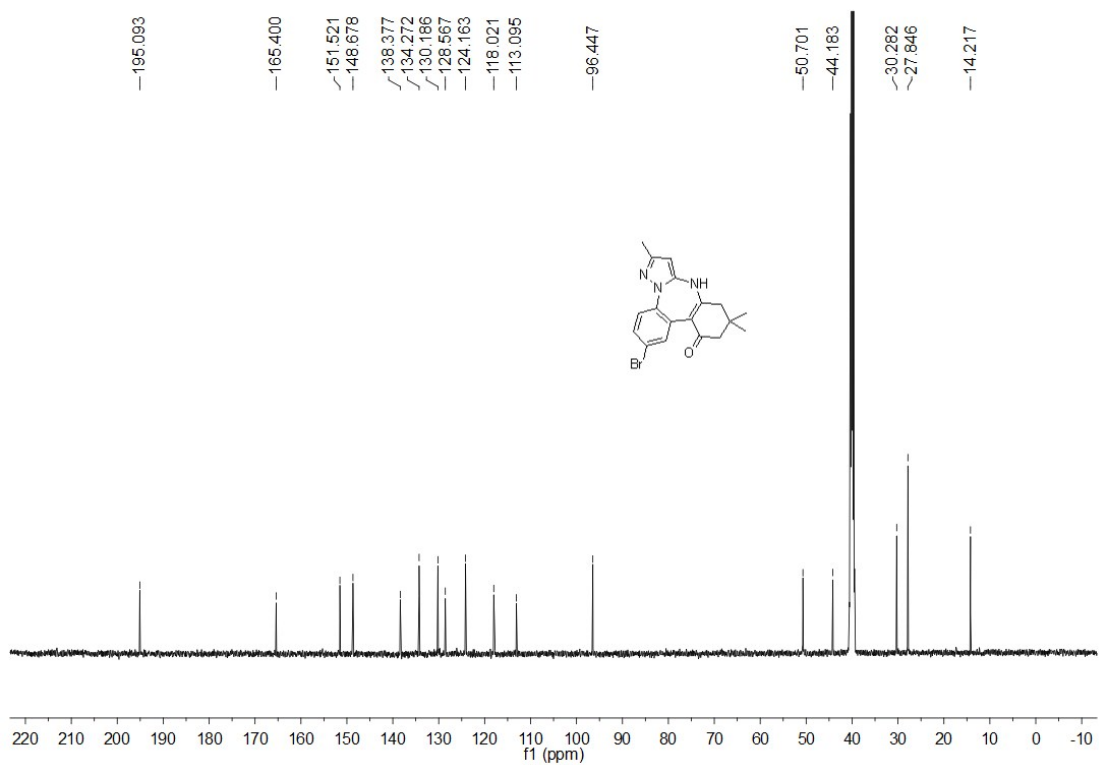
¹H NMR Spectrum of Compound 3g



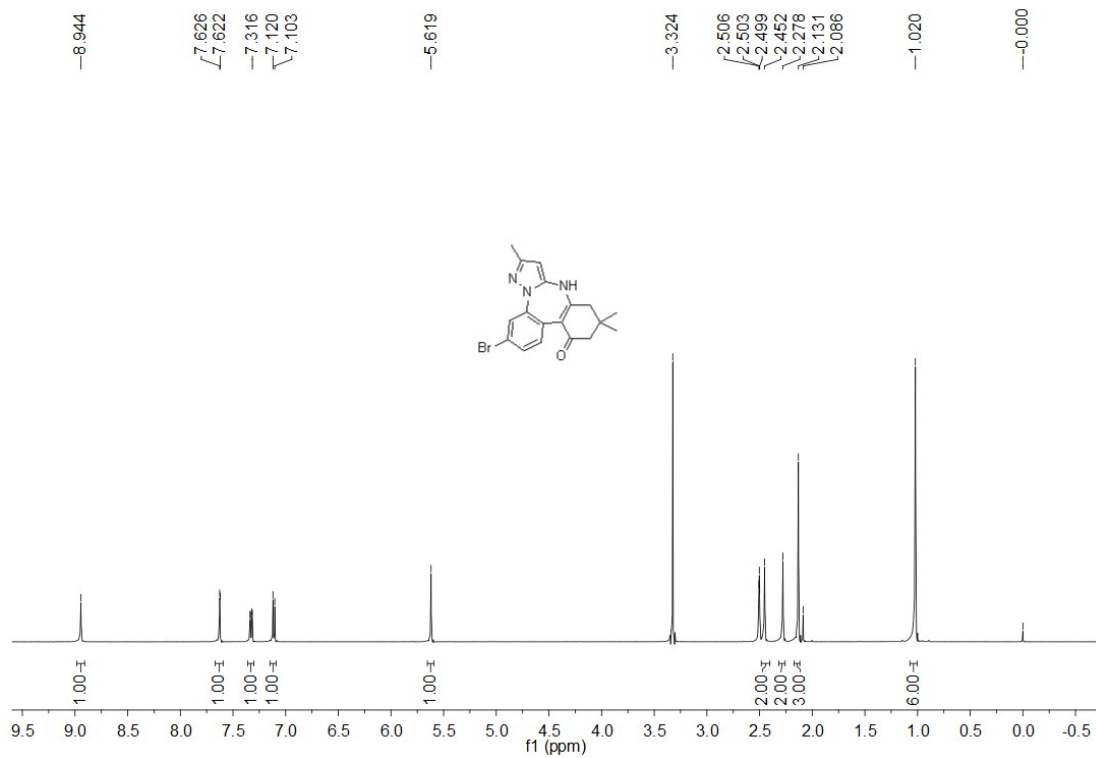
¹³C NMR Spectrum of Compound 3g



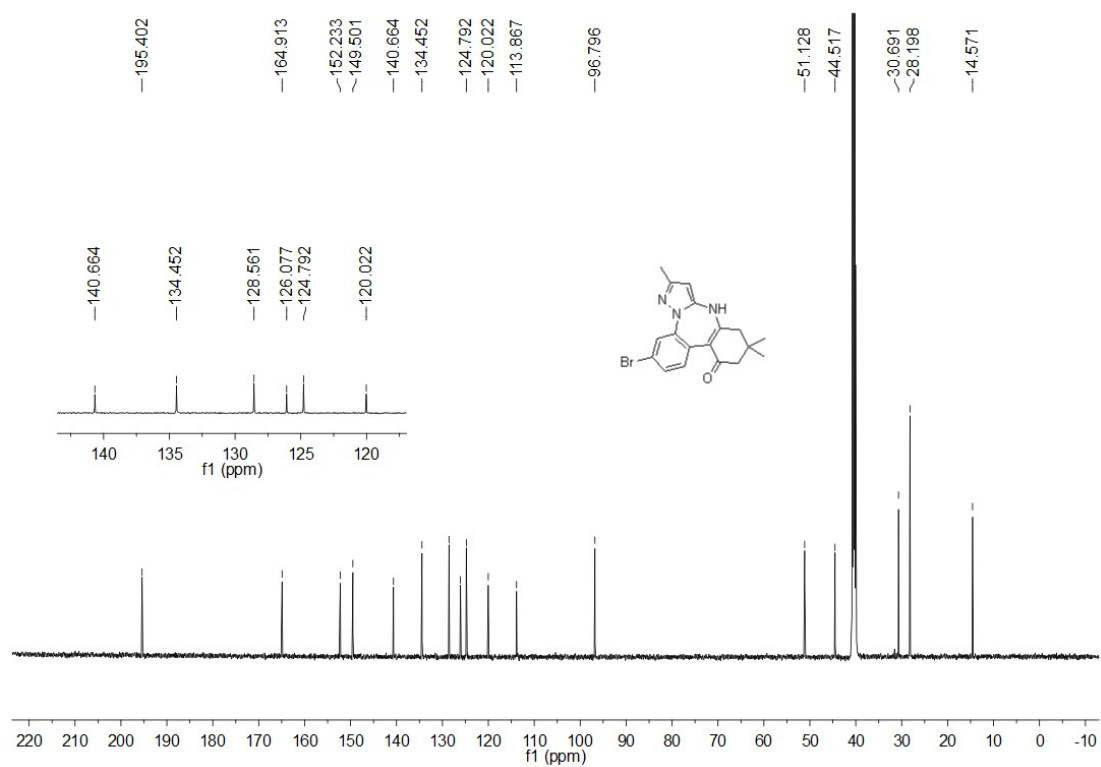
¹H NMR Spectrum of Compound 3h



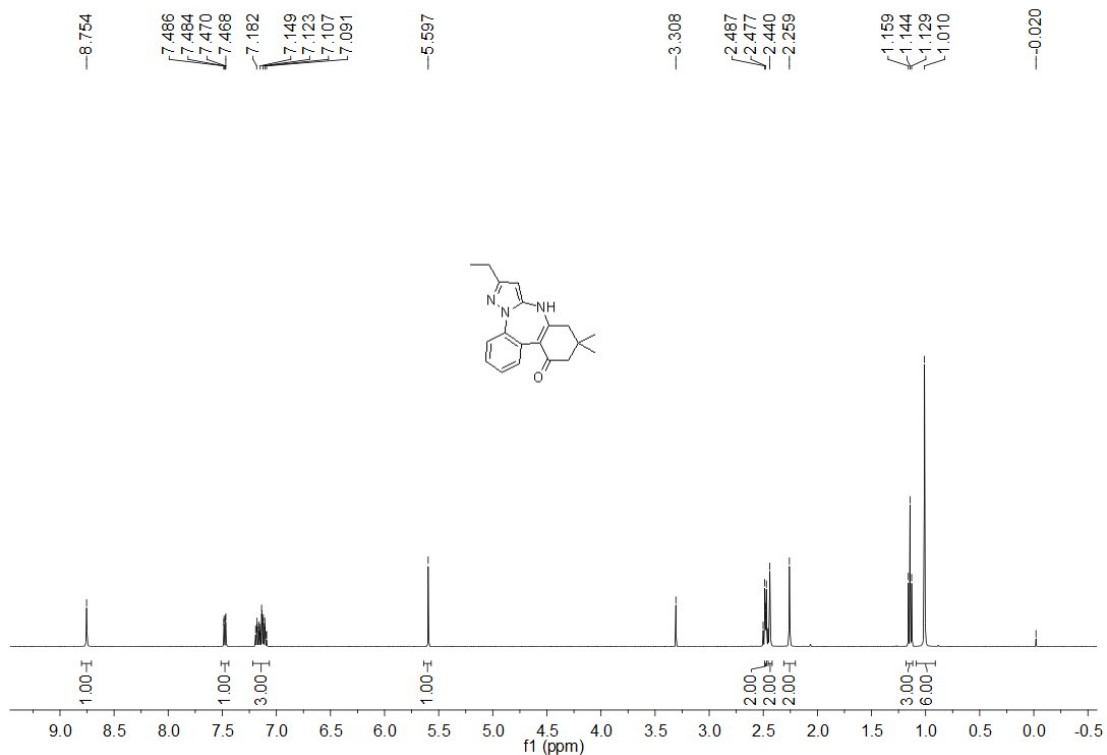
¹³C NMR Spectrum of Compound 3h



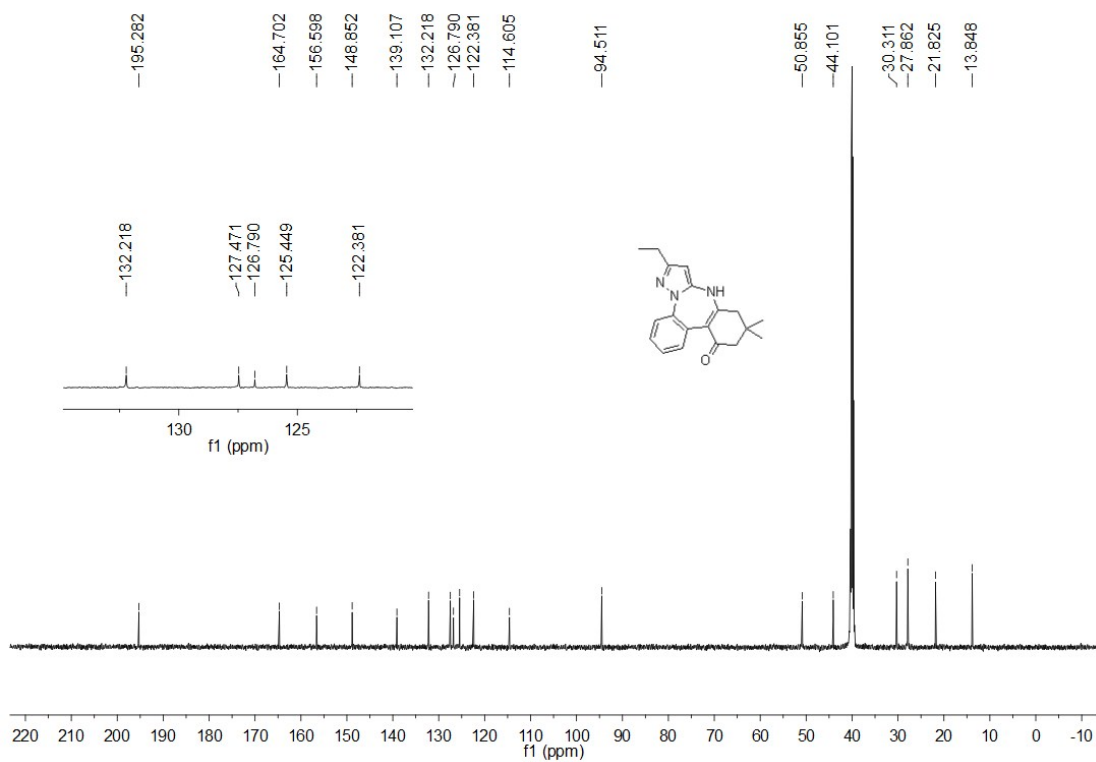
¹H NMR Spectrum of Compound 3i



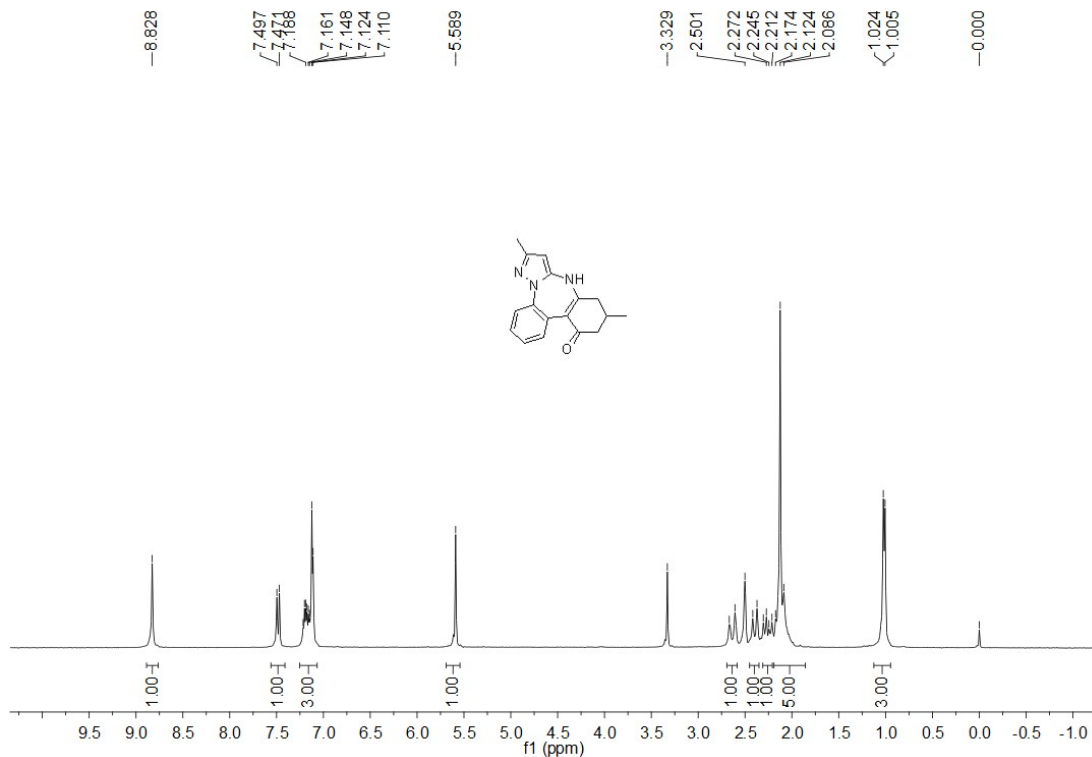
¹³C NMR Spectrum of Compound 3i



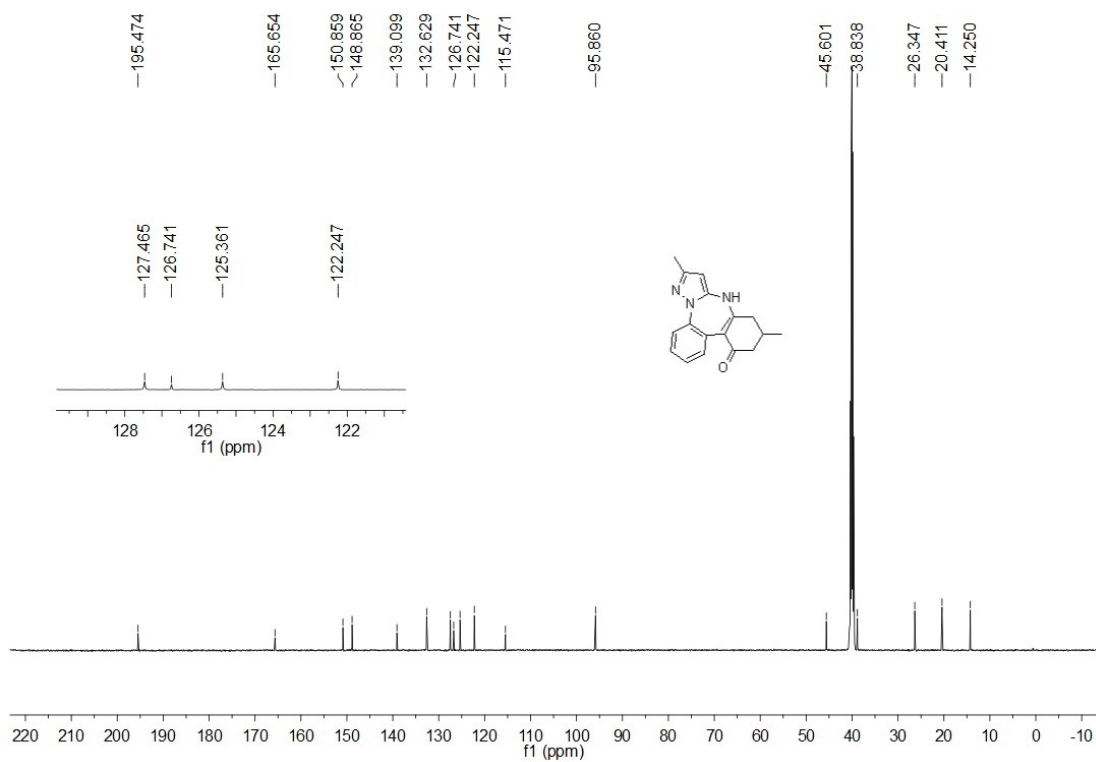
¹H NMR Spectrum of Compound 3j



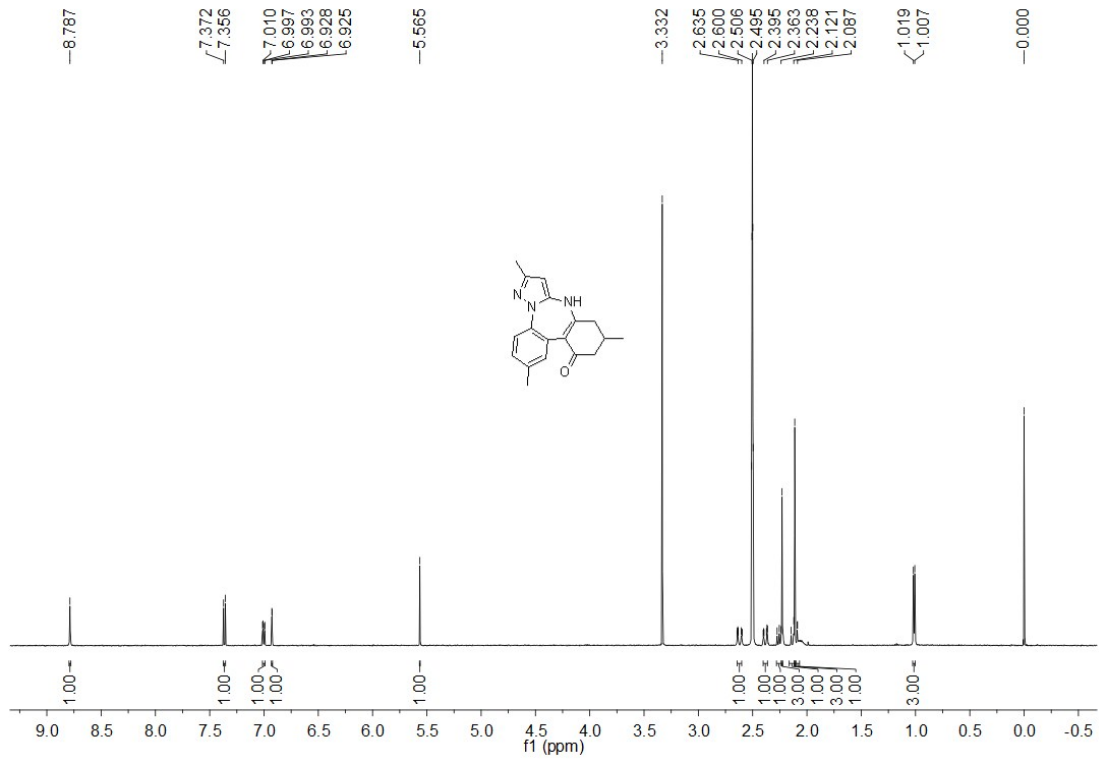
¹³C NMR Spectrum of Compound 3j



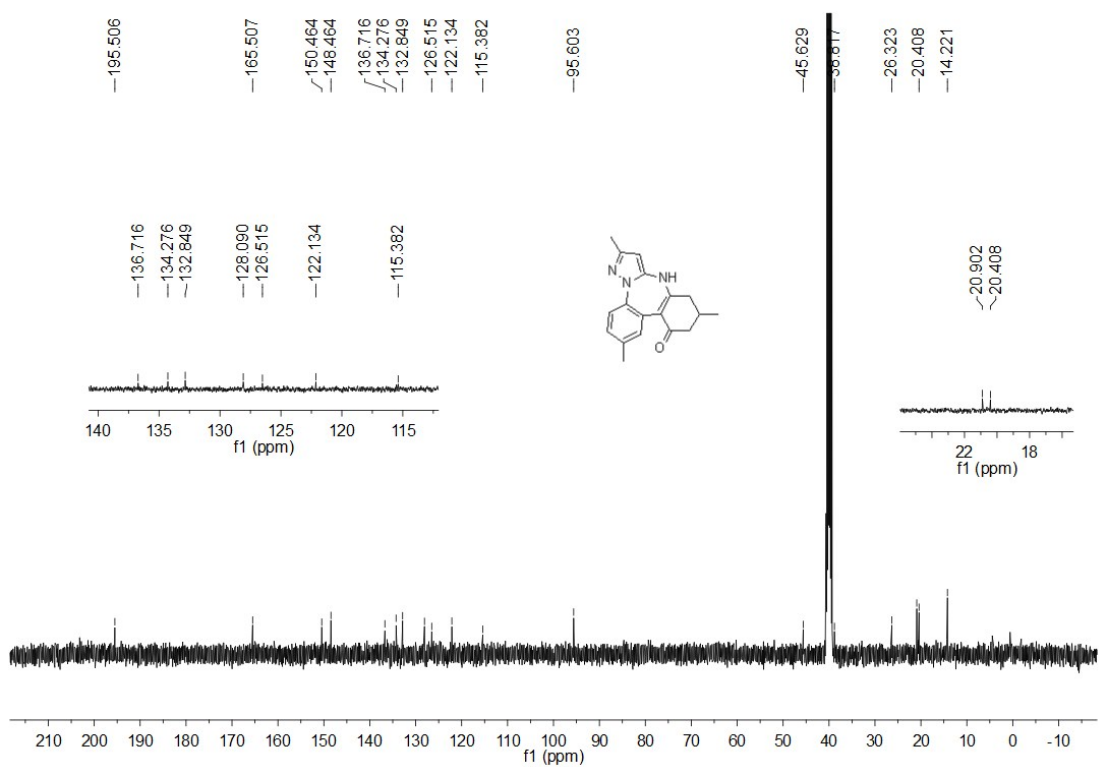
¹H NMR Spectrum of Compound 3n



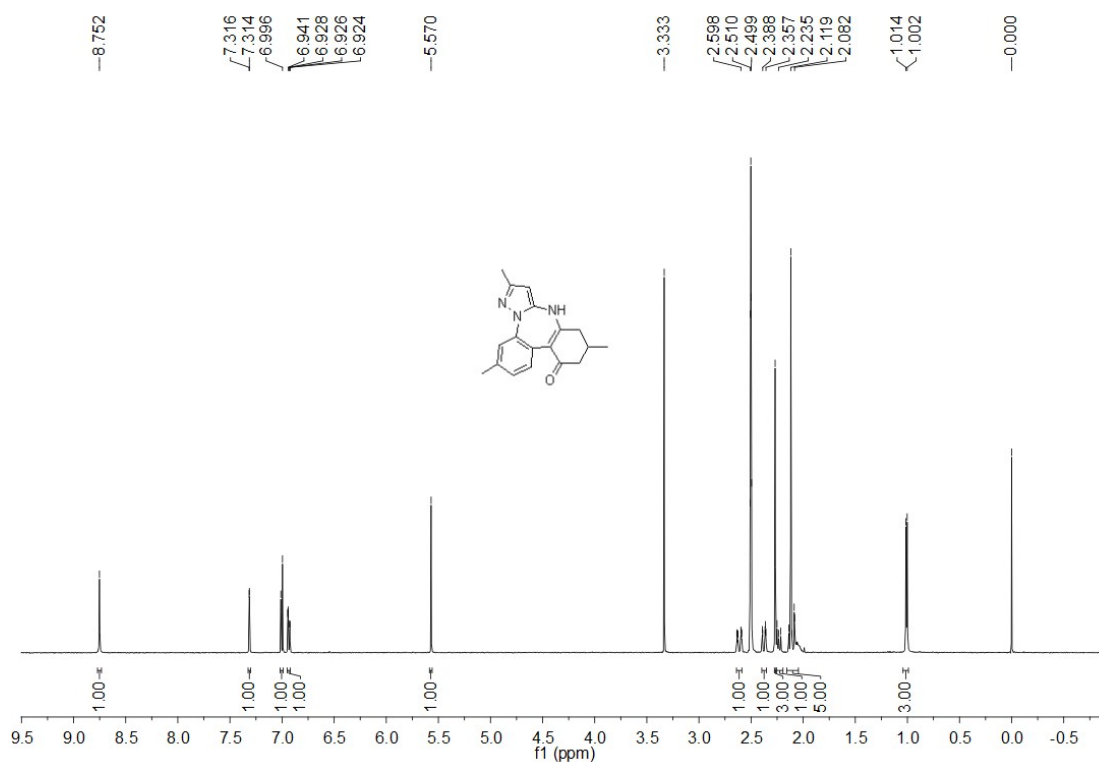
¹³C NMR Spectrum of Compound 3n



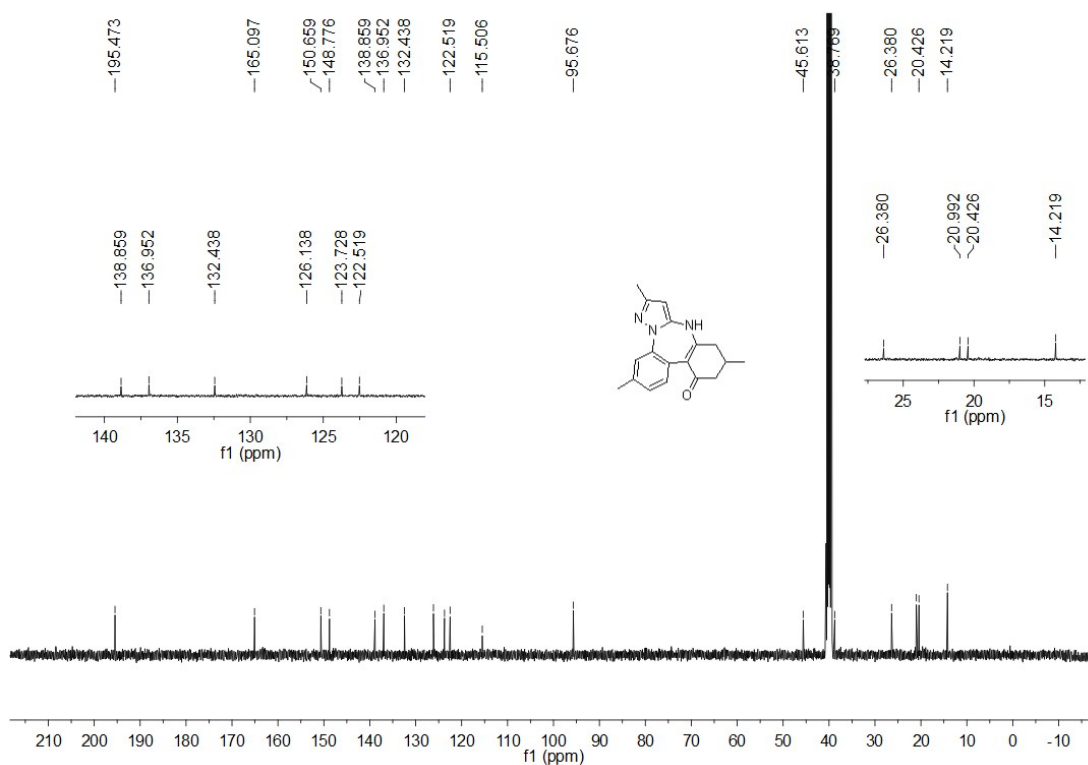
¹H NMR Spectrum of Compound 3o



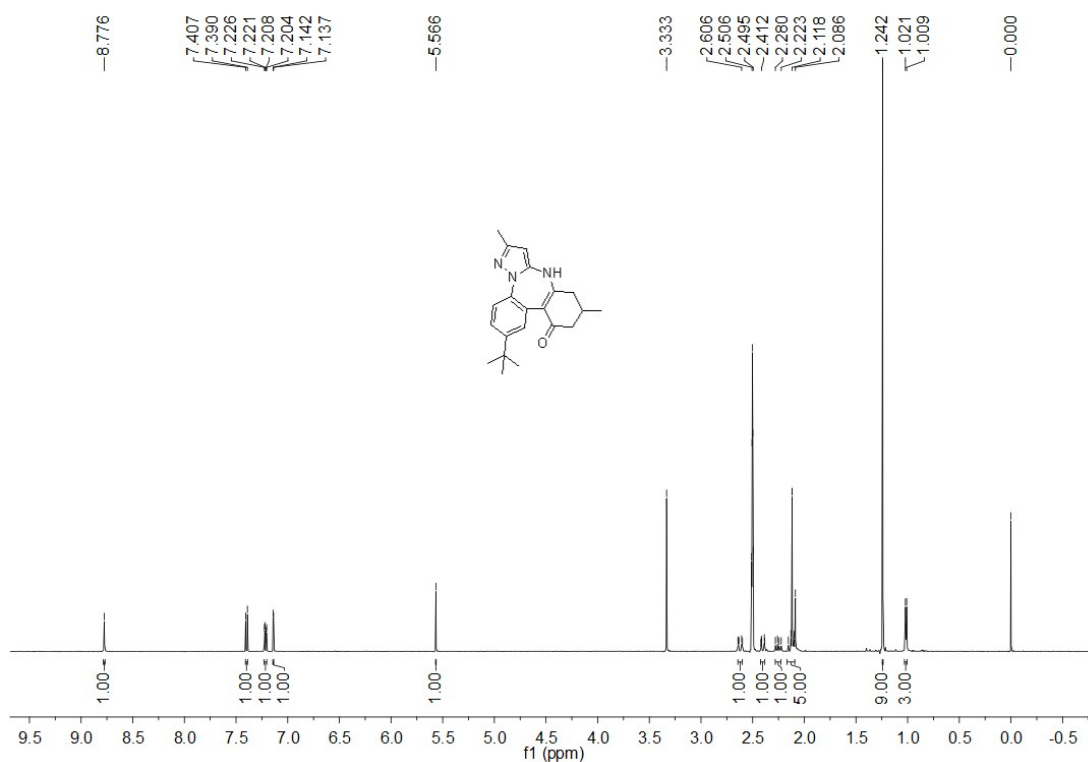
¹³C NMR Spectrum of Compound 3o



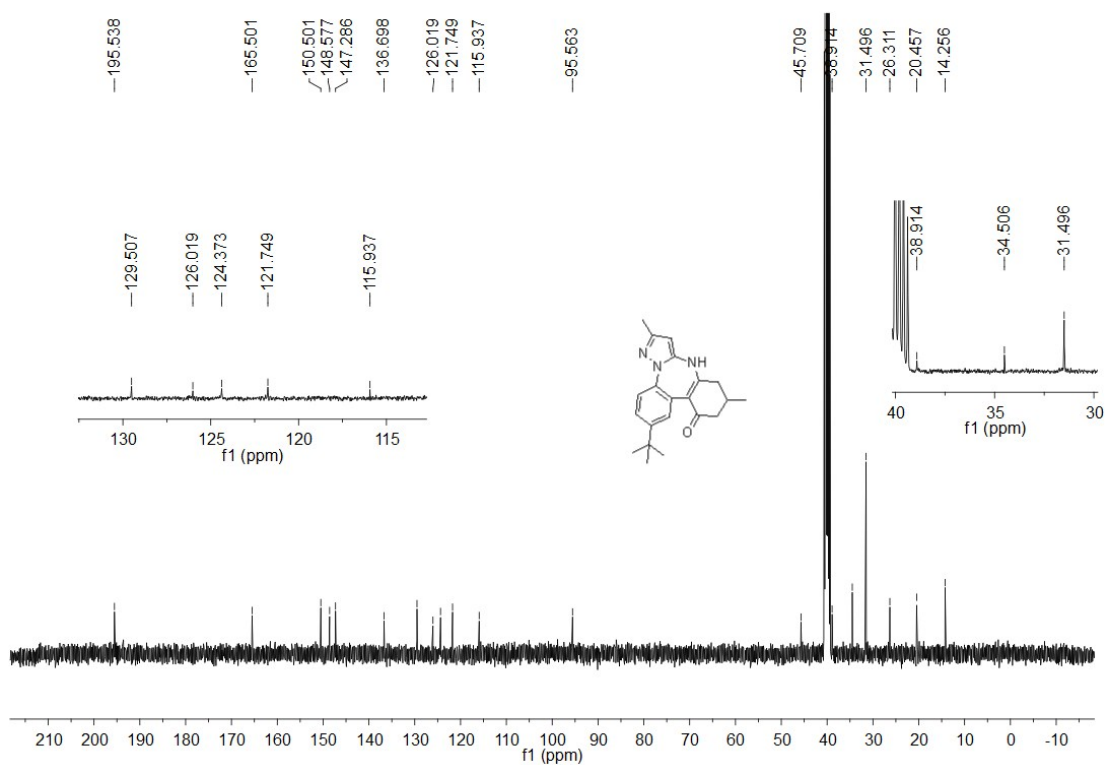
¹H NMR Spectrum of Compound 3p



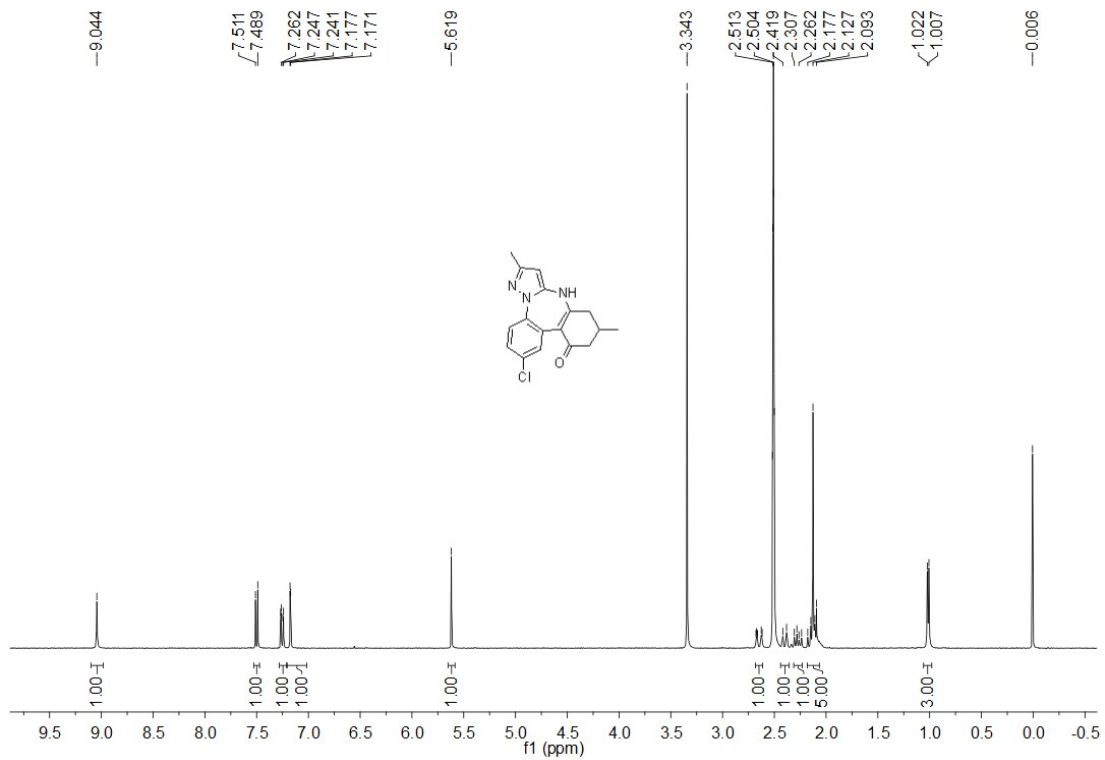
¹³C NMR Spectrum of Compound 3p



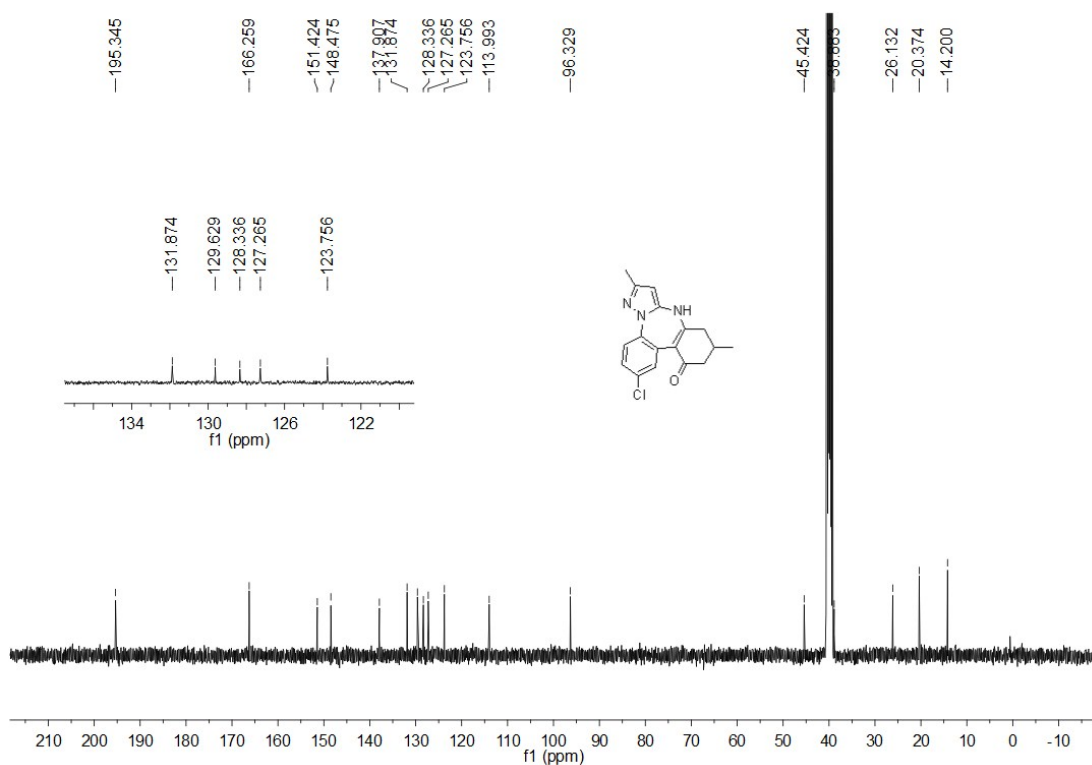
¹H NMR Spectrum of Compound 3q



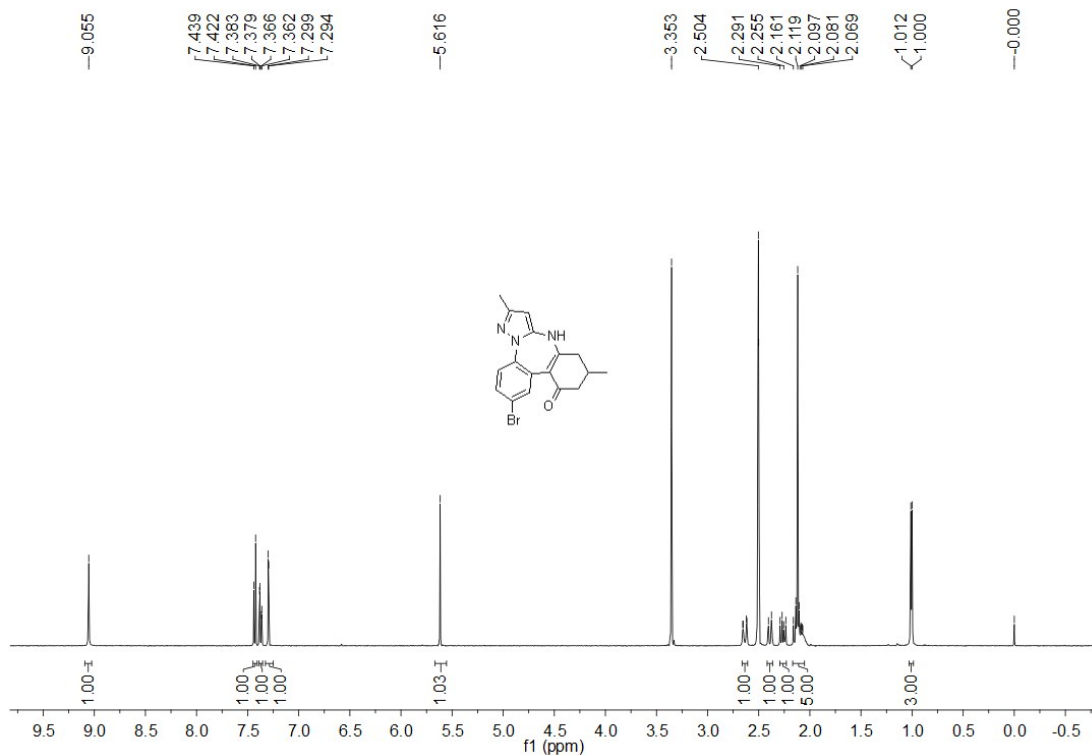
¹³C NMR Spectrum of Compound 3q



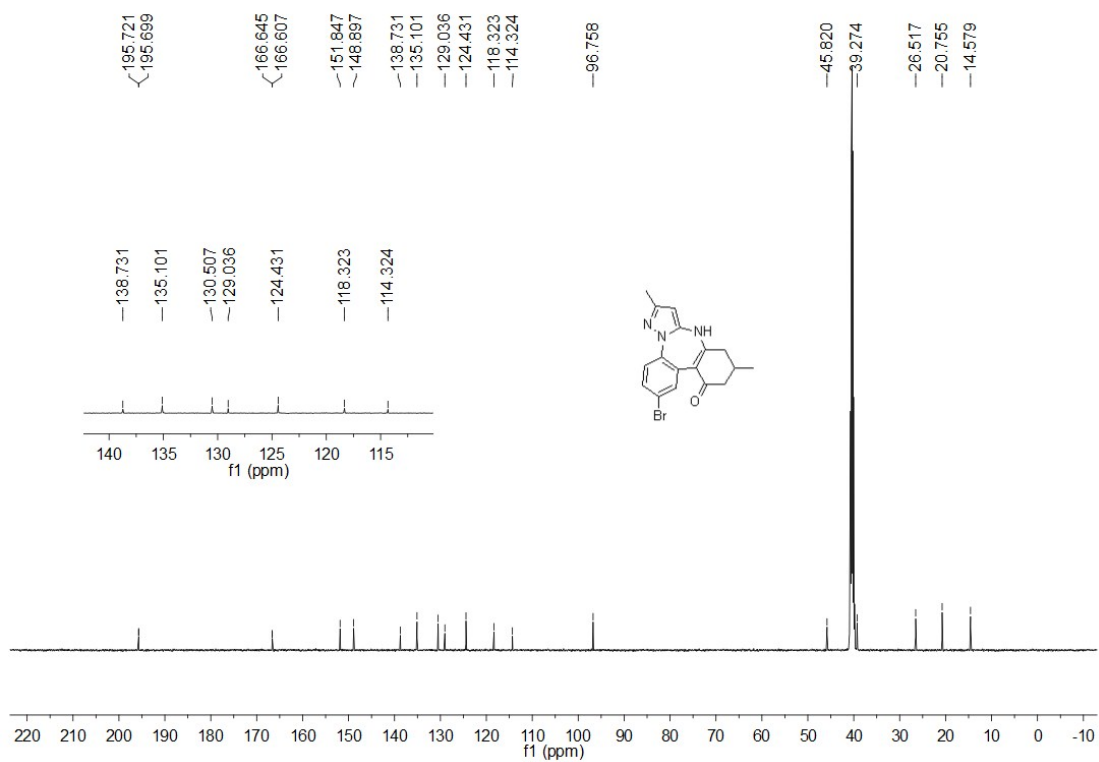
¹H NMR Spectrum of Compound 3r



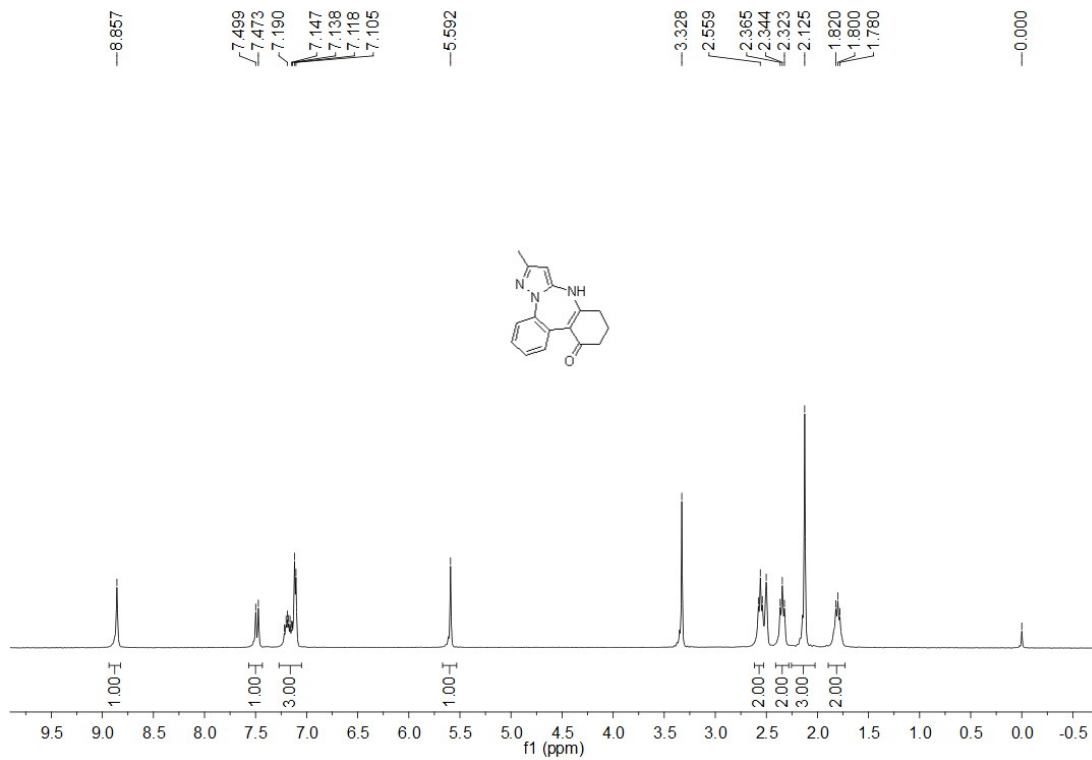
¹³C NMR Spectrum of Compound 3r



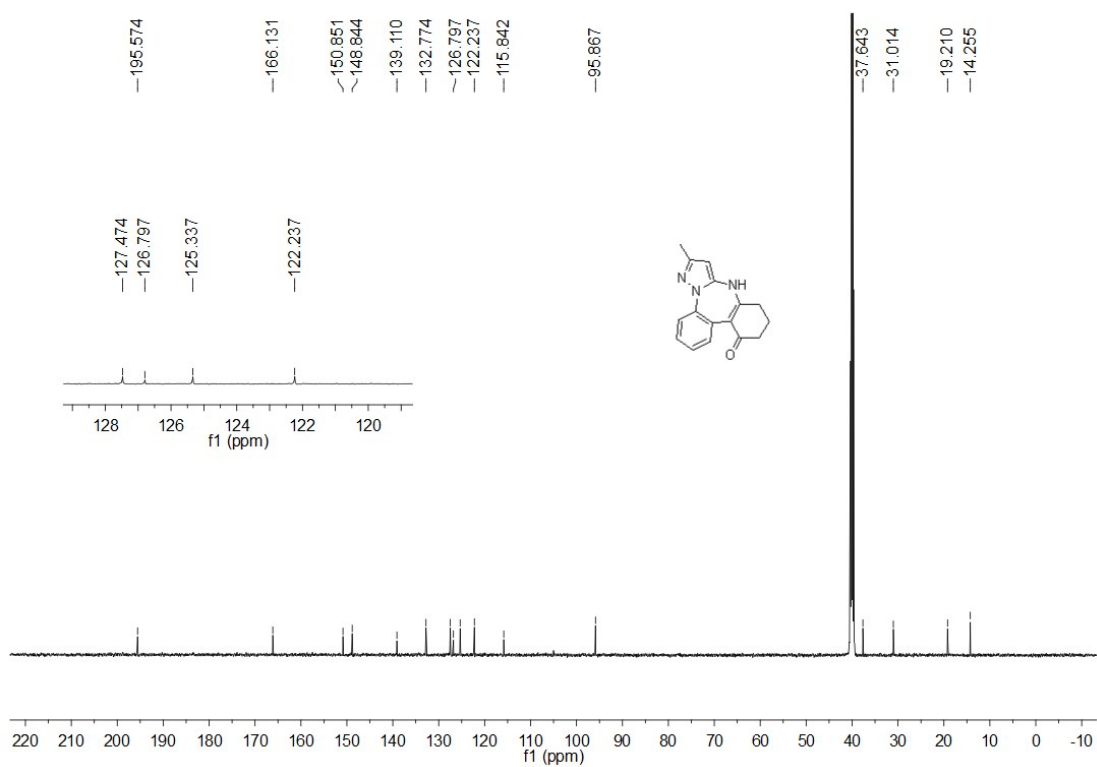
¹H NMR Spectrum of Compound 3s



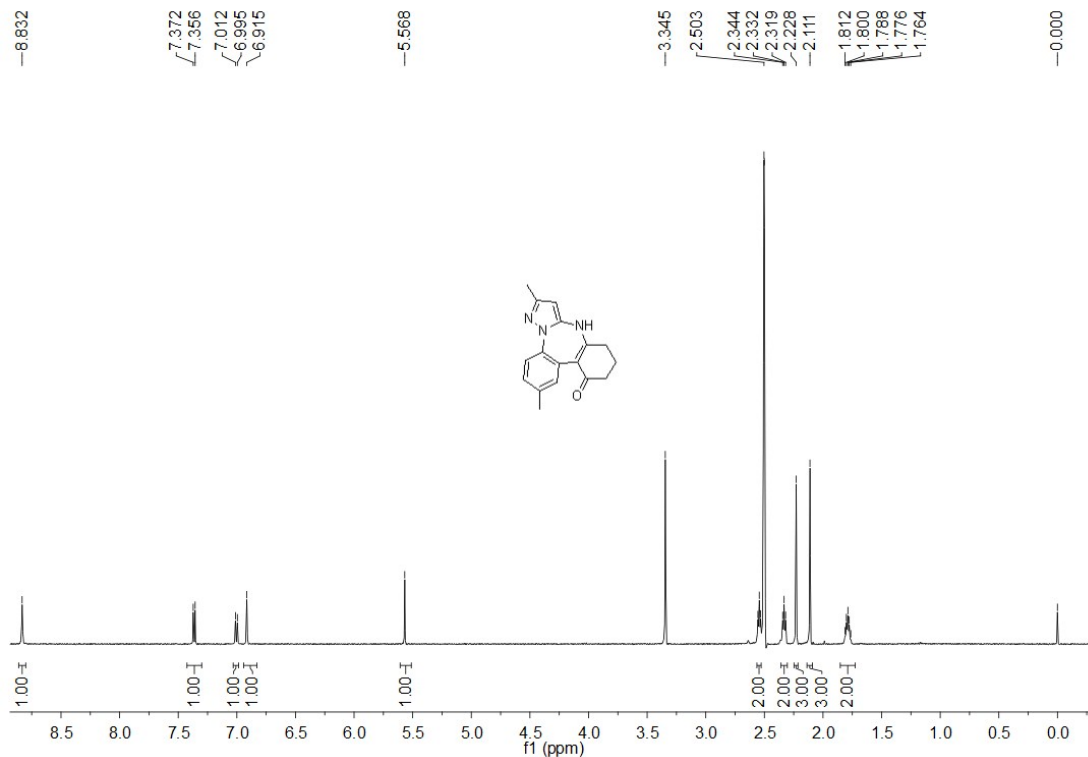
¹³C NMR Spectrum of Compound 3s



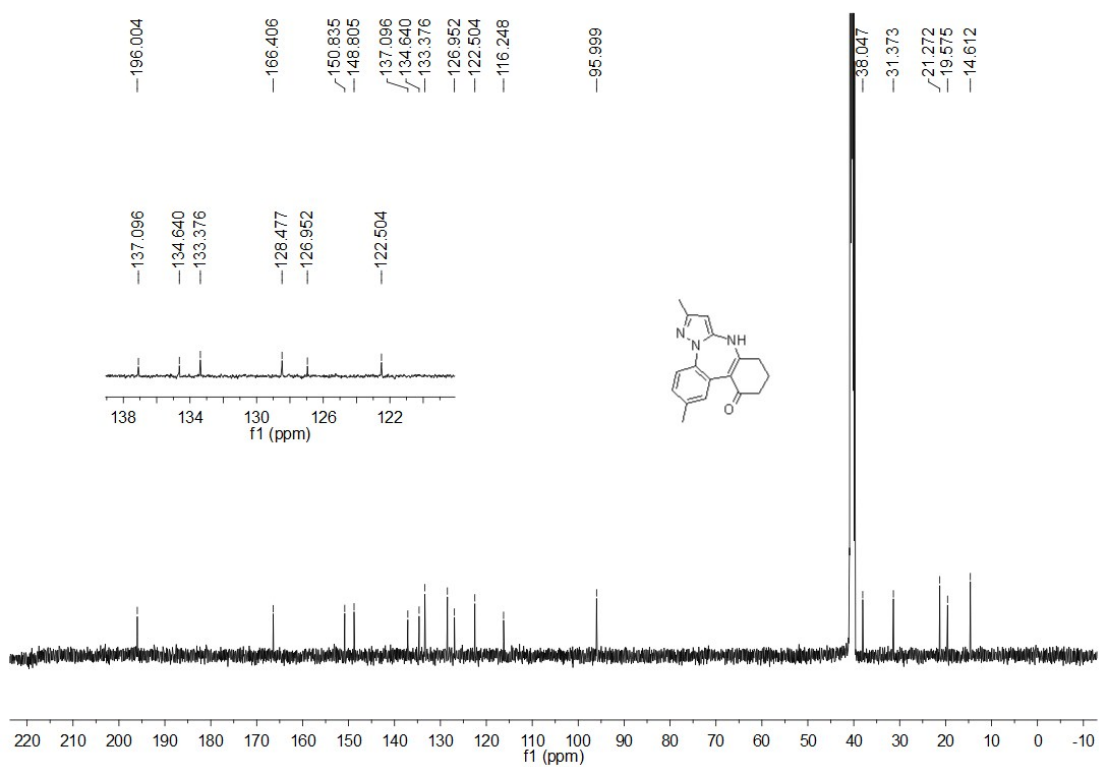
¹H NMR Spectrum of Compound 3t



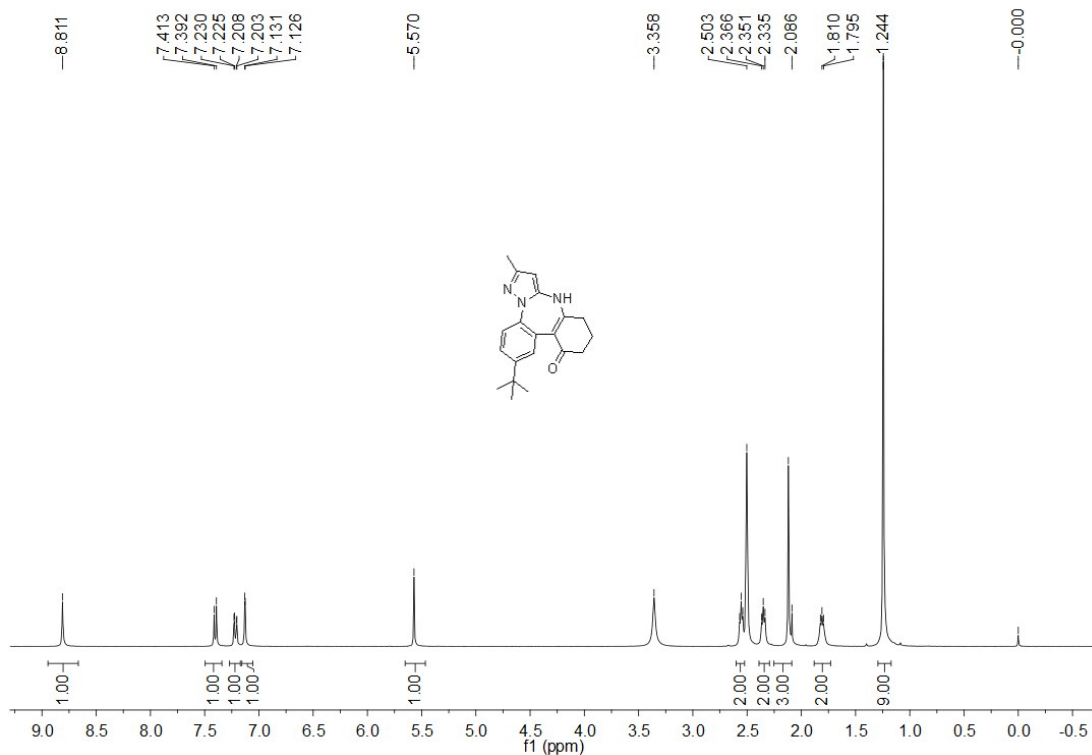
¹³C NMR Spectrum of Compound 3t



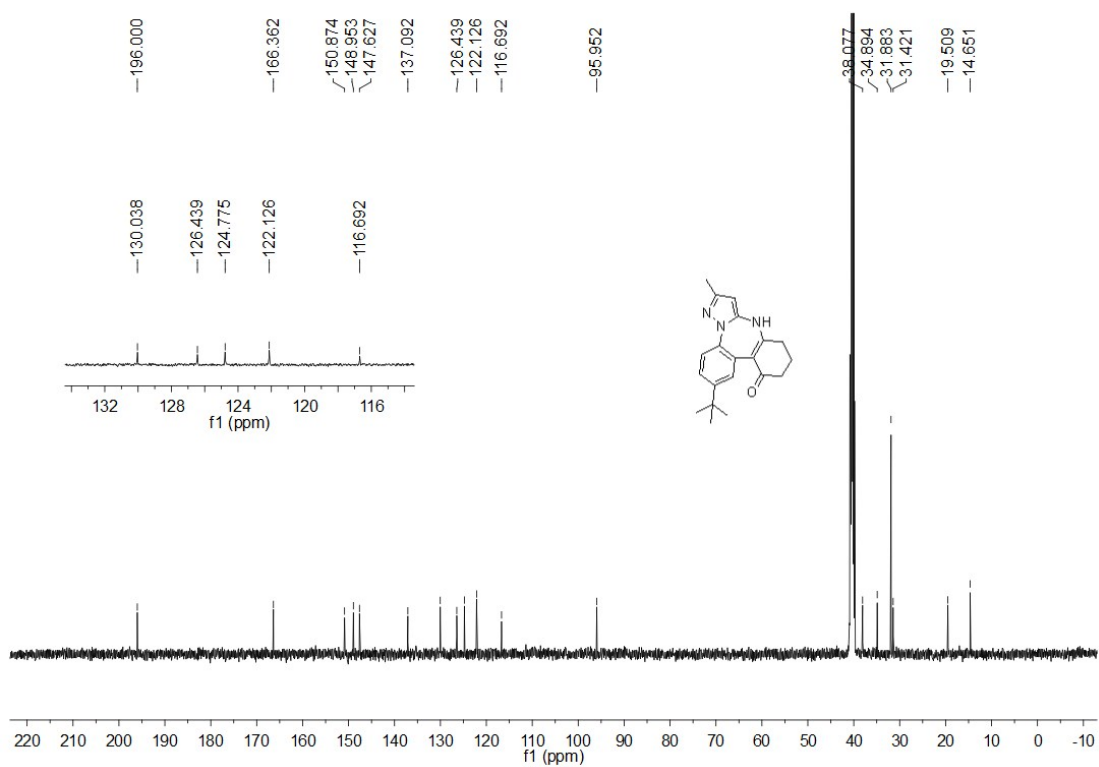
¹H NMR Spectrum of Compound 3u



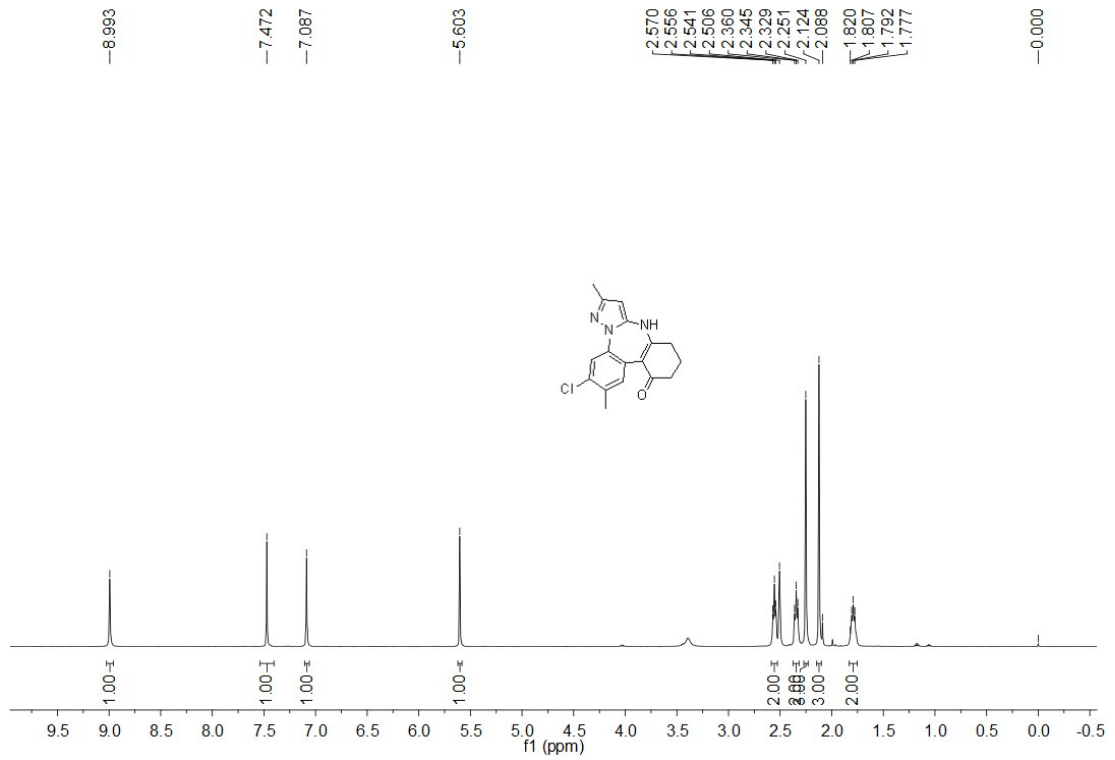
¹³C NMR Spectrum of Compound 3u



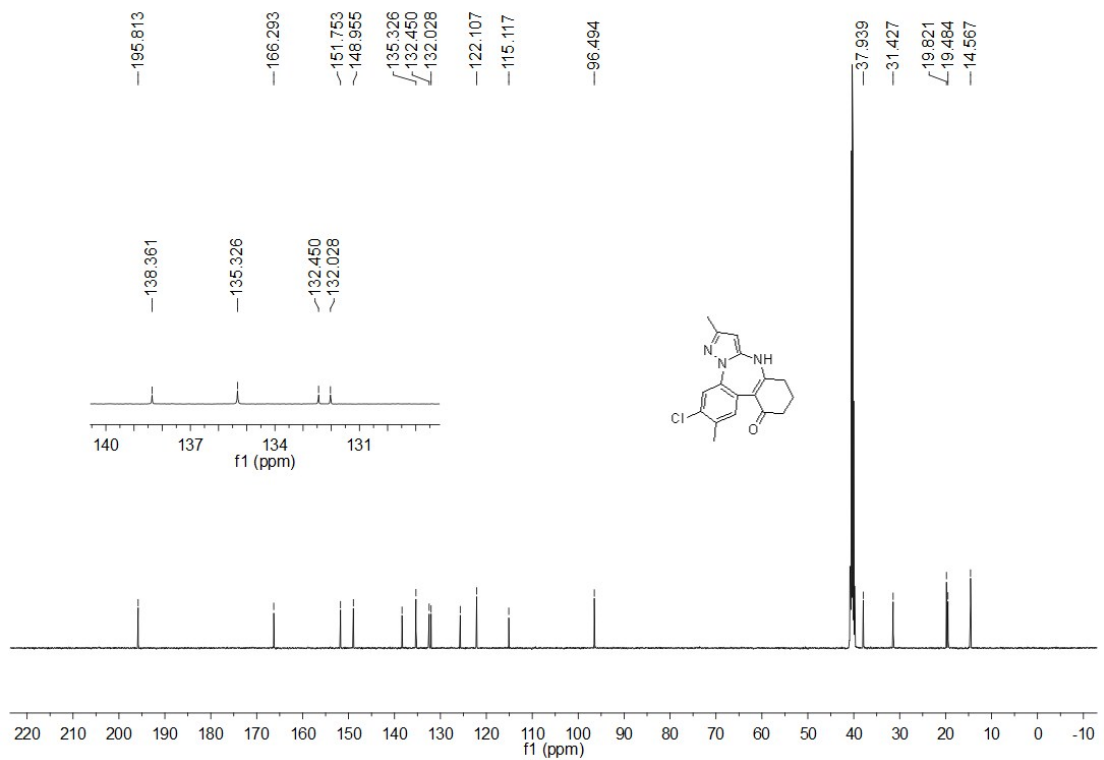
¹H NMR Spectrum of Compound 3v



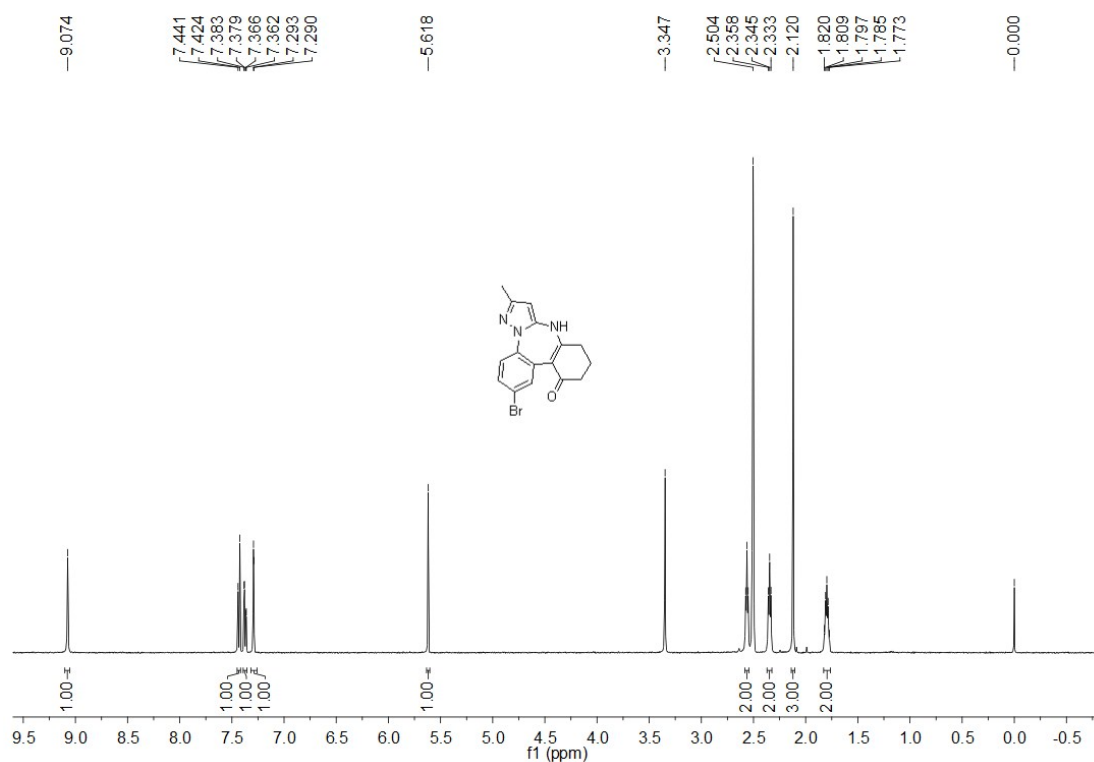
¹³C NMR Spectrum of Compound 3v



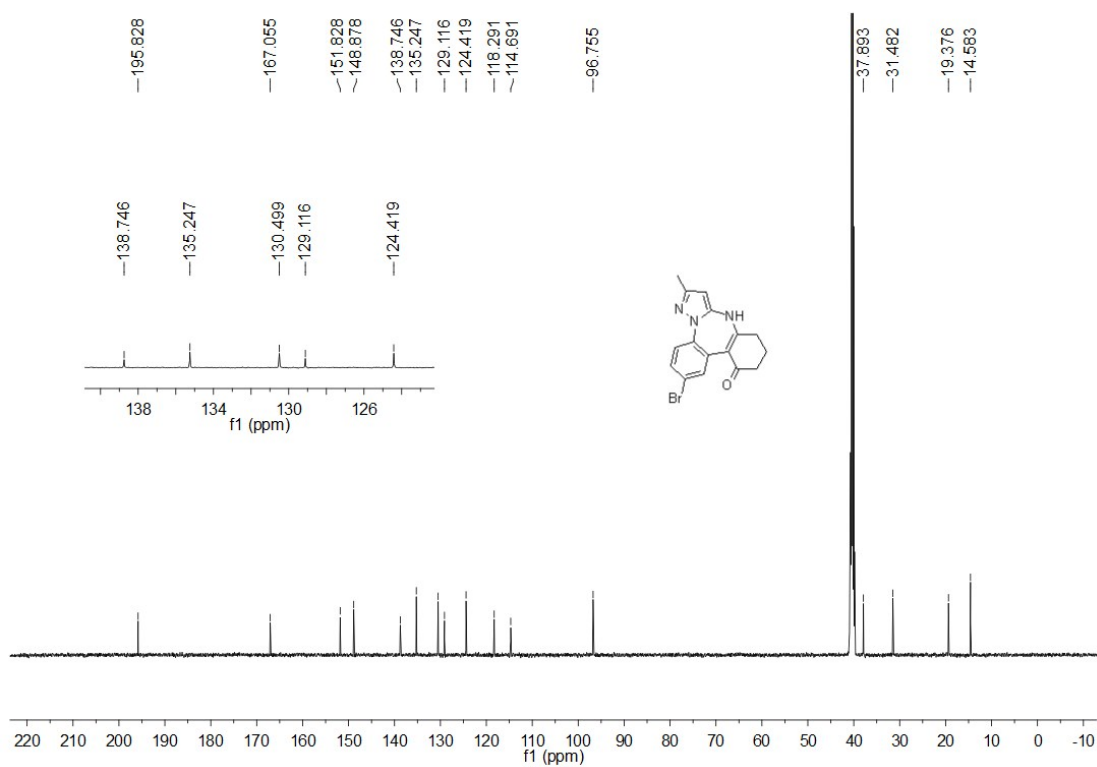
¹H NMR Spectrum of Compound 3w



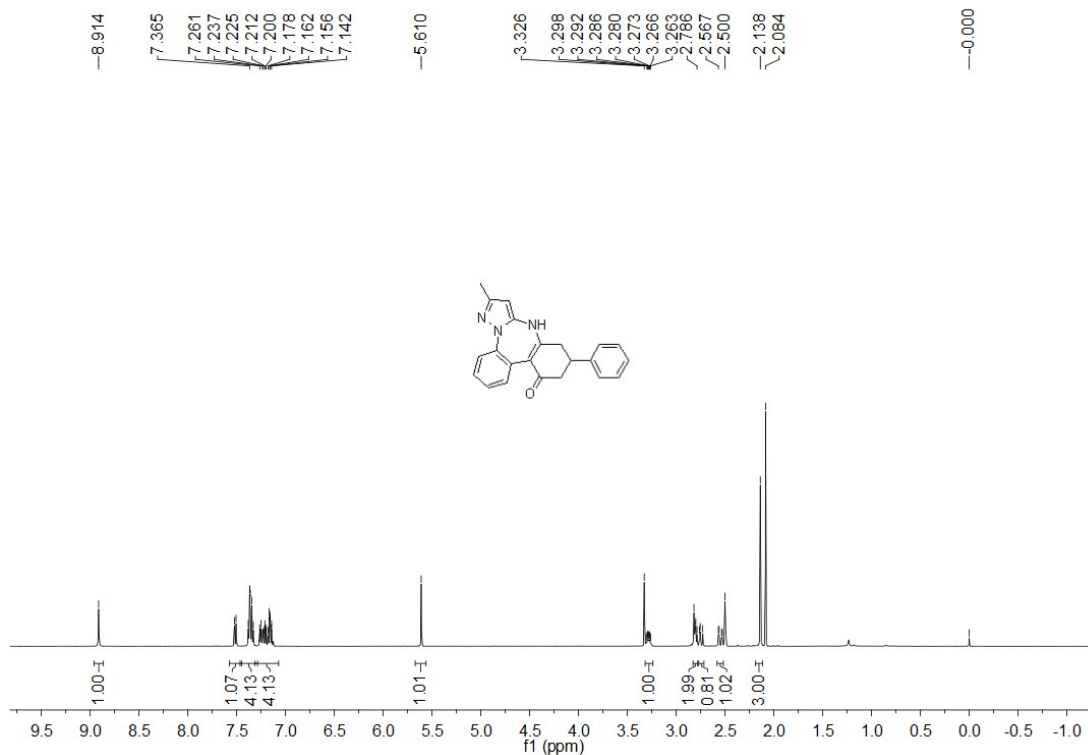
¹³C NMR Spectrum of Compound 3w



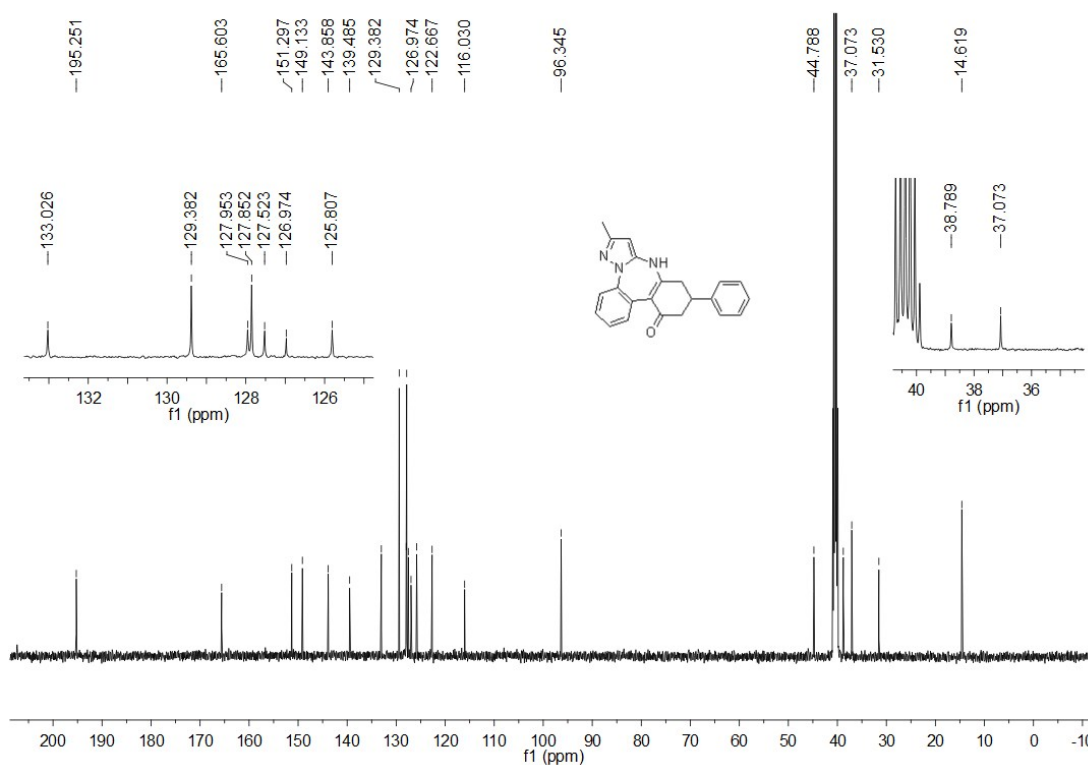
¹H NMR Spectrum of Compound 3x



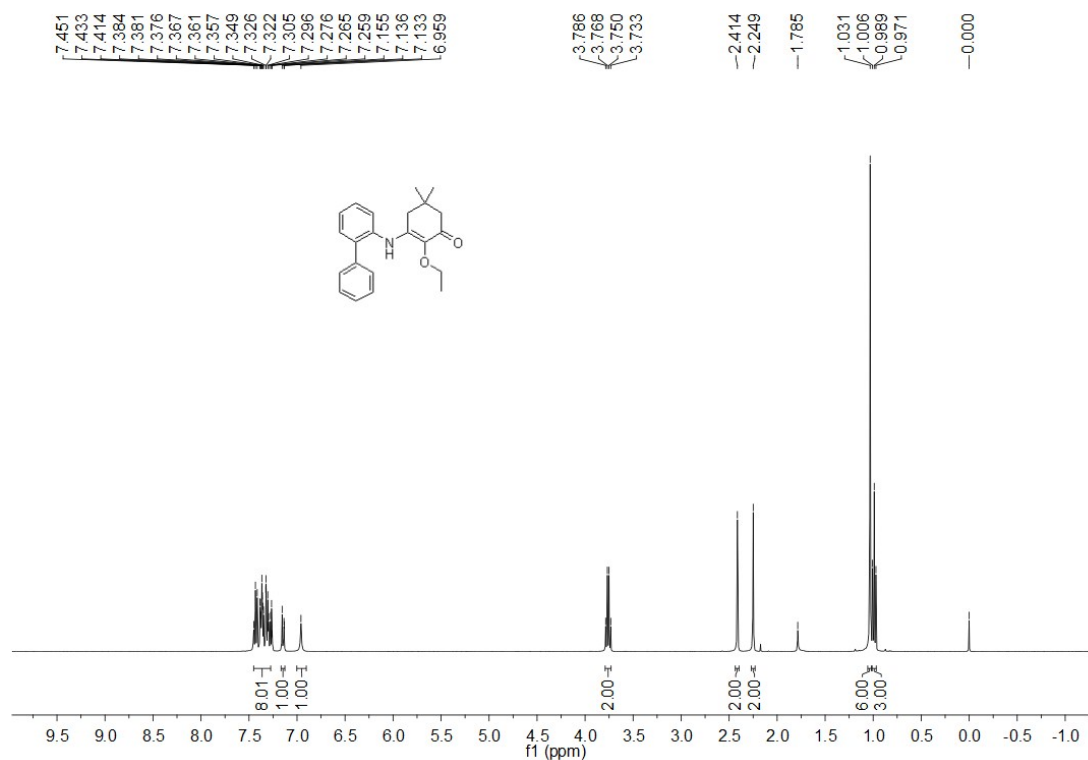
¹³C NMR Spectrum of Compound 3x



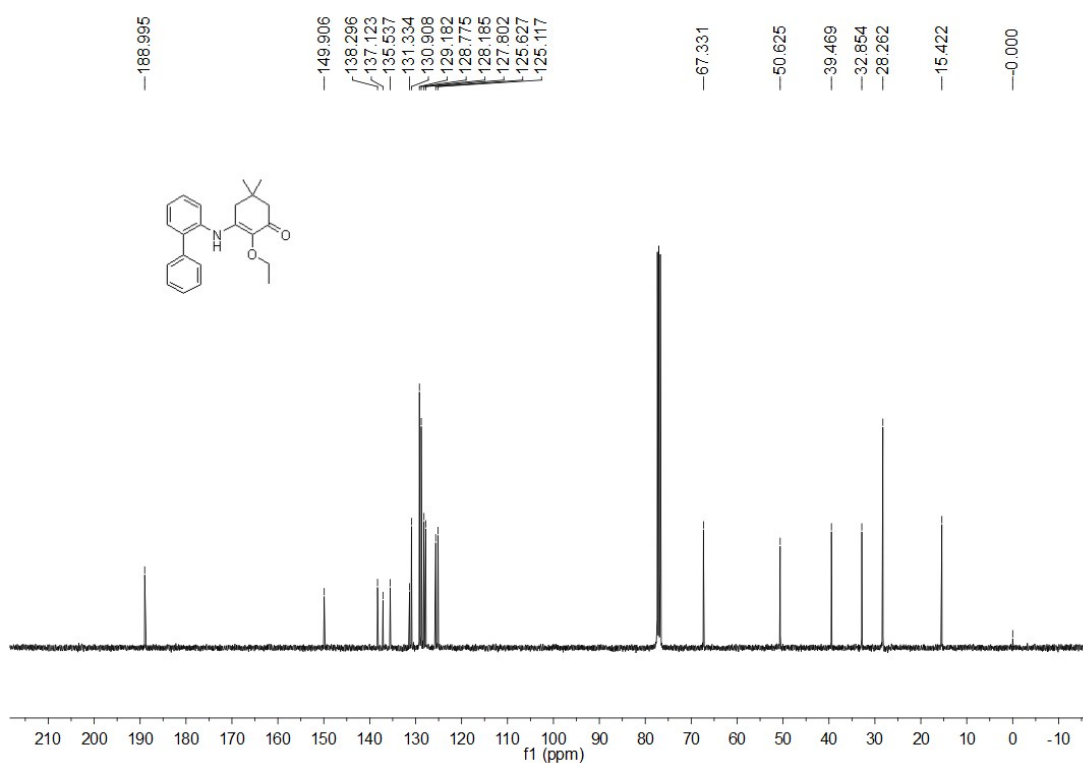
¹H NMR Spectrum of Compound 3y



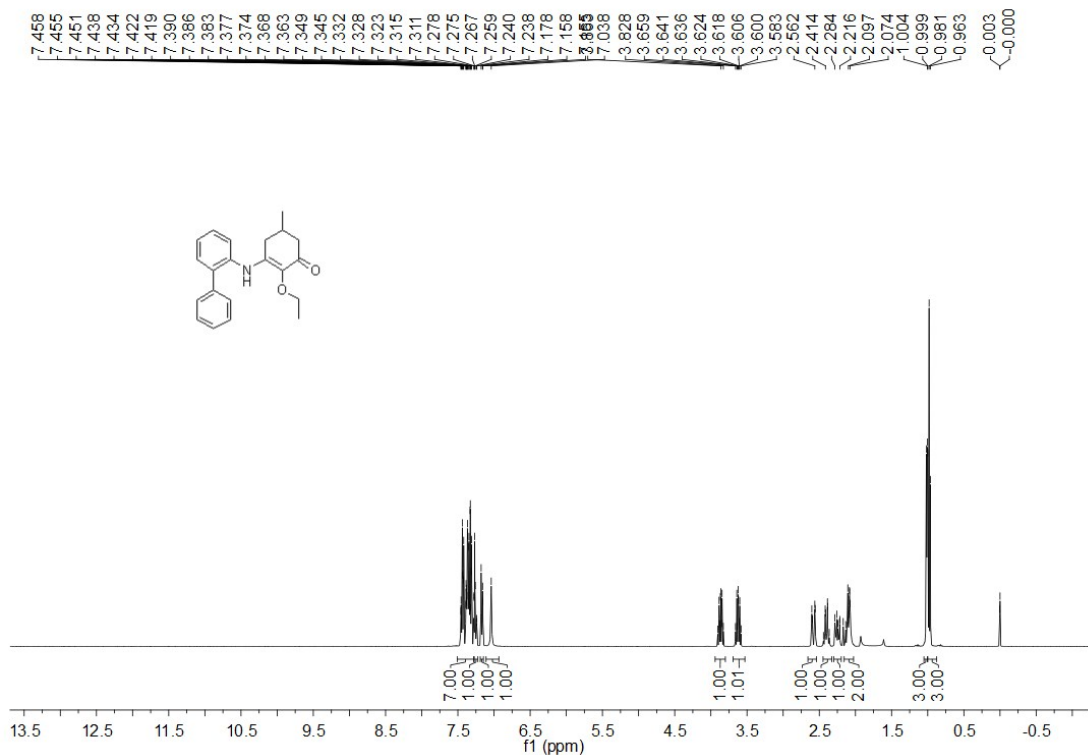
¹³C NMR Spectrum of Compound 3y



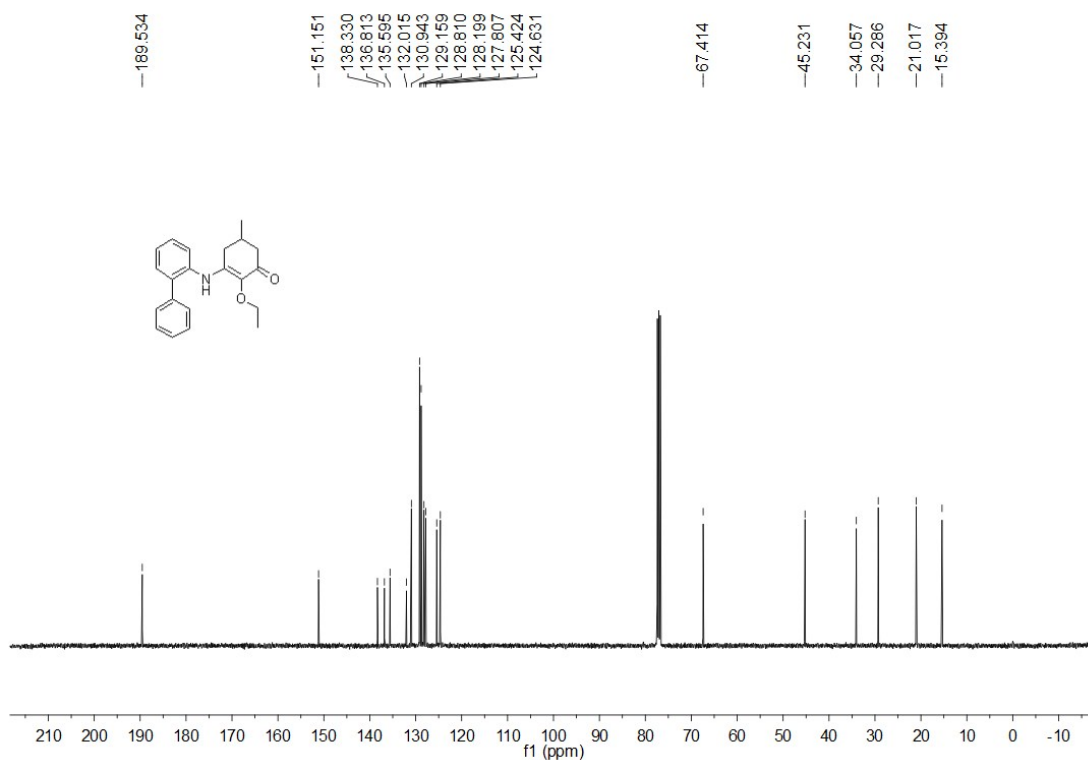
¹H NMR Spectrum of Compound 5a



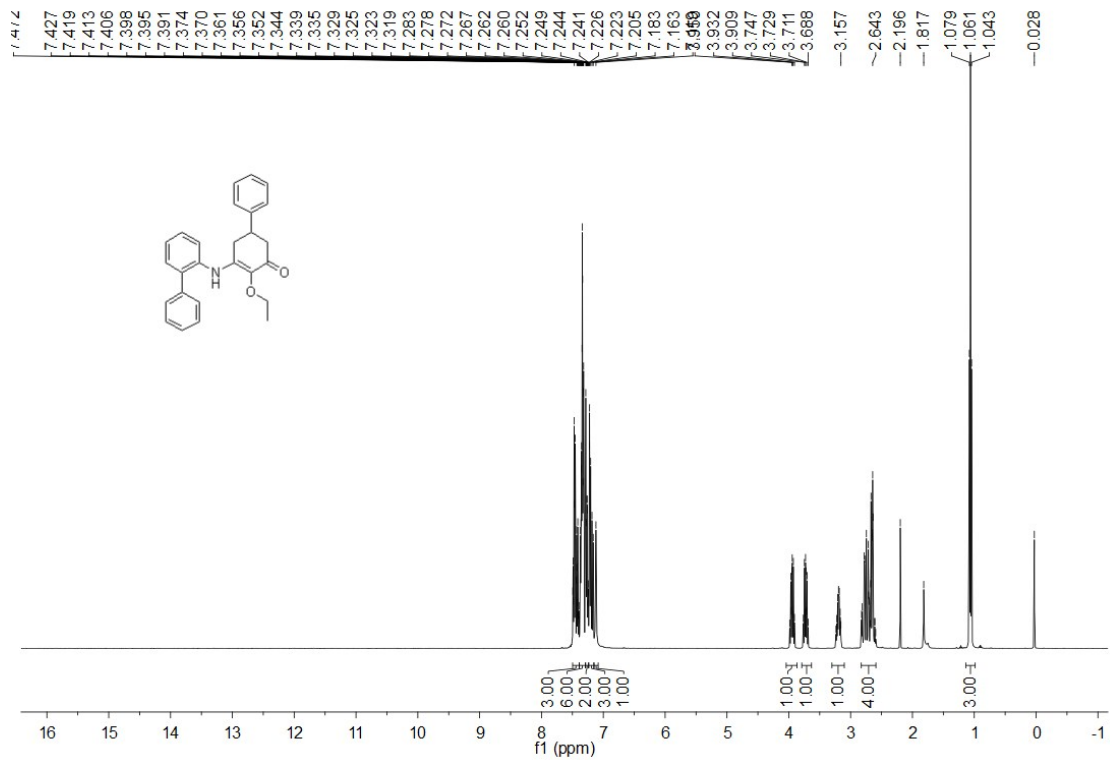
¹³C NMR Spectrum of Compound 5a



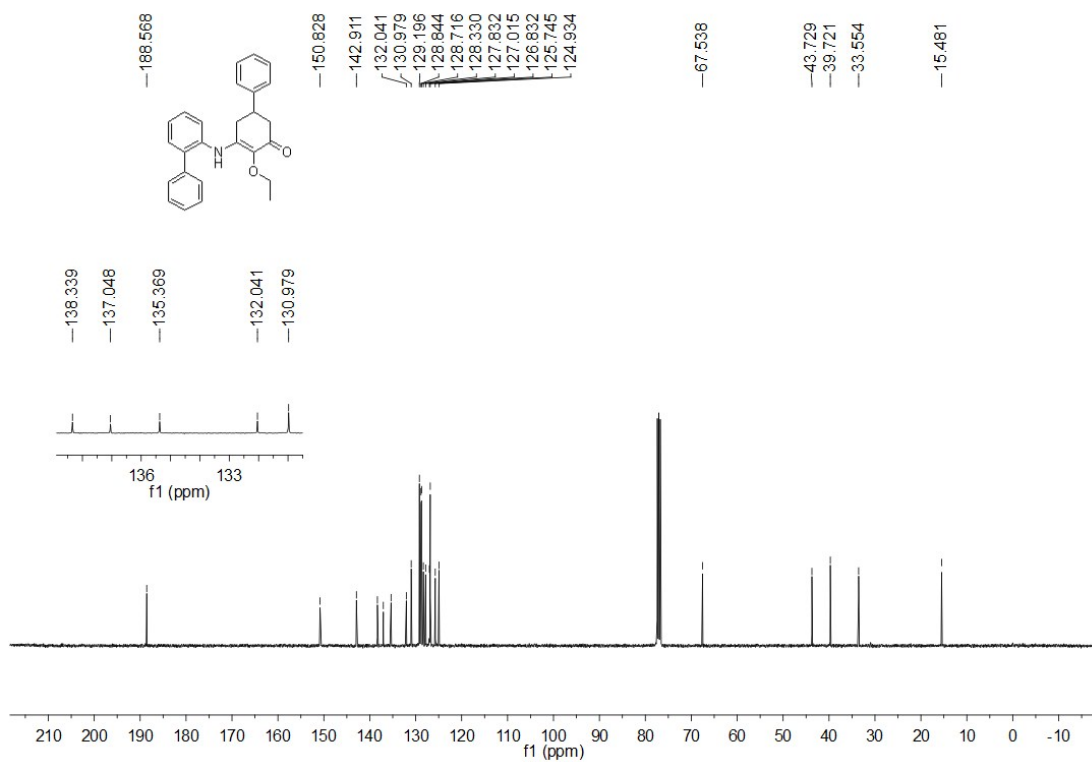
¹H NMR Spectrum of Compound 5b



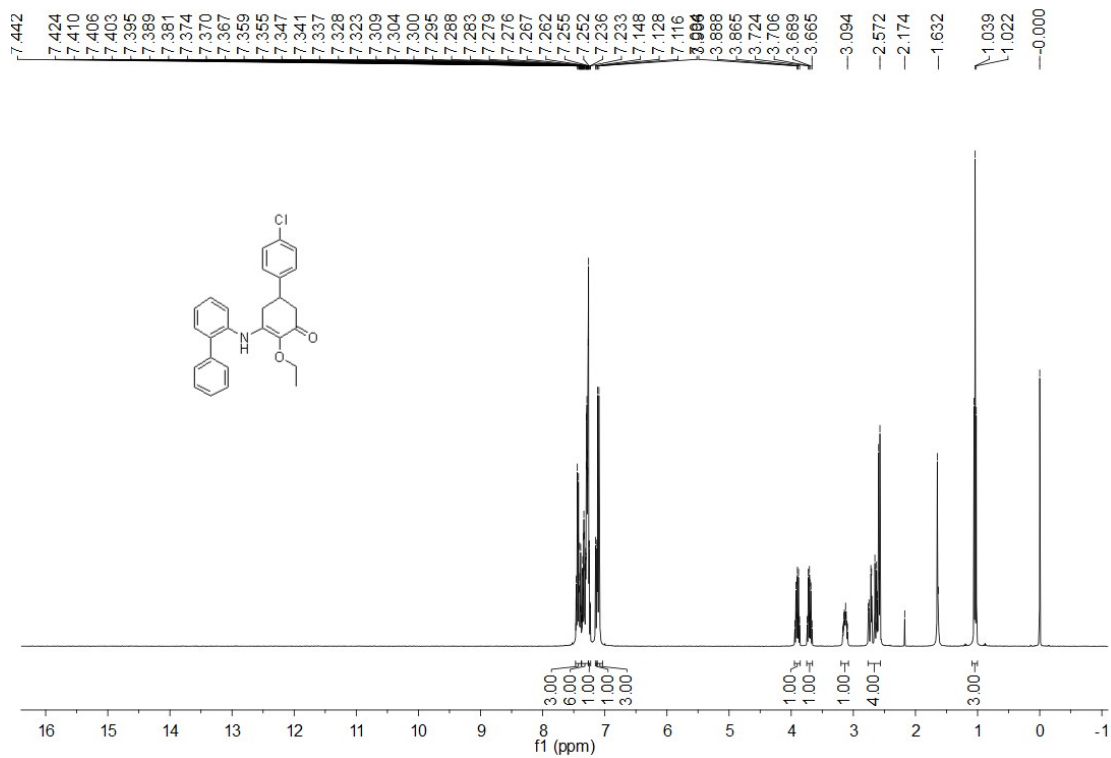
¹³C NMR Spectrum of Compound 5b



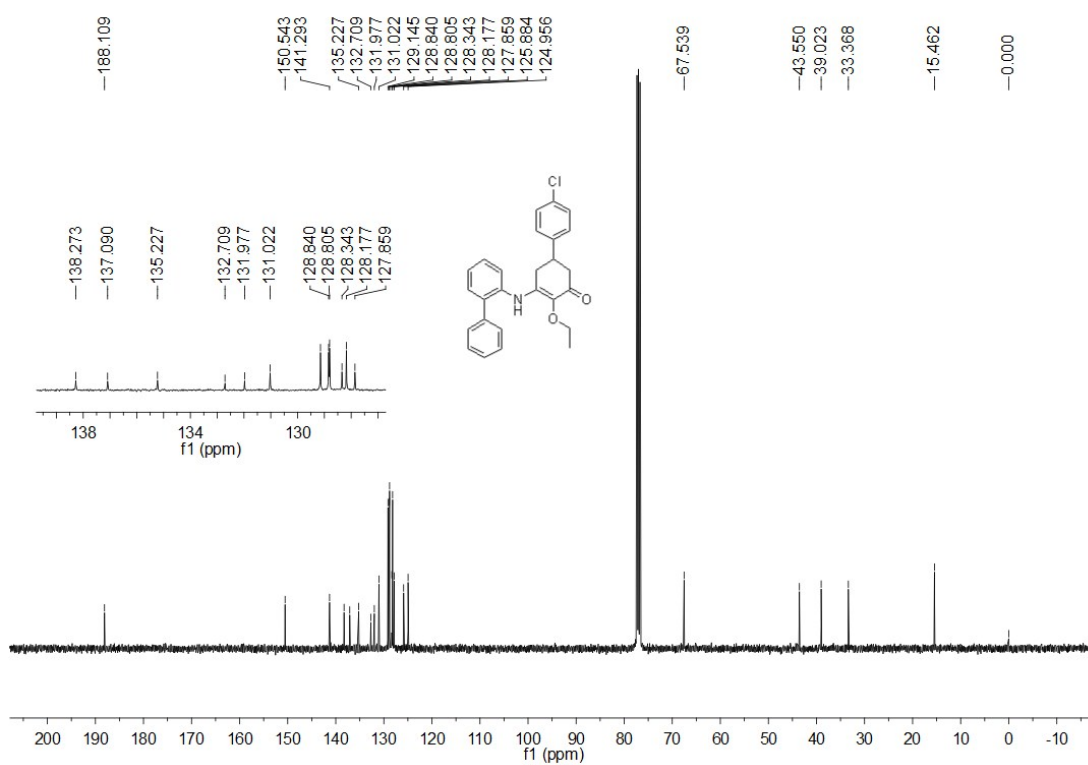
¹H NMR Spectrum of Compound 5c



¹³C NMR Spectrum of Compound 5c



¹H NMR Spectrum of Compound 5d



¹³C NMR Spectrum of Compound 5d

X-ray structure of 3a

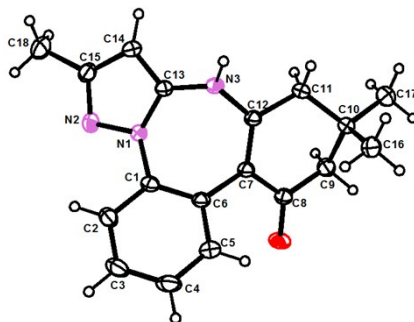


Table S1. Crystal Data for Compound **3a**

CCDC number	1976950
Formula	C ₁₈ H ₁₉ N ₃ O
Formula weight	293.36
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	<i>P</i> 2 (1)/ <i>c</i>
Unit cell dimensions	<i>a</i> = 7.2409(13) Å <i>α</i> = 90 deg. <i>b</i> = 19.433(4) Å <i>β</i> = 95.667(2) deg. <i>c</i> = 10.923(2) Å <i>γ</i> = 90 deg.
Volume	1529.4(5) Å ³
<i>Z</i>	4
Density (calculated)	1.274 Mg/m ³
Absorption coefficient	0.081 mm ⁻¹
<i>F</i> (000)	624
Crystal	0.23 x 0.21 x 0.20 mm
Theta range for data collection	2.10 to 25.37 deg.
Limiting indices	-8 ≤ <i>h</i> ≤ 8, -23 ≤ <i>k</i> ≤ 23, -13 ≤ <i>l</i> ≤ 13
Reflections collected	14728
Independent reflections	2801 [R(int) = 0.0408]
Data / restraints / parameters	2801 / 0 / 202
Goodness-of-fit on <i>F</i> ²	1.042
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0472, <i>wR</i> ₂ = 0.1181
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0636, <i>wR</i> ₂ = 0.1283
Largest diff. peak and hole	0.420 and -0.366 e. Å ⁻³

X-ray structure of 5b

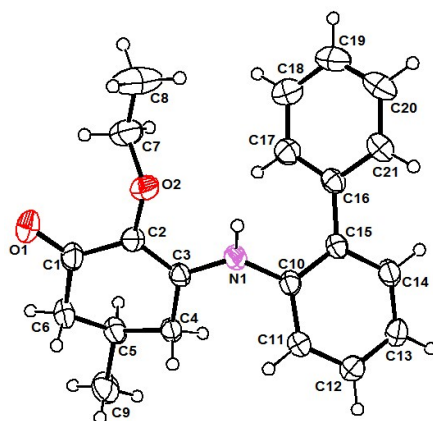


Table S1. Crystal Data for Compound **5b**

CCDC number	1976897
Formula	C ₂₁ H ₂₃ NO ₂
Formula weight	321.40
Temperature	298.15 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /n
Unit cell dimensions	$a = 13.583(3)$ Å $\alpha = 90$ deg. $b = 8.561(2)$ Å $\beta = 97.03(3)$ deg. $c = 15.116(3)$ Å $\gamma = 90$ deg.
Volume	1744.5(7) Å ³
<i>Z</i>	4
Density (calculated)	1.224 Mg/m ³
Absorption coefficient	0.078 mm ⁻¹
<i>F</i> (000)	688
Crystal	0.23 x 0.21 x 0.20 mm
Theta range for data collection	5.638 to 55.07 deg.
Limiting indices	-17 ≤ <i>h</i> ≤ 17, -11 ≤ <i>k</i> ≤ 11, -19 ≤ <i>l</i> ≤ 19
Reflections collected	32906
Independent reflections	4008 [R(int) = 0.0353]
Data / restraints / parameters	4008 / 0 / 219
Goodness-of-fit on <i>F</i> ²	1.036
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	$R_1 = 0.0495$, $wR_2 = 0.1225$
<i>R</i> indices (all data)	$R_1 = 0.0695$, $wR_2 = 0.1402$
Largest diff. peak and hole	0.20 and -0.20 e. Å ⁻³