Electronic Supporting Information (ESI)

for

Regioselectivity of the trifluoroethanol-promoted intramolecular *N*-Boc – epoxide cyclization towards 1,3-oxazolidin-2-ones and 1,3-oxazinan-2-ones

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1. X-ray crystallography data

X-ray reflections were collected on a Bruker APEX-II, CCD diffractometer using Mo Kα (λ = 0.71073 Å) radiation. Data reduction was performed using Bruker SAINT Software.[1] Intensities for absorption were corrected using SADABS. Structures were solved and refined using SHELXL-2014 with anisotropic displacement parameters for non-H atoms. Hydrogen atom on O was experimentally located in the crystal structure. All C–H atoms were fixed geometrically using the HFIX command in SHELX-TL.[2] A check of the final CIF file using PLATON did not show any missed symmetry.[3,4] The crystallographic parameters for **5d** and **6d** are summarized in Table ESI-1. X-ray crystallographic structures of **5e** and **5f** are shown in the Figures ESI-1 and ESI-1, respectively.

Table ESI-1. Crystal data parameters of **5e** and **6e**

Crystal Data	**5e**	**6e**
Formula unit	$C_{16}H_{15}NO_3$	$C_{16}H_{15}NO_3$
Formula wt.	269.29	269.29
Crystal system	Triclinic	Orthorhombic
T [K]	100	100
a [Å]	7.3130(10)	14.3884(13)
b [Å]	9.4042(12)	26.944(3)
c [Å]	9.8866(13)	6.9828(6)
α [°]	97.320(7)	90
β [°]	95.213(7)	96
γ [°]	94.533(7)	90
Volume [Å^3]	668.77(15)	2707.1(4)
Space group	*P-1*	*Pccn*
Z	2	8
D_{calc} [g cm^{-3}]	1.337	1.321
μ/mm^{-1}	0.093	0.092
Reflns. Collected	22687	21415

Unique reflns.	3653	3356
Observed reflns.	2689	1667
R_1 [I>2σ(I)], wR_2	0.0451, 0.1199	0.0620, 0.1681
GOF	0.780	0.767
Instrument	Bruker APEX-II CCD	Bruker APEX-II CCD
X-ray	MoK\a	MoK\a
CCDC Reference No.	1970676	1970675

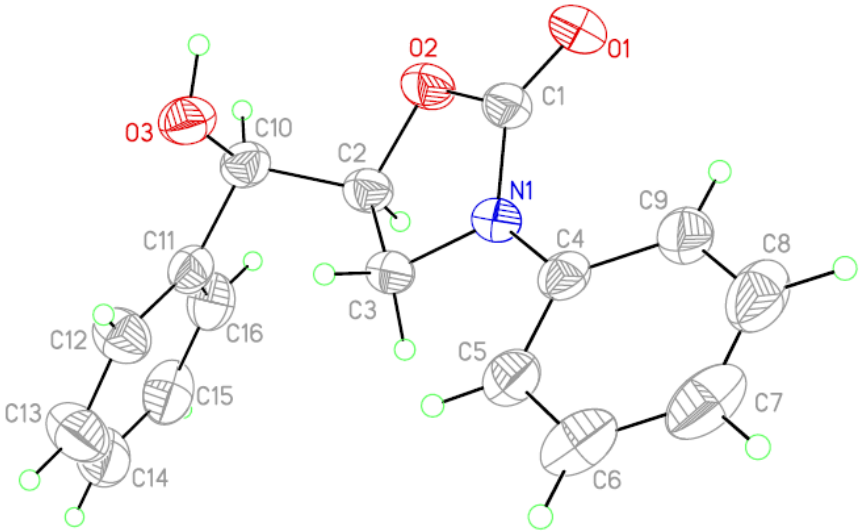


Figure ESI-1. X-ray crystallographic structure of **5e.**

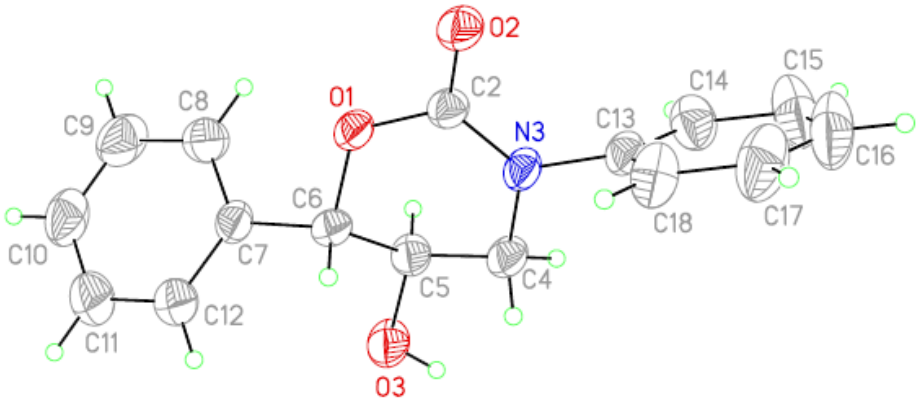
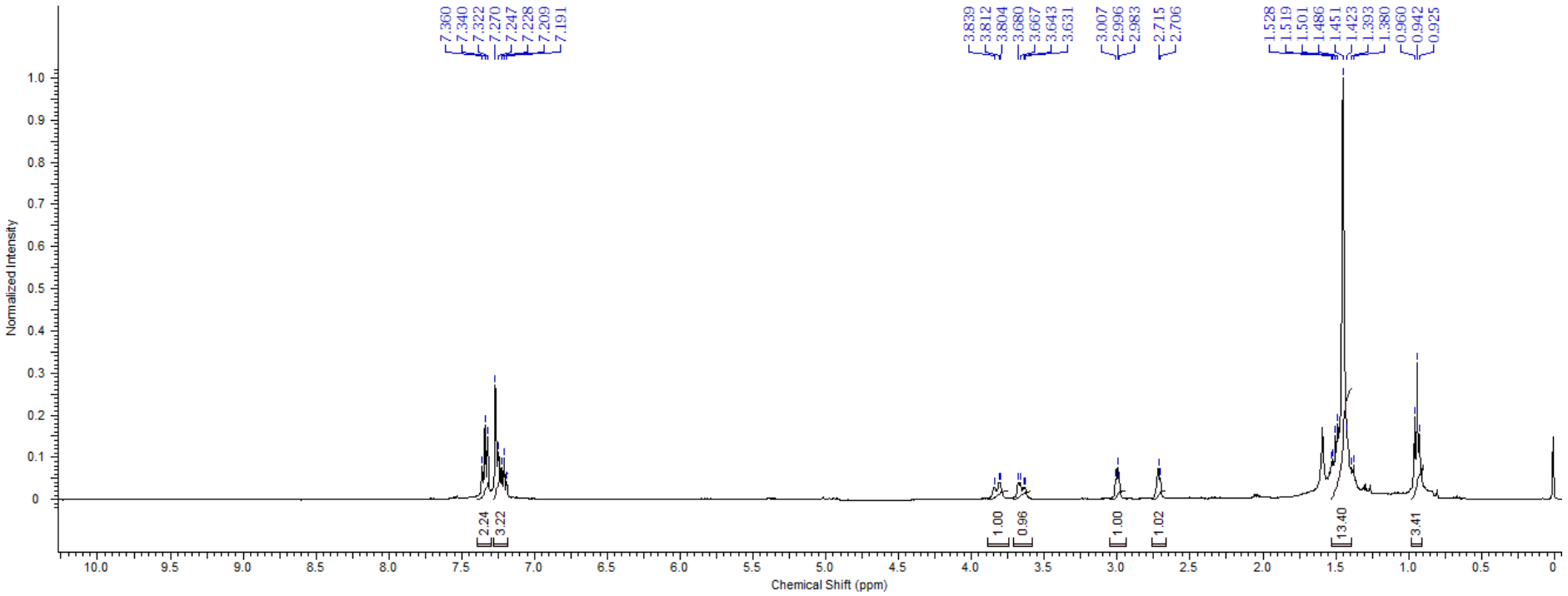


Figure ESI-2. X-ray crystallographic structure of **6e.**

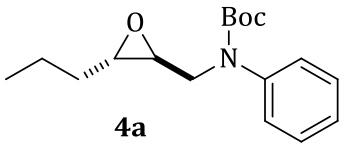
2. References:

1. SAINT Plus, Bruker AXS Inc.: Madison, WI, 2008; BRUKER AXS (v 6.14).
2. Bruker AXS Inc.: Madison, WI, 2008.
3. PLATON, A Multipurpose Crystallographic Tool; A. L. Spek, Utrecht University: Utrecht, Netherland, 2002.
4. Spek, A. L. *J. Appl. Crystallogr.*, **2003**, *36*, 7–13.

3. Copies of ^{1}H and ^{13}C NMR spectra of compounds



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4a**.



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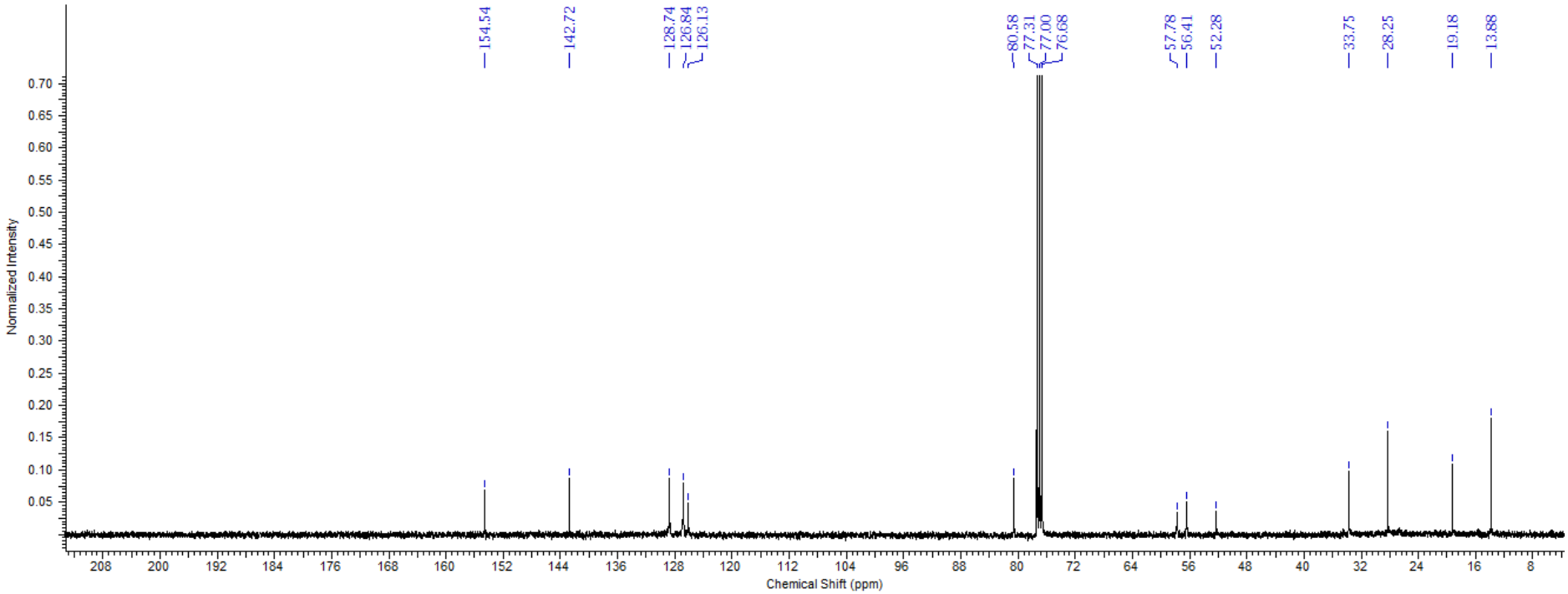
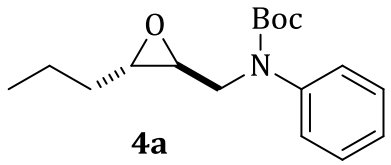


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4a**.



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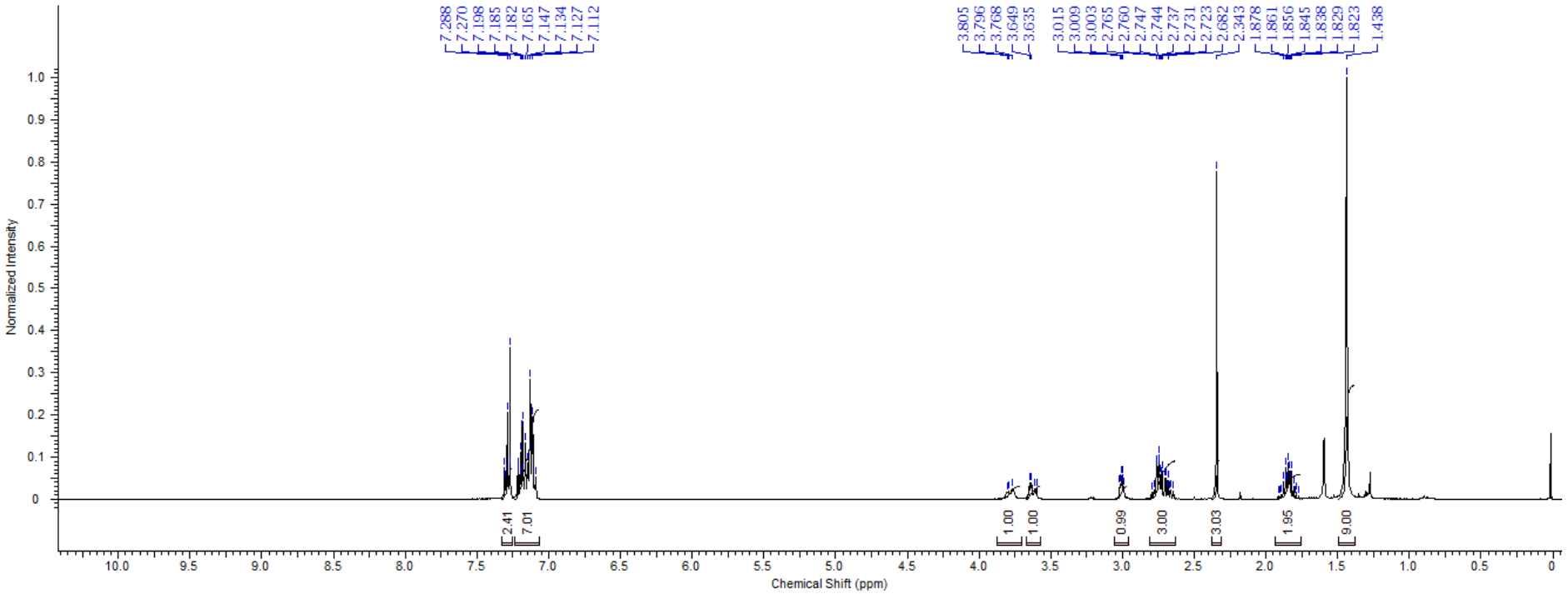
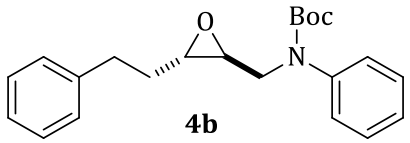


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4b**.



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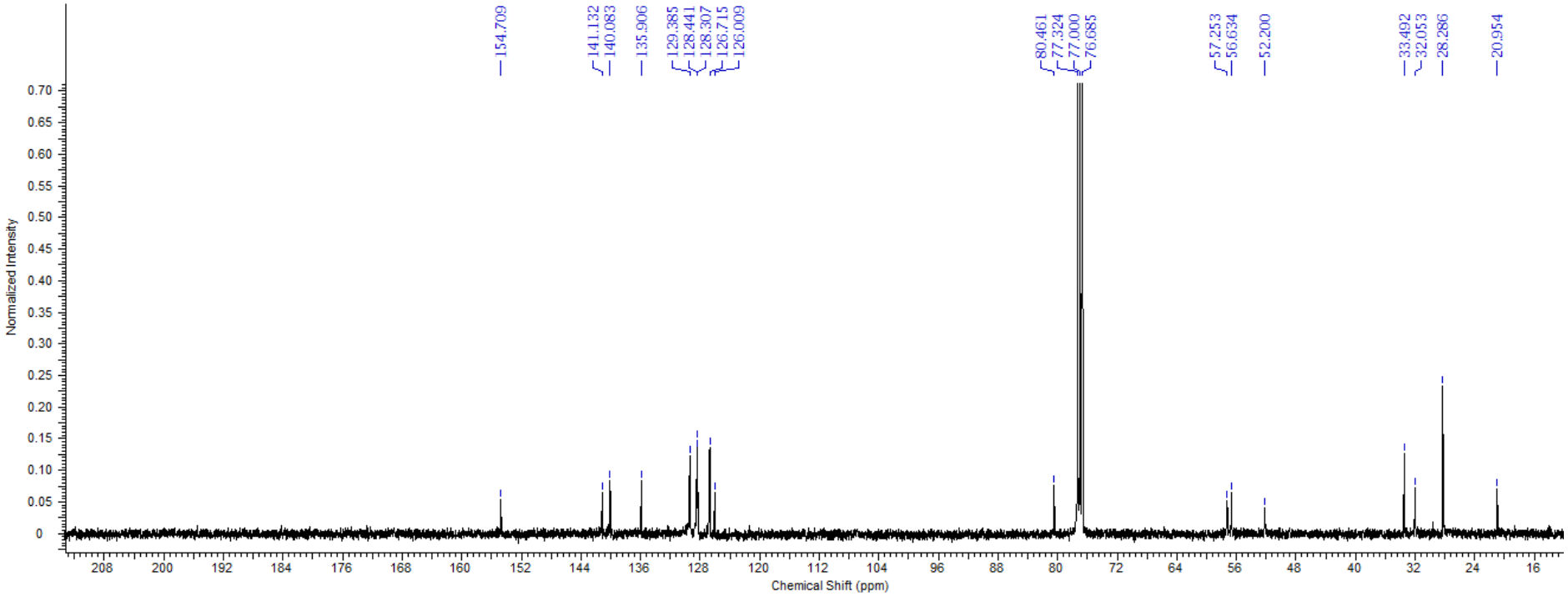
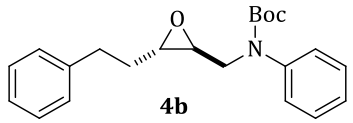


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4b**.



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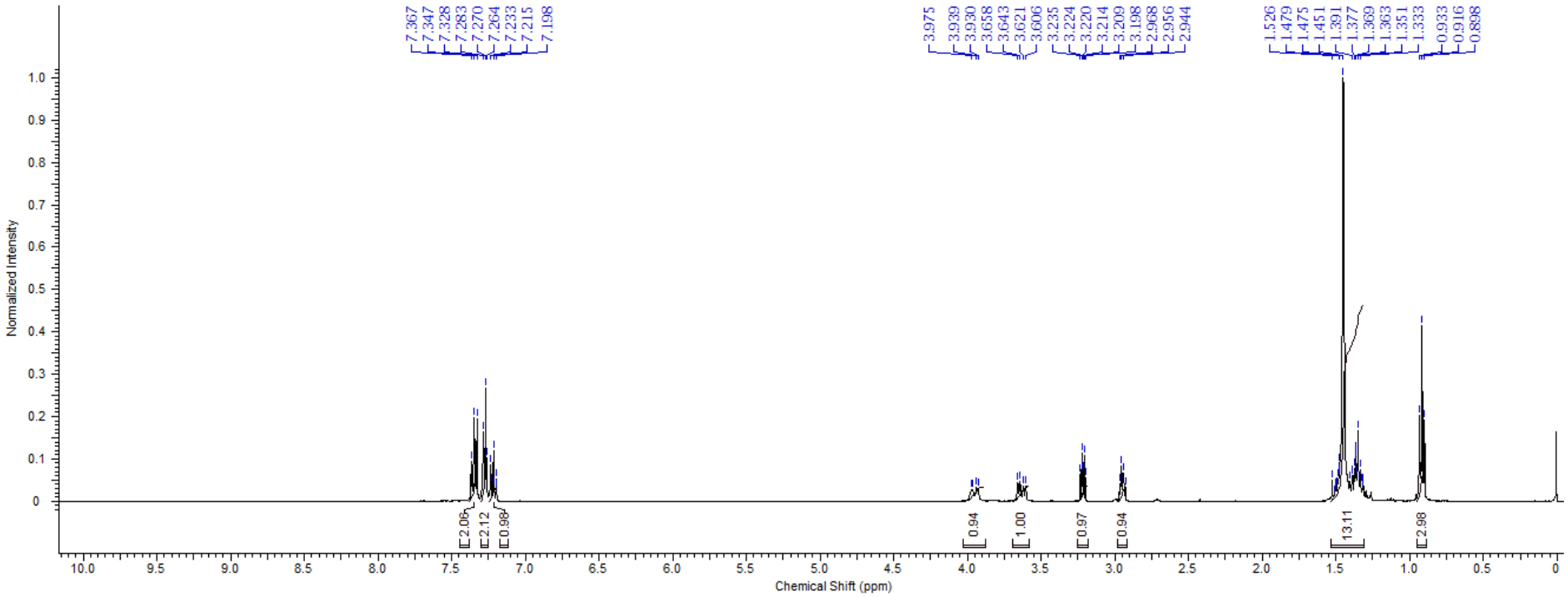
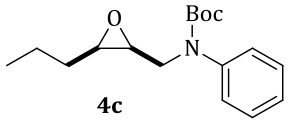


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4c**.



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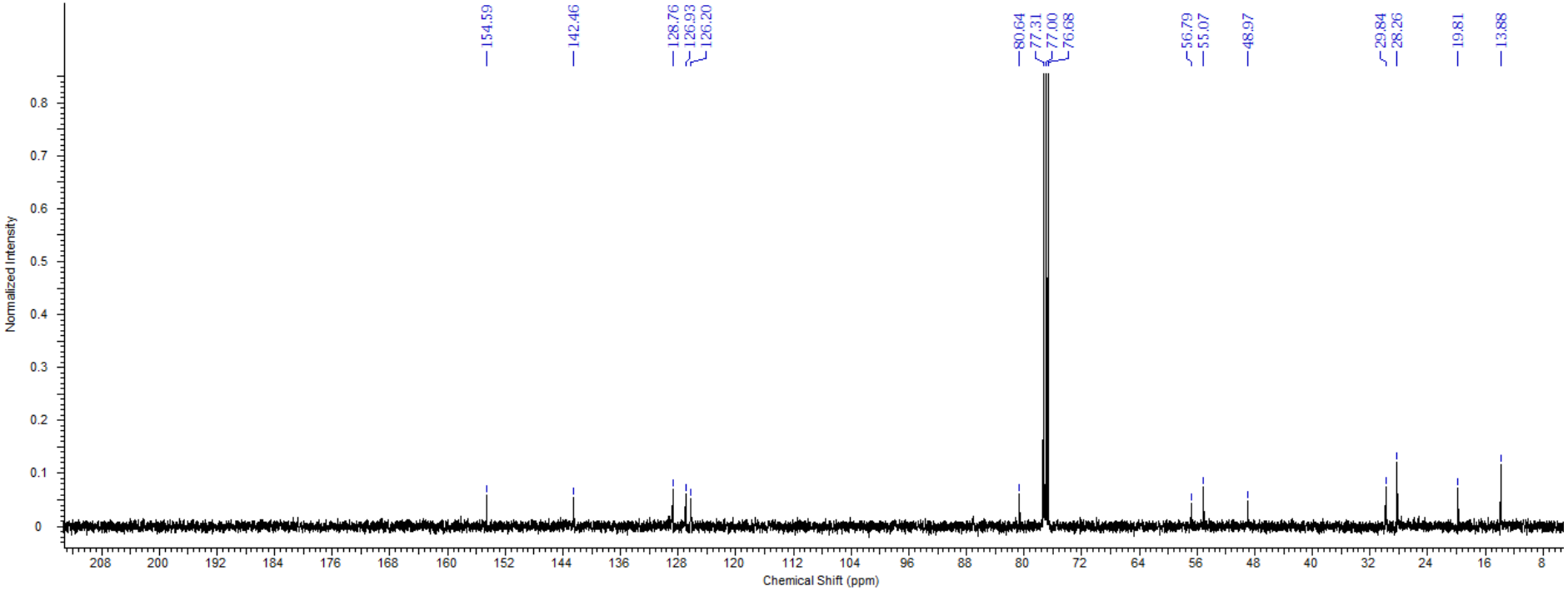
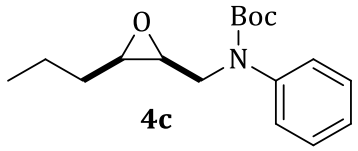


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4c**.



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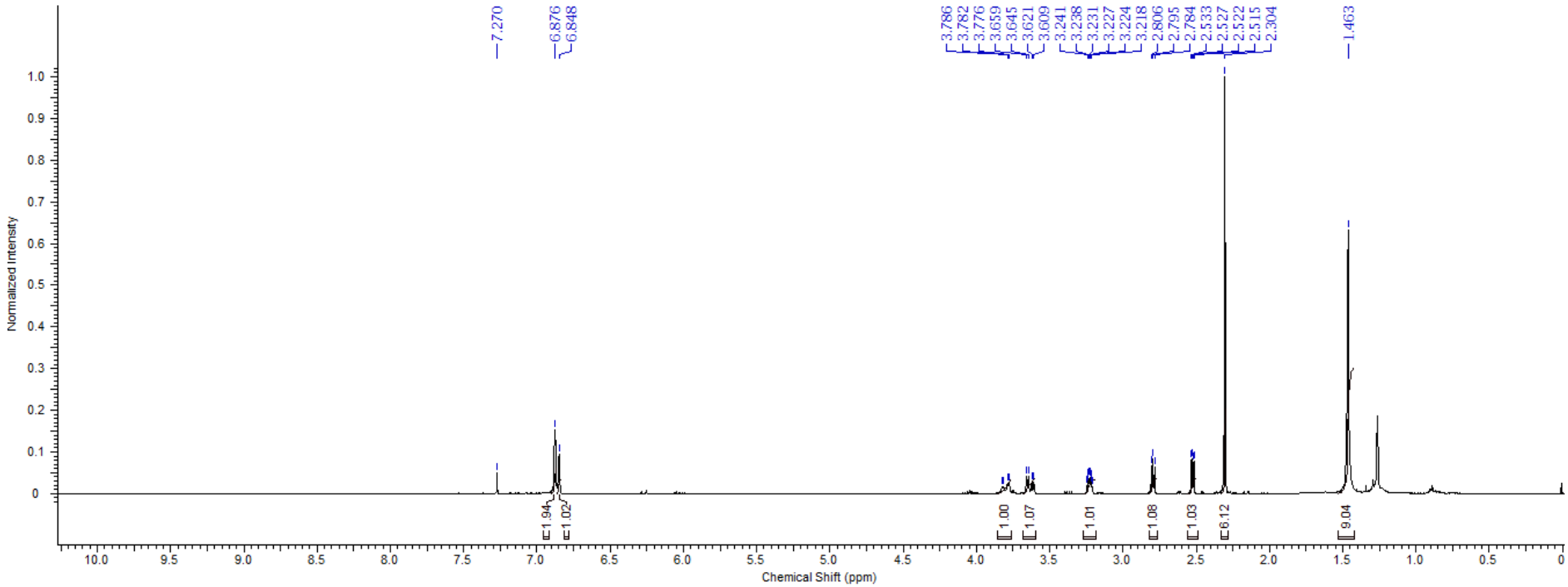

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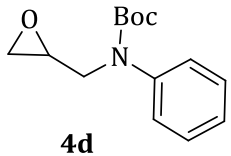

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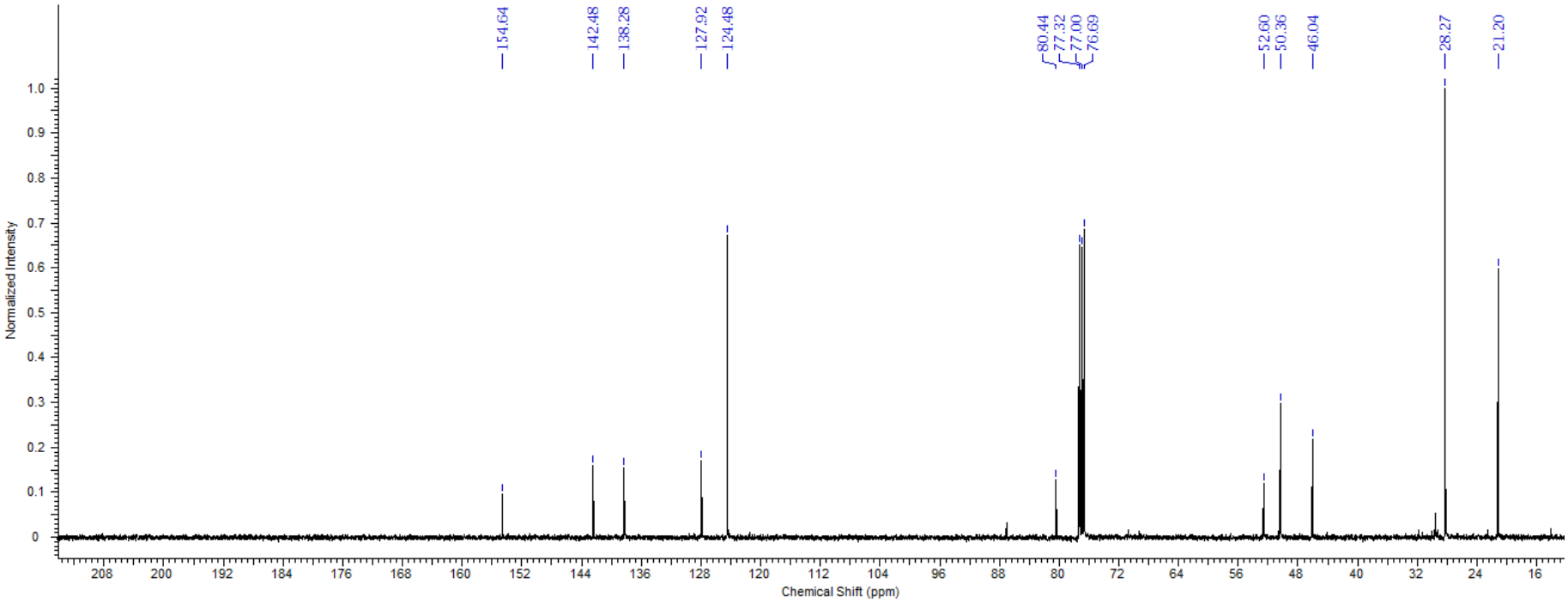

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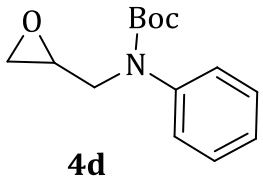

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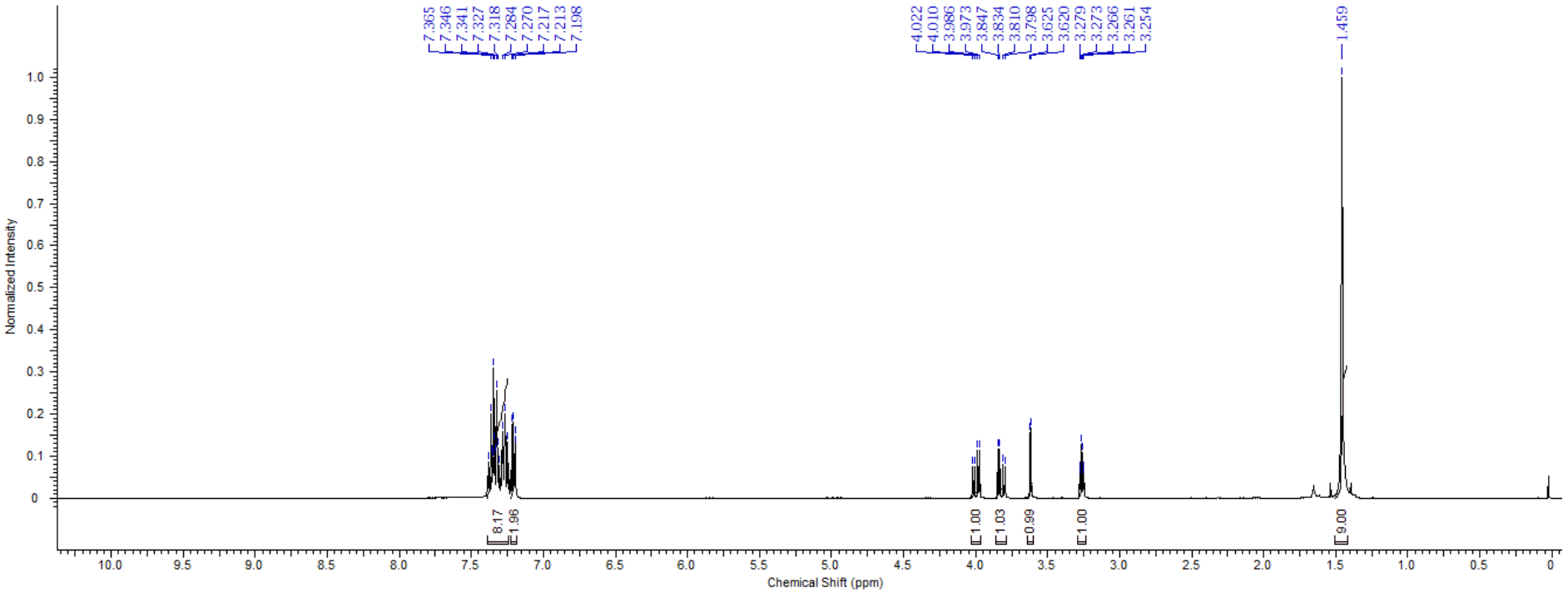

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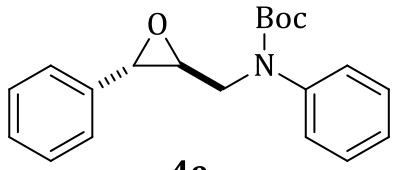

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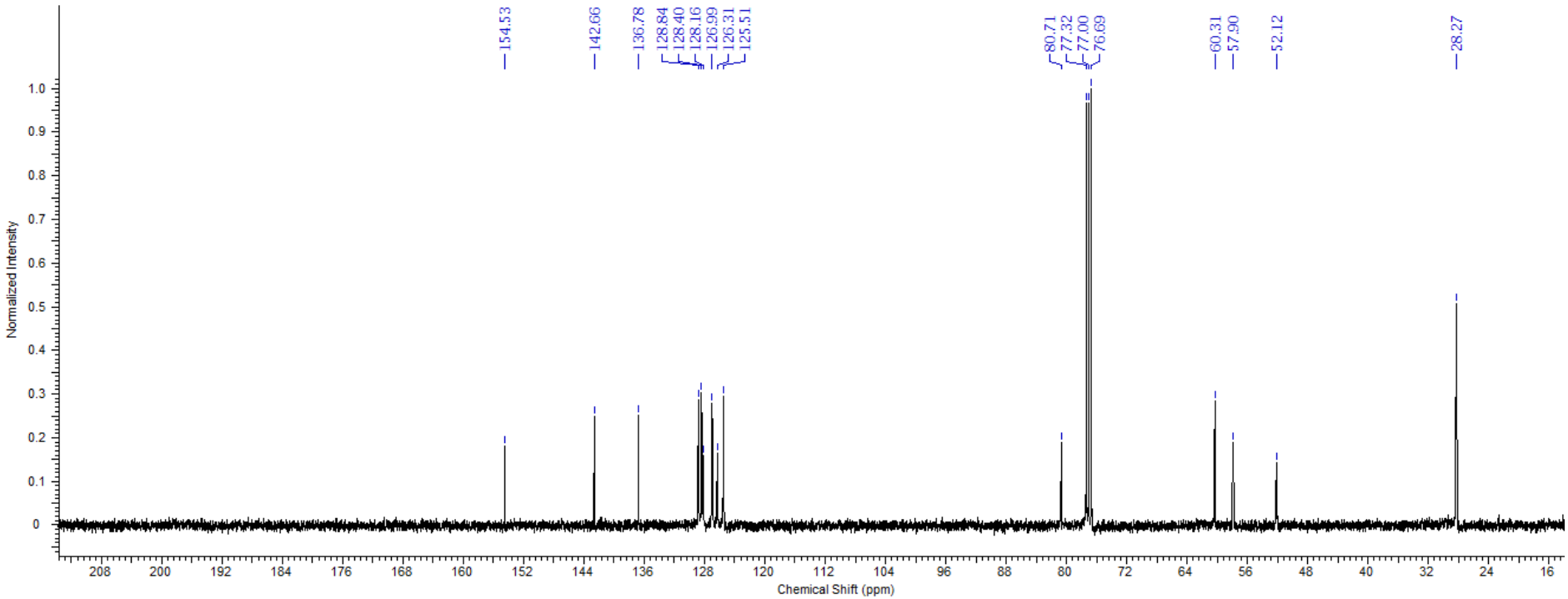

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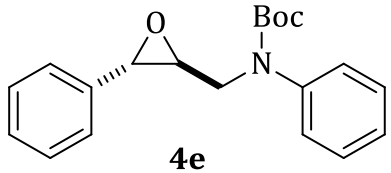

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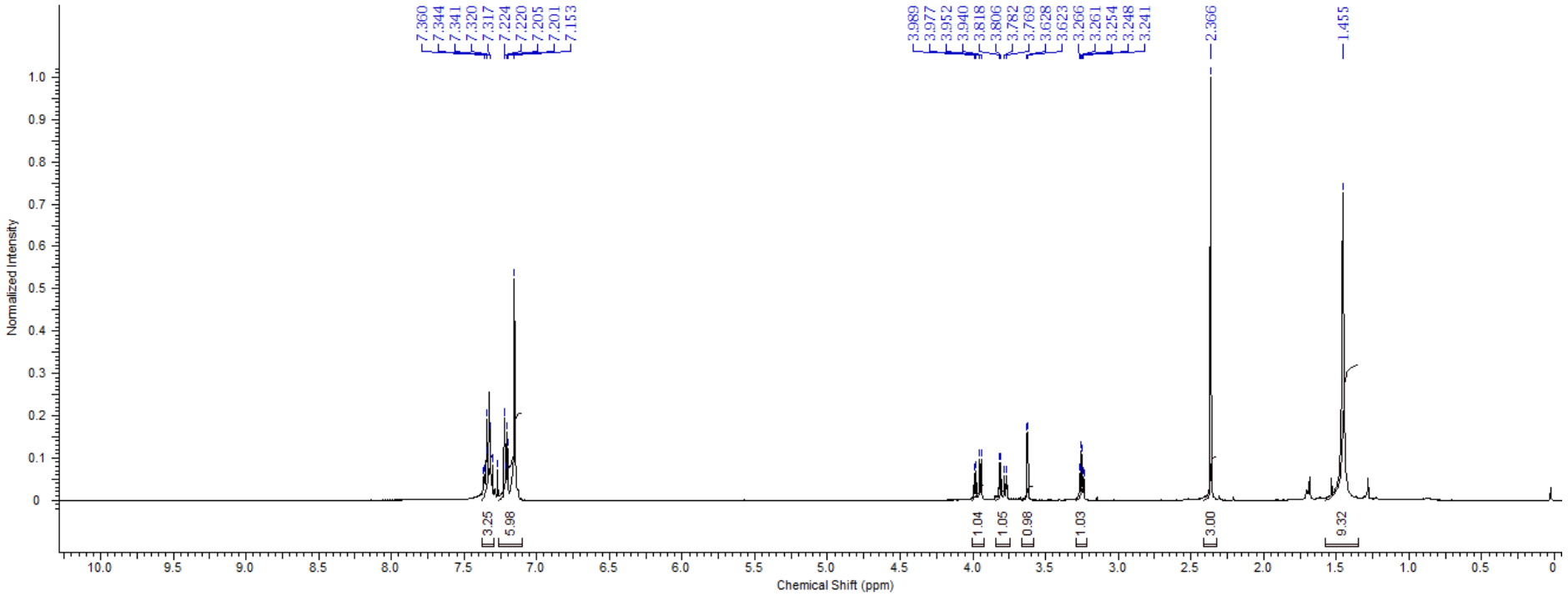
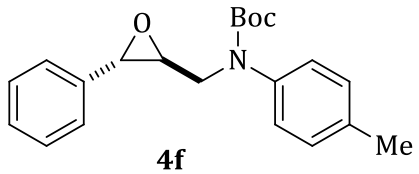


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4f**.



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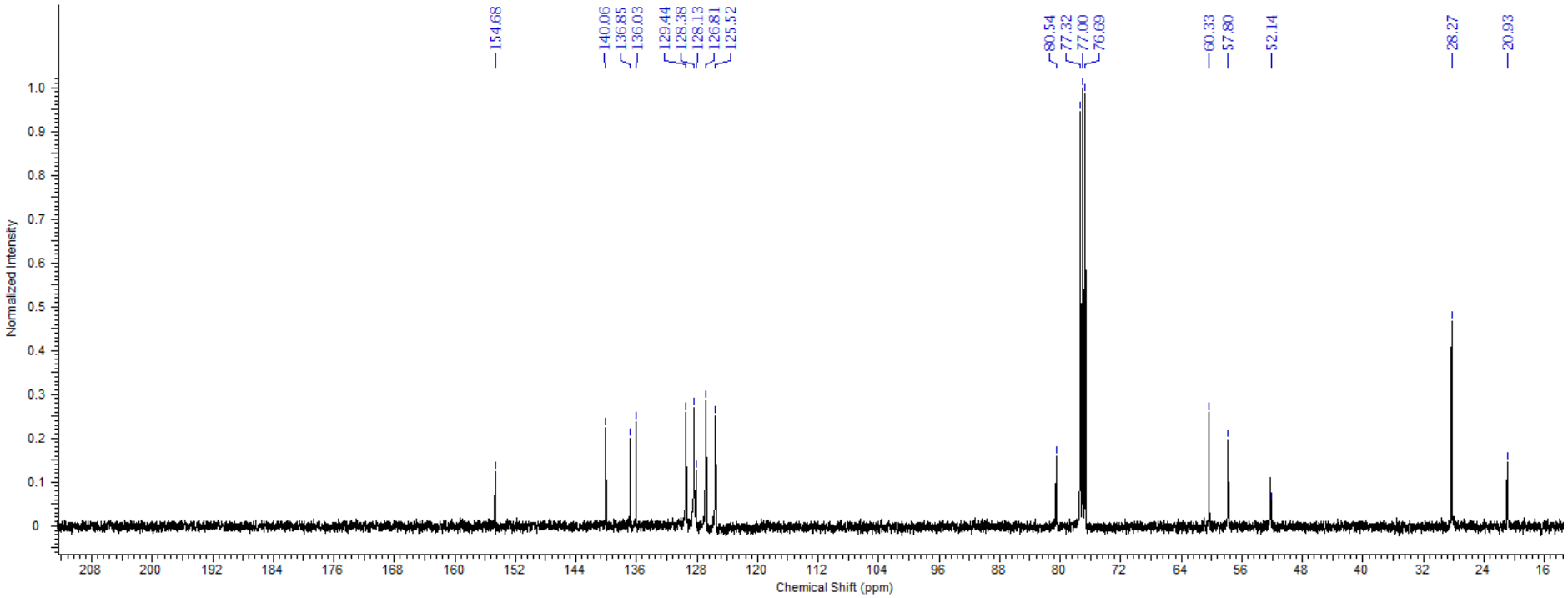

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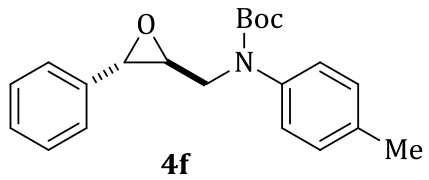

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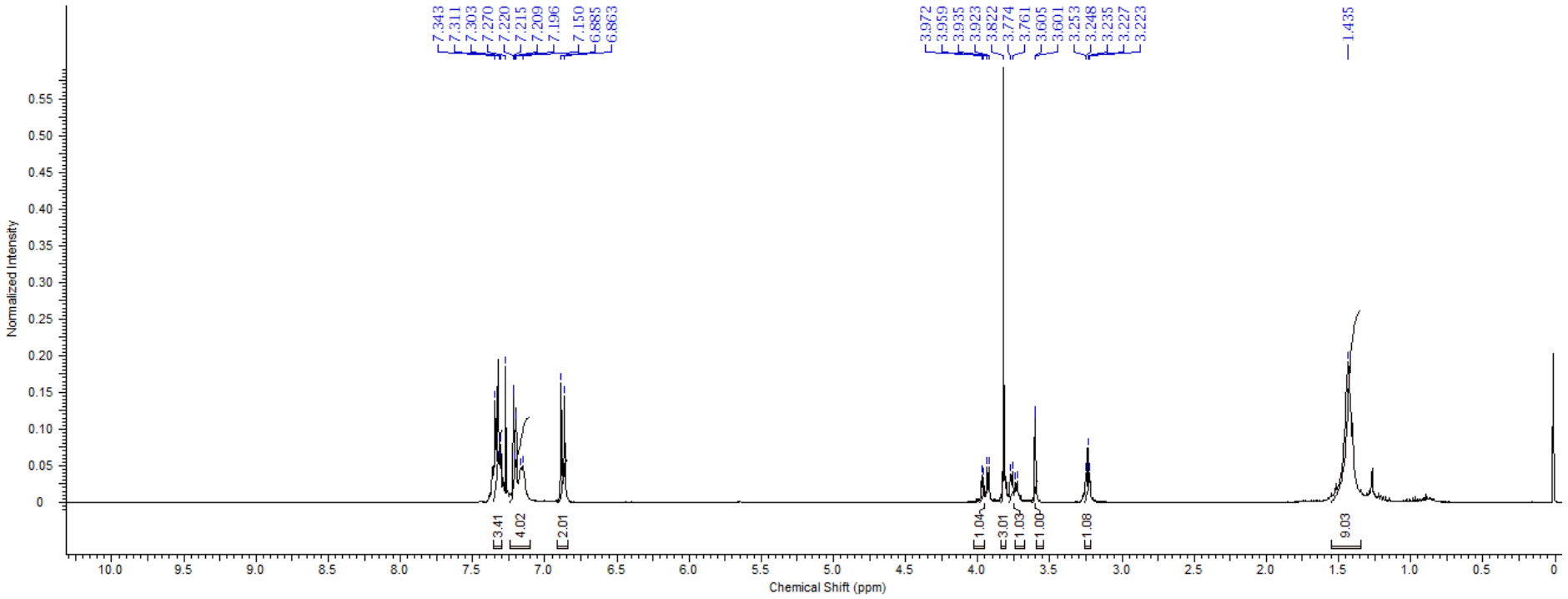
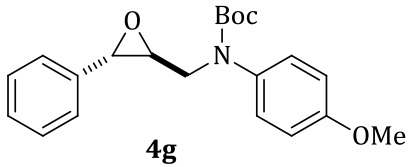


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4g**.



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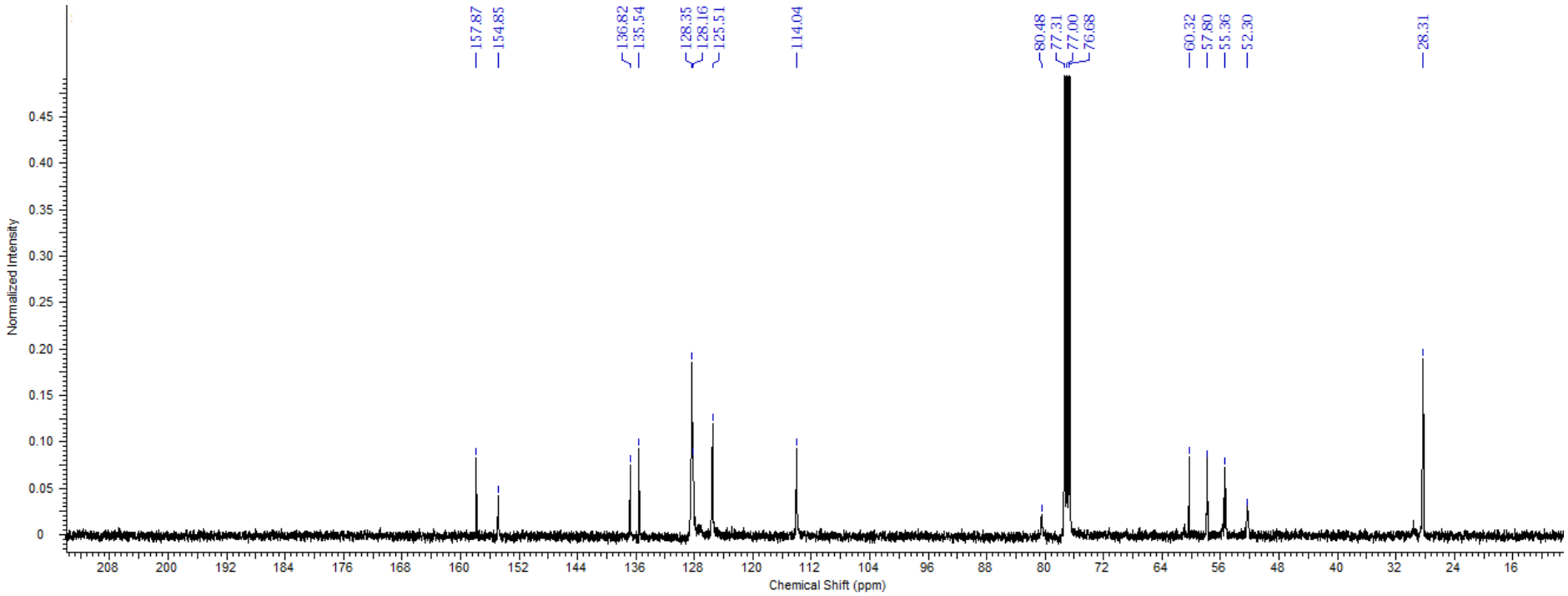

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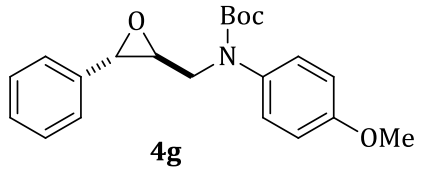

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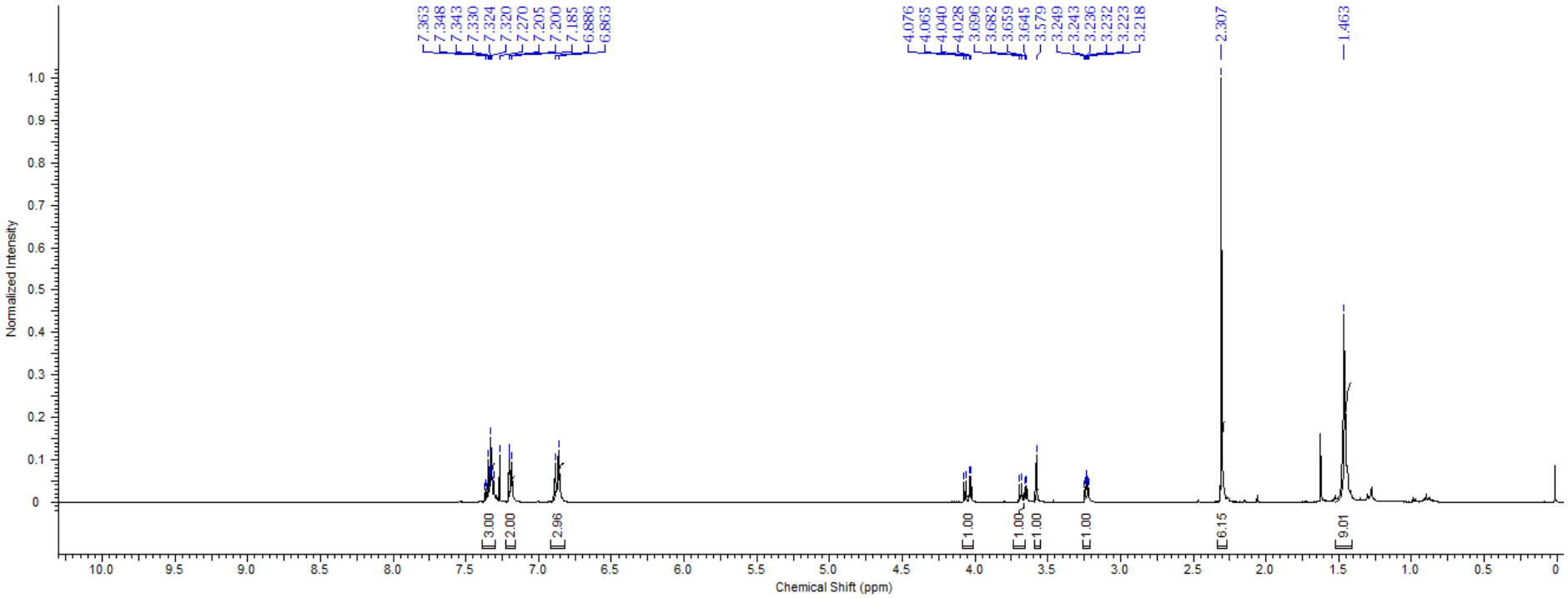

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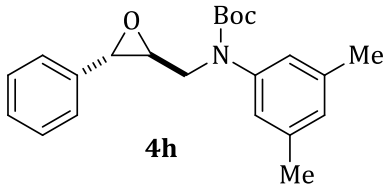

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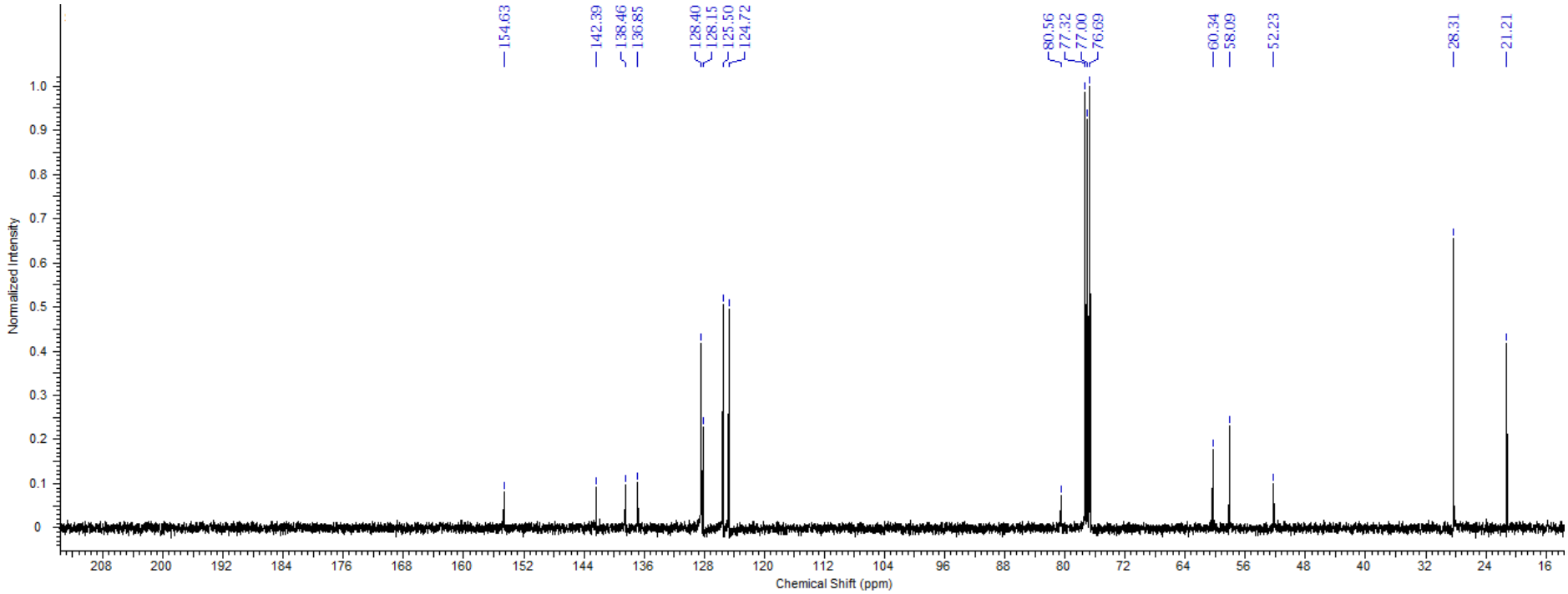

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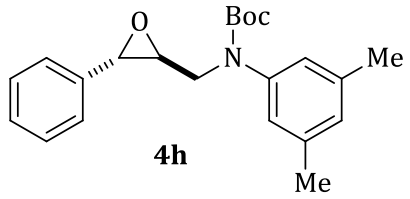

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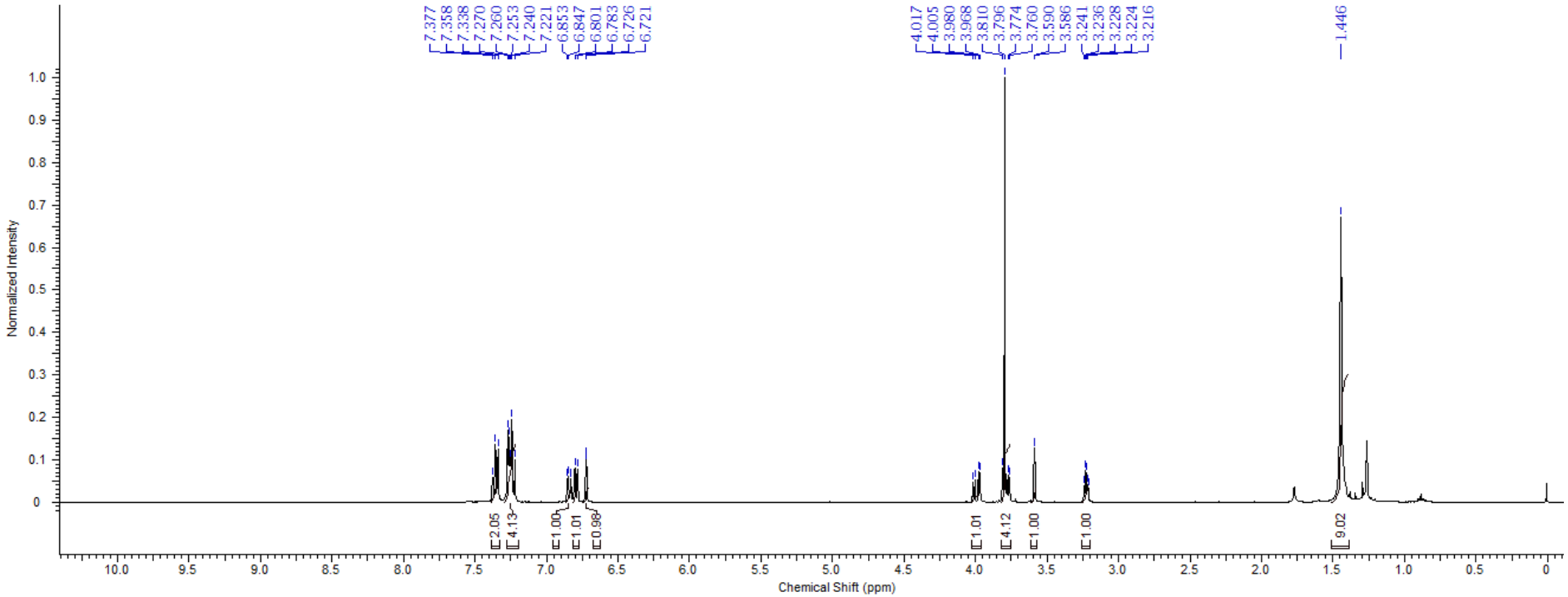

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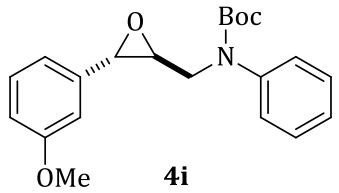

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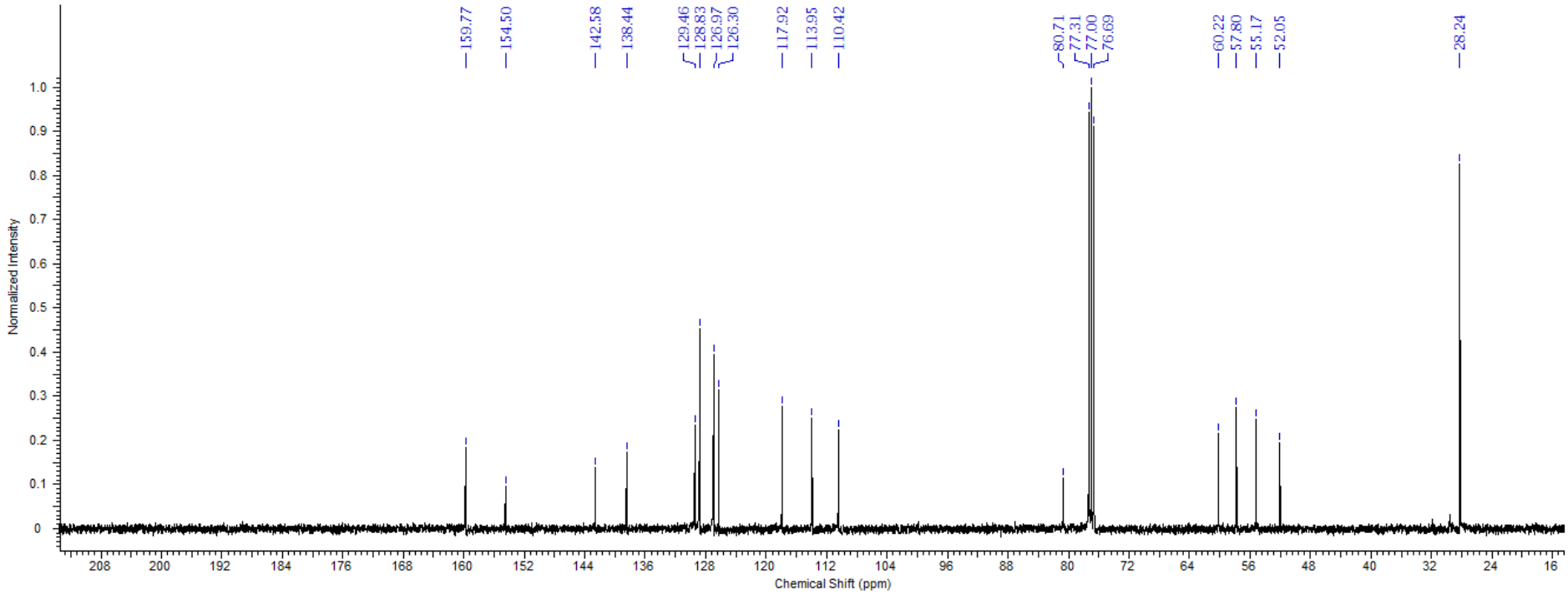

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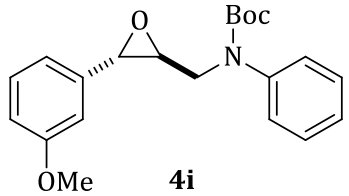

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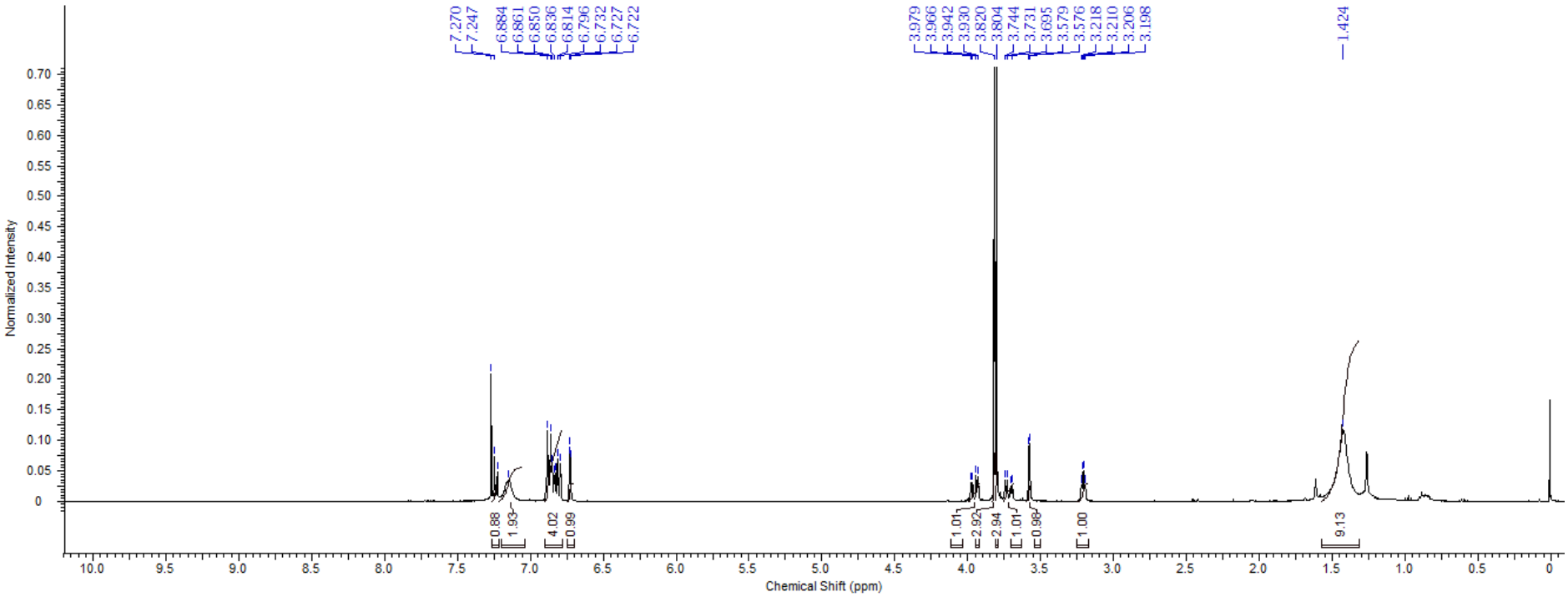

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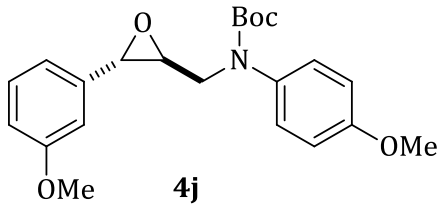

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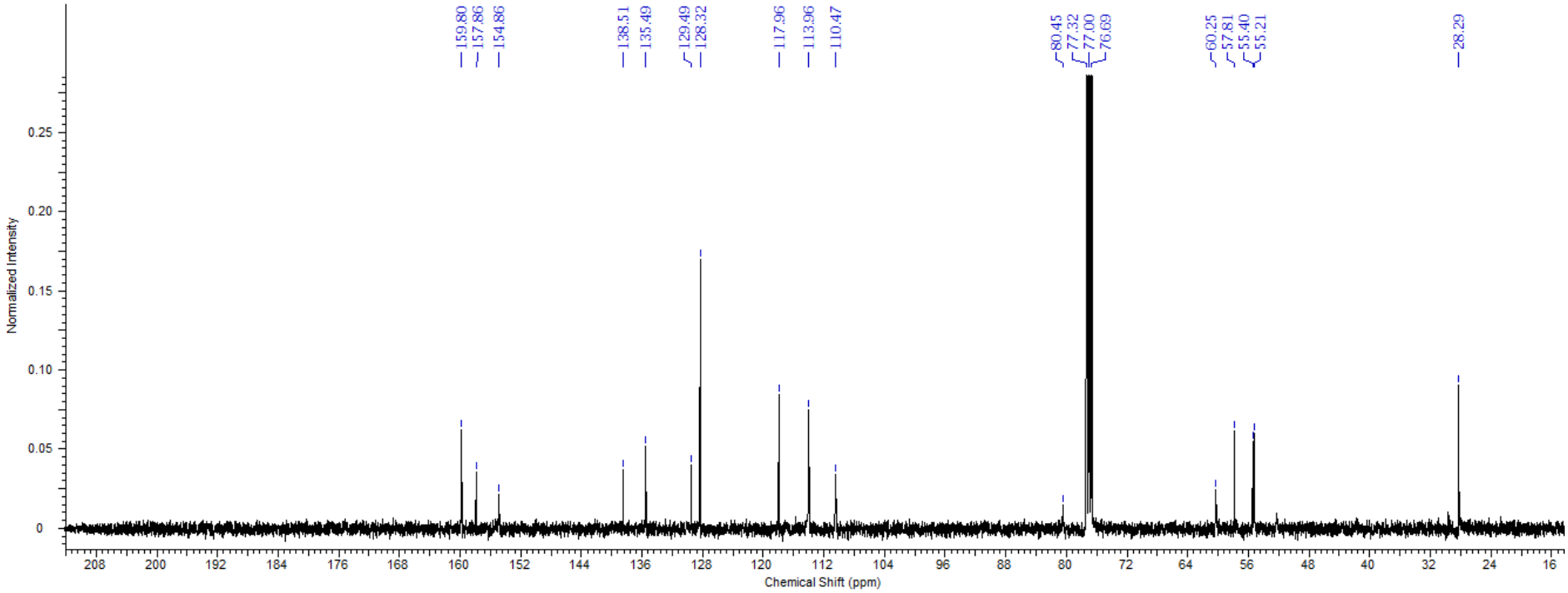

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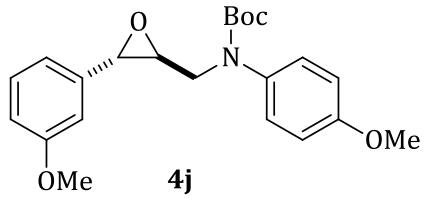

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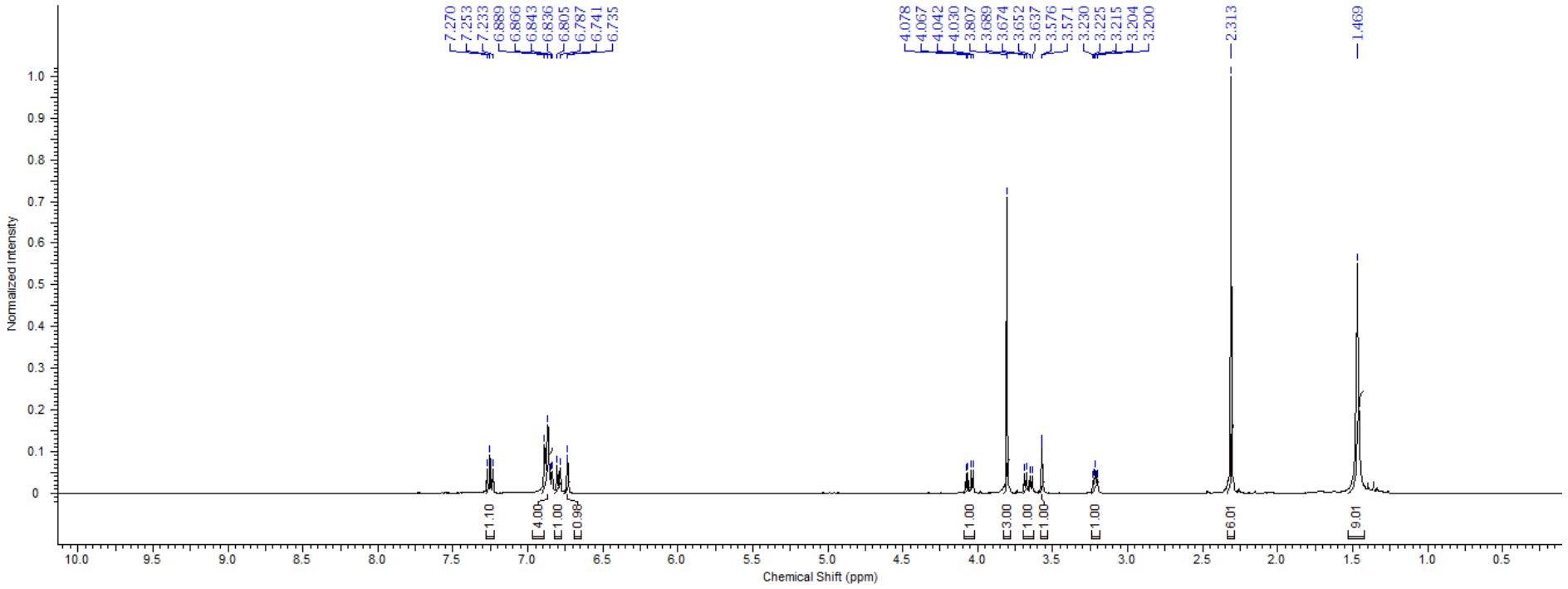

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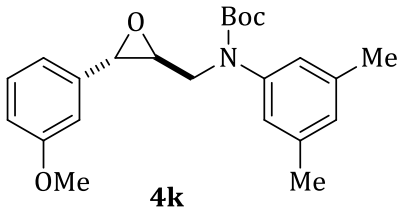

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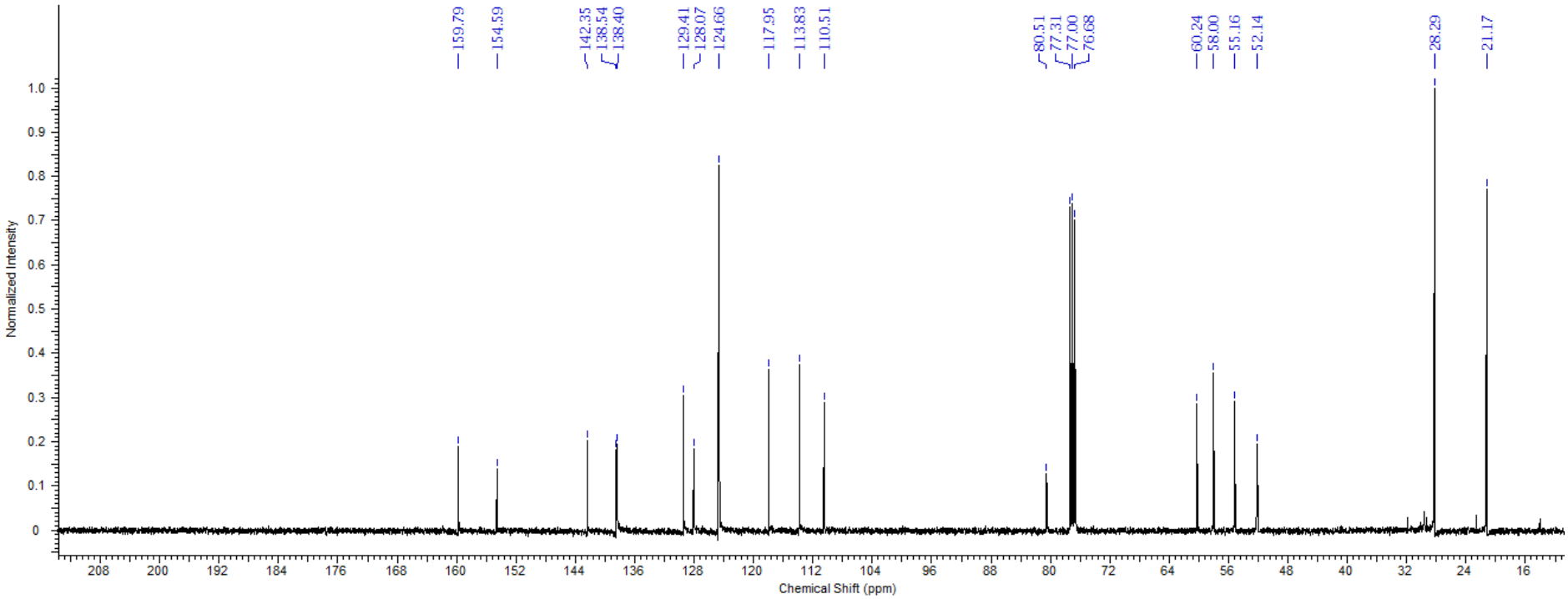

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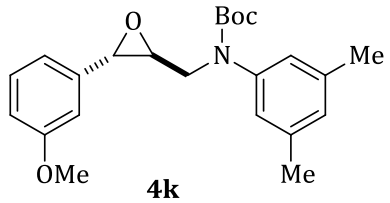

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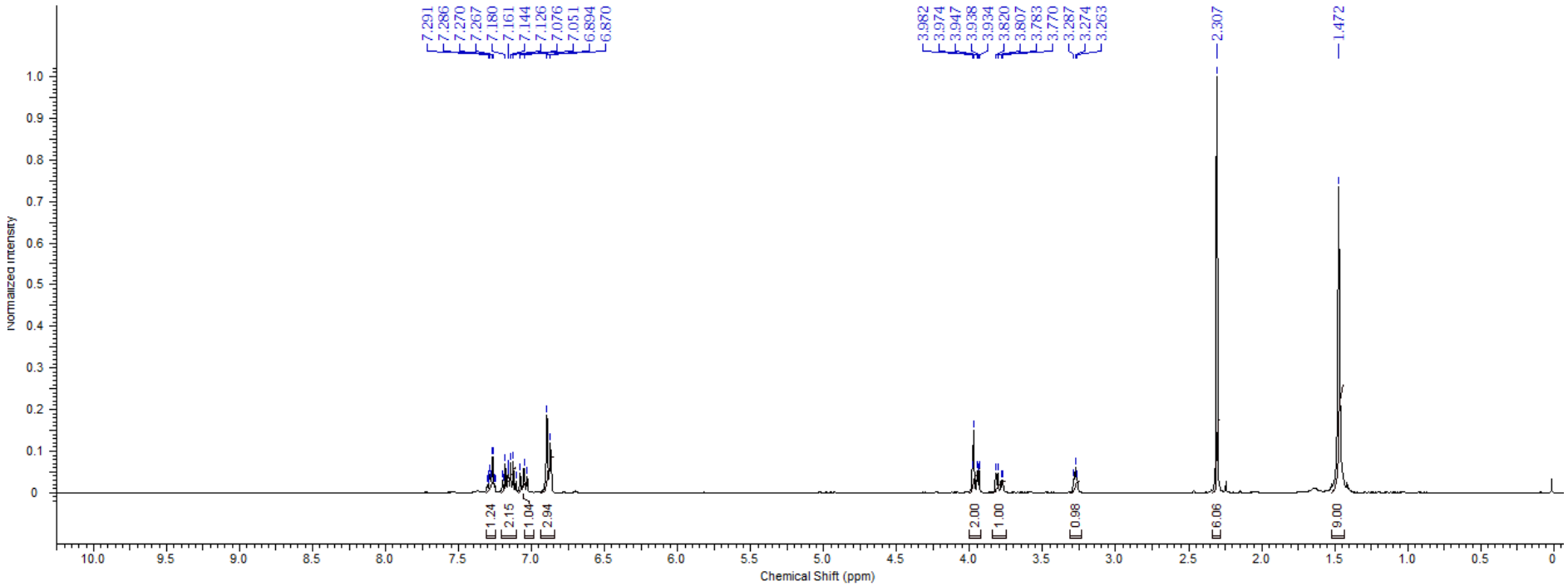

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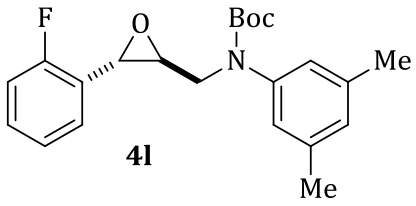

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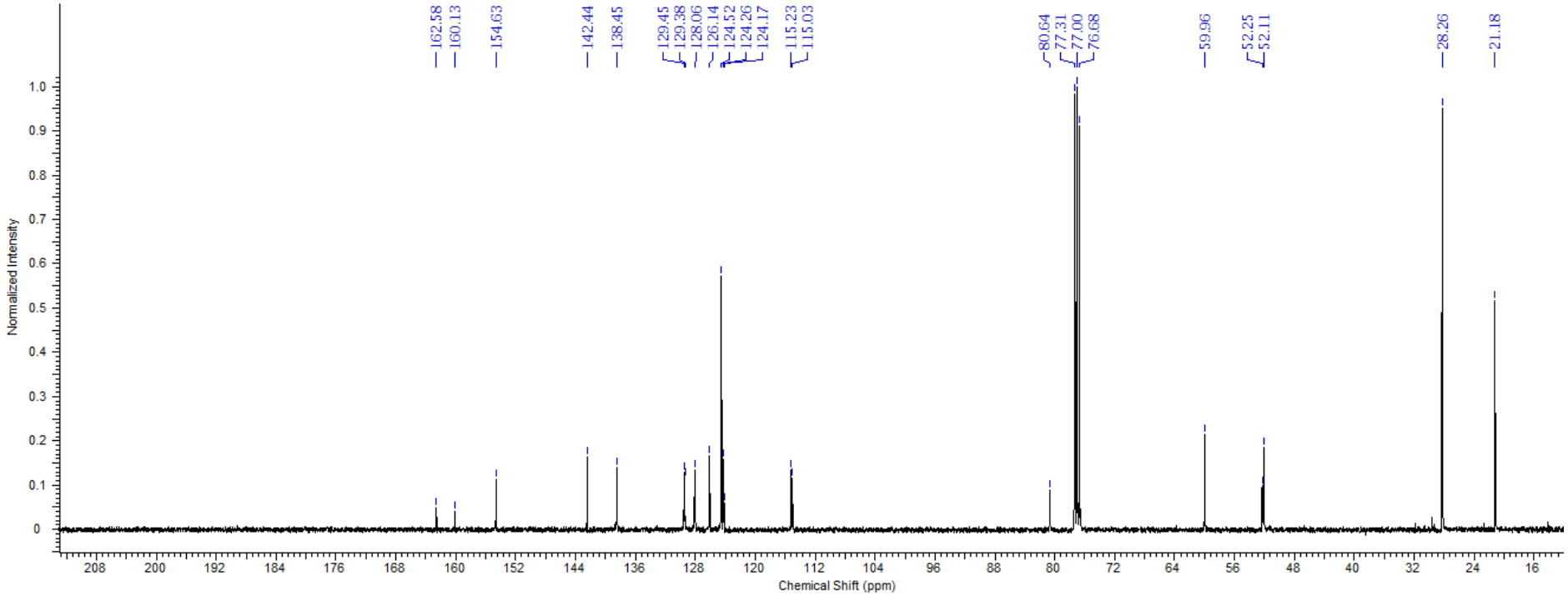
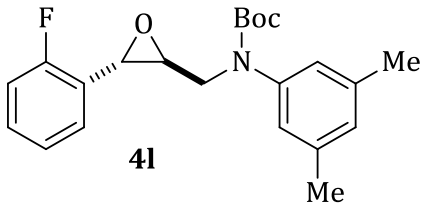
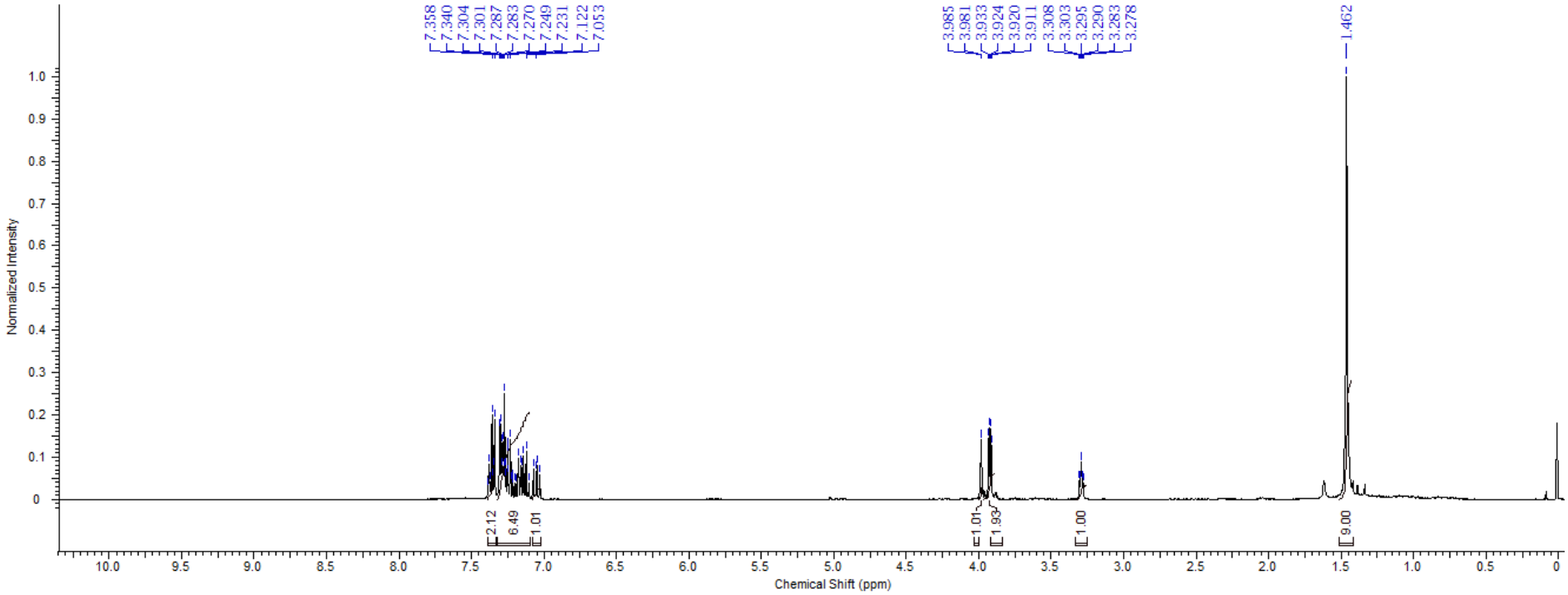


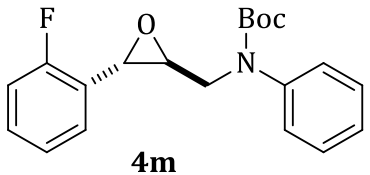
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4l**.



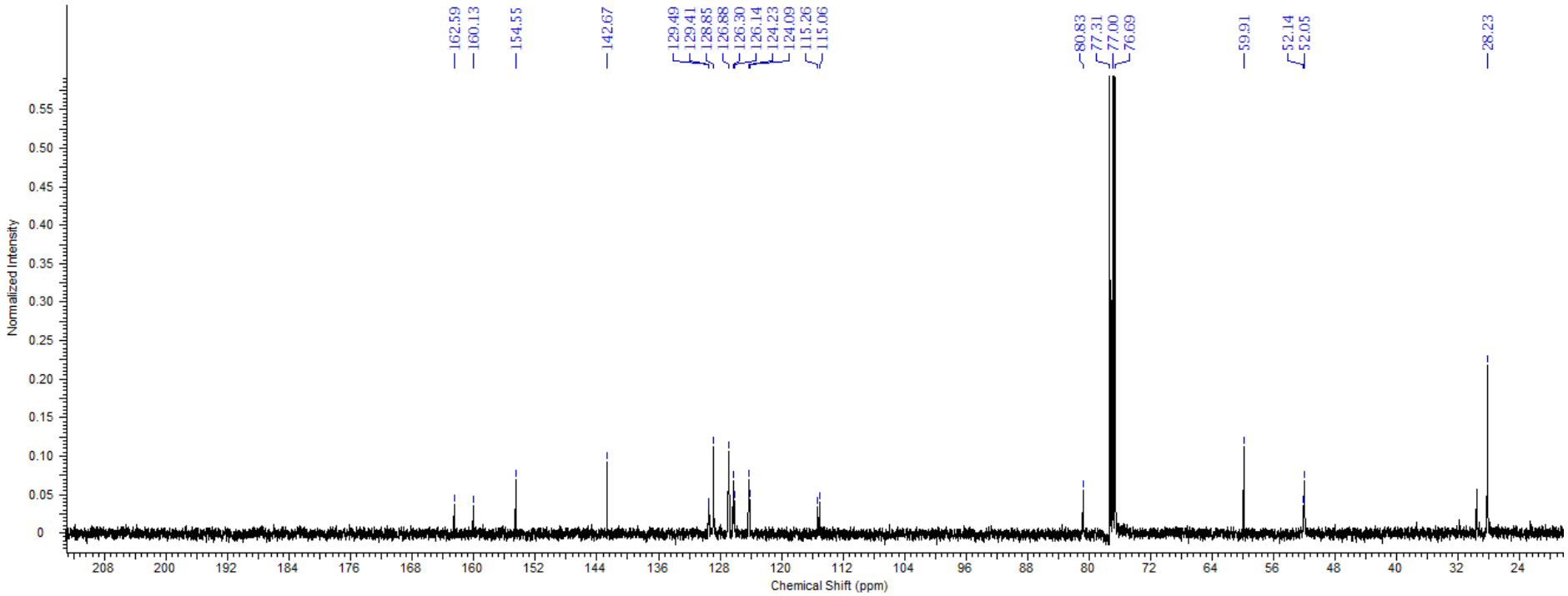
4l



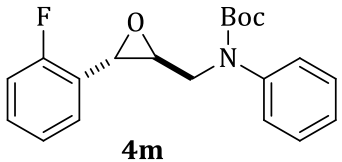
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4m**.



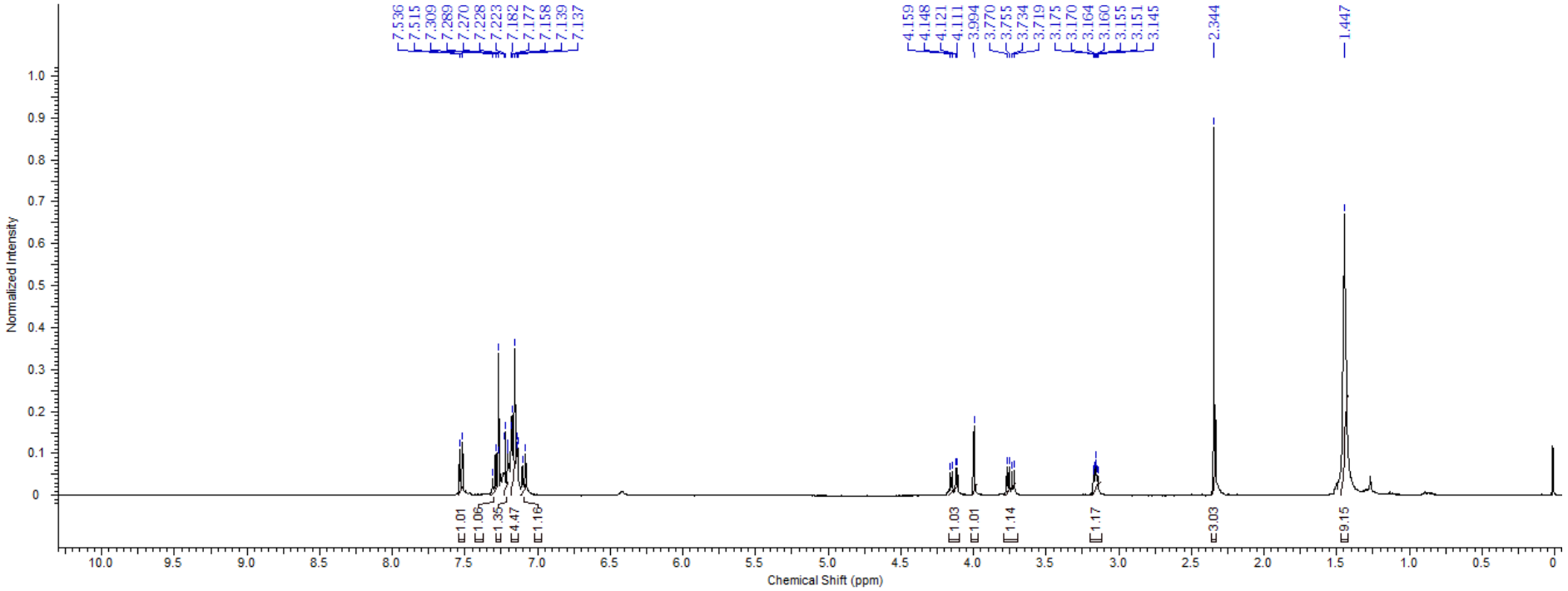
4m



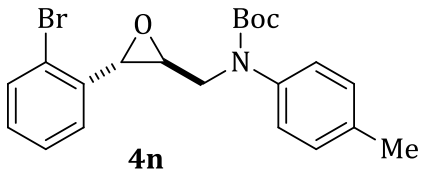
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4m**.



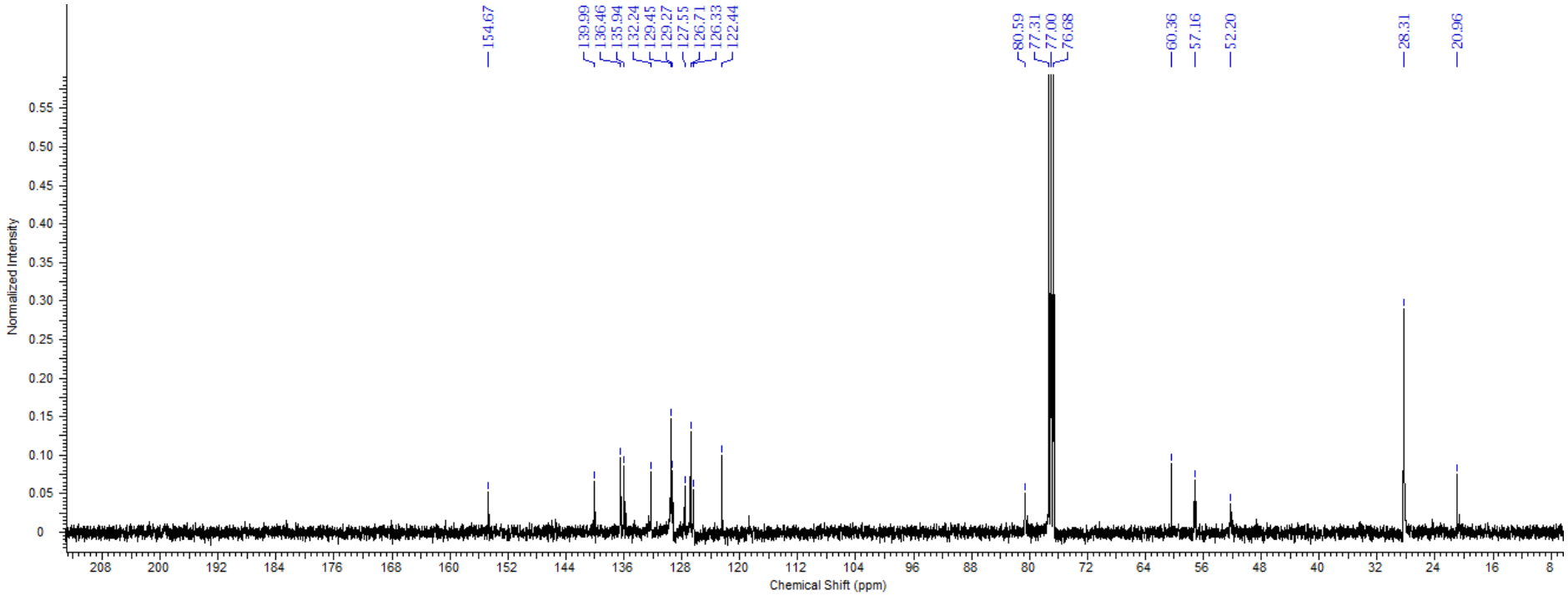
4m



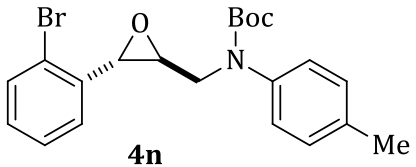
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4n**.



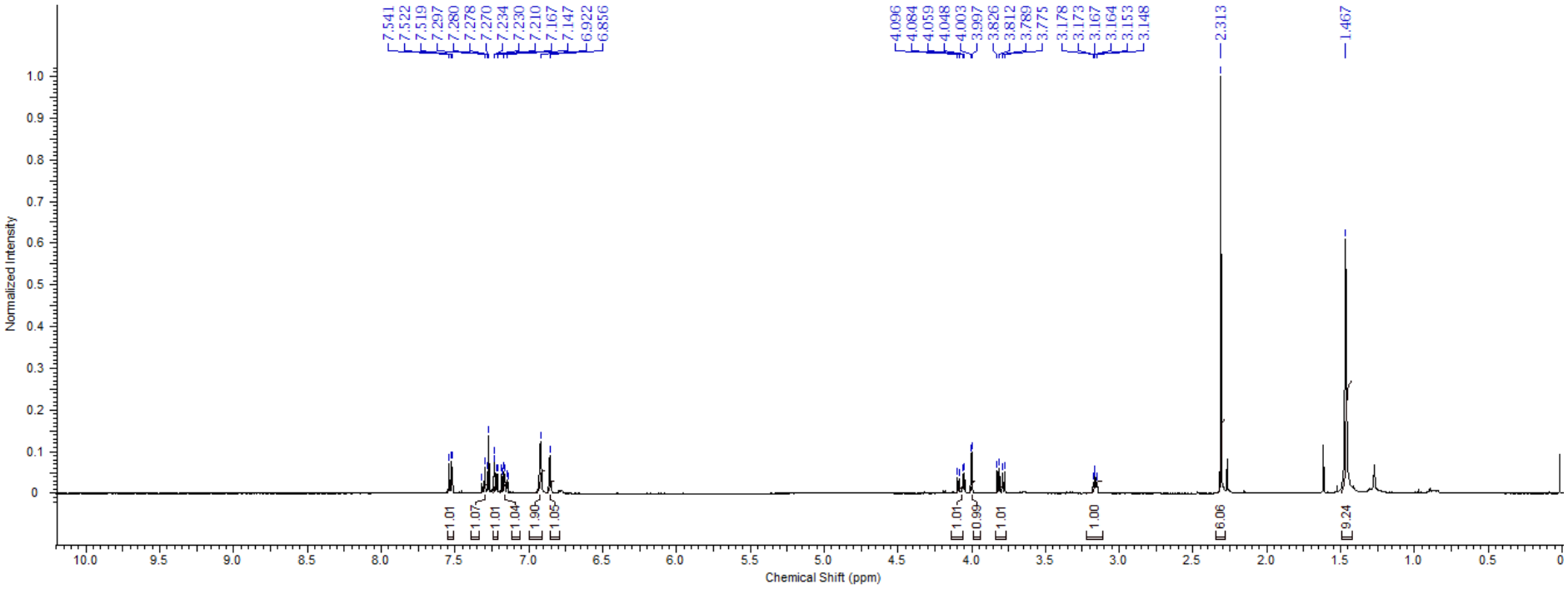
4n



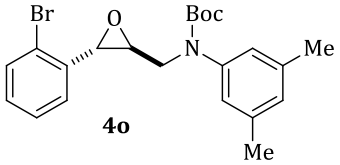
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4n**.



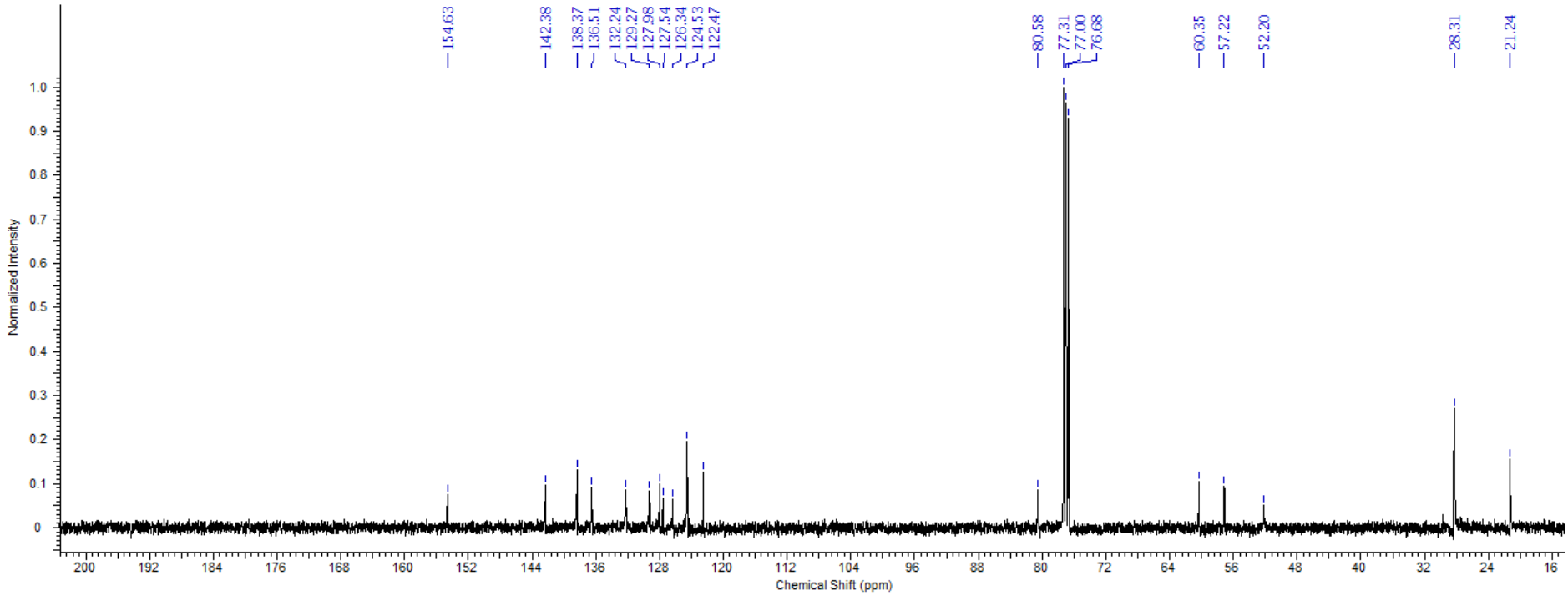
4n



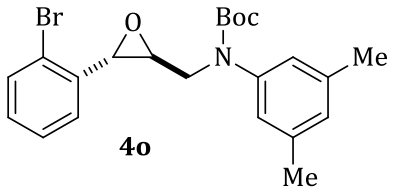
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4o**.



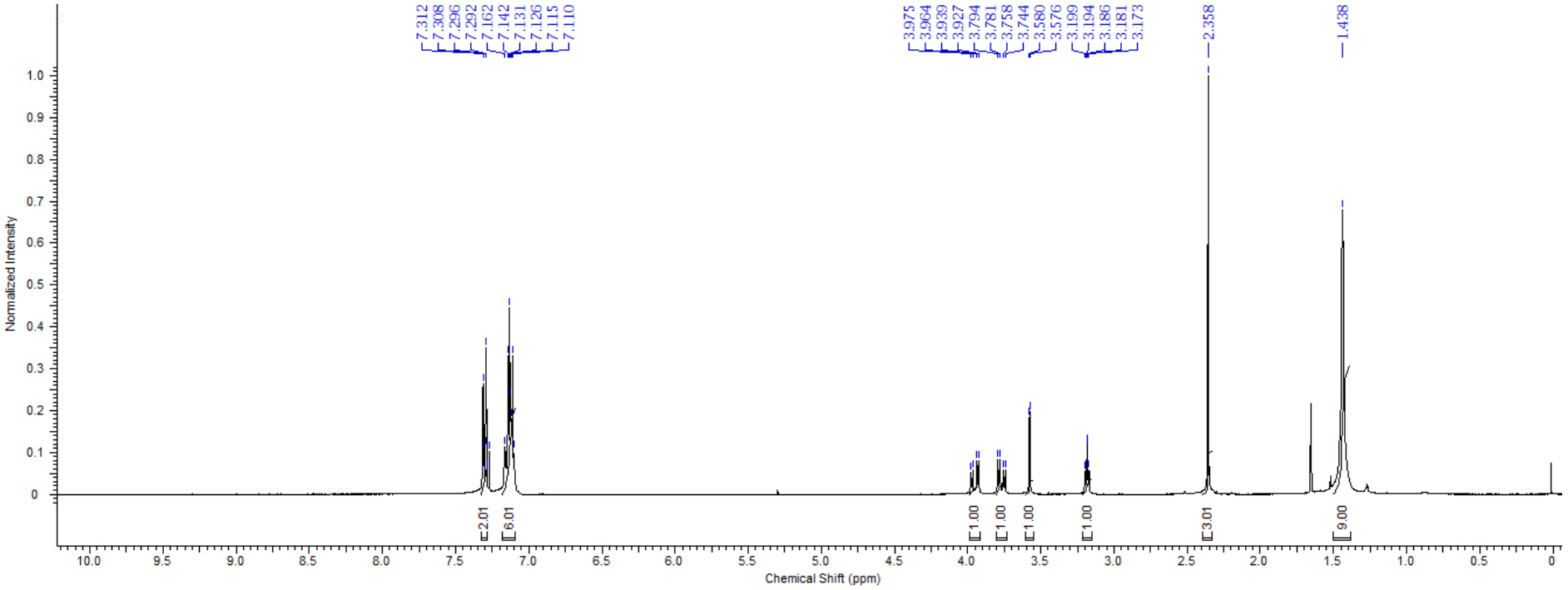
4o



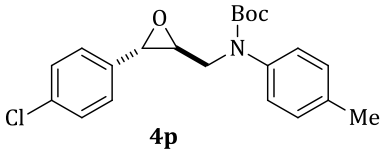
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4o**.



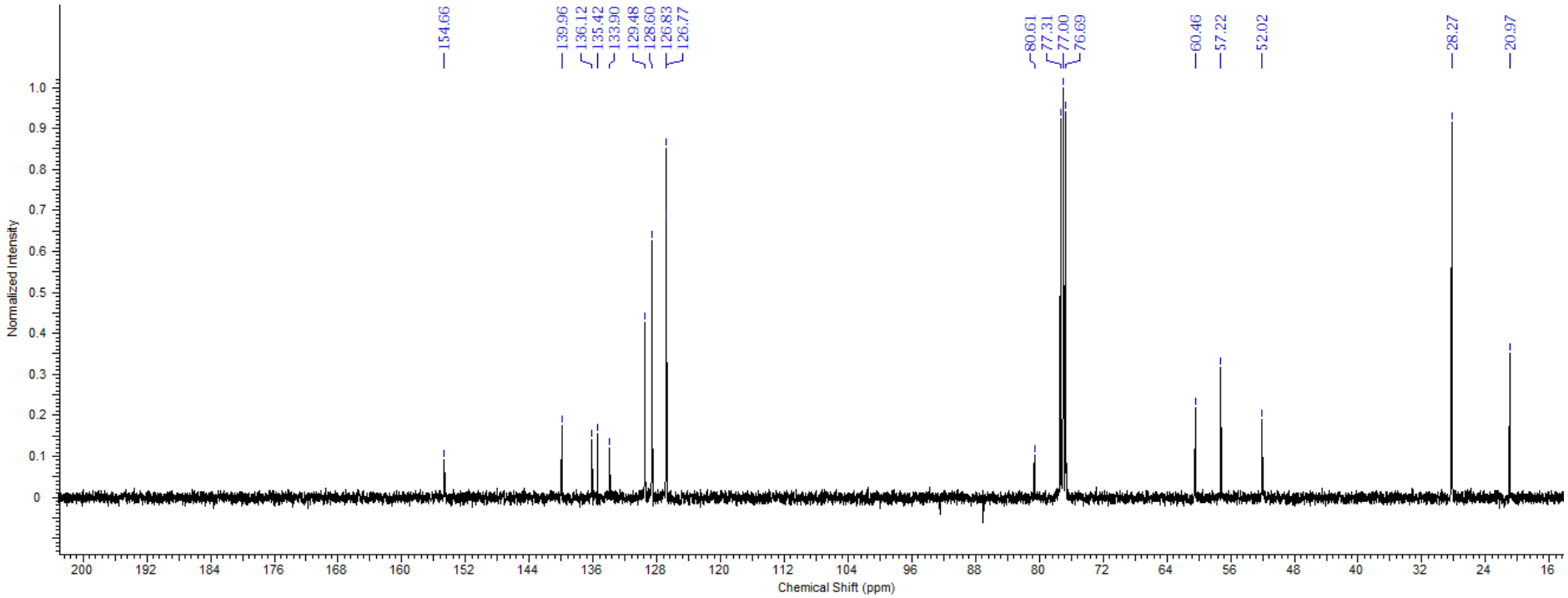
4o



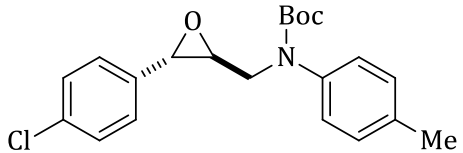
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4p**



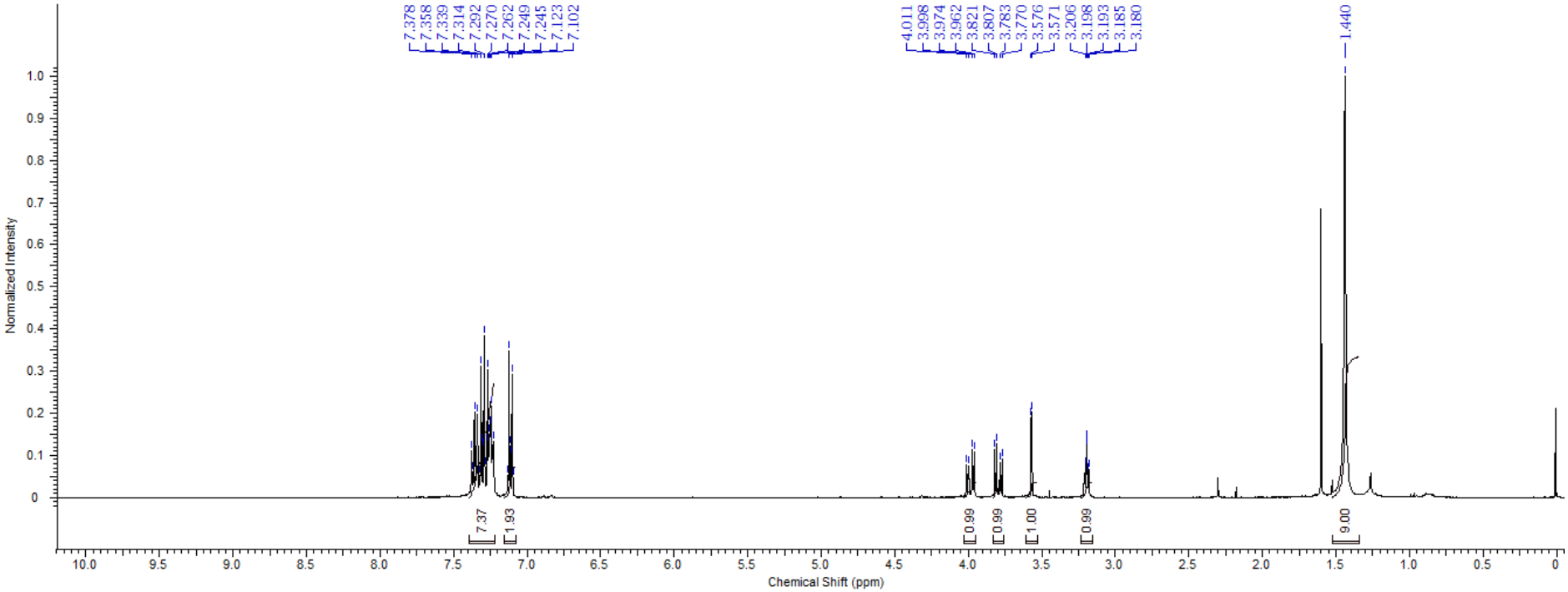
4p



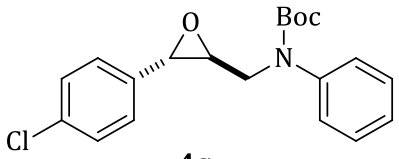
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4p**.



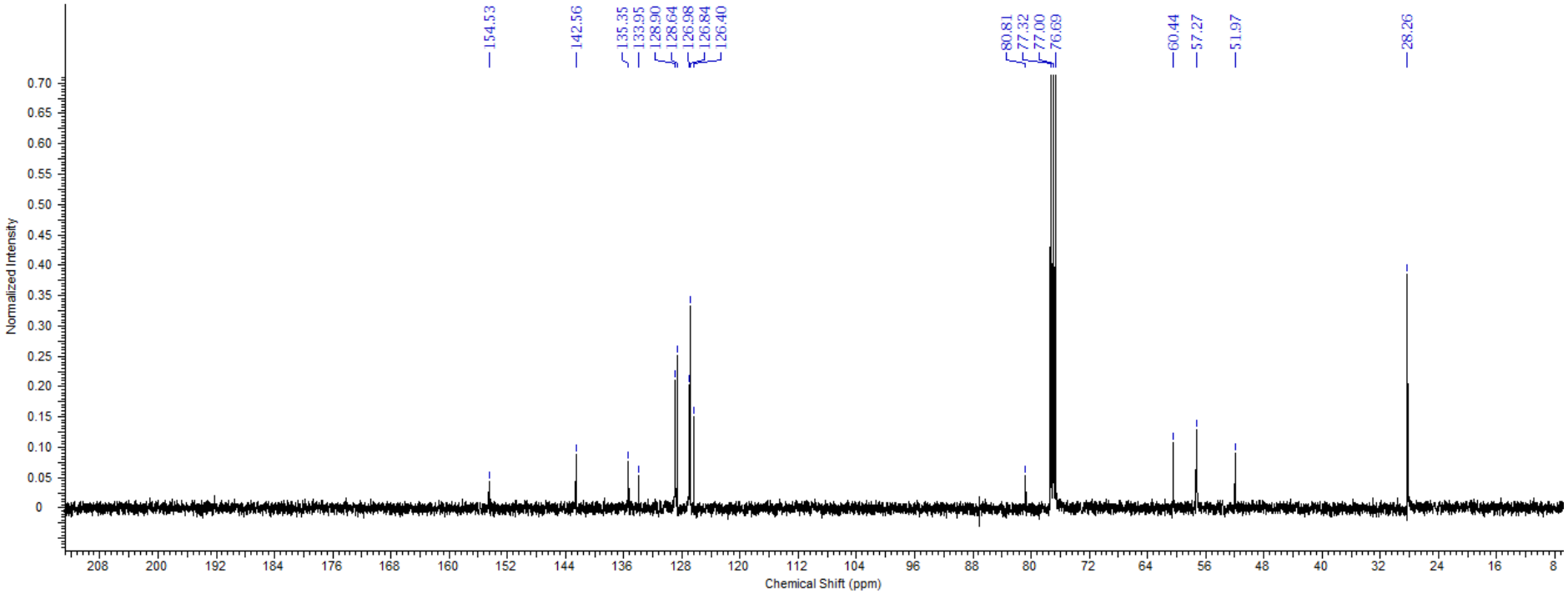
4p



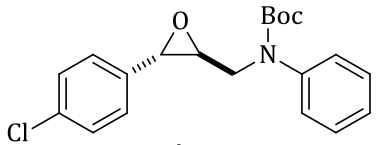
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4q**.



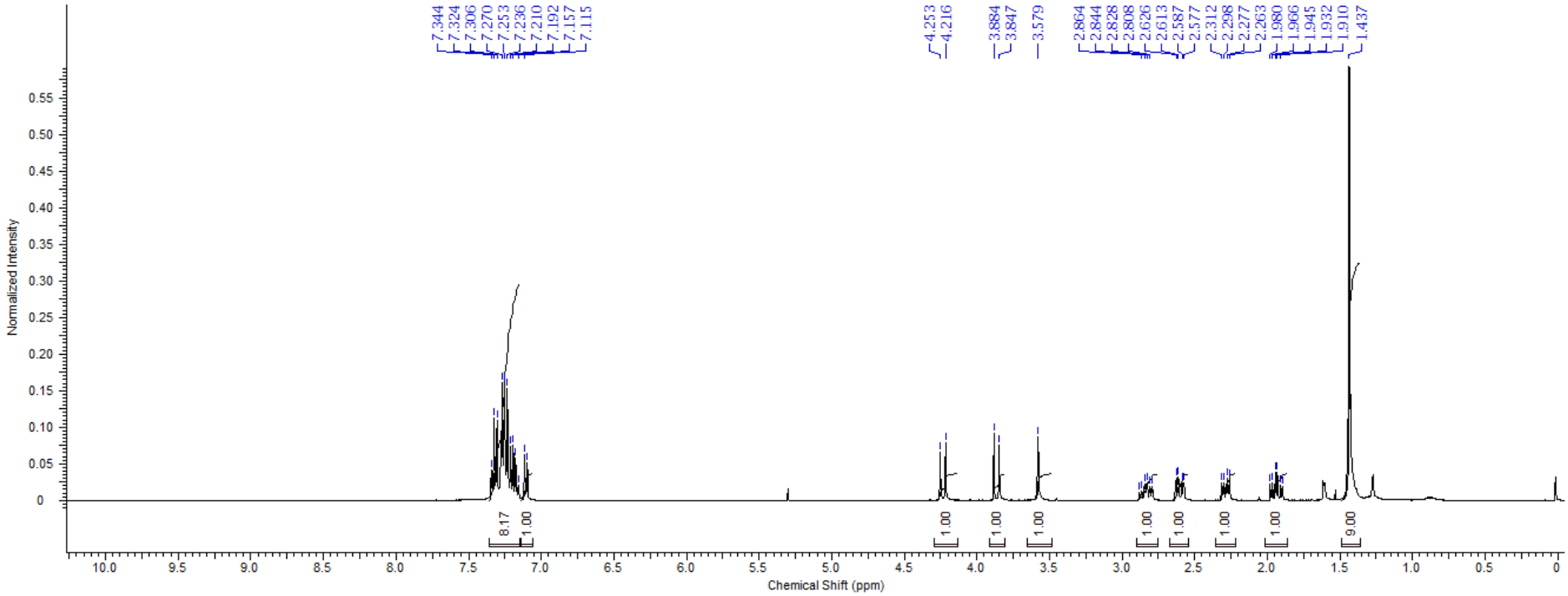
4q

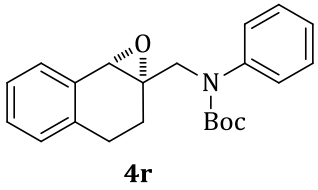


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4q**.

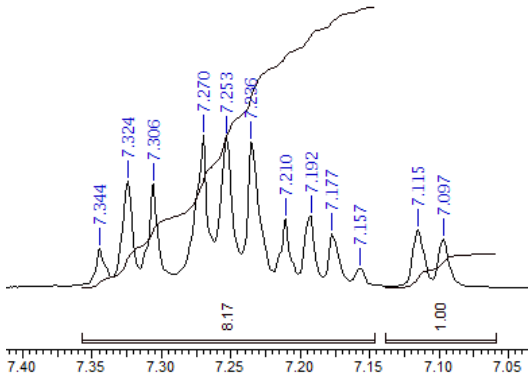


4q

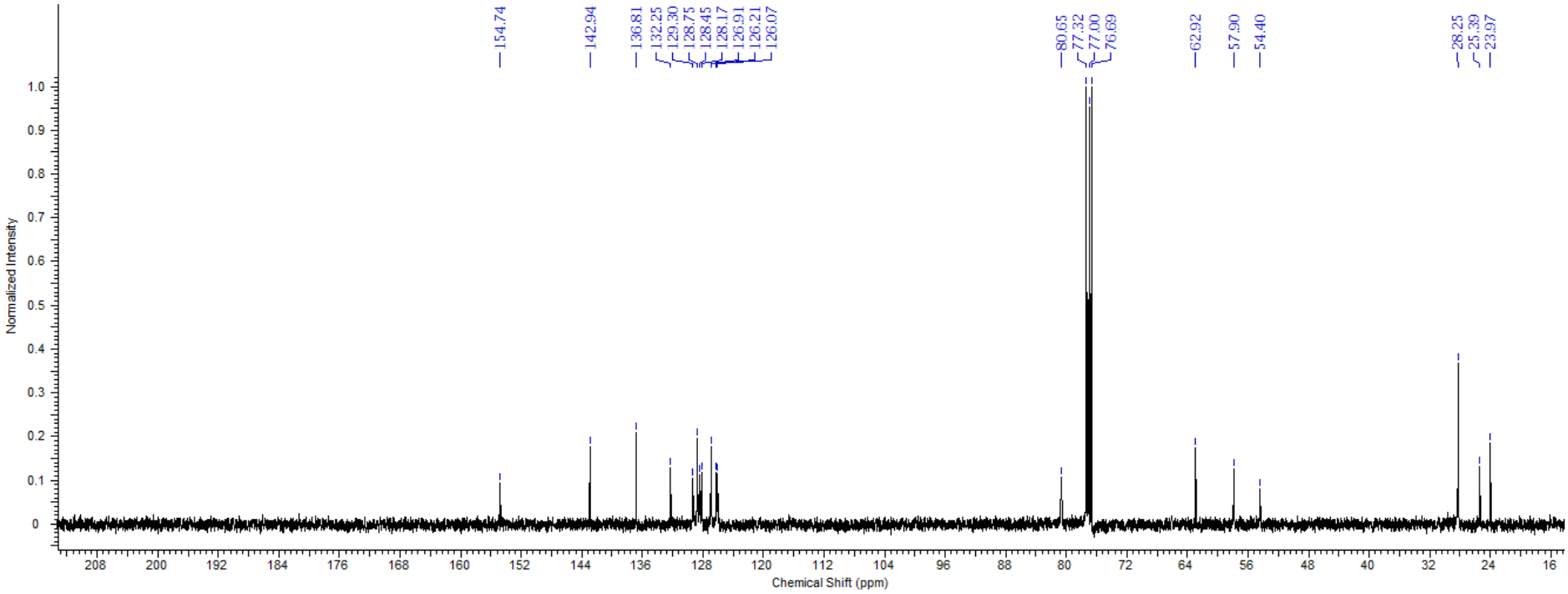


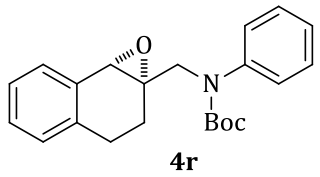


4r

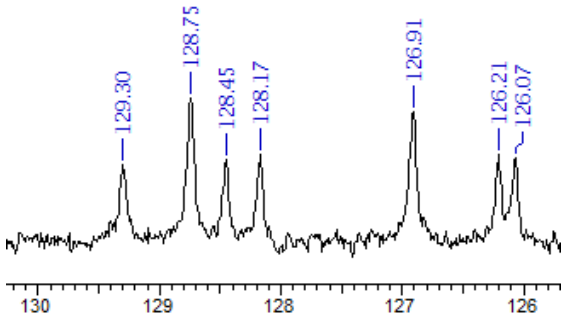


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4r**.

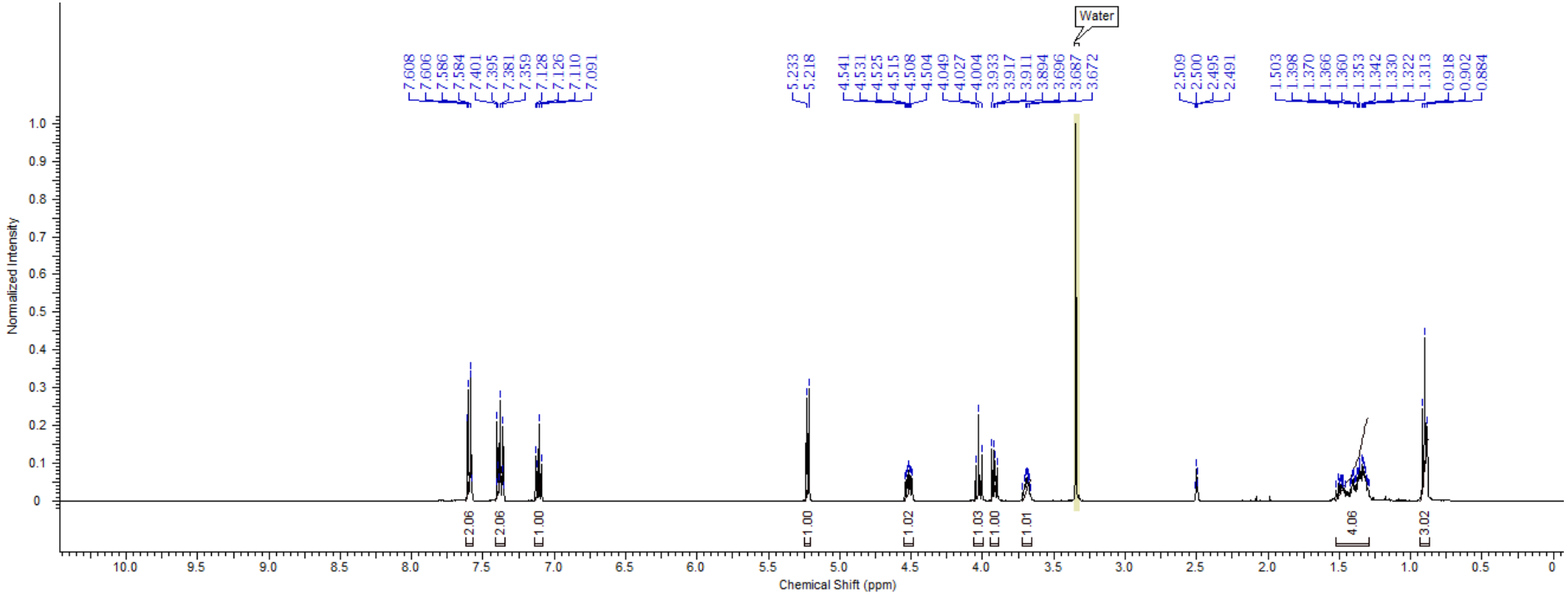




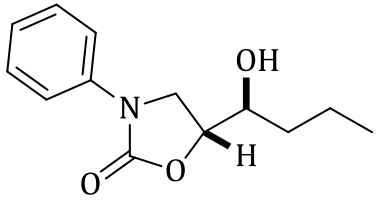
4r



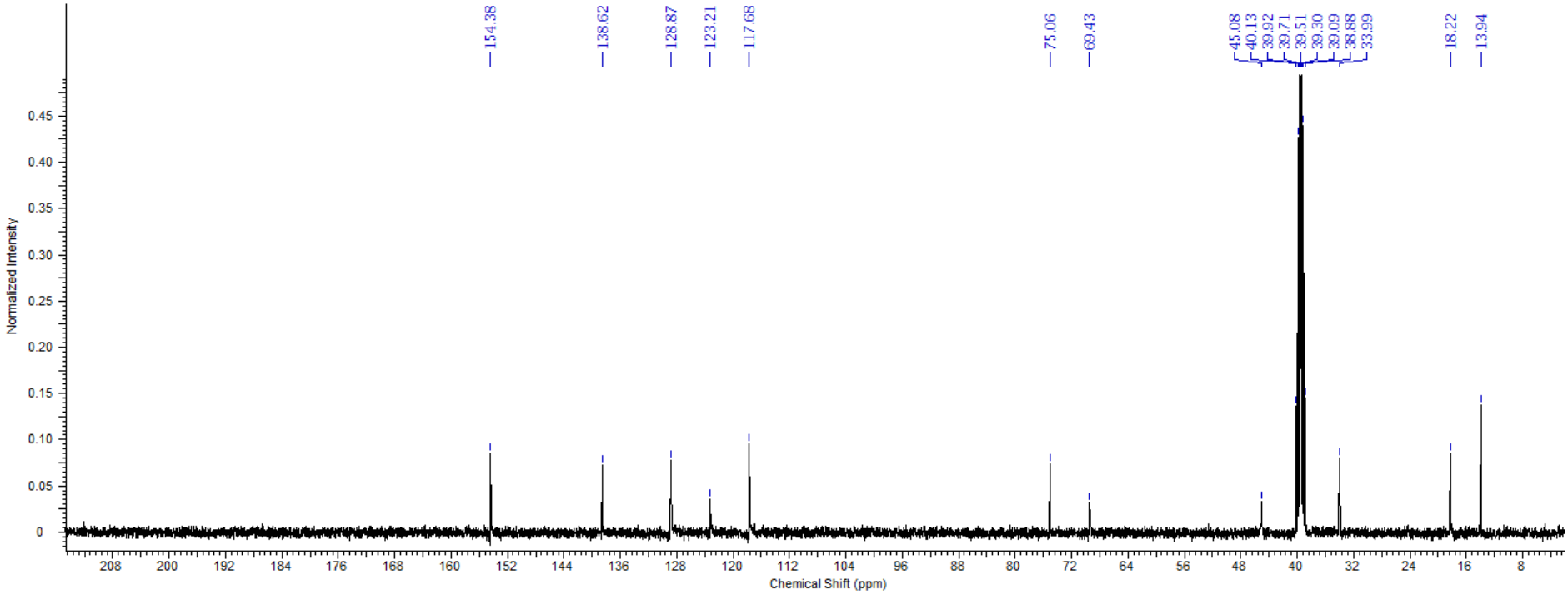
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **4r**.



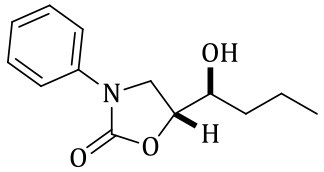
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5a**.



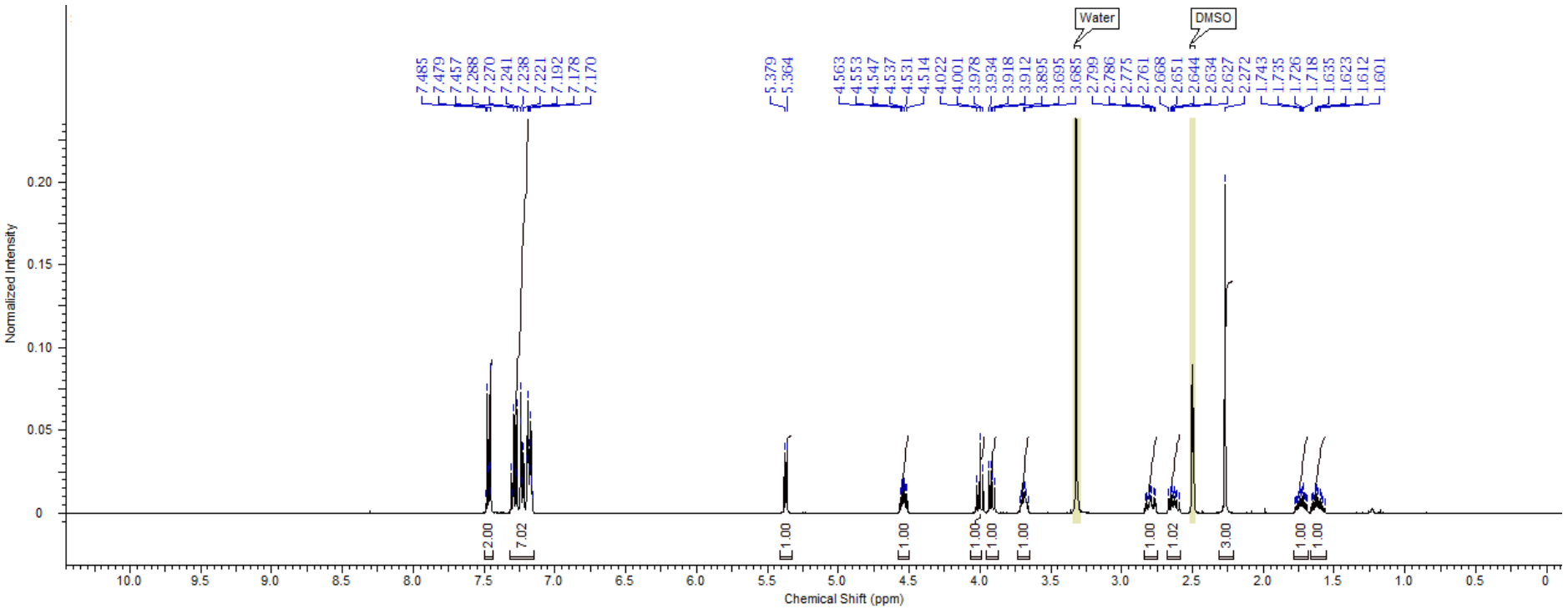
5a



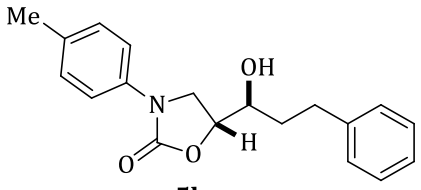
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **5a**.



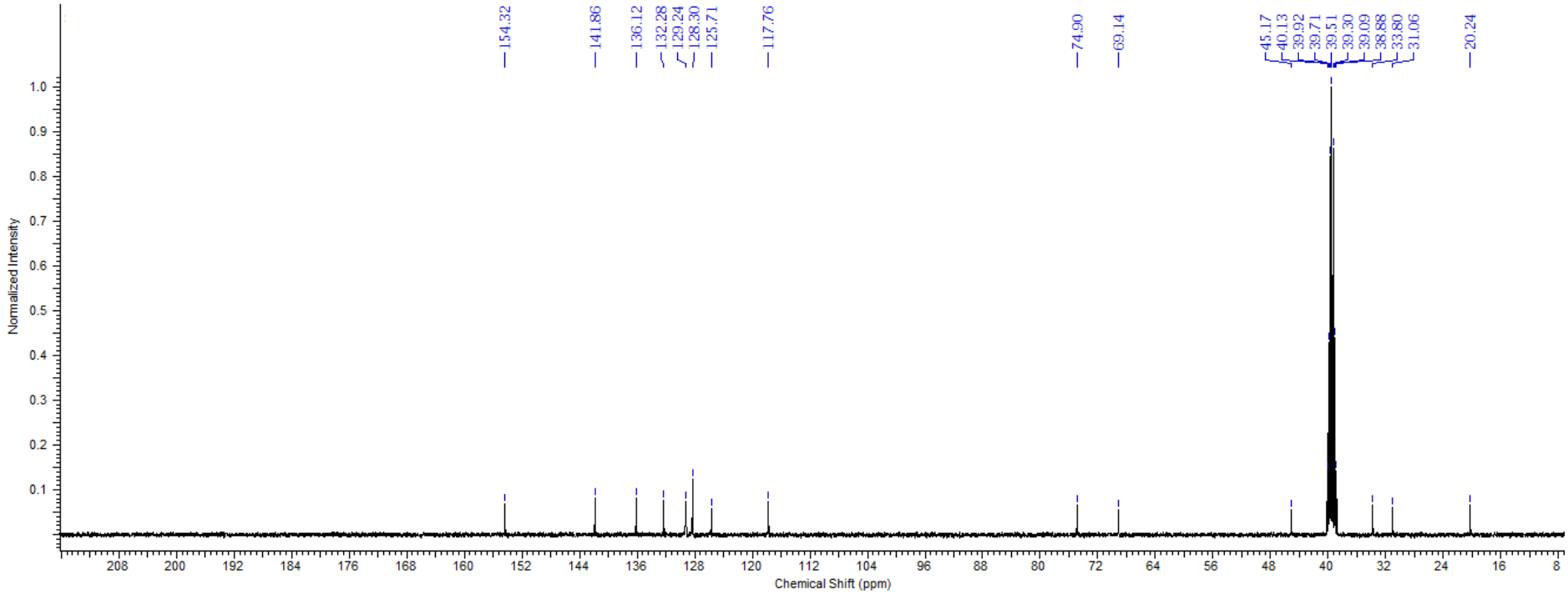
5a



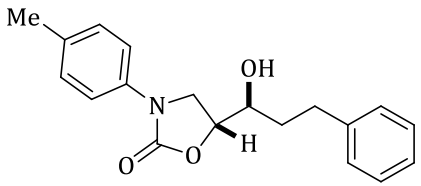
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5b**.



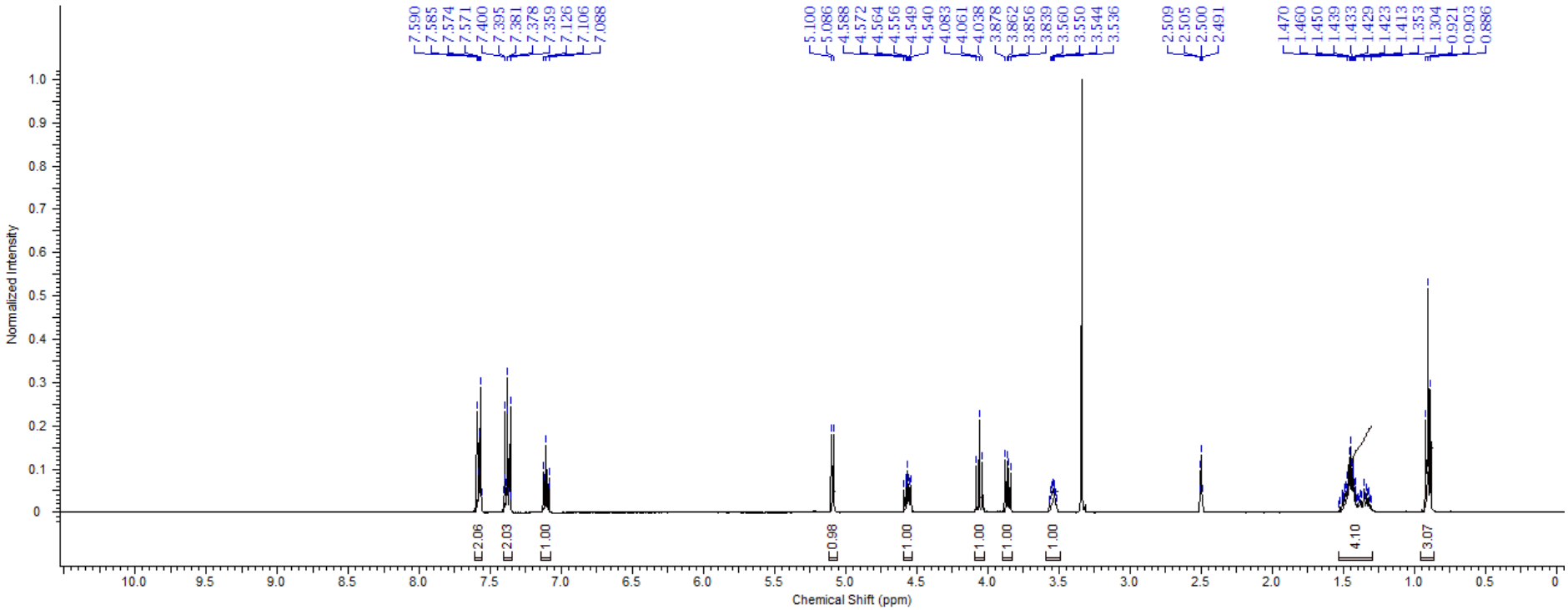
5b



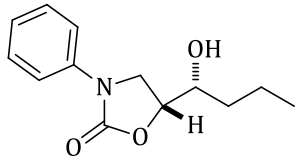
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **5b**.



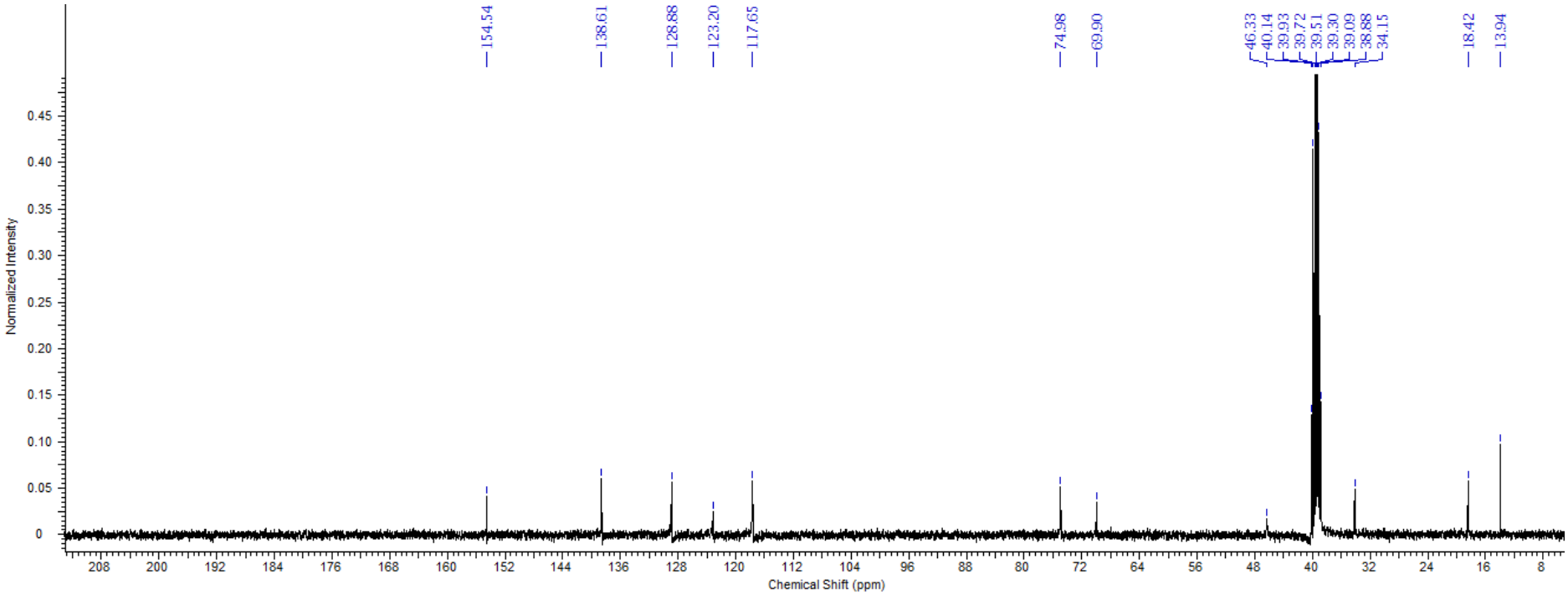
5b



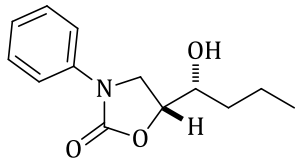
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5c**.



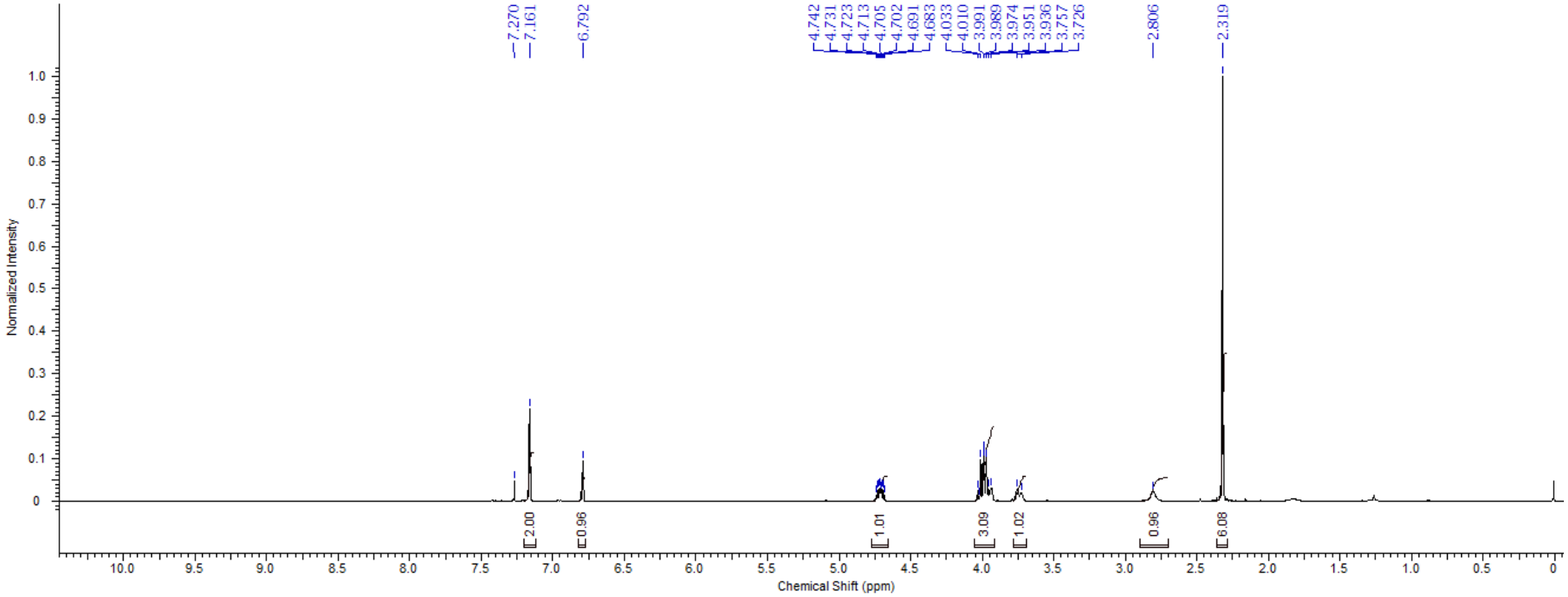
5c



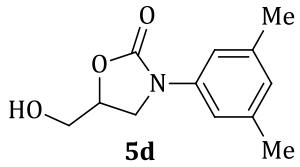
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **5c**.



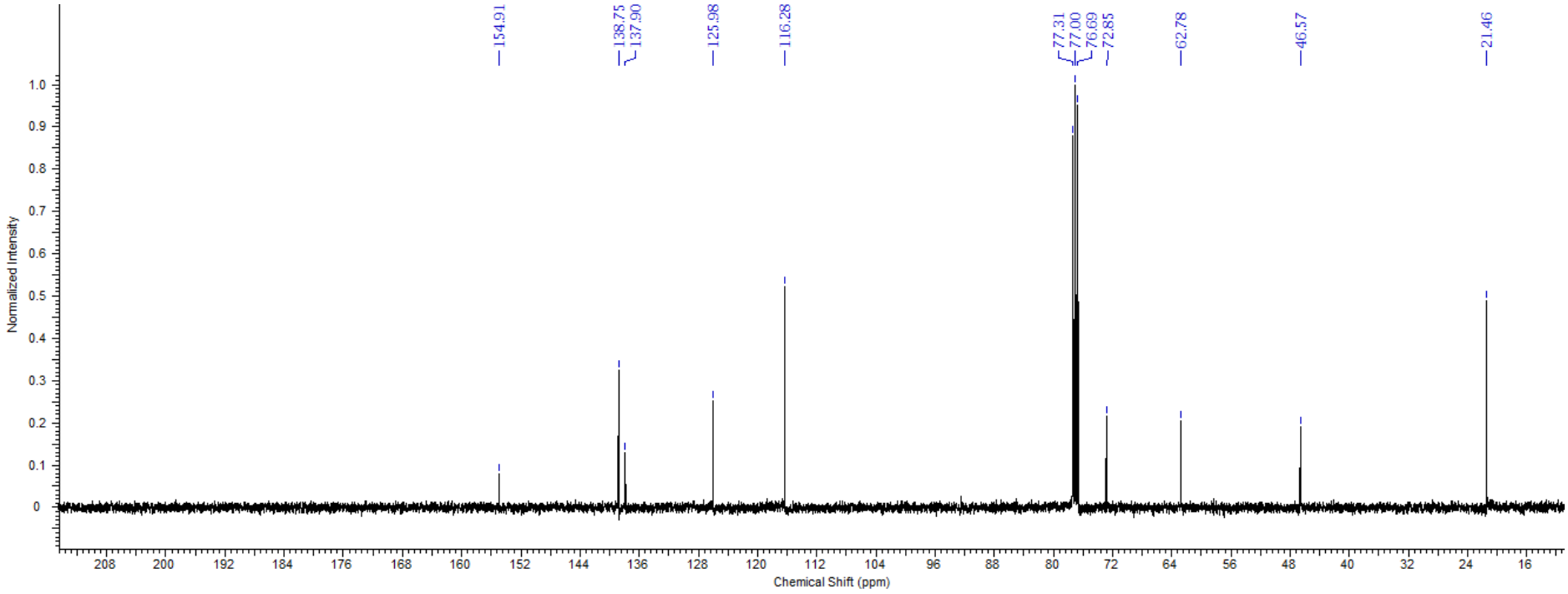
5c



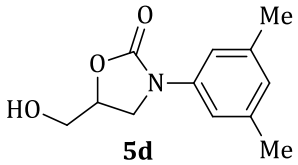
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5d**.



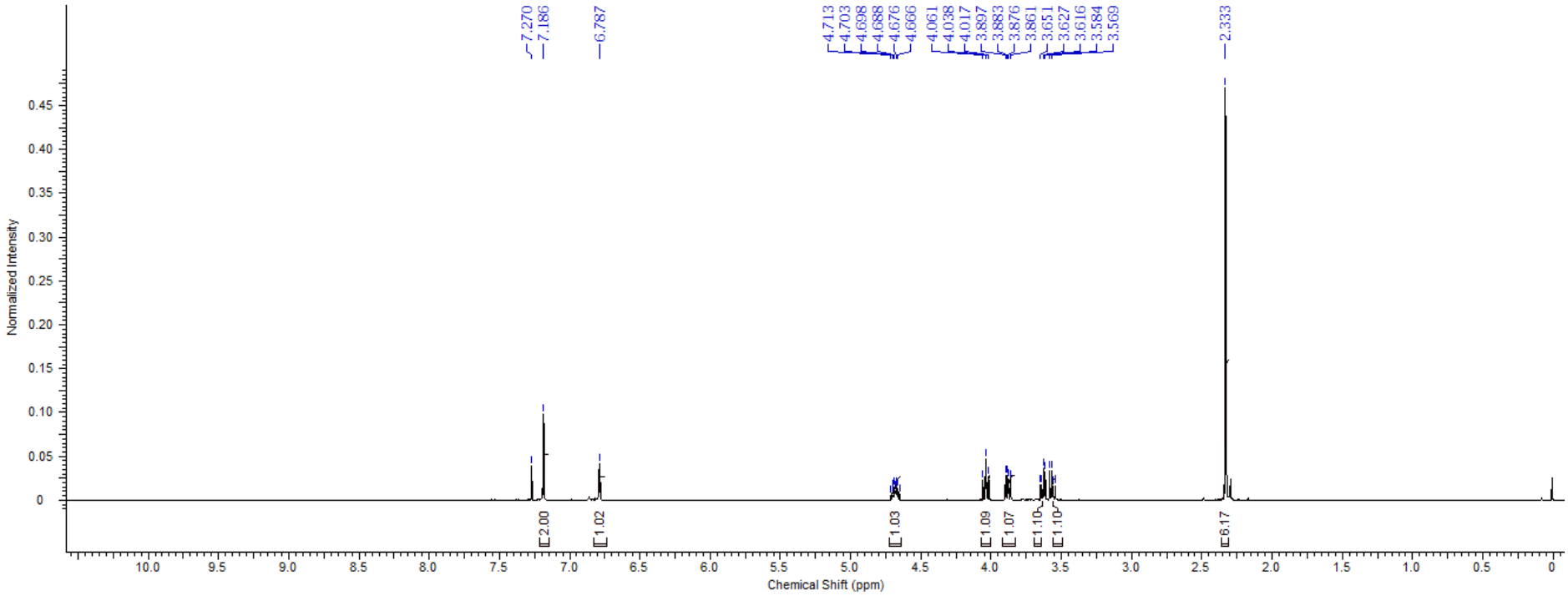
5d



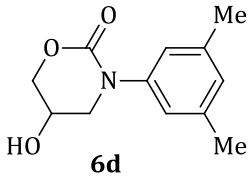
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5d**.



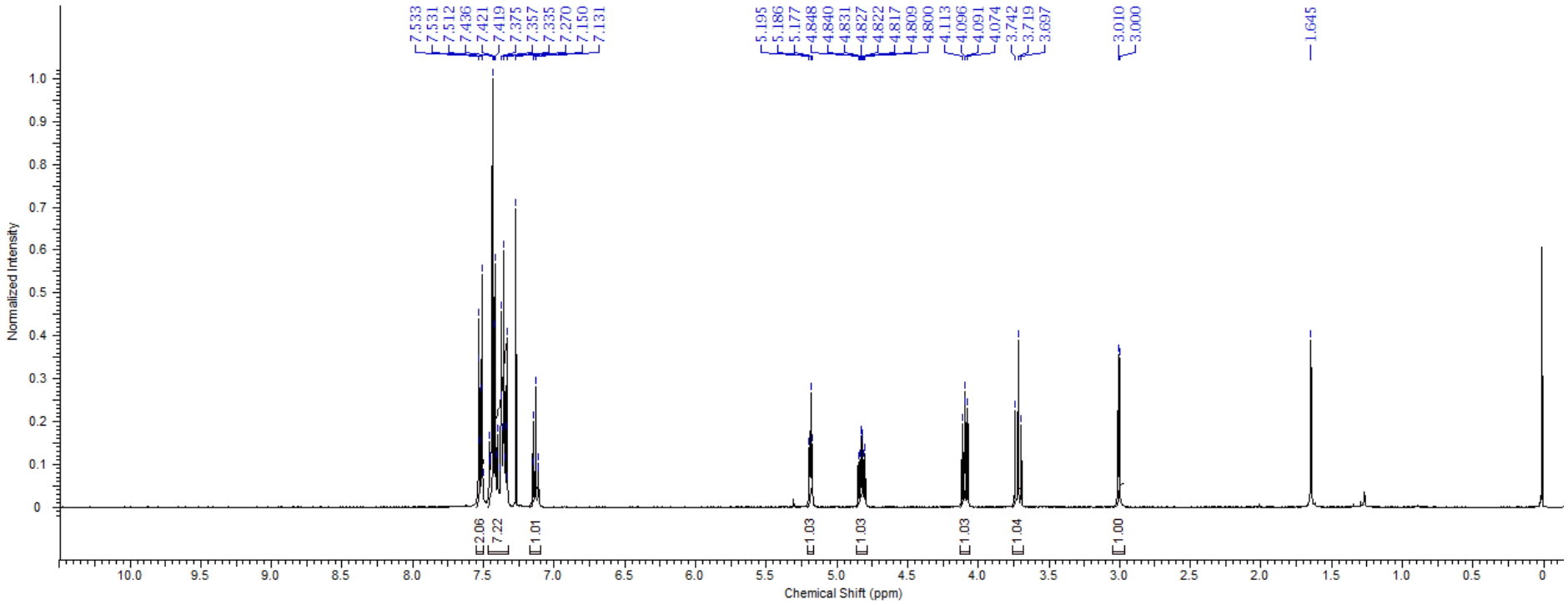
5d



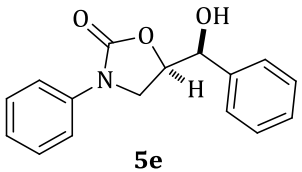
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **6d**.



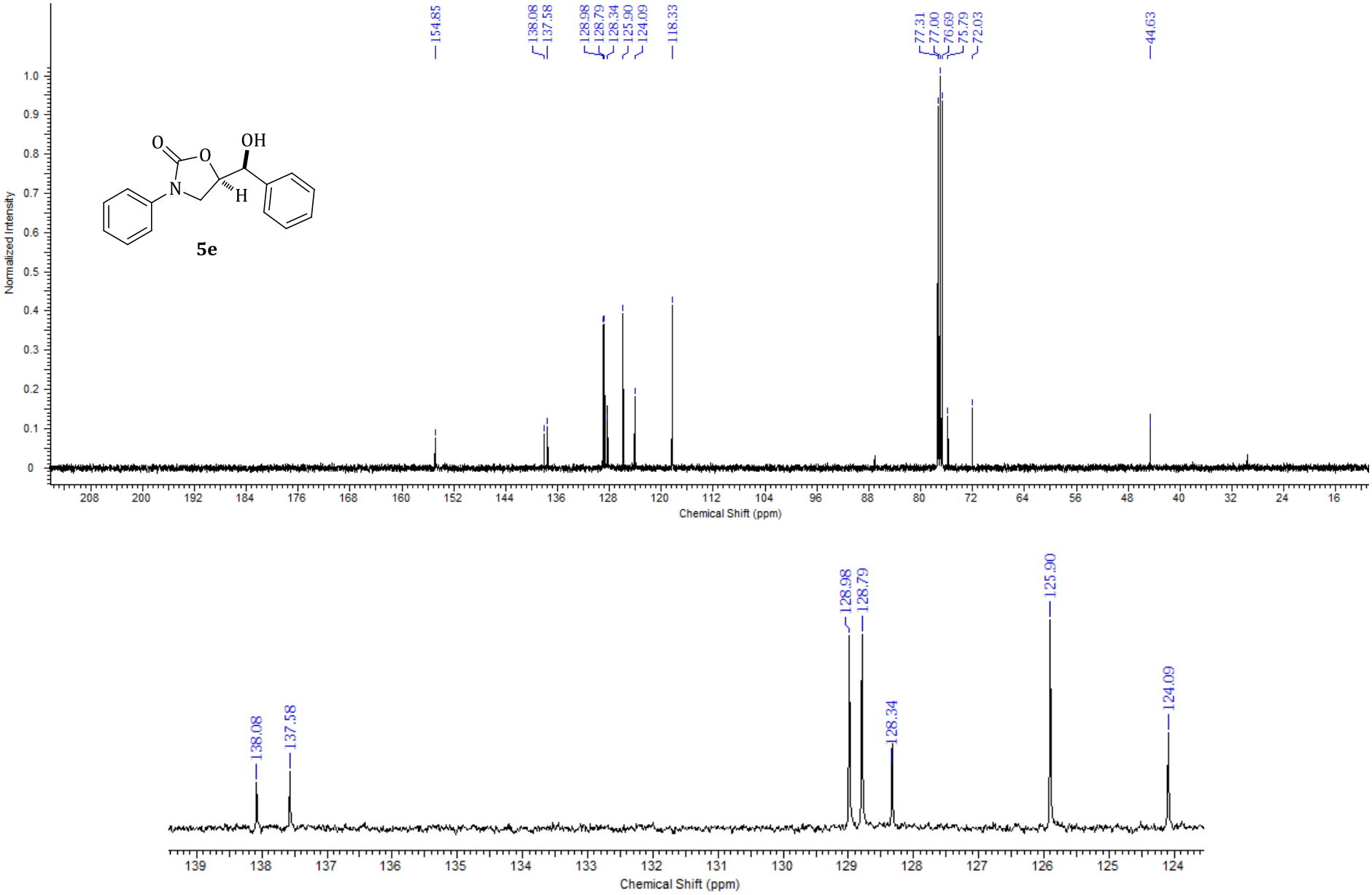
6d



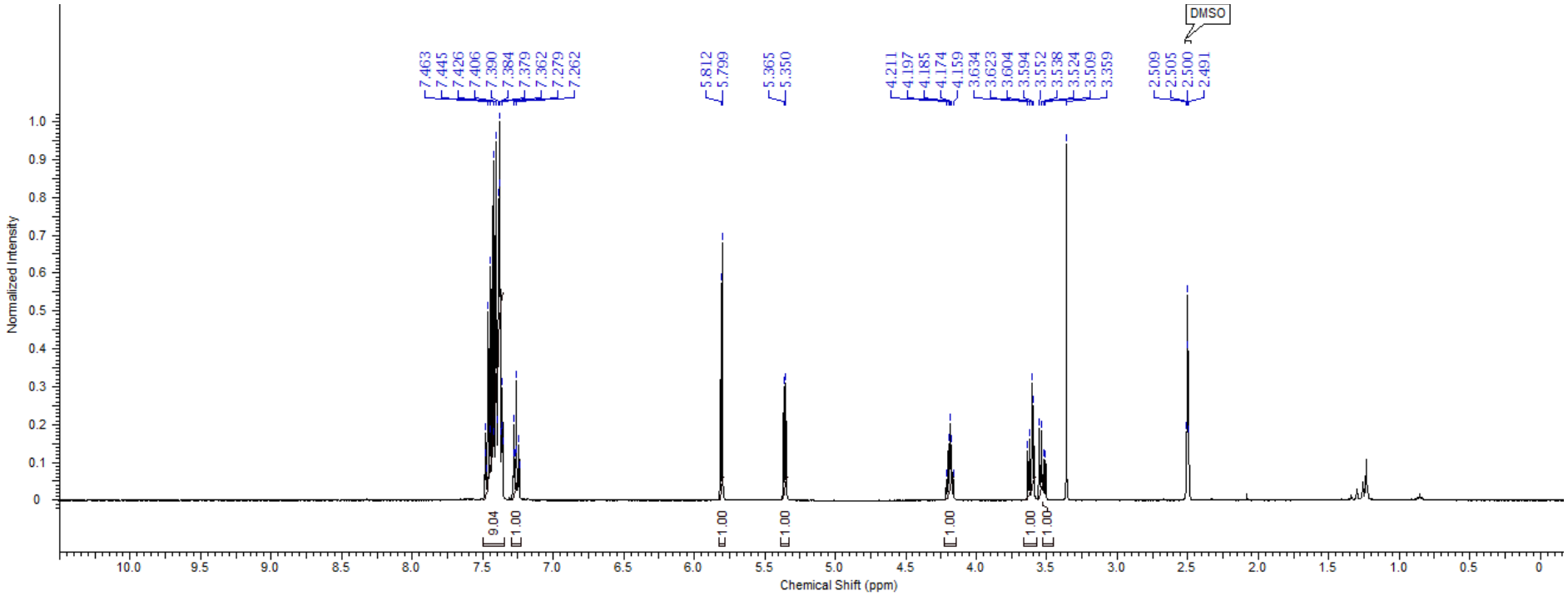
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5e**.



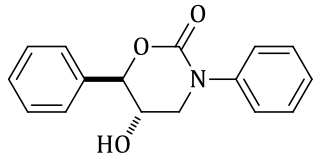
5e



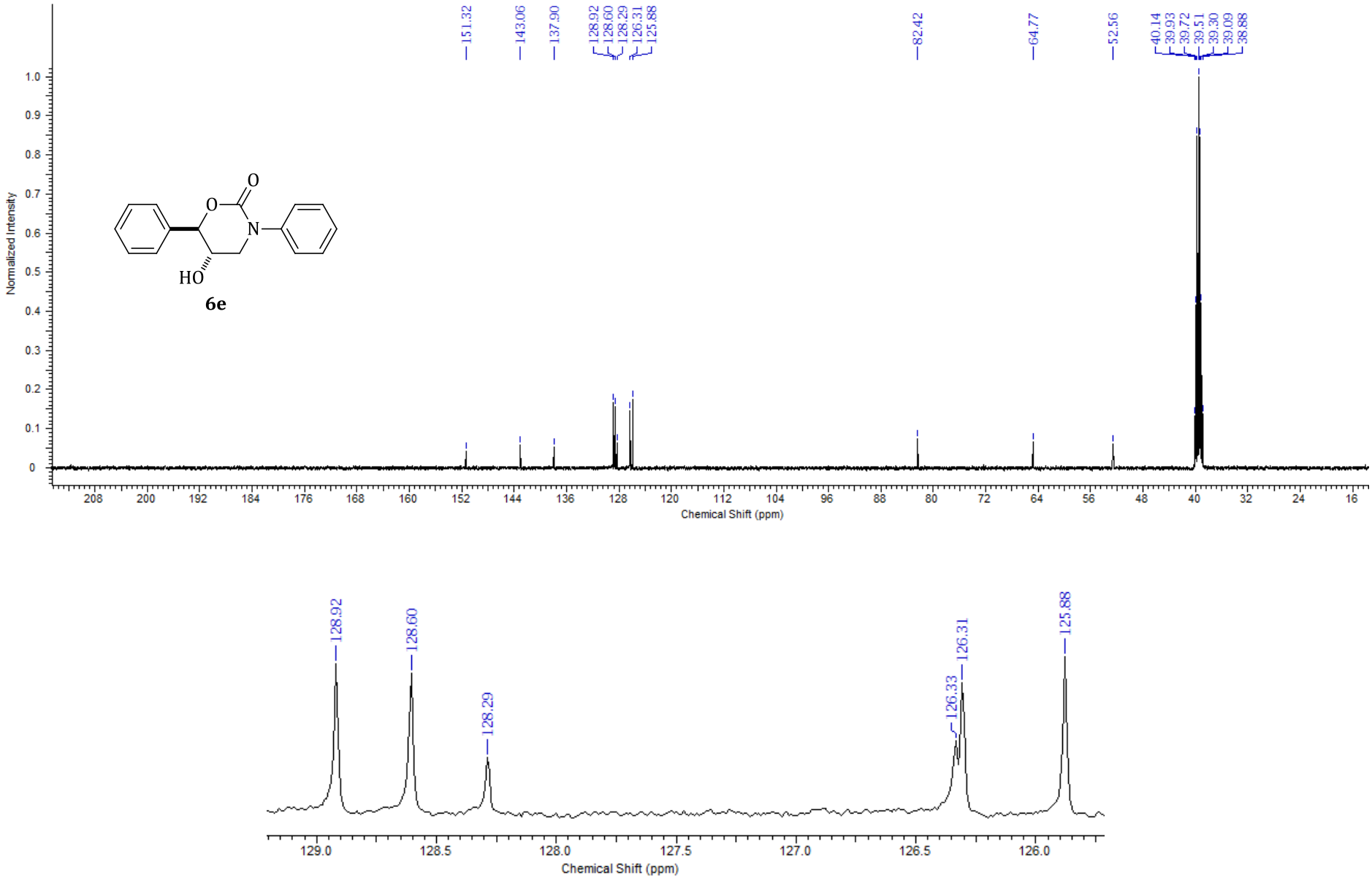
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5e**.



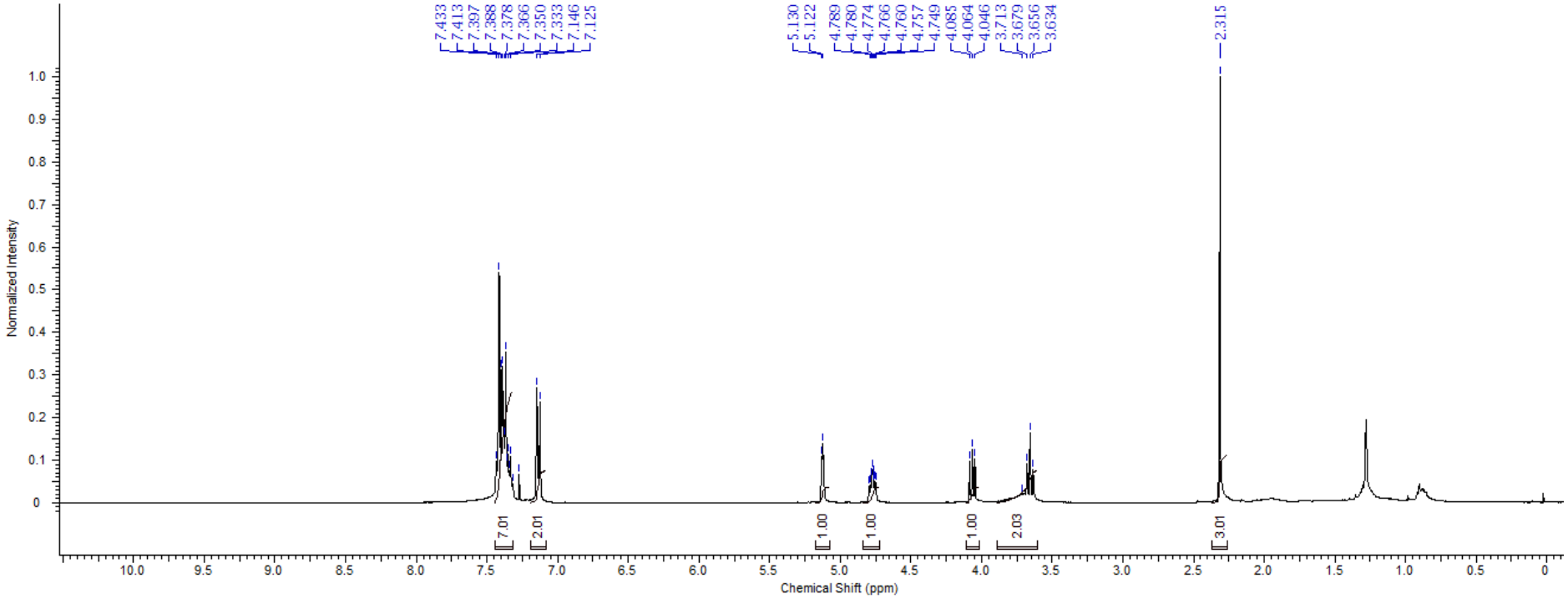
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **6e**.



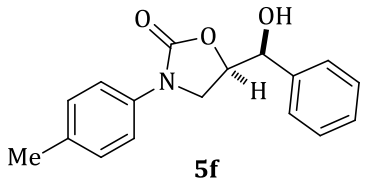
6e



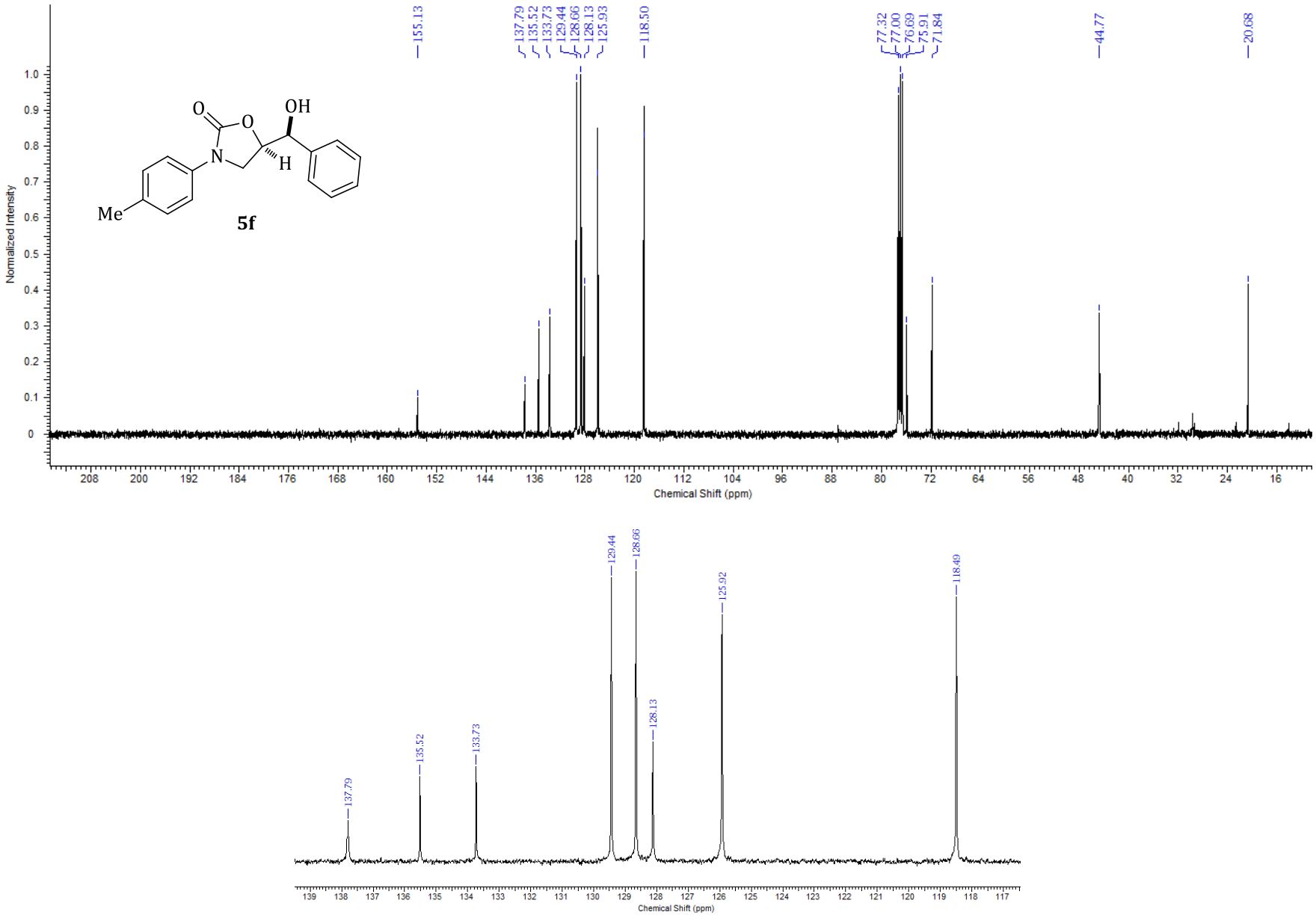
^{13}C NMR (DMSO-d_6, 400 MHz) spectrum of **6e**.



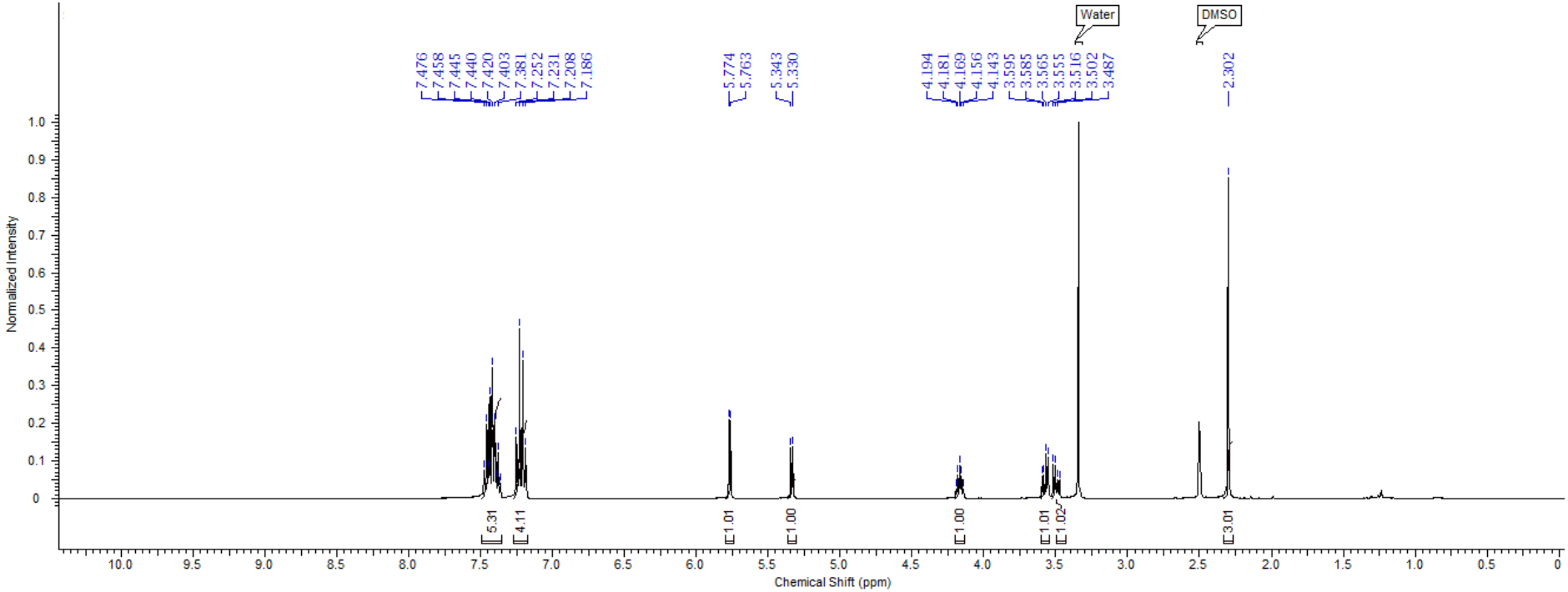
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5f**.



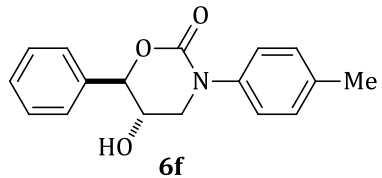
5f



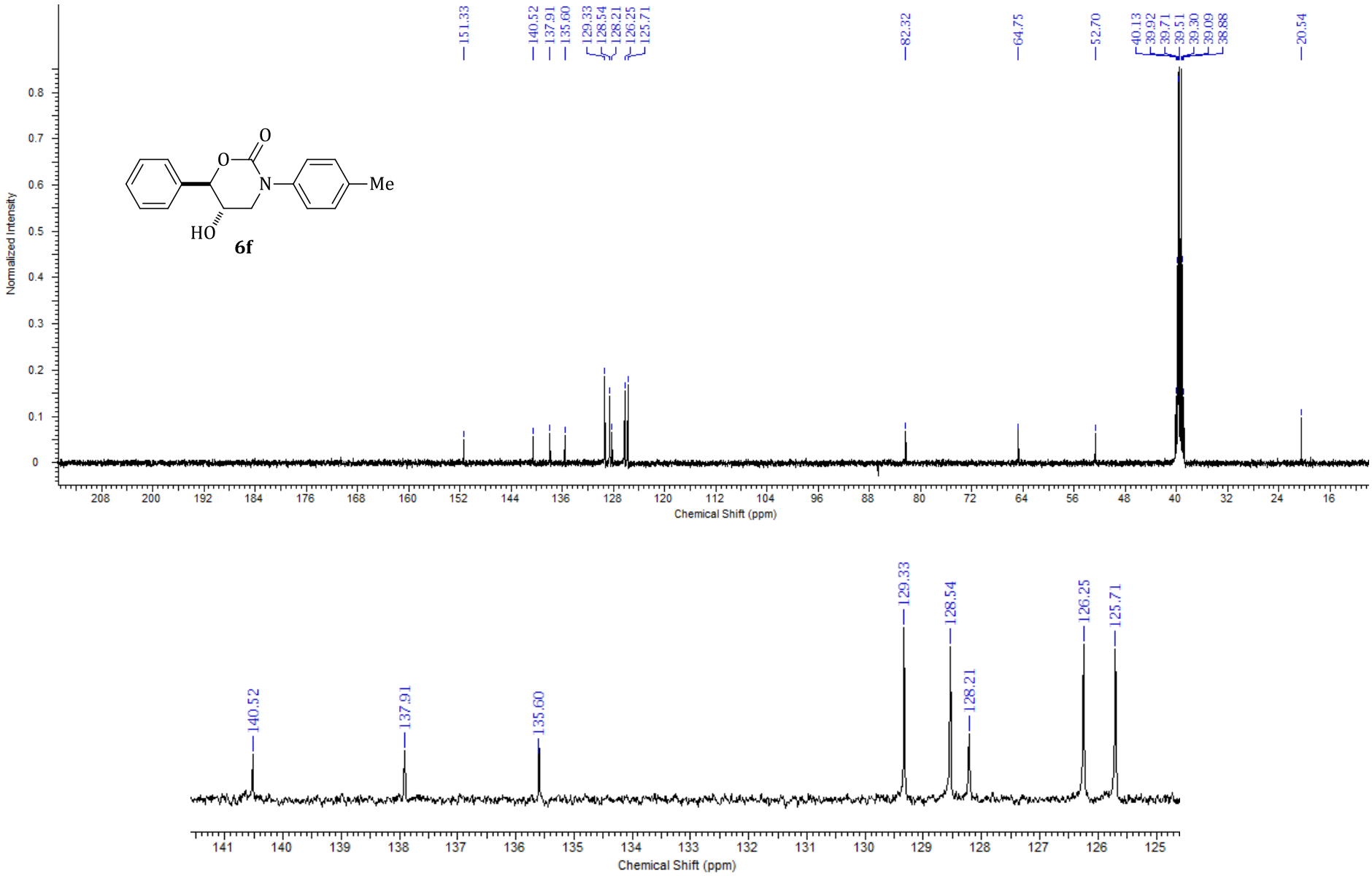
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5f**.



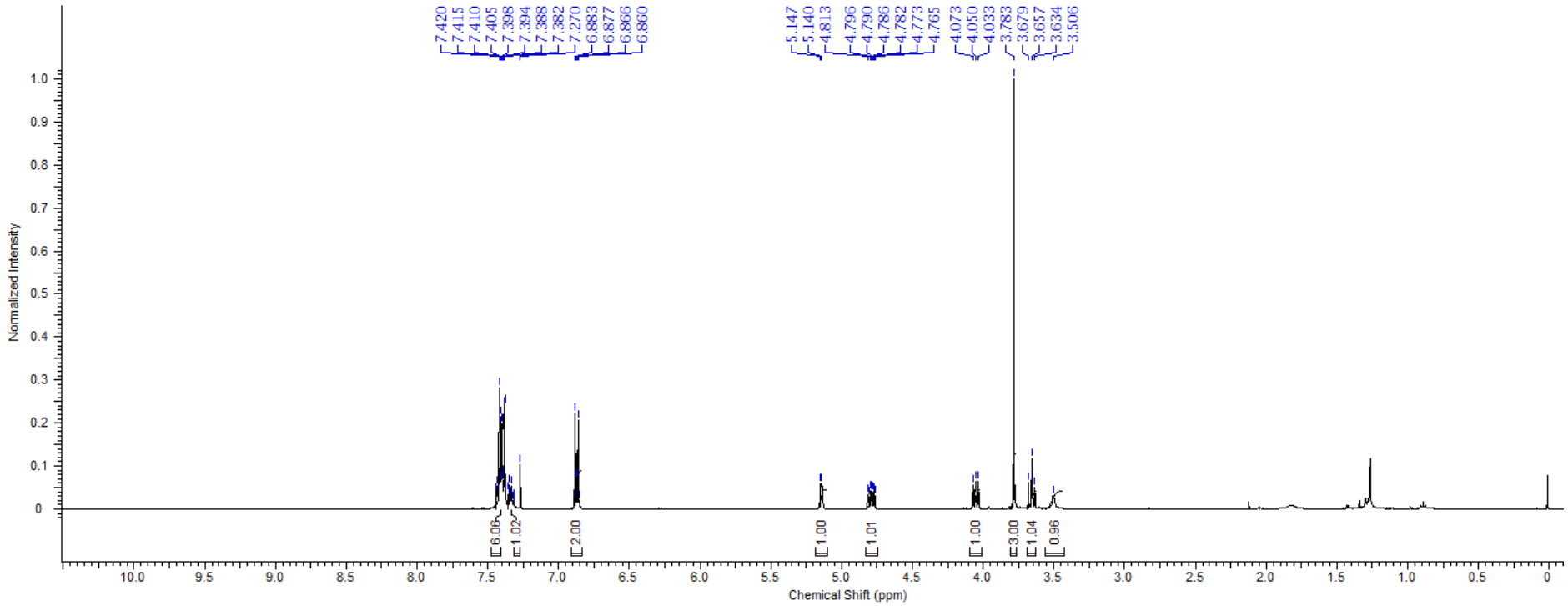
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **6f**.



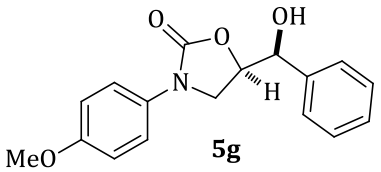
6f



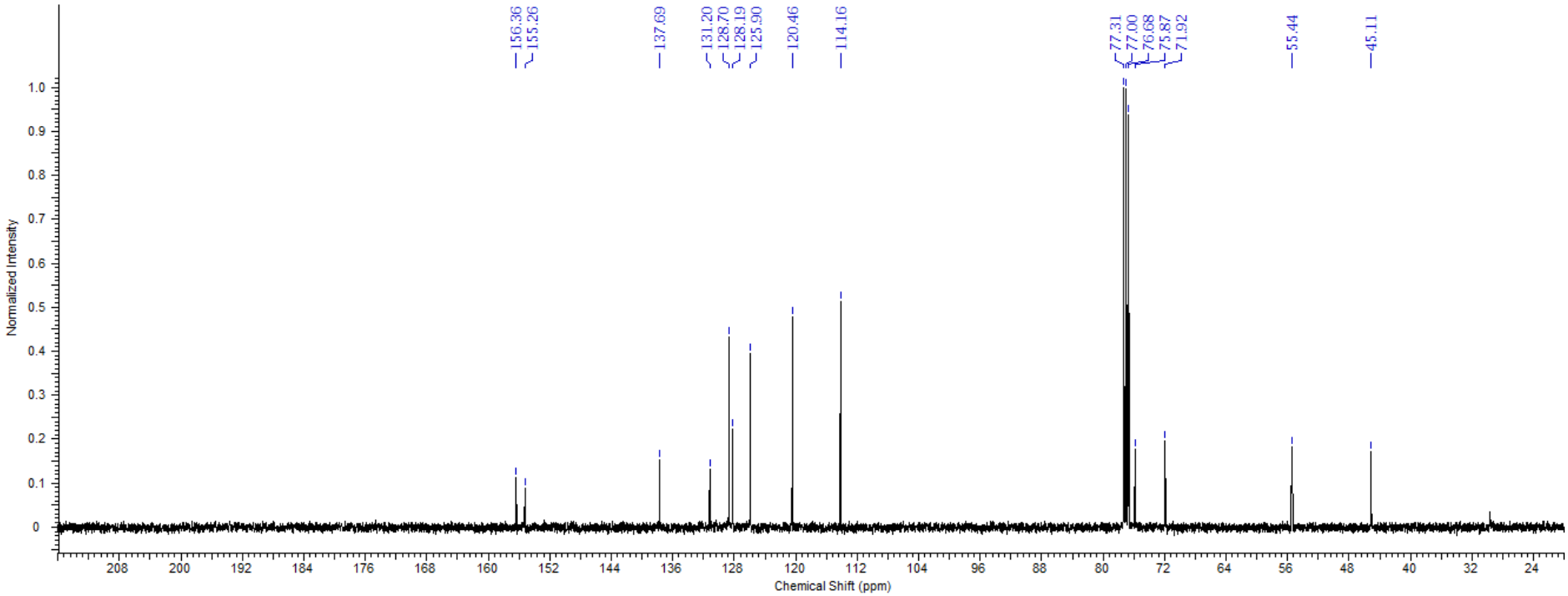
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6f**.



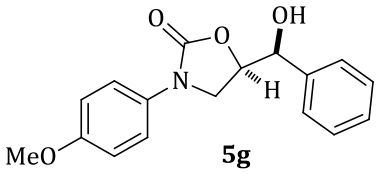
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5g**.



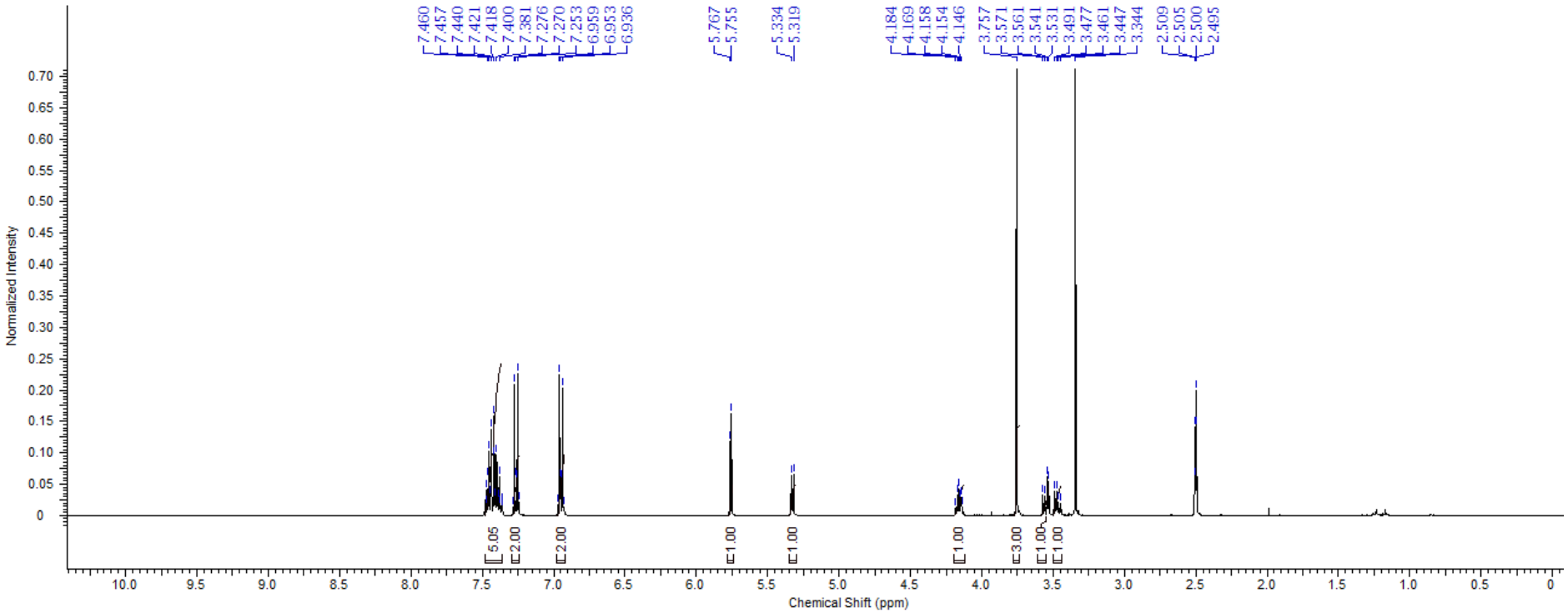
5g



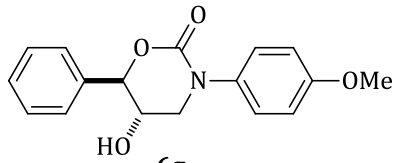
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5g**.



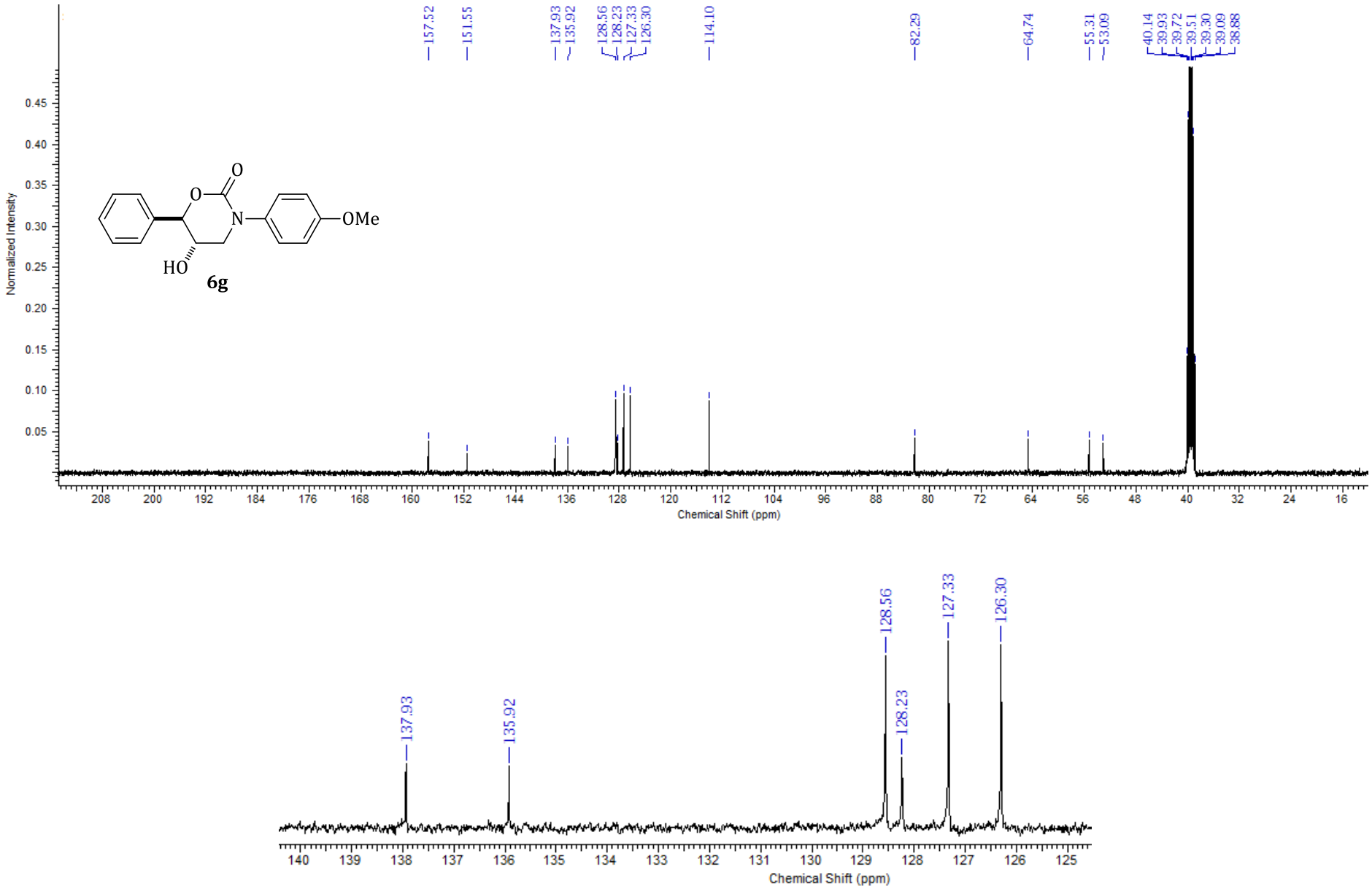
5g



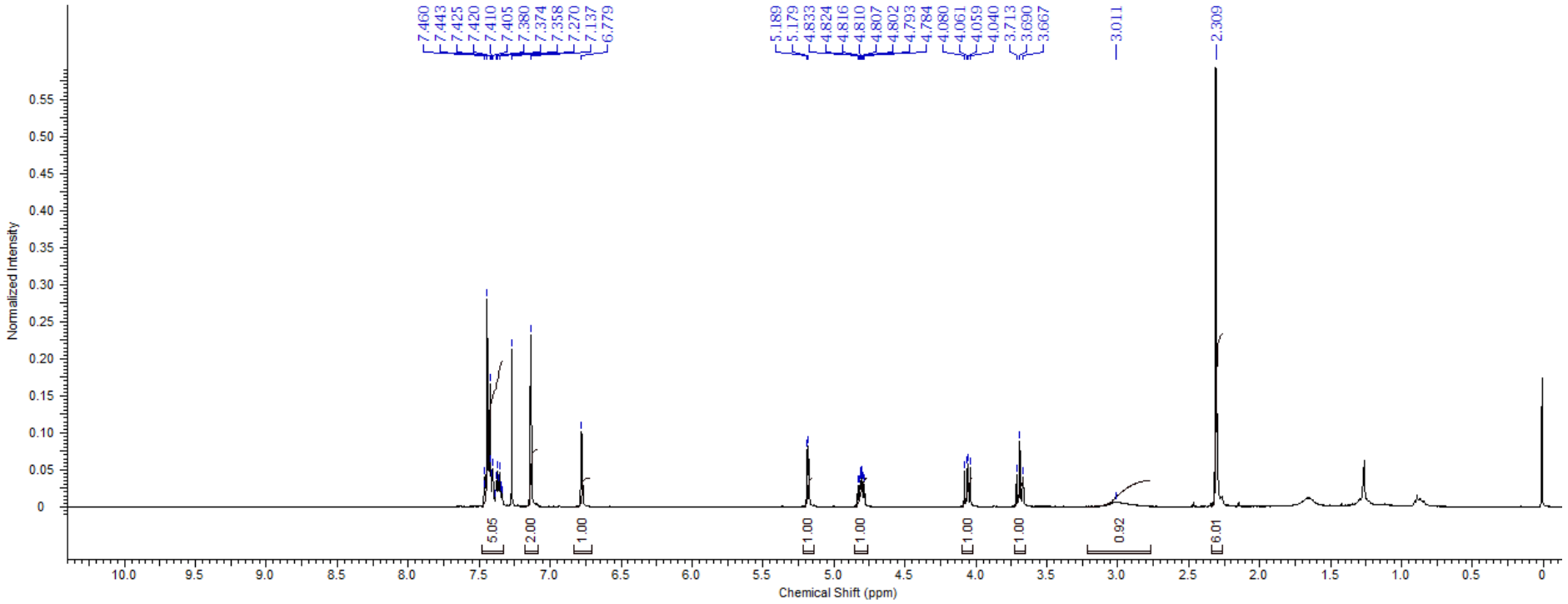
^{1}H NMR (DMSO-d_6, R00 MHz) spectrum of **6g**.



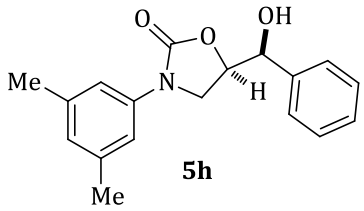
6g



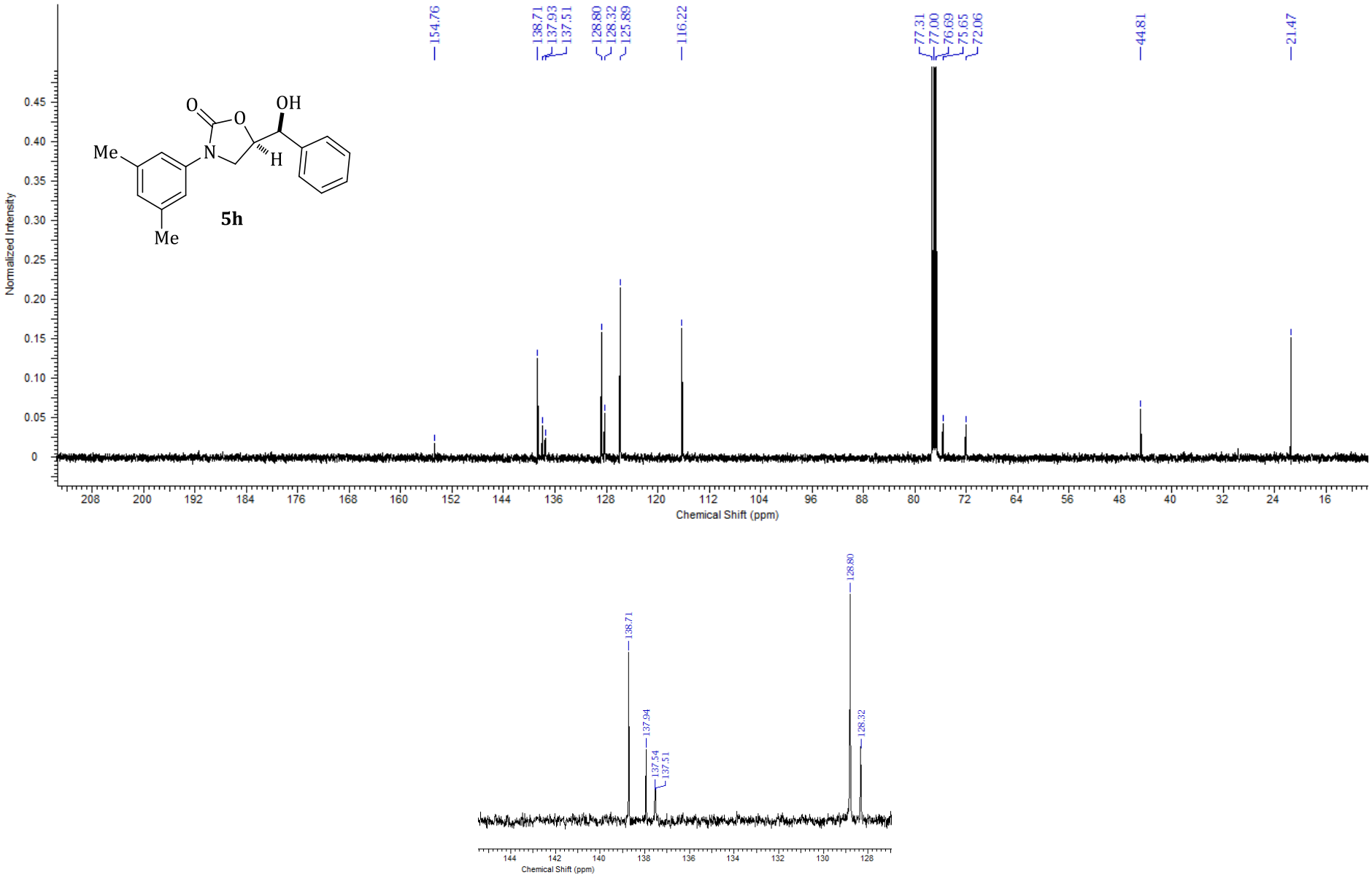
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6g**.



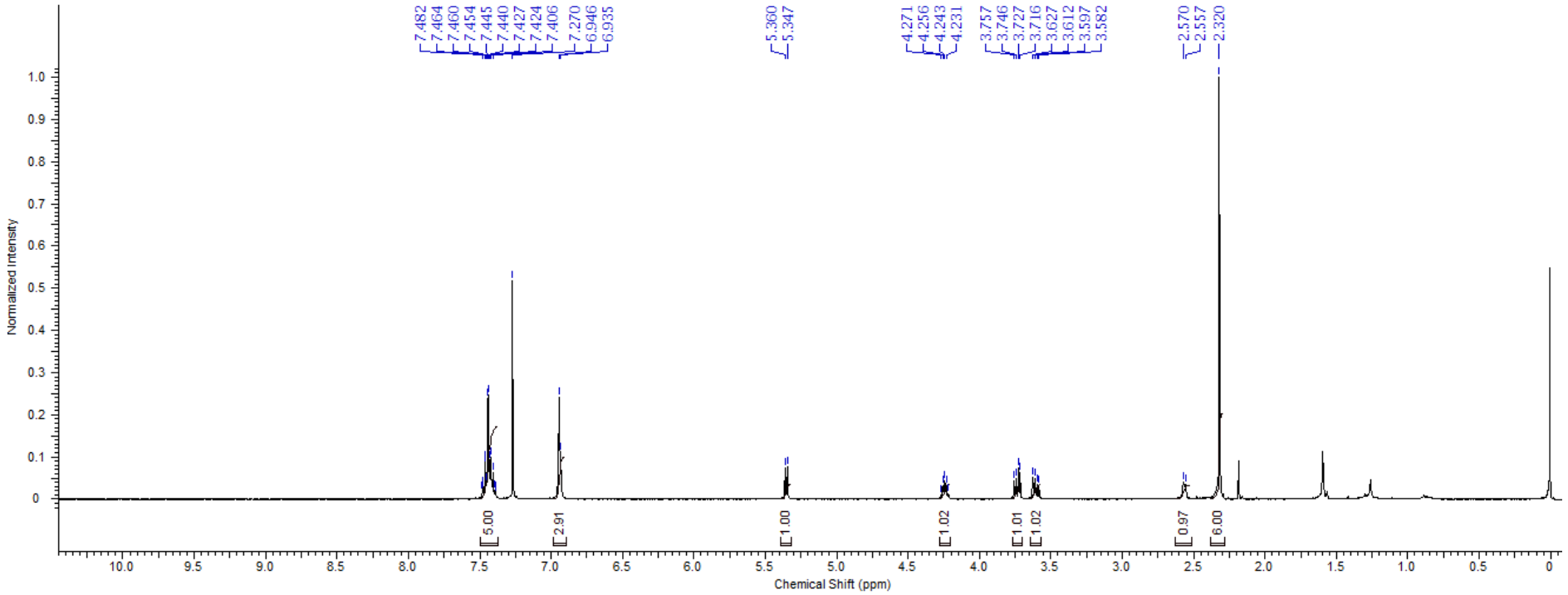
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5h**.



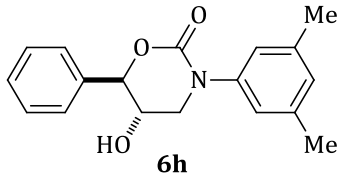
5h



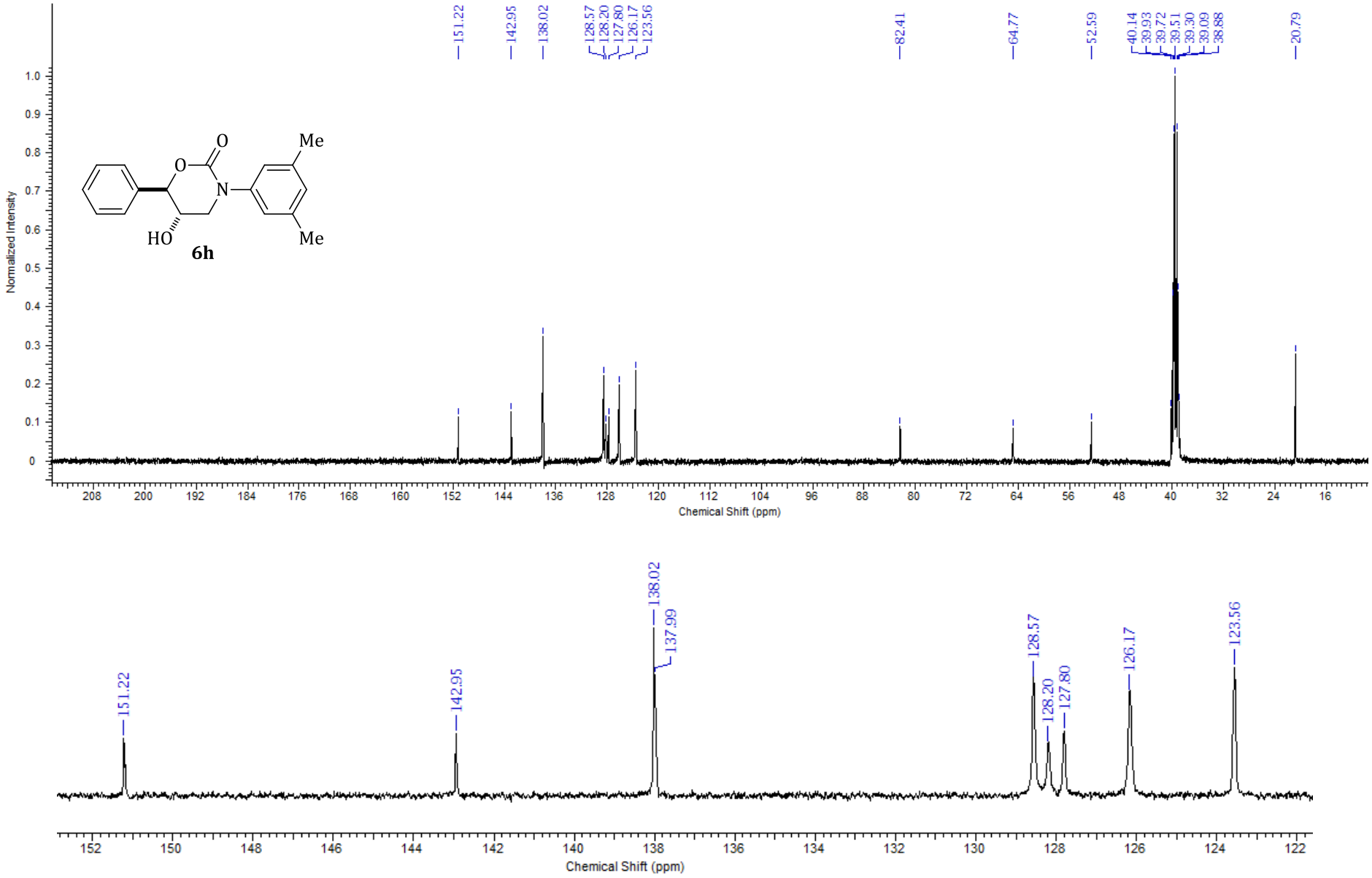
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5h**.



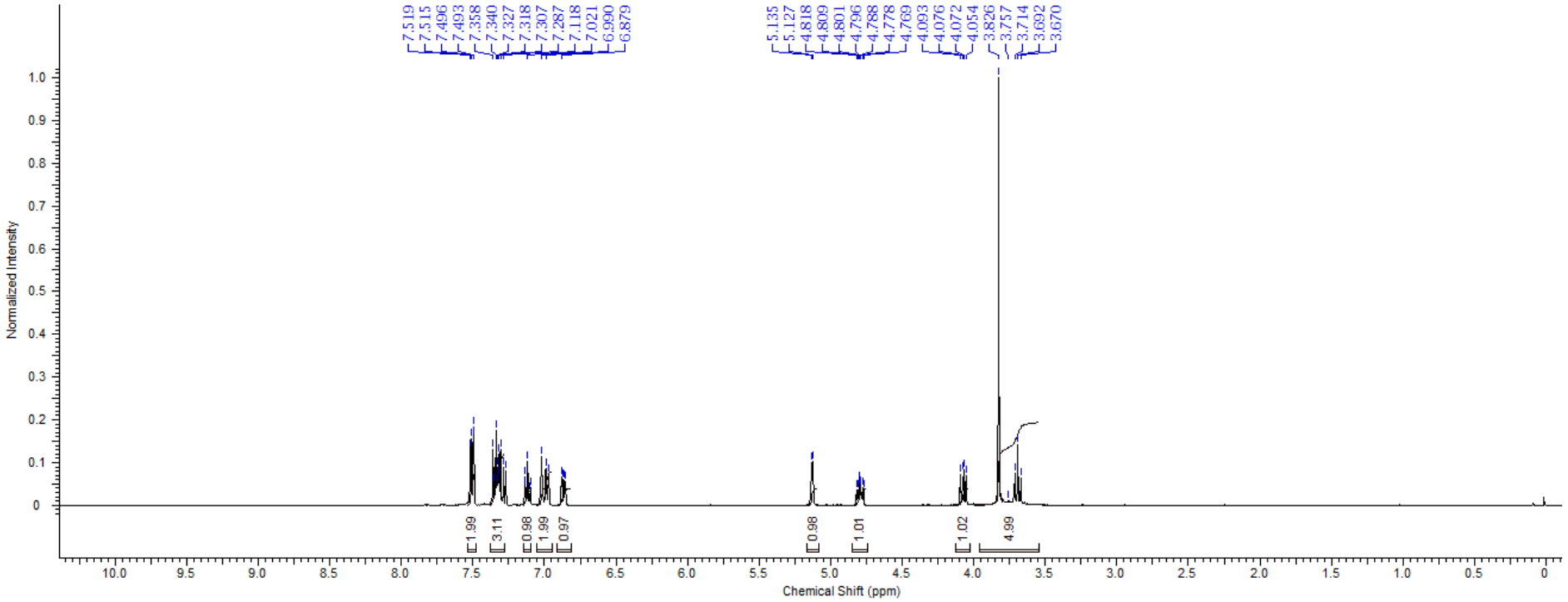
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **6h**.



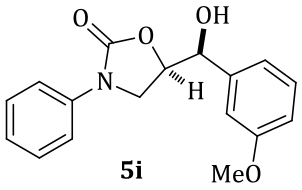
6h



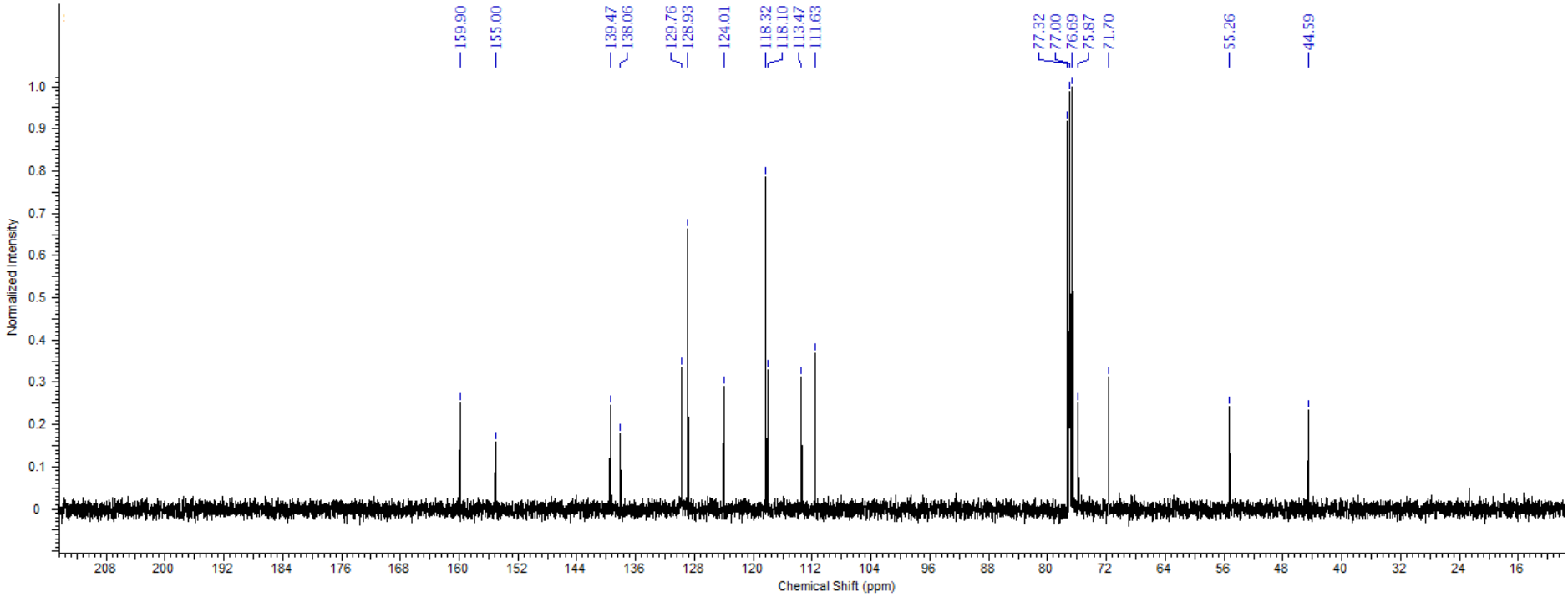
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6h**.



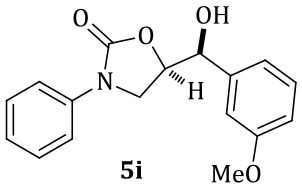
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5i**.



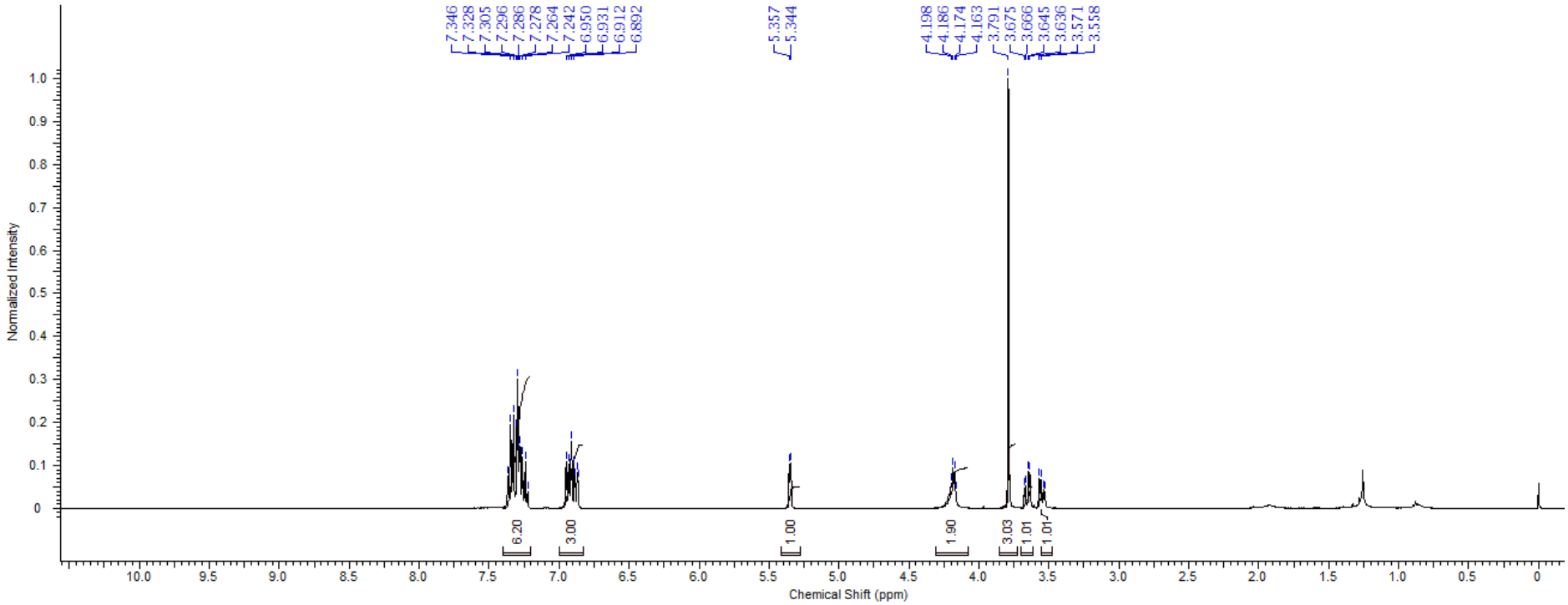
5i



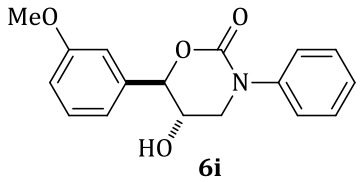
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5i**.



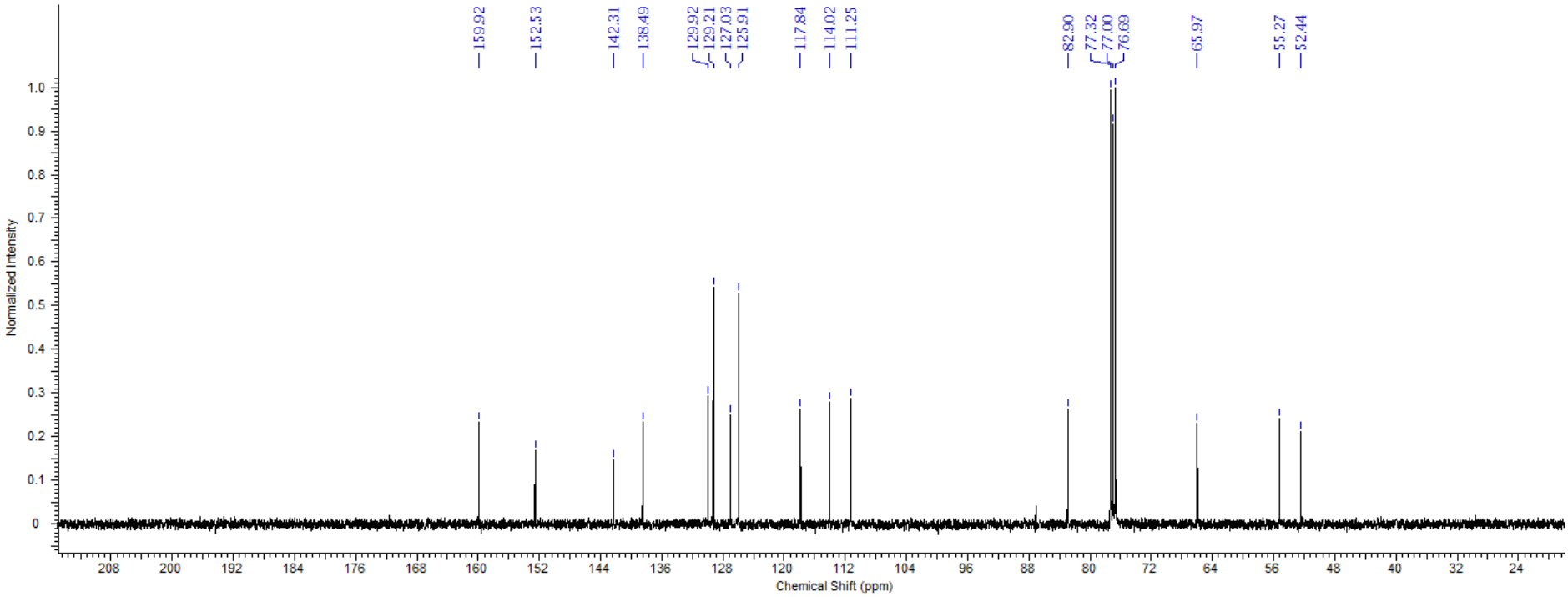
5i



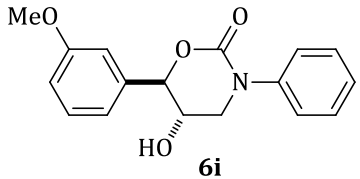
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **6i**.



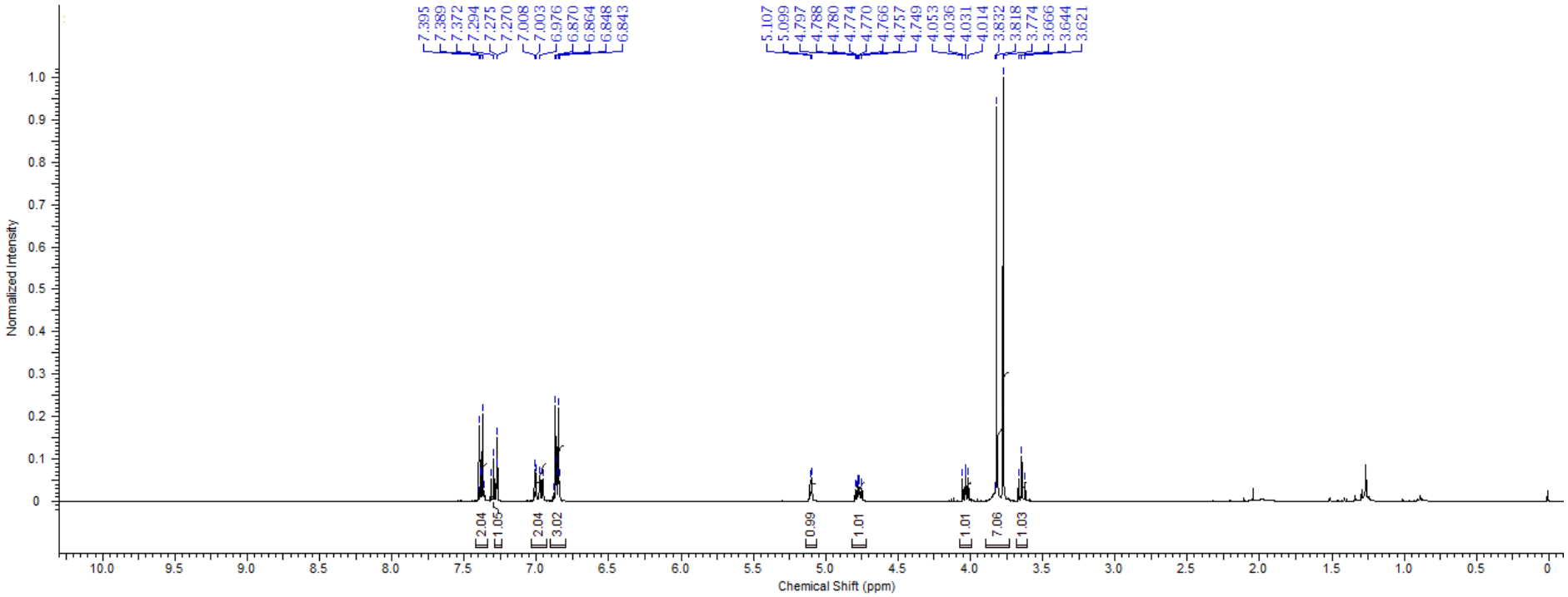
6i



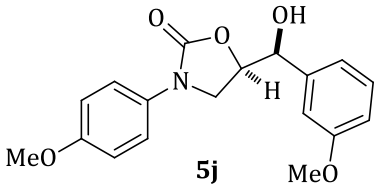
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **6i**.



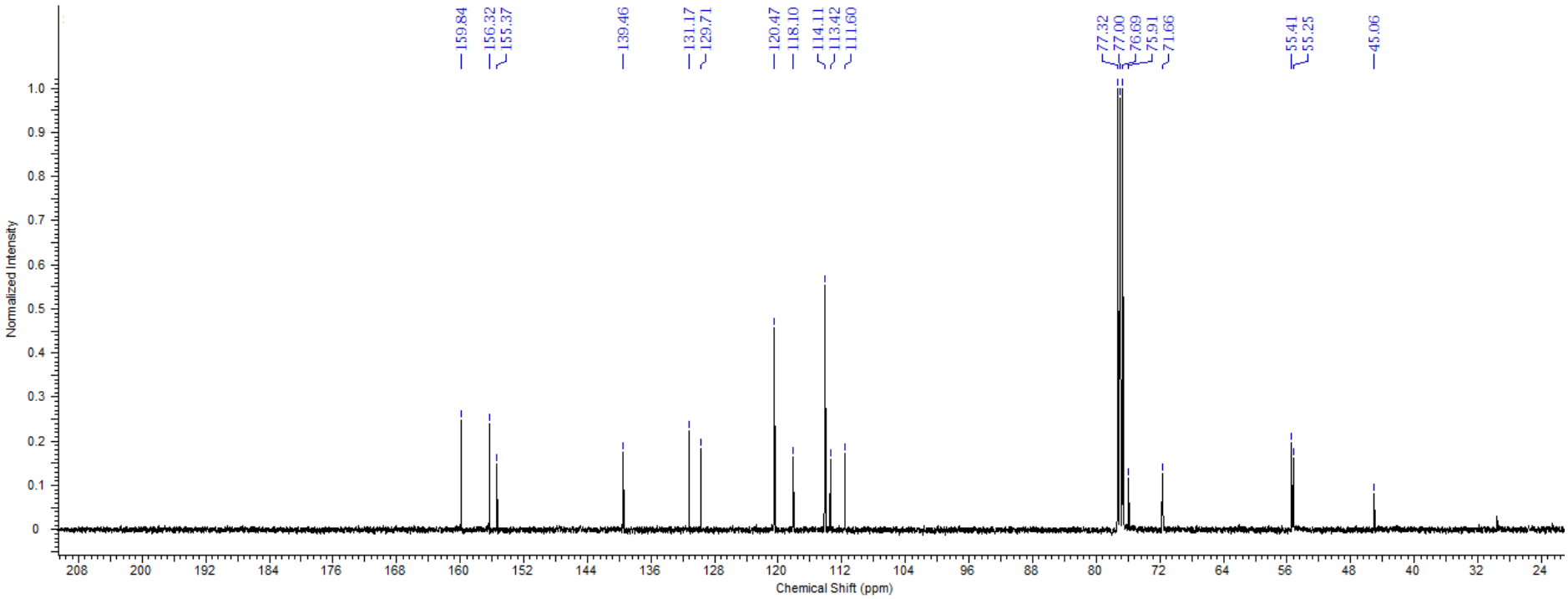
6i



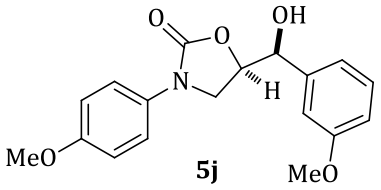
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5j**.



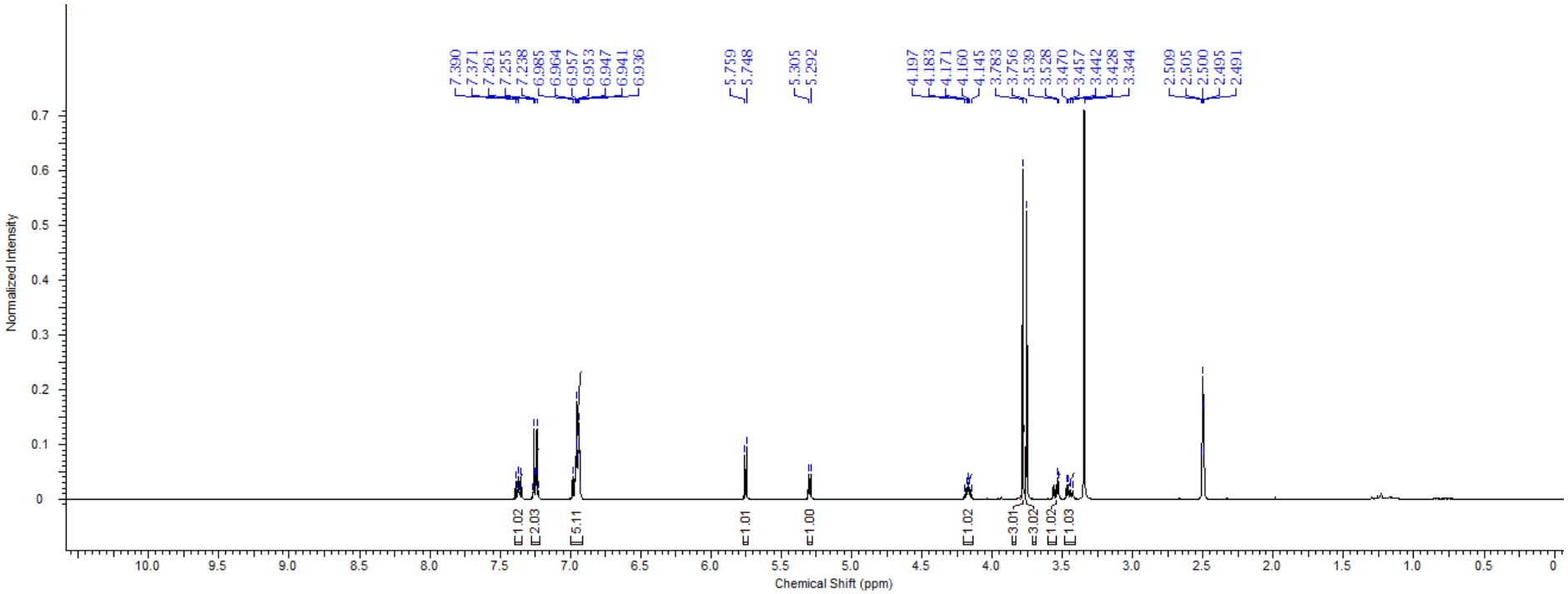
5j



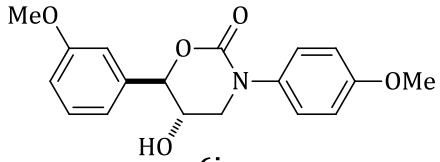
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5j**.



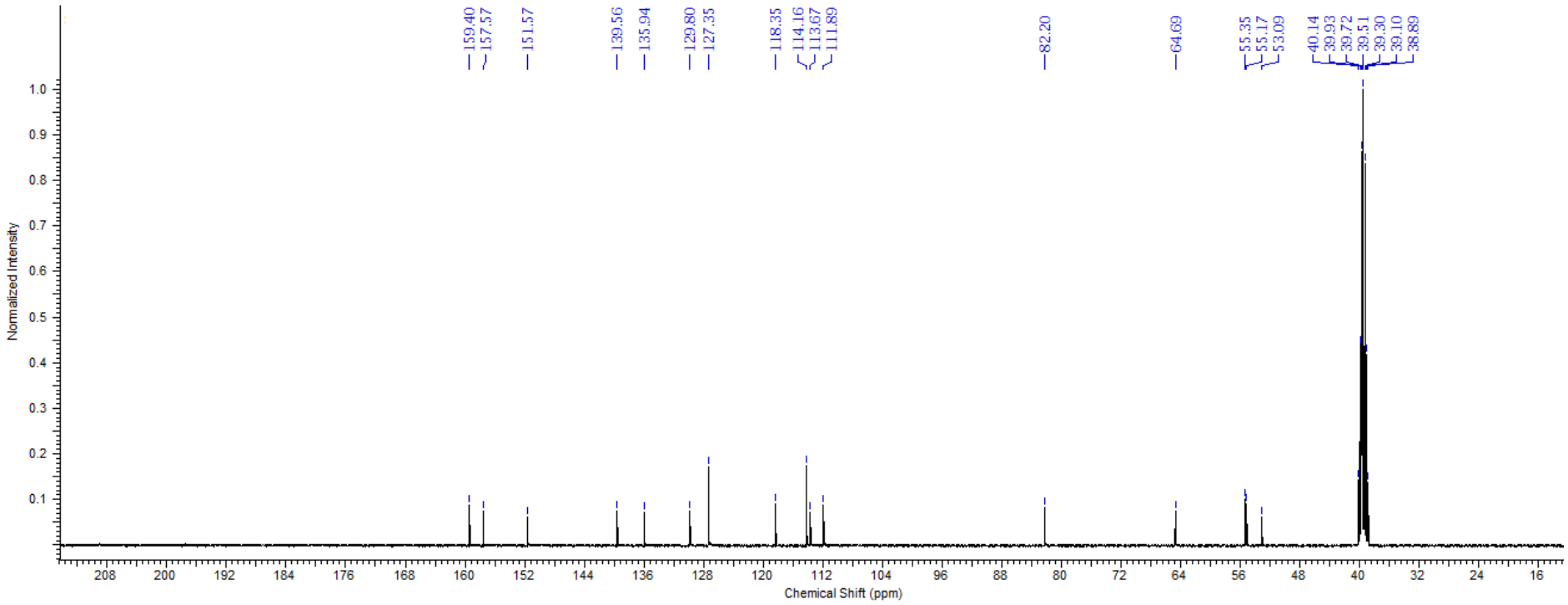
5j



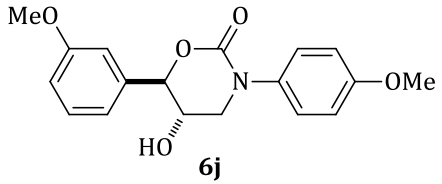
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **6j**.



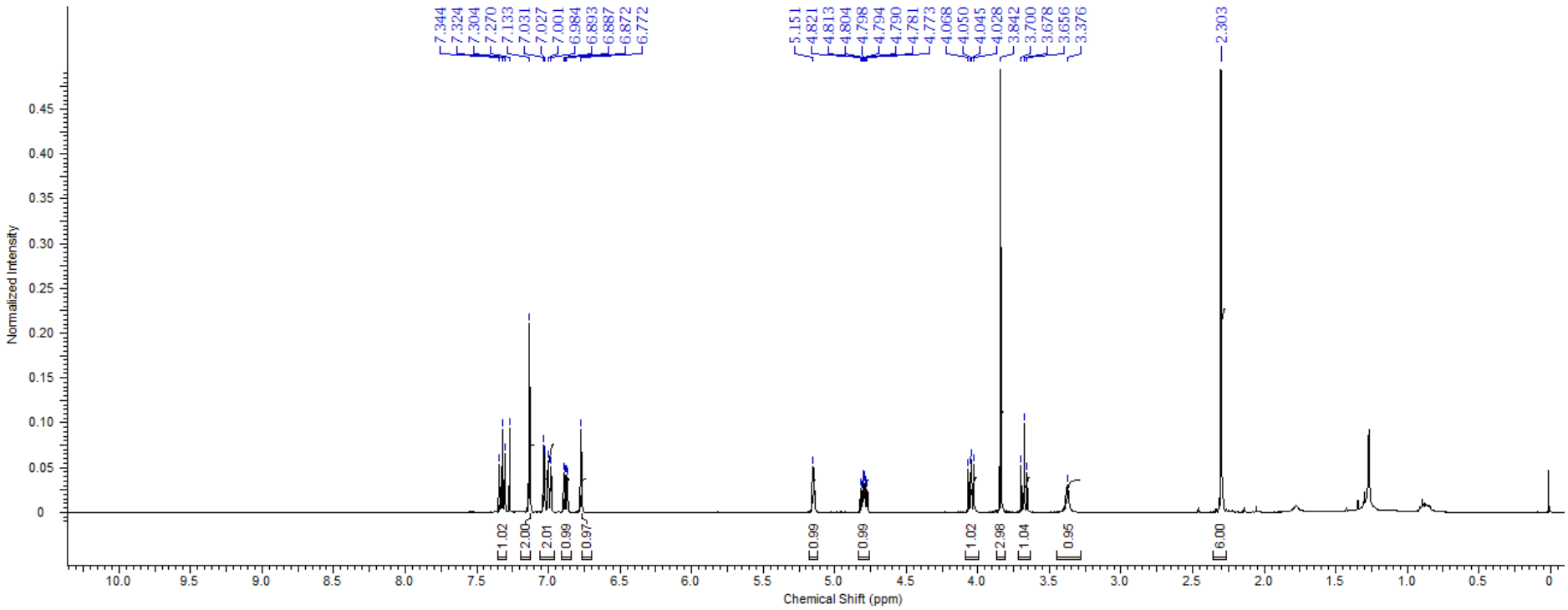
6j



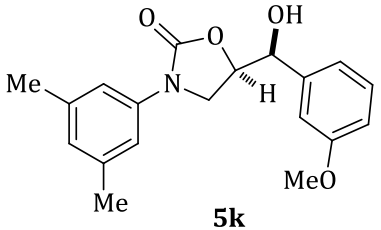
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6j**.



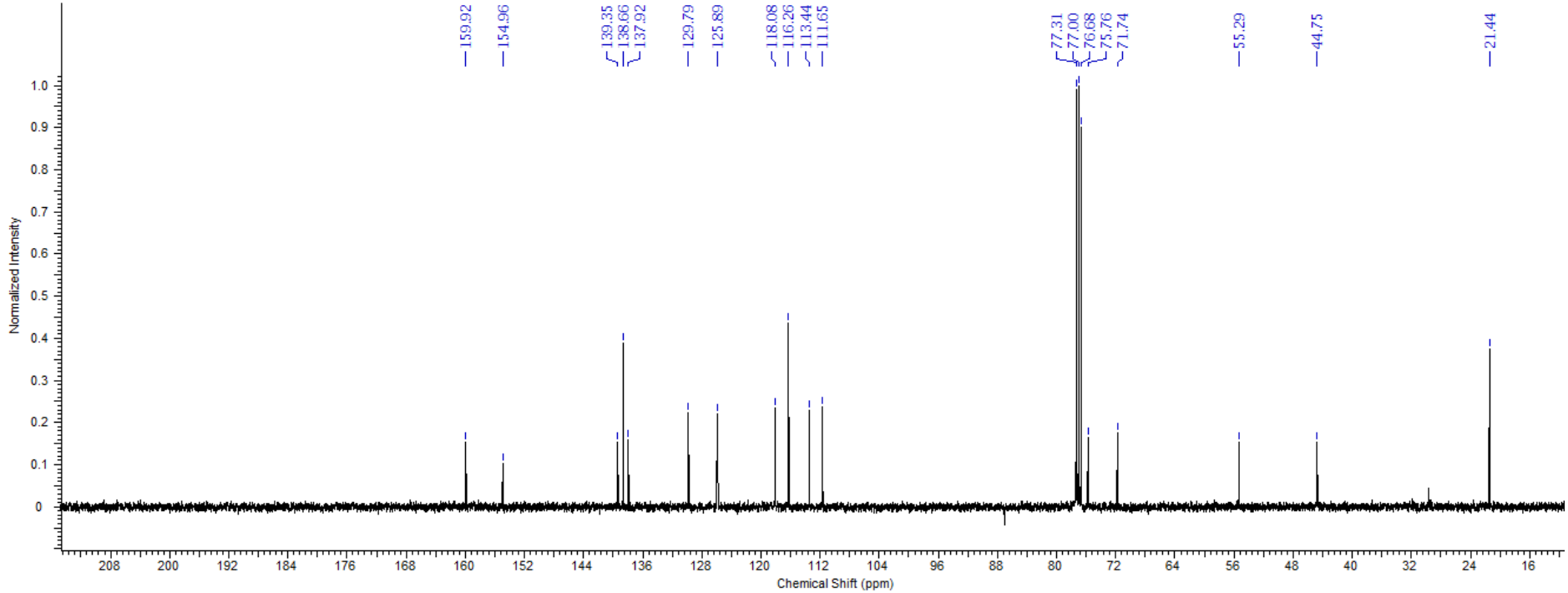
6j



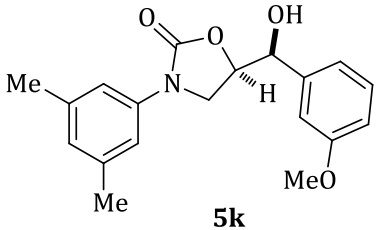
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **5k**.



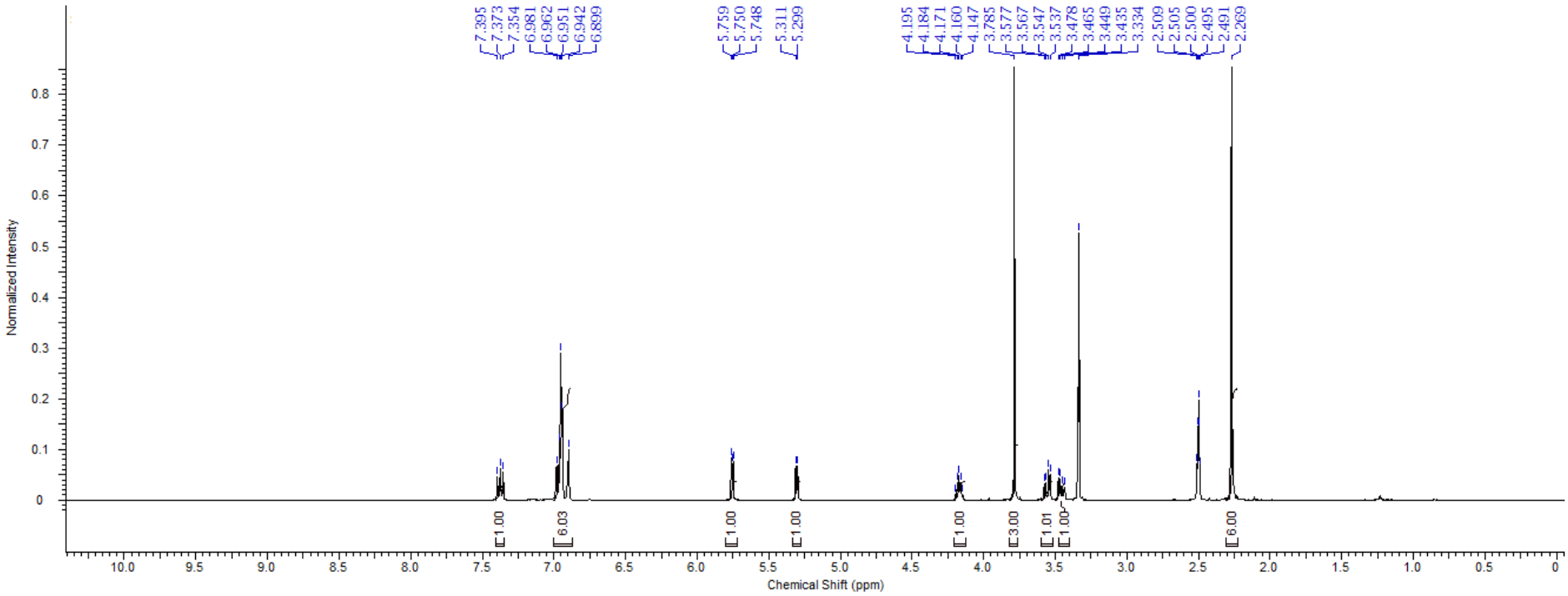
5k



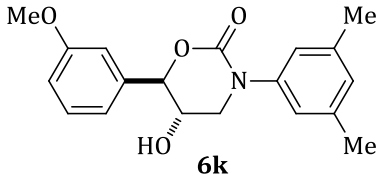
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5k**.



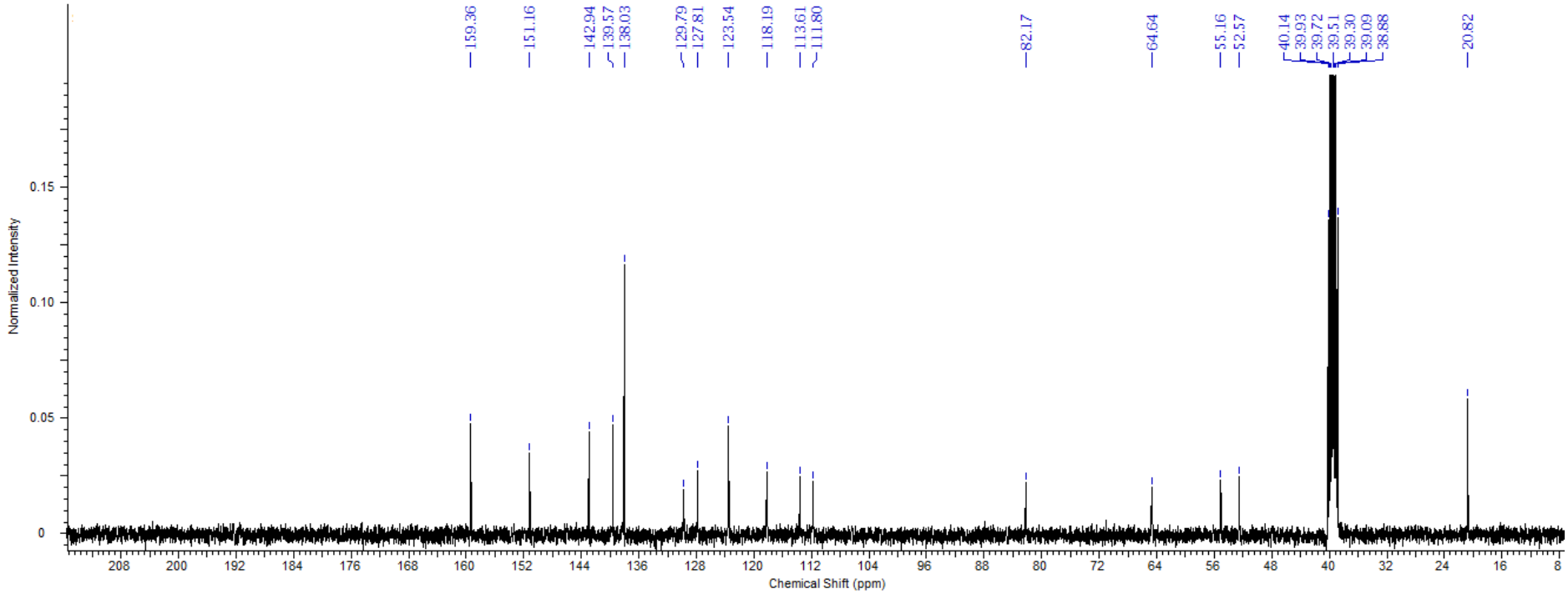
5k



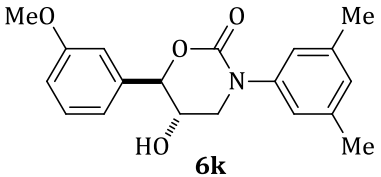
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **6k**.



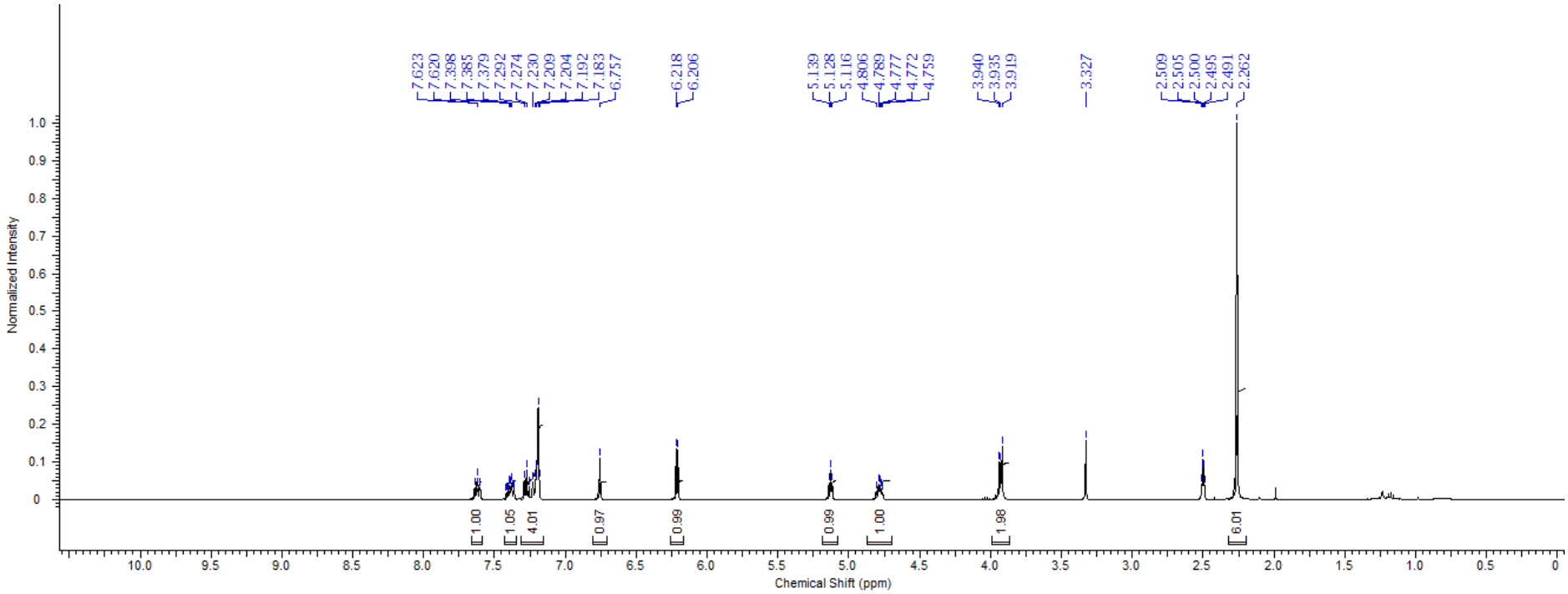
6k



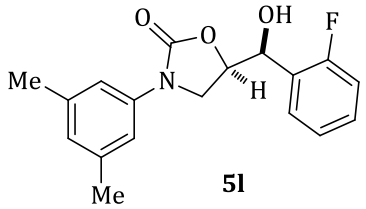
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6k**.



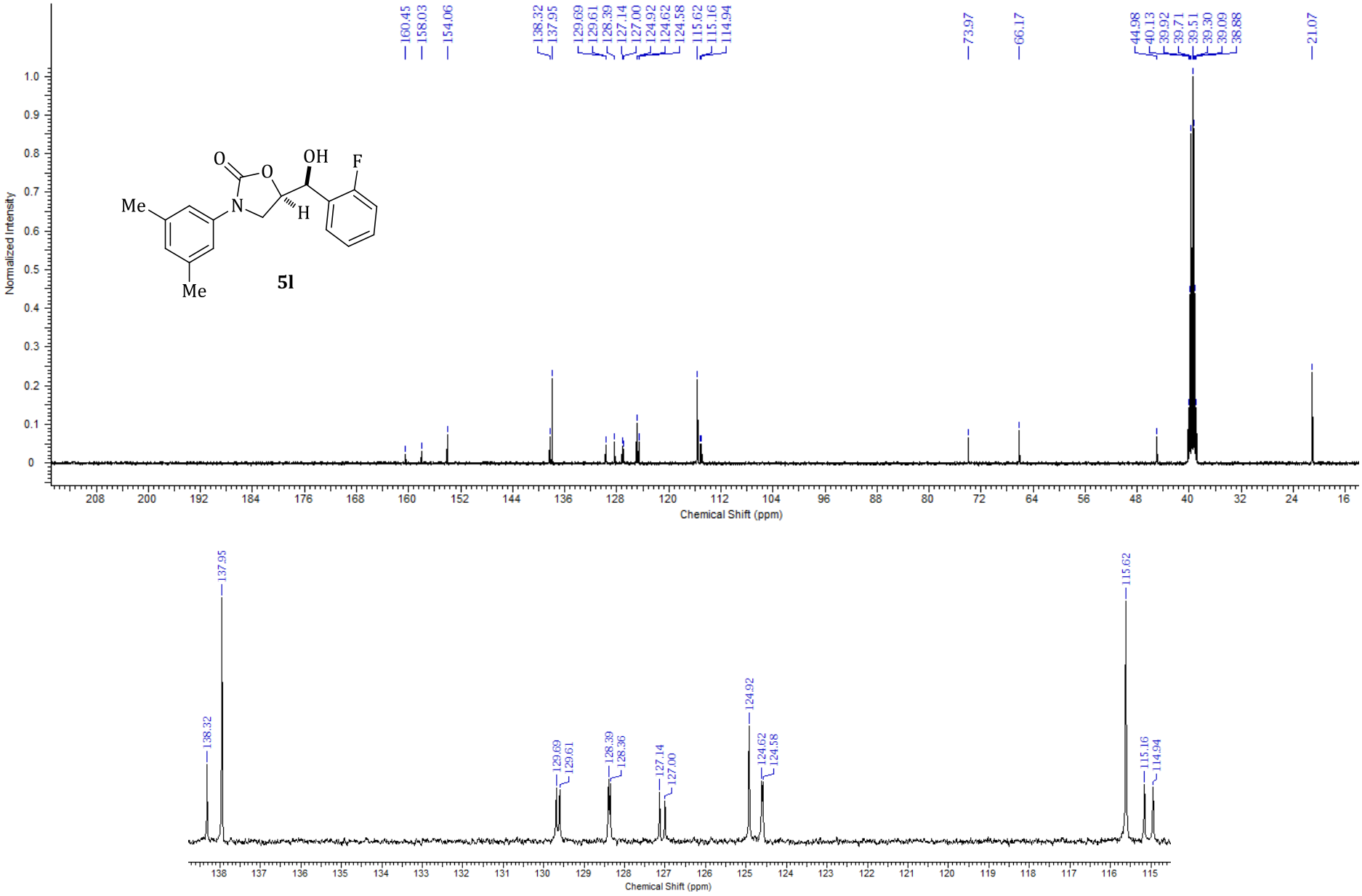
6k



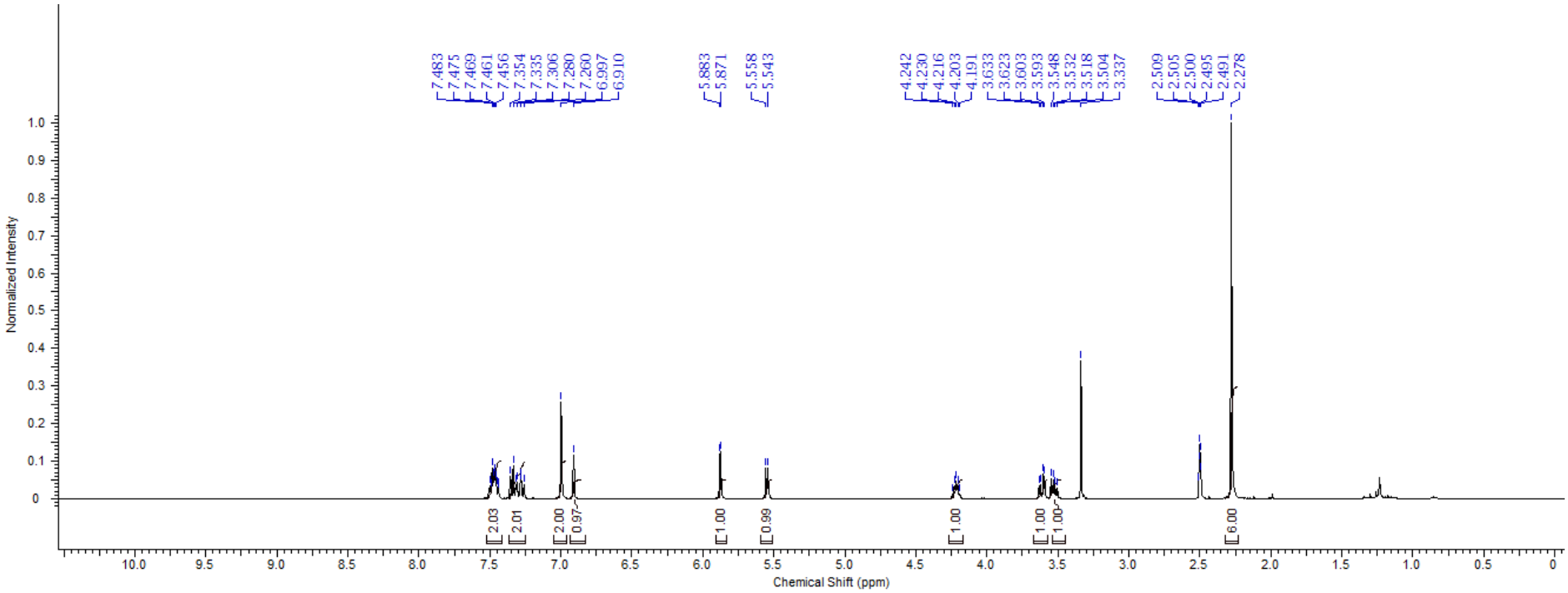
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5l**.



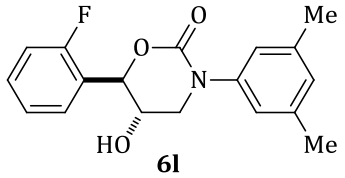
5l



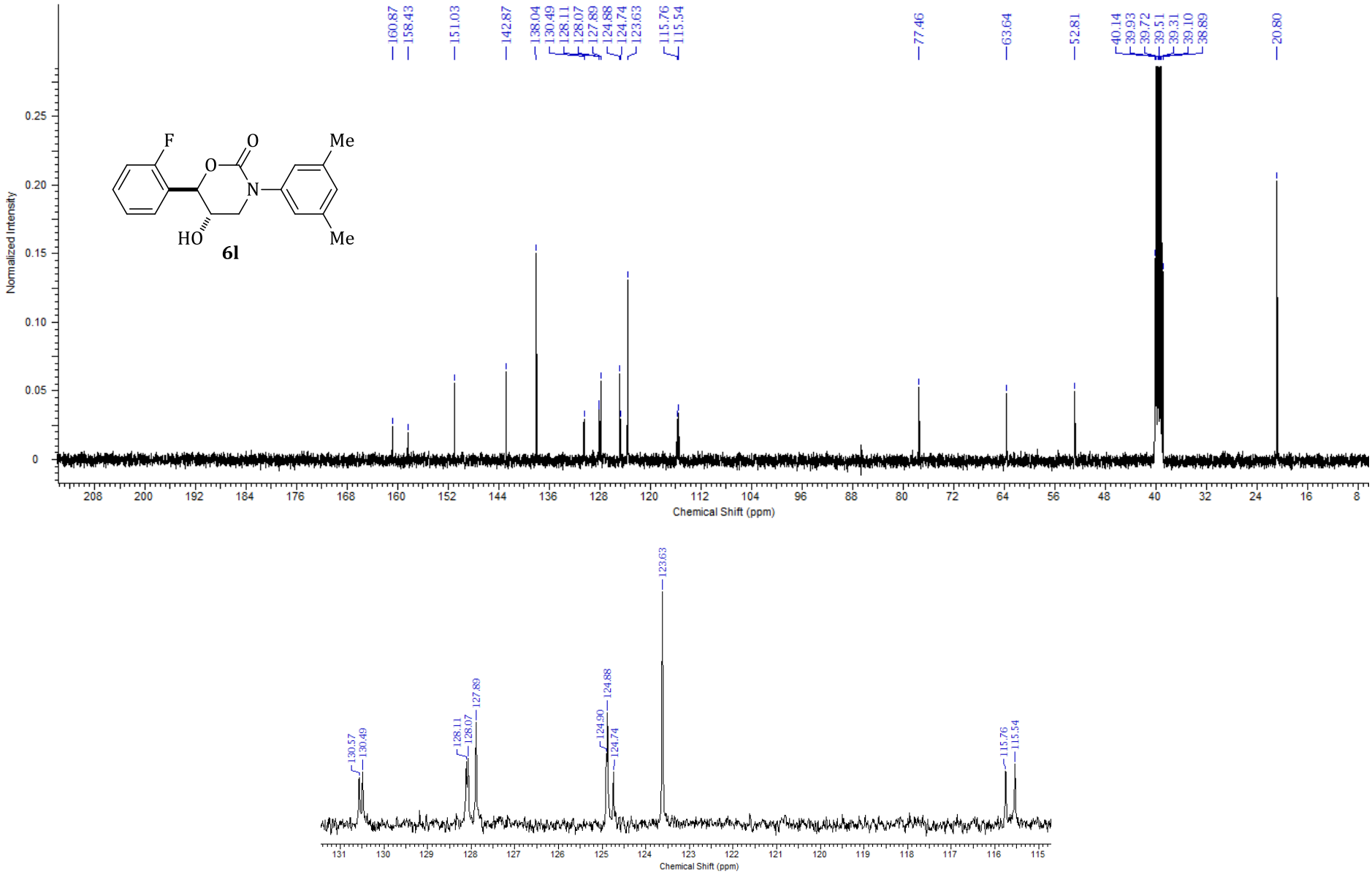
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **5l**.



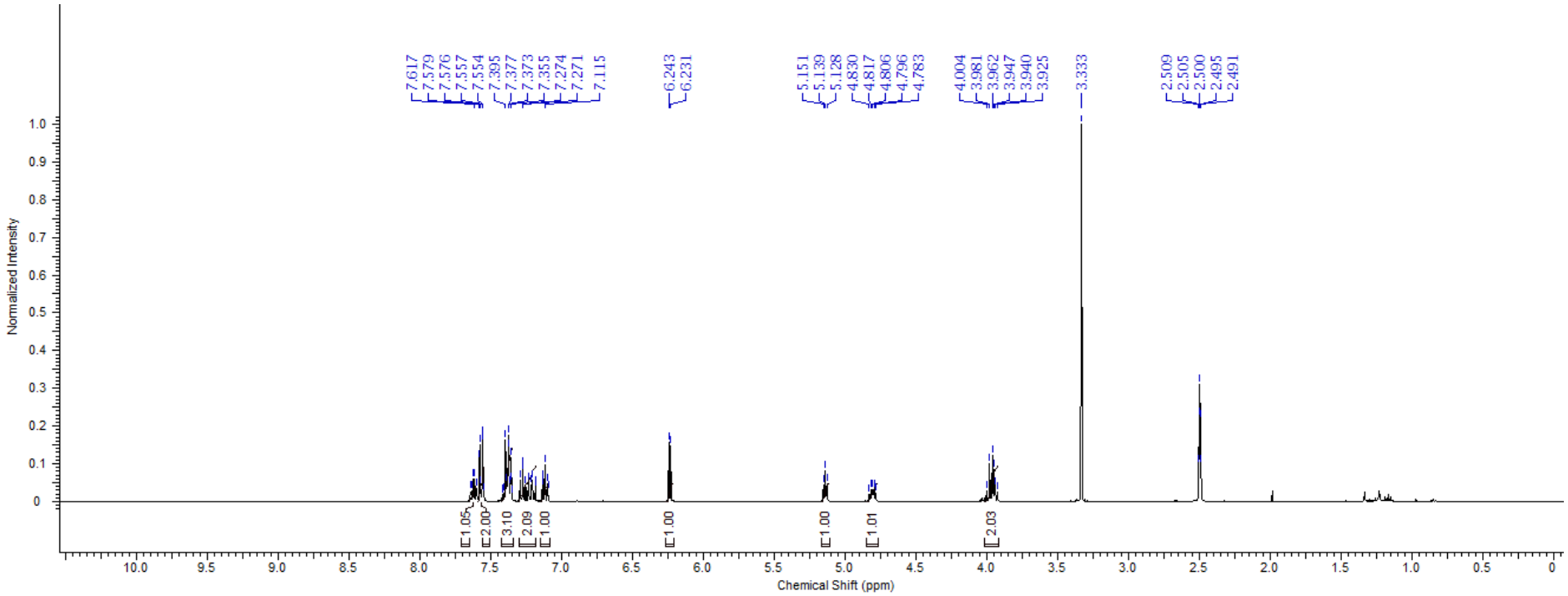
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **6l**.



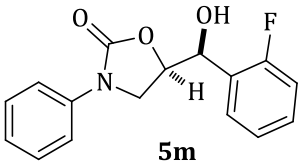
6l



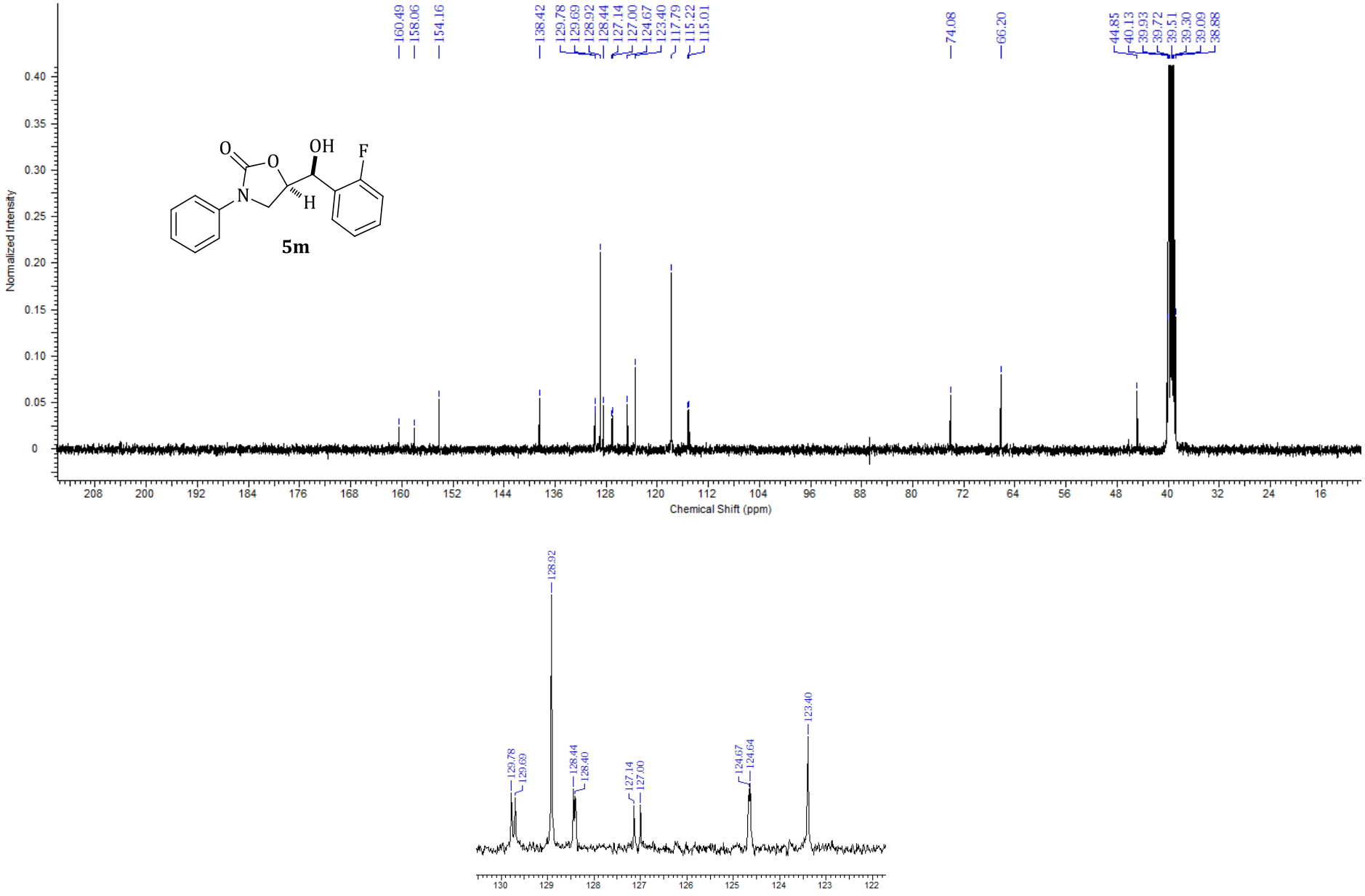
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6l**.



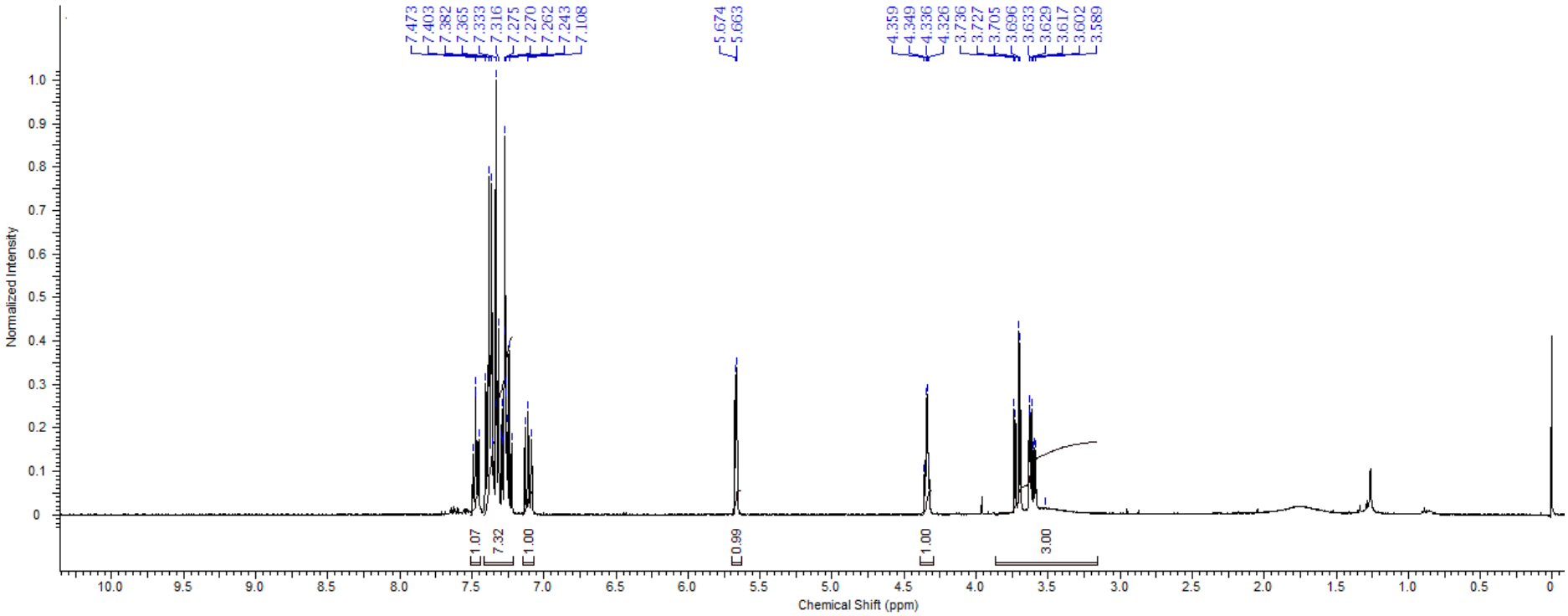
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5m**.



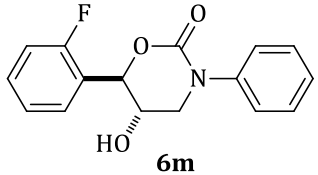
5m



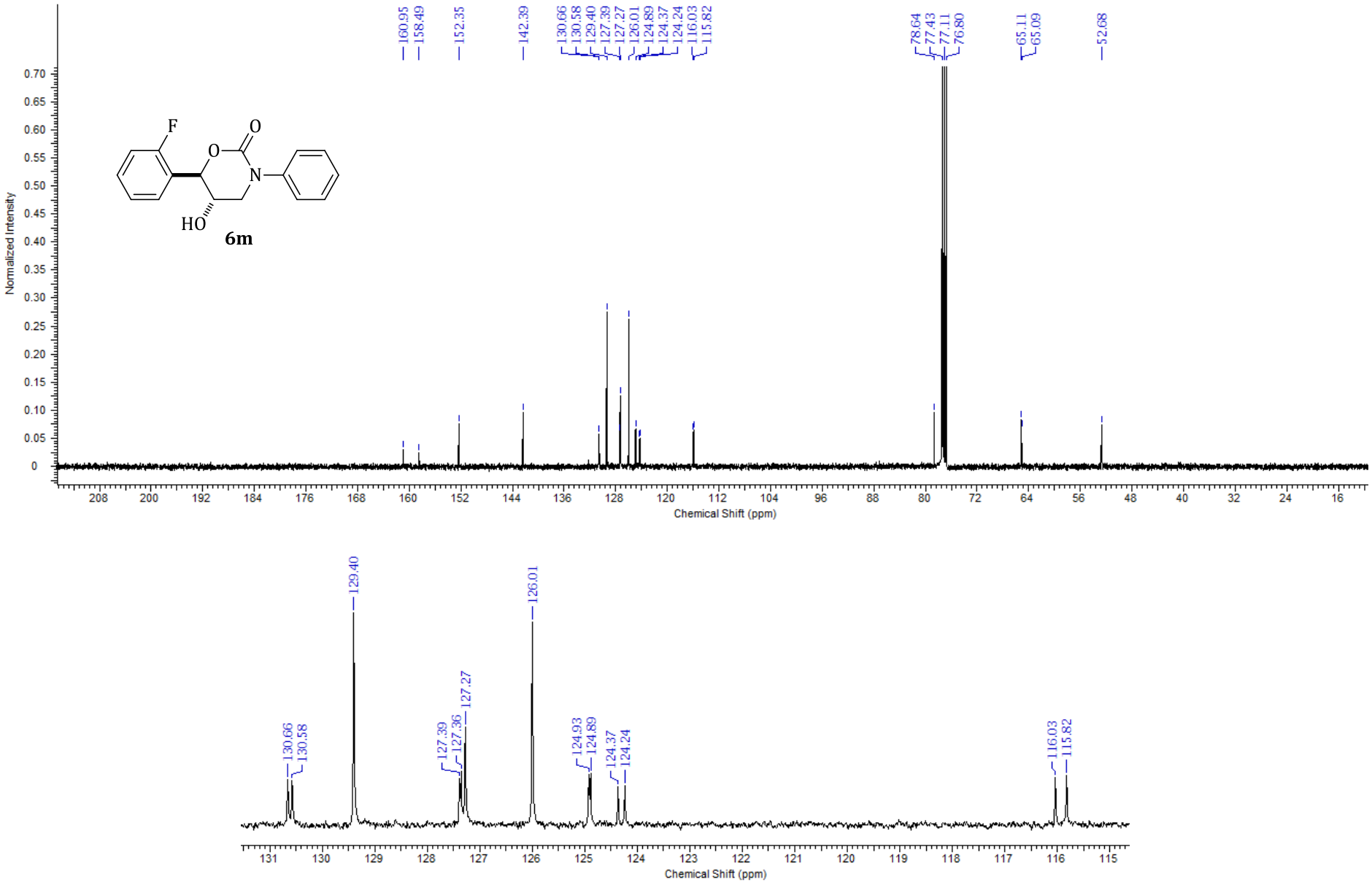
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **5m**.



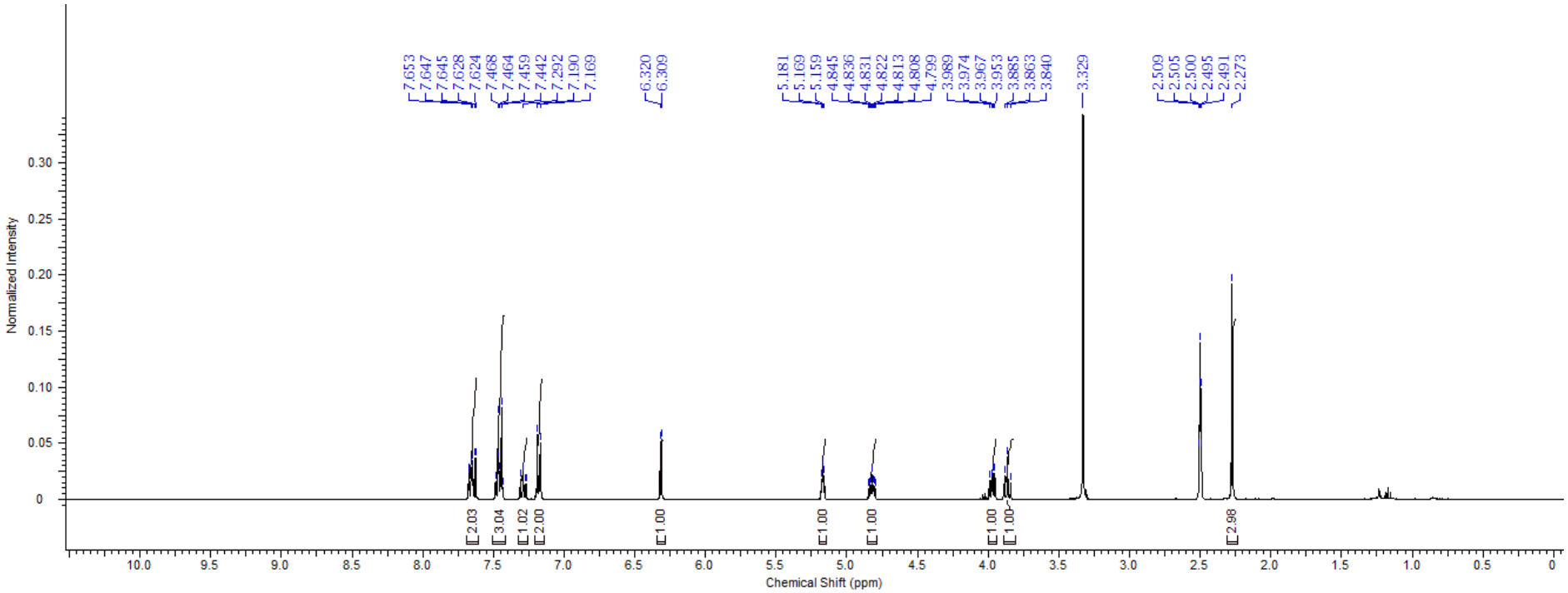
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **6m**.



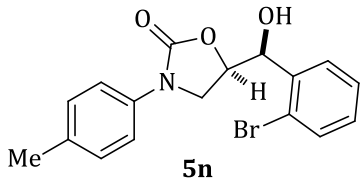
6m



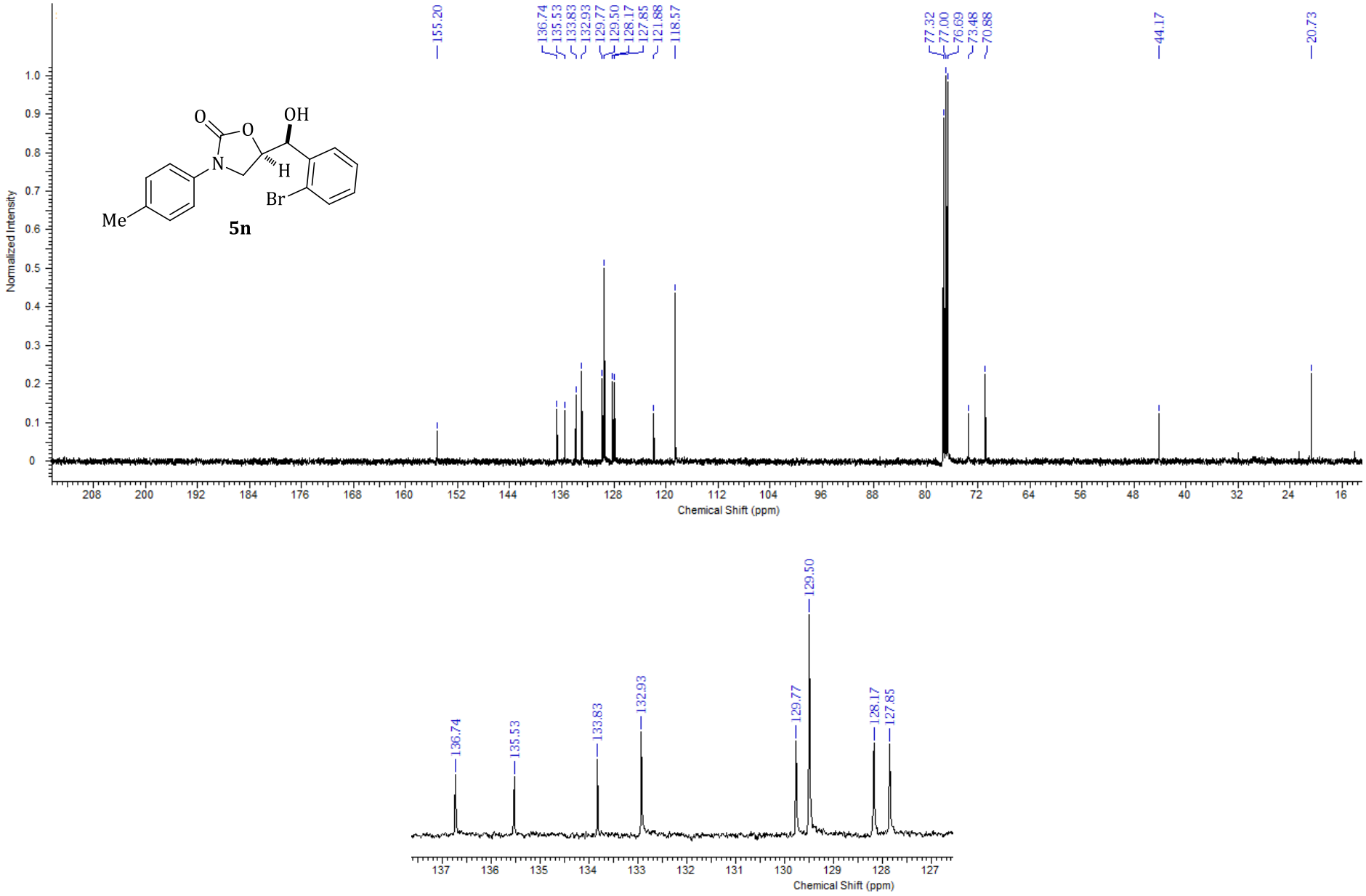
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **6m**.



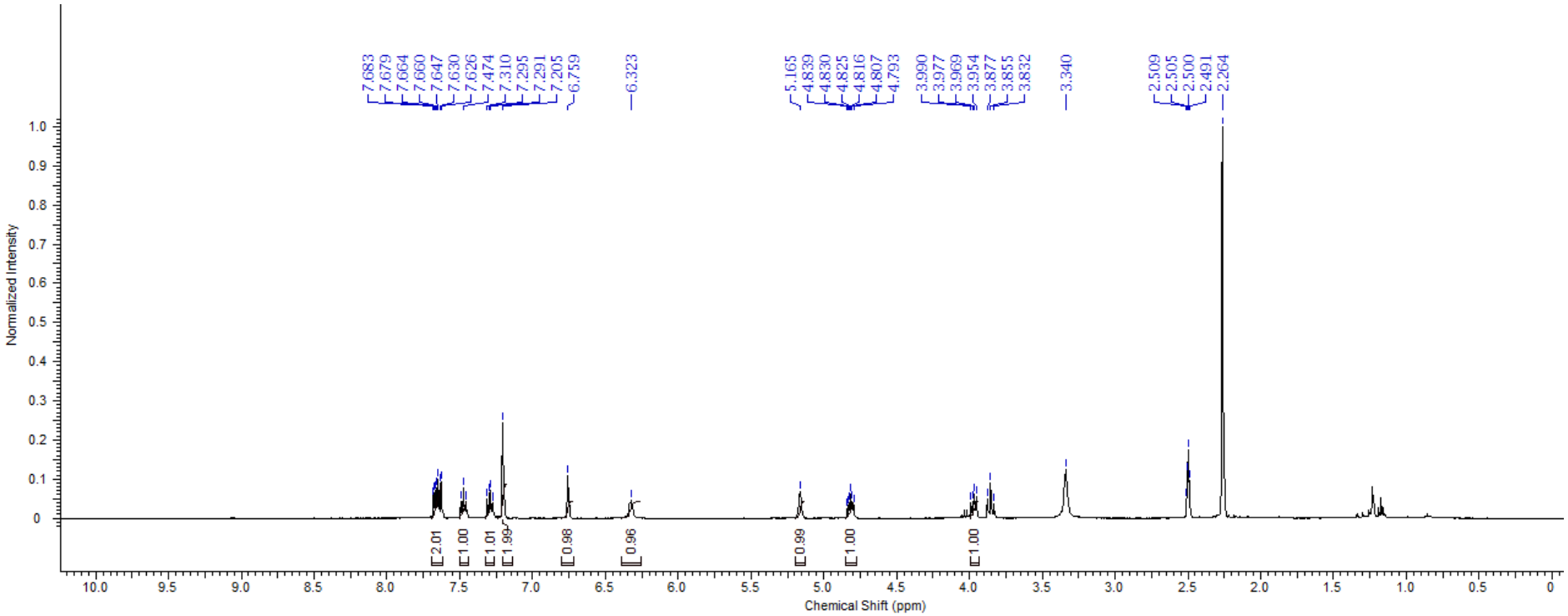
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5n**.



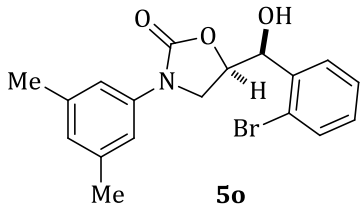
5n



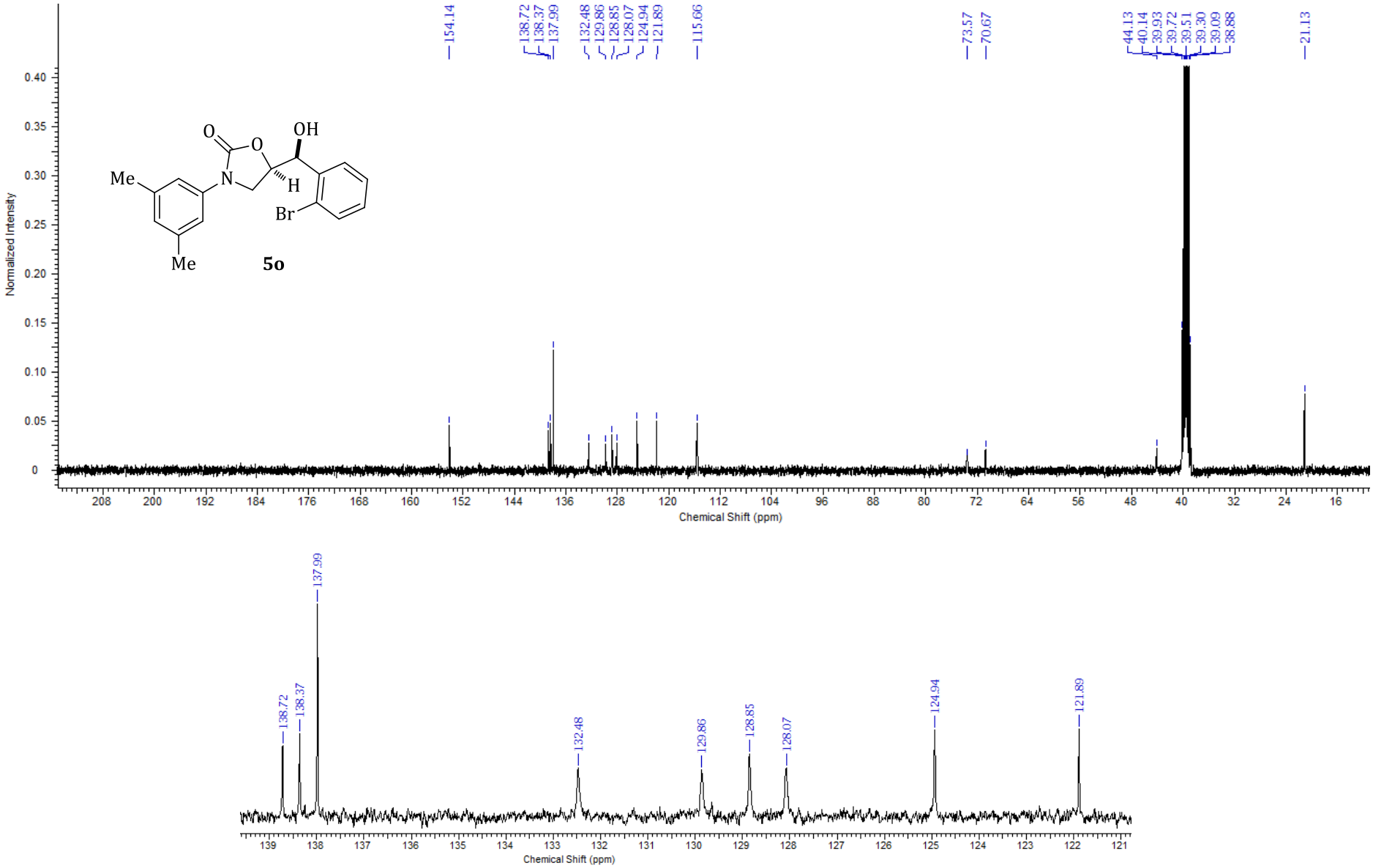
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5n**.



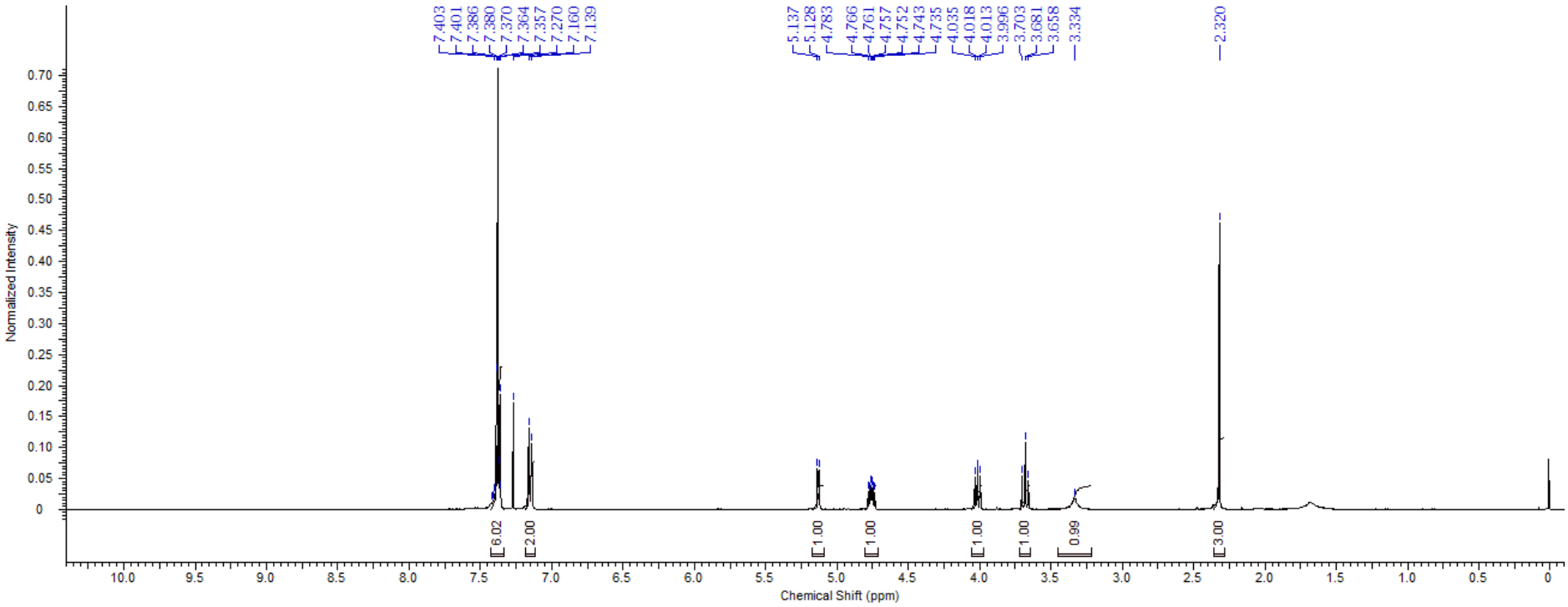
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5o**.



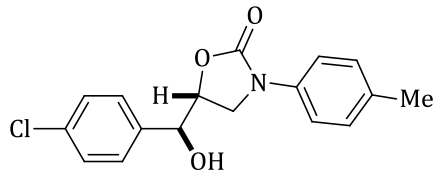
5o



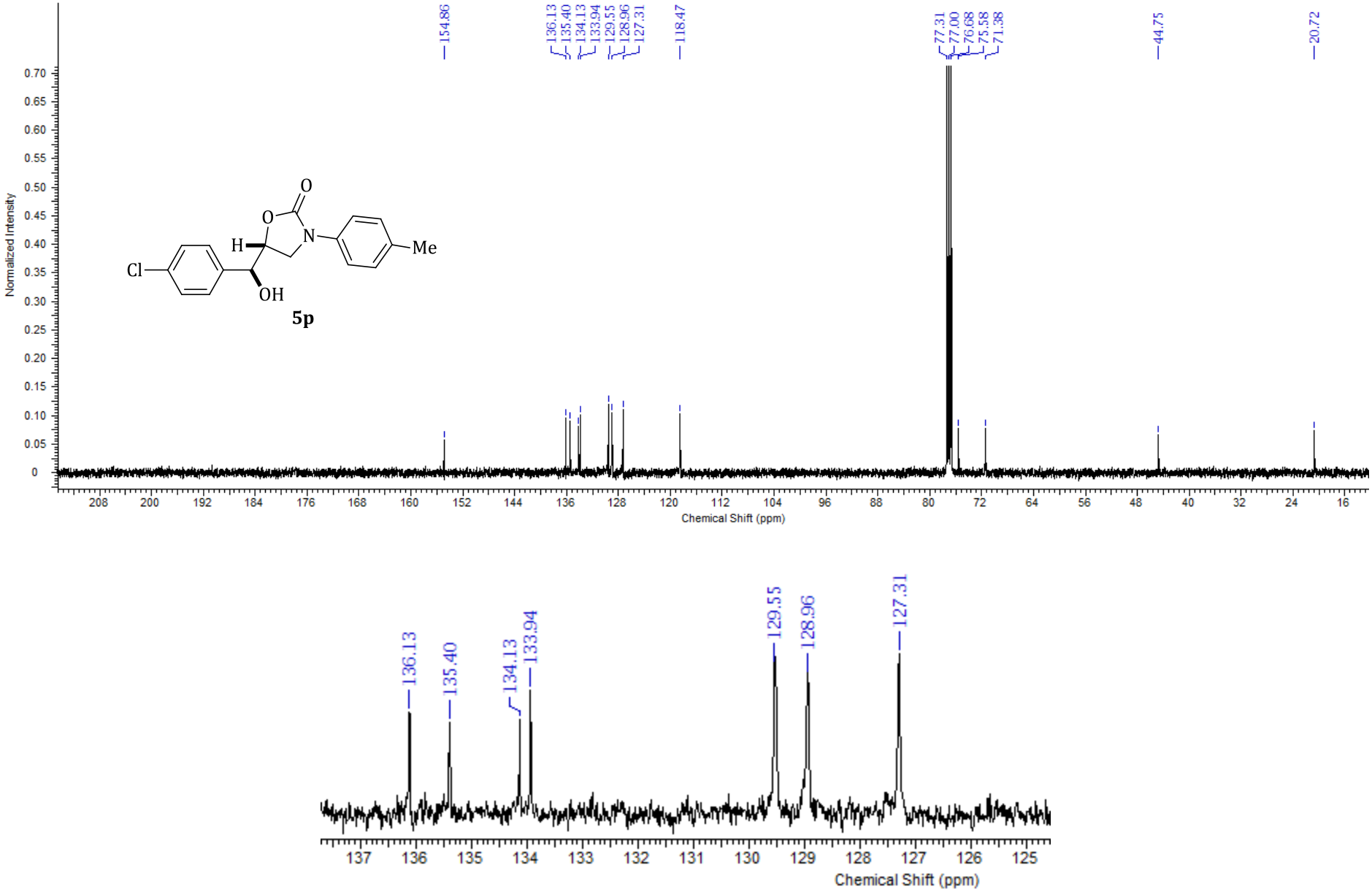
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **5o**.



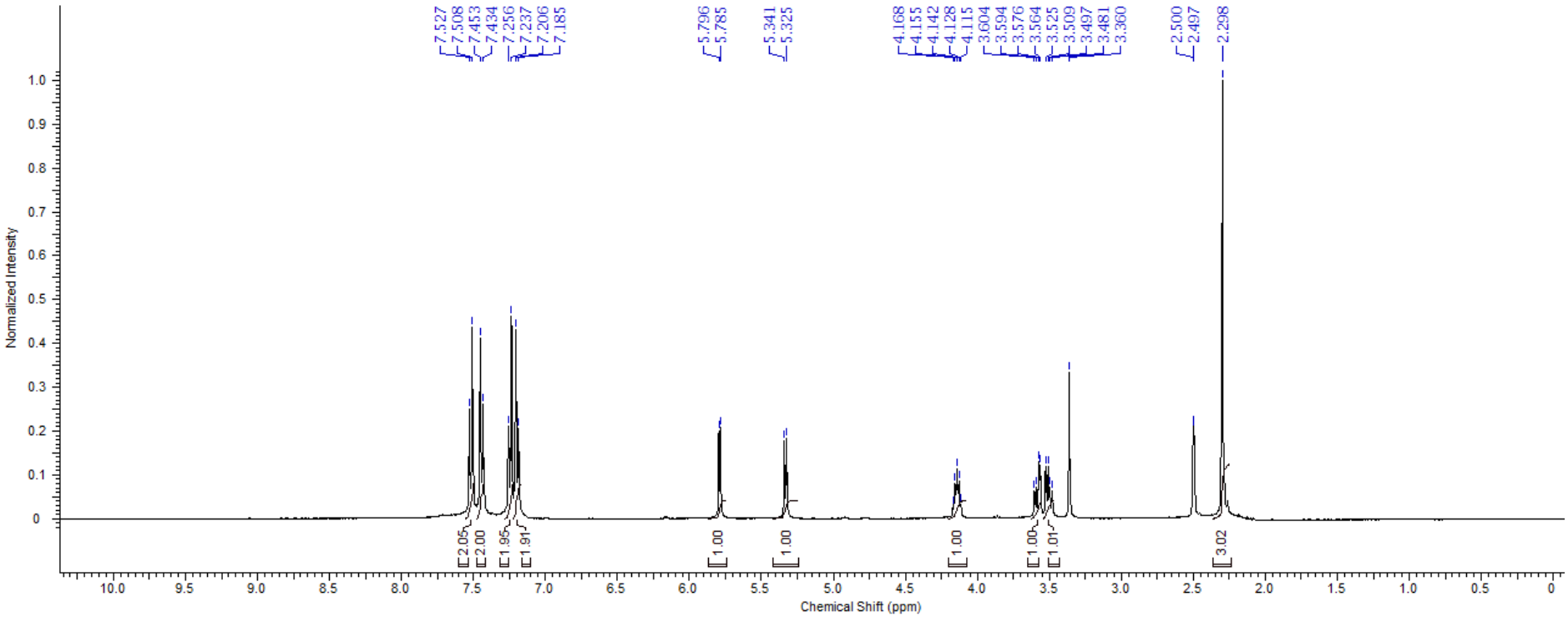
^{1}H NMR ($CDCl_3$, 100 MHz) spectrum of **5p**.



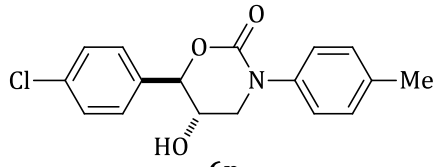
5p



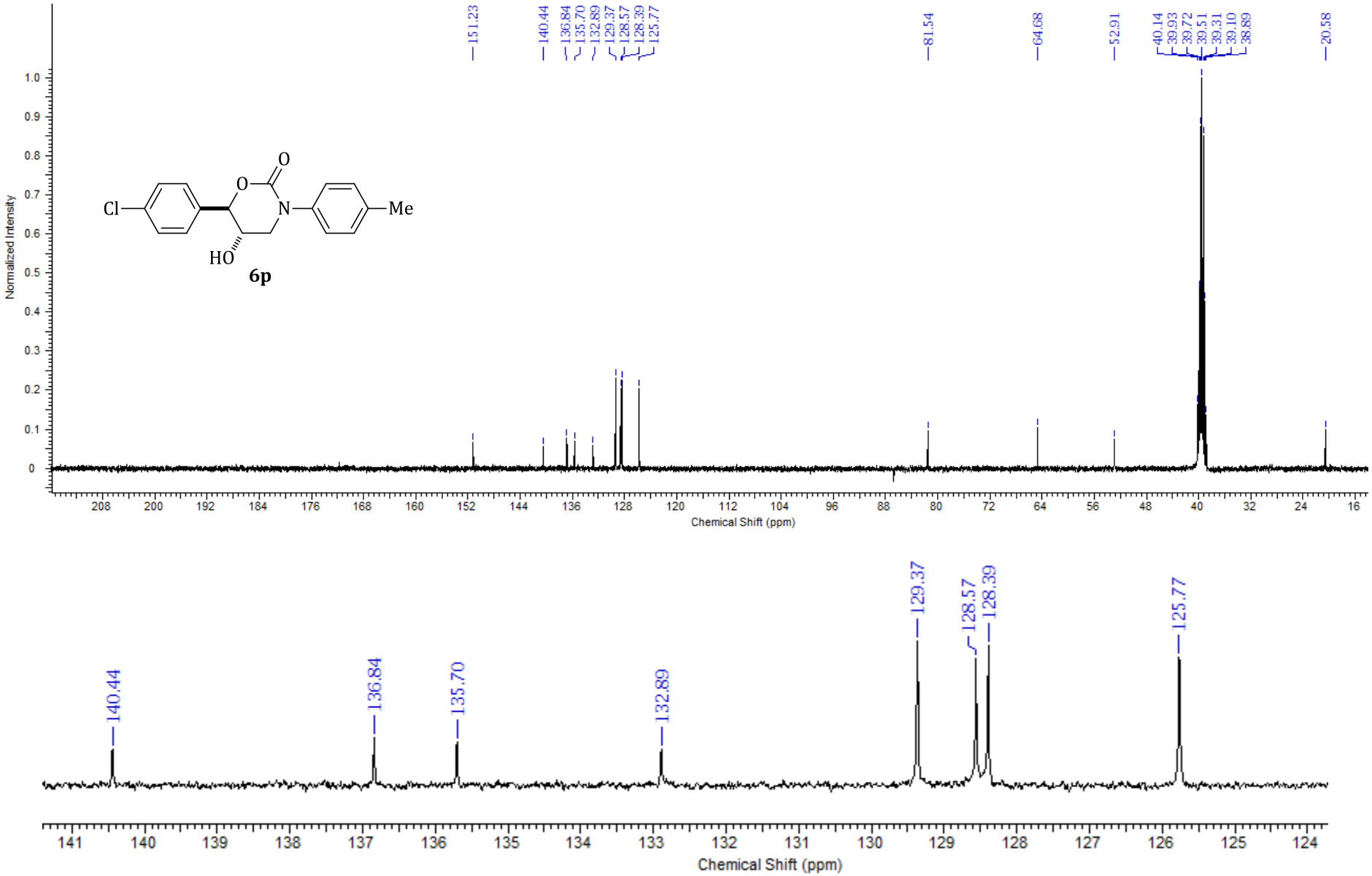
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **5p**.



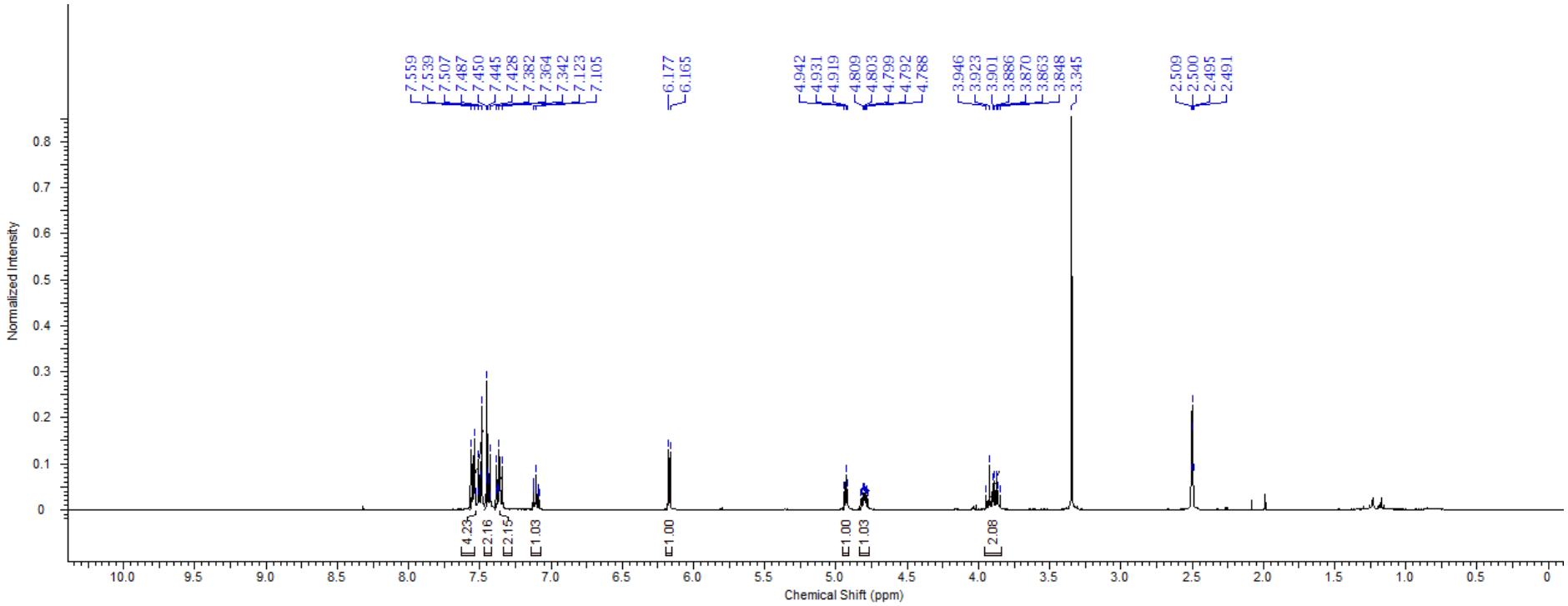
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **6p**.



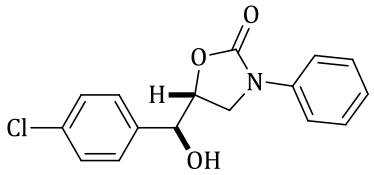
6p



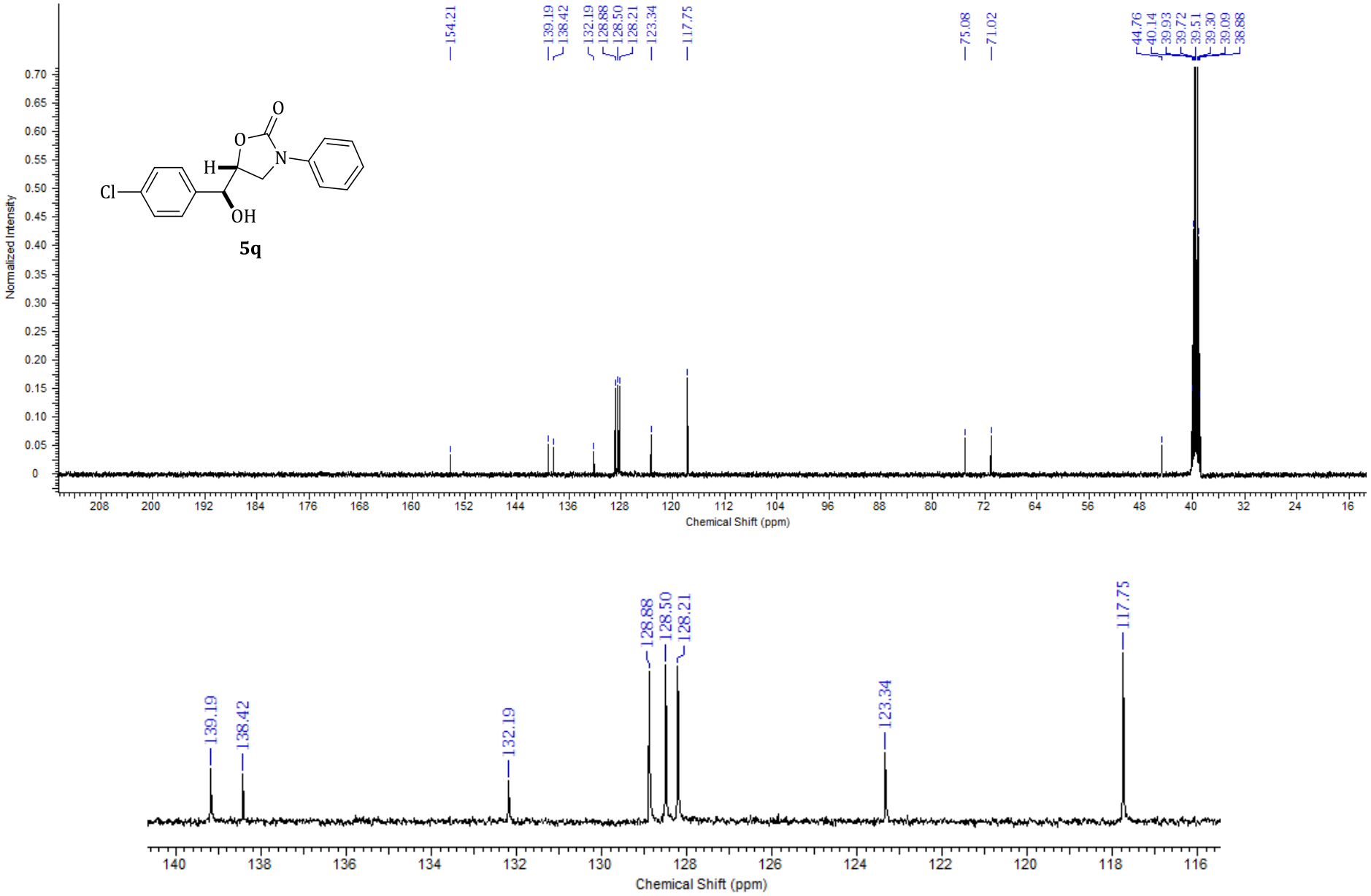
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6p**.



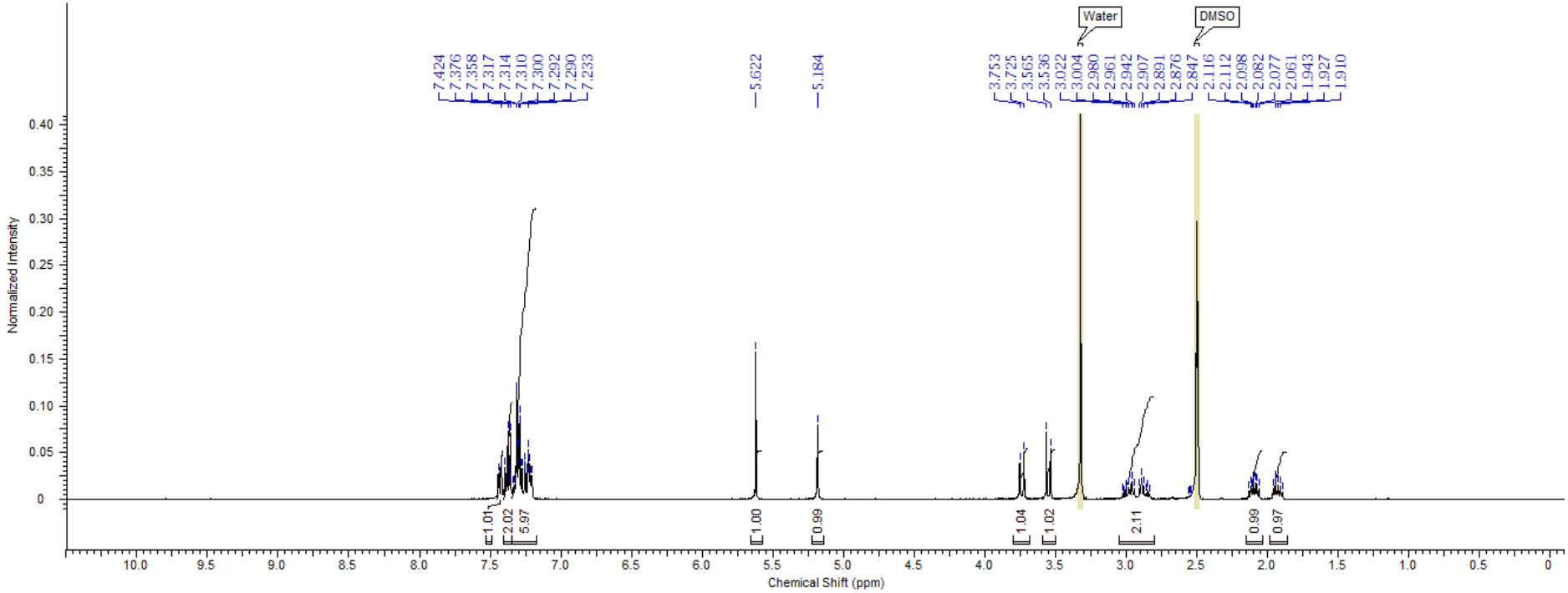
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **5q**.



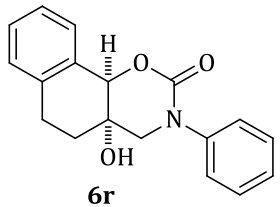
5q



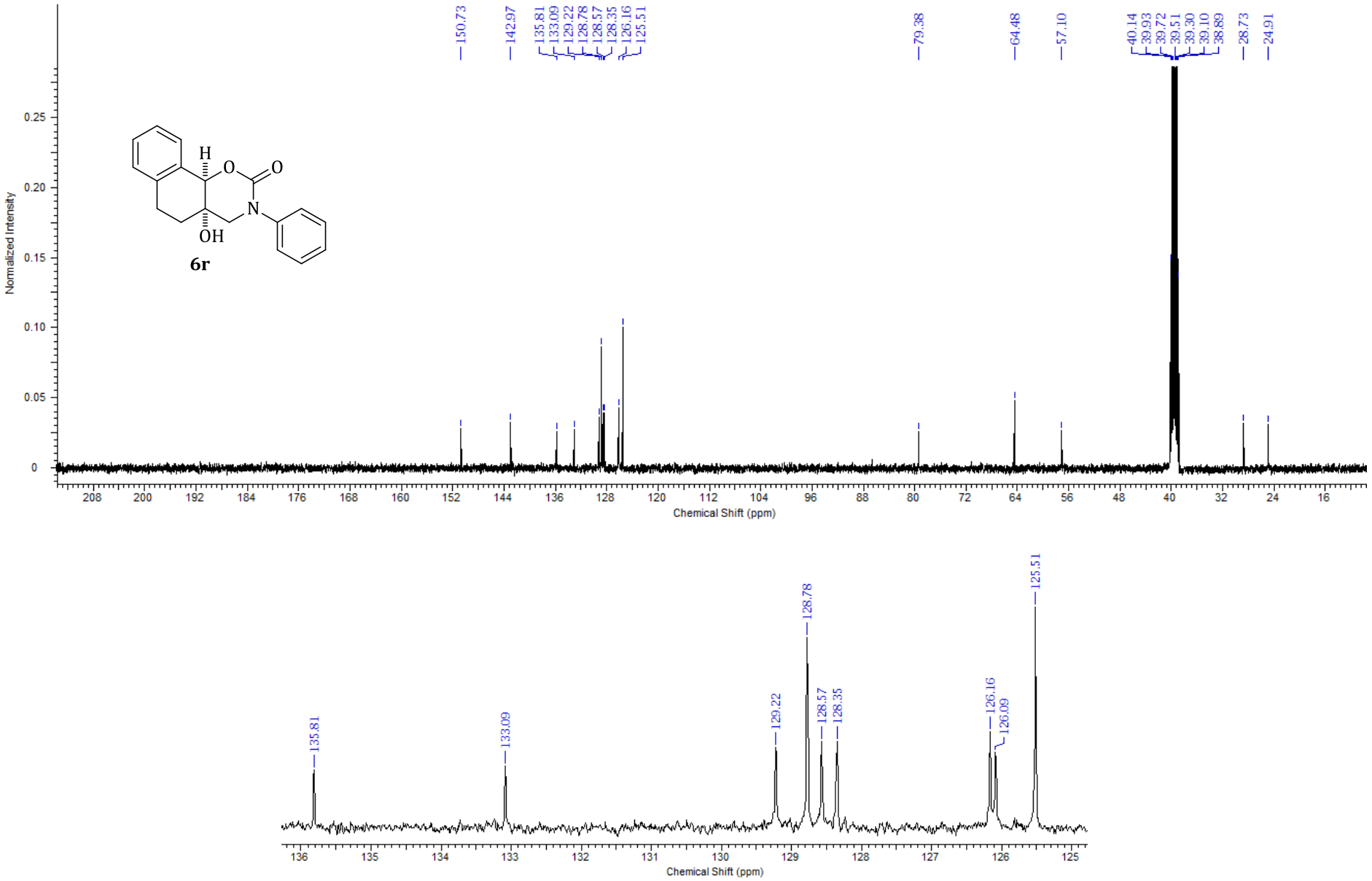
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **5q**.



^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **6r**.



6r



^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **6r**.