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Electronic supplementary information (ESI)

Phenolate-induced intramolecular ring-opening cyclization of *N*-tosylaziridines: access to functionalized benzoxacycles

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1. X-ray crystallography

X-ray crystallography: 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 are solved and refined using SHELXL-2014 with anisotropic displacement parameters for non-H atoms. Hydrogen atoms on O and N are experimentally located in all crystal structures. All C–H atoms are fixed geometrically using the HFIX command in SHELX-TL.[2] A check of the final CIF file using PLATON have not shown any missed symmetry.[3,4] The crystallographic parameters for all structures are summarized in Table ESI-1. ORTEP is generated using XP-software[2] with 35% probability ellipsoid (Figure ESI-1) and hydrogen bond parameters are available in Table ESI-2.

Compound **12e** was crystallized (from its solution in ethyl acetate/hexane) in non-enantiogenic orthogonal space group $Pna2_1$. Crystal structure is solved and refined with two symmetry independent molecules. The ORTEP is shown in Figure ESI-1. Two 2-fold screw axis related molecules form a dimer via strong N−H···O hydrogen bonding between the amine NH of first molecule to the second molecules OH group. The dangling OH groups form O−H···O hydrogen bonds with the sulfonamide oxygen of nearby dimer extending the structure into a one dimensional molecular tapes along [001] crystallographic axis (Figure ESI-2). These tapes are connected primarily via C−H···π interactions that completes the 3D packing of the molecules. The crystallographic data and hydrogen bond matrices are shown in Table ESI-1 and Table ESI-2.

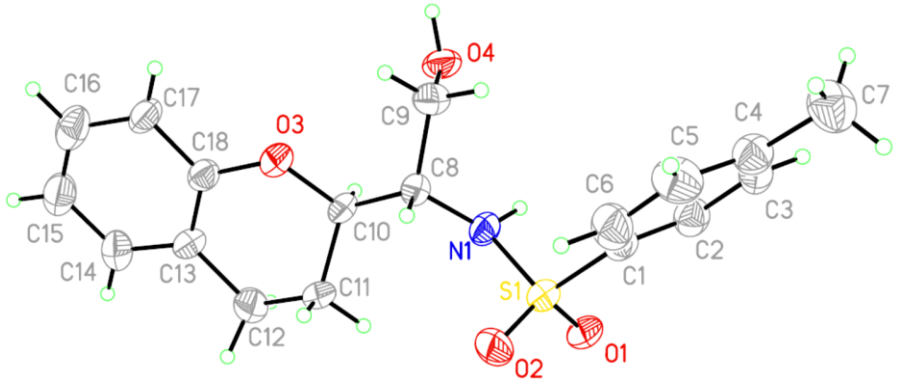


Figure ESI-1 ORTEP of chroman derivative **12e** with 35% probability ellipsoid [only one asymmetric molecule is displayed for clarity]

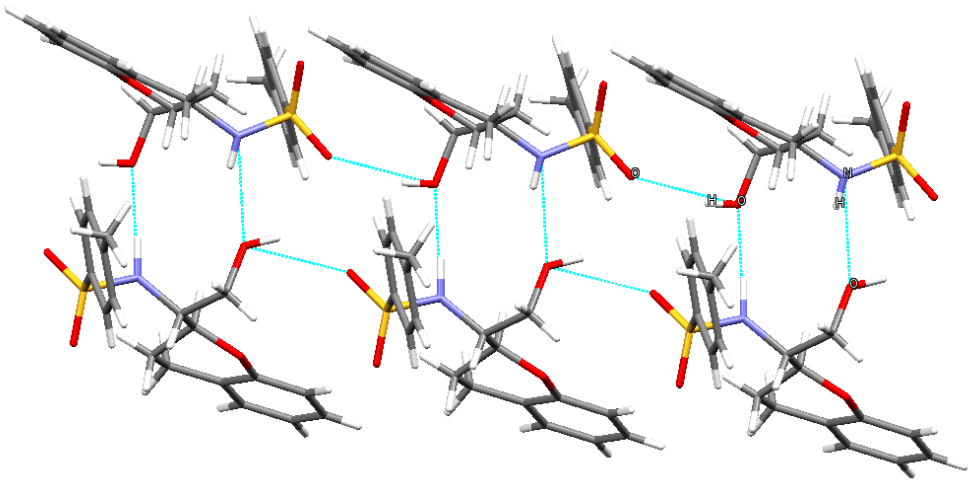


Figure ESI-2 Molecules are arranged in one dimensional tape like structure in chroman derivative **12e** via N−H···O and O−H···O hydrogen bonds along [001] crystallographic axis.

Table ESI-1: Crystallographic data of chroman derivative **12e**

Crystal Data	**12e**
Formula unit	$C_{18}H_{21}NO_4S$
Formula wt.	347.42
Crystal system	Orthorhombic
T [K]	100
a [Å]	19.409 (11)
b [Å]	22.804 (14)
c [Å]	7.899 (5)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	3496 (4)
Space group	*Pna*2$_1$
Z	8
D_{calc} [g cm^{-3}]	1.320
μ/mm^{-1}	0.206
Reflns. Collected	36469
Unique reflns.	7968
Observed reflns.	3221
R_1 [I>2σ(I)], wR_2	0.0692; 0.1375
GOOF	0.933
Instrument	Bruker APEX-II CCD
X-ray	MoK\α; λ=0.71073
CCDC Reference	1840365

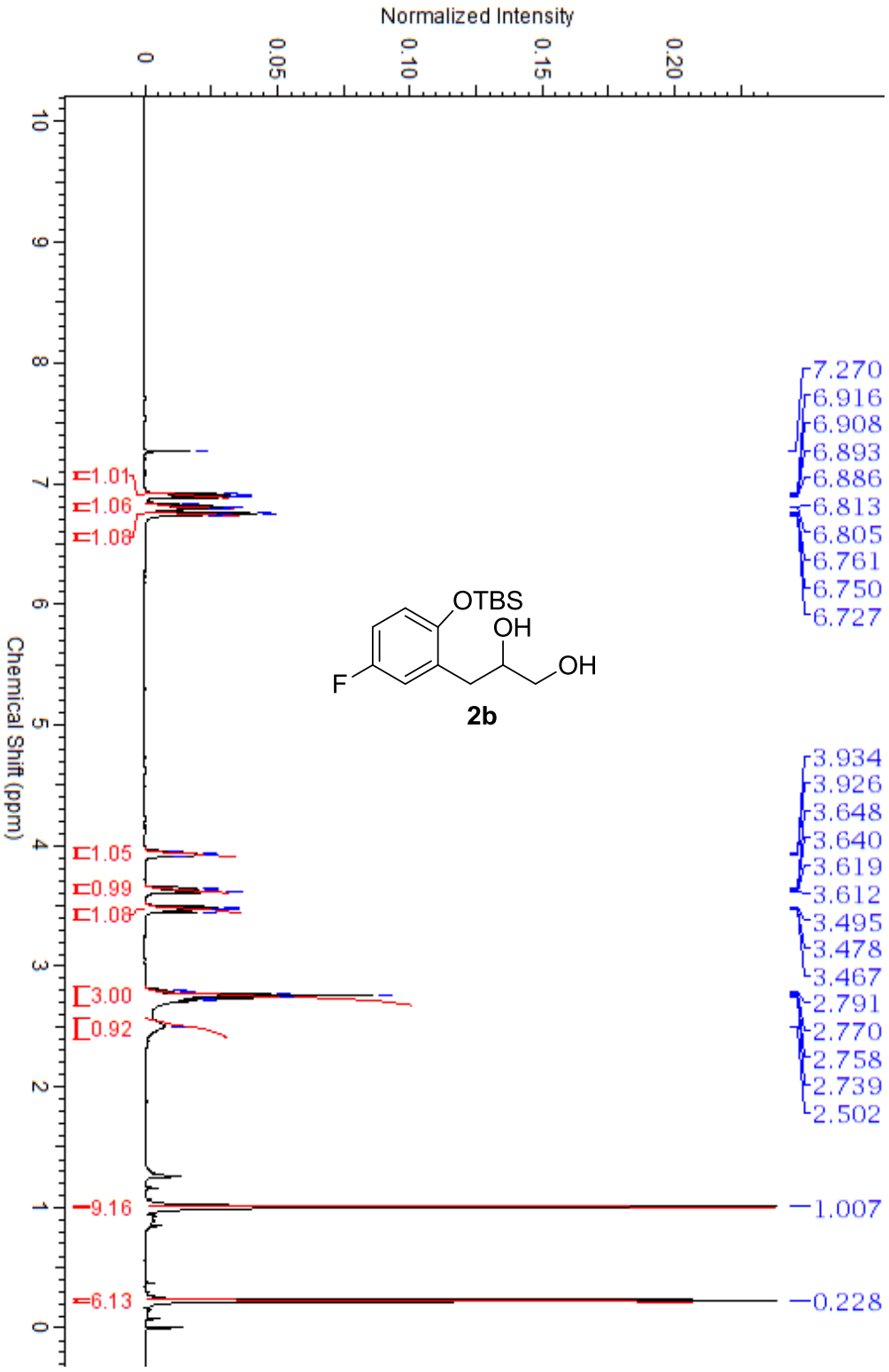
Table ESI-2: Hydrogen bond matrices of **12e**

Interaction	H···A (Å)	D···A (Å)	D–H···A (º)	Symmetry Code
N_1–H_{1A}···O_8	1.98(9)	2.957(7)	176(10)	1/2-x,-1/2+y,-1/2+z
N_2–H_{2A}···O_4	2.16(7)	2.923(7)	157(7)	1/2-x,1/2+y,1/2+z
O_4–H_{4A}···O_1	2.12(11)	2.854(6)	138(8)	x,y,-1+z
O_4–H_{4A}···O_6	2.50(10)	3.202(6)	135(8)	1/2-x,-1/2+y,-1/2+z
O_8–H_{8A}···O_6	2.14(6)	2.889(6)	161(7)	x,y,1+z
C_{35}–H_{35}···O_5	2.45(5)	3.369(8)	168(6)	x,y,1+z
C_{21}–H_{21}···O_2	2.54(5)	3.435(8)	161(6)	-
Intra C_2–H_2···O_1	2.60(4)	2.932(7)	102(6)	-
Intra C_8–H_8···O_2	2.52(6)	2.977(8)	108(4)	-
Intra C_{20}–H_{20}···O_5	2.58(6)	2.928(7)	103(6)	-
Intra C_{26}–H_{26}···O_5	2.52(6)	2.997(8)	109(4)	-

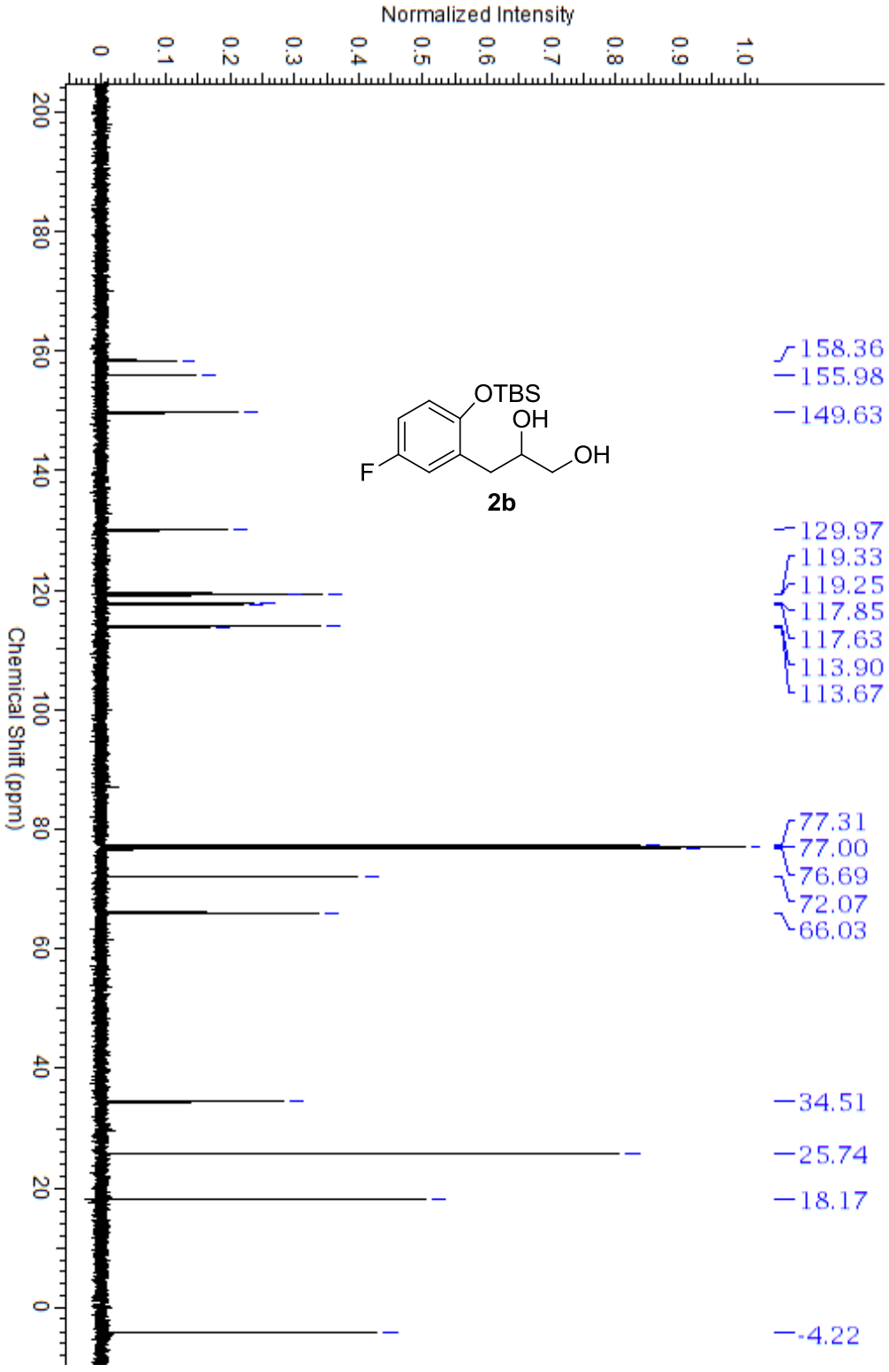
2. References

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. A. L. Spek, *J. Appl. Crystallogr.*, **2003**, *36*, 7–13.

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

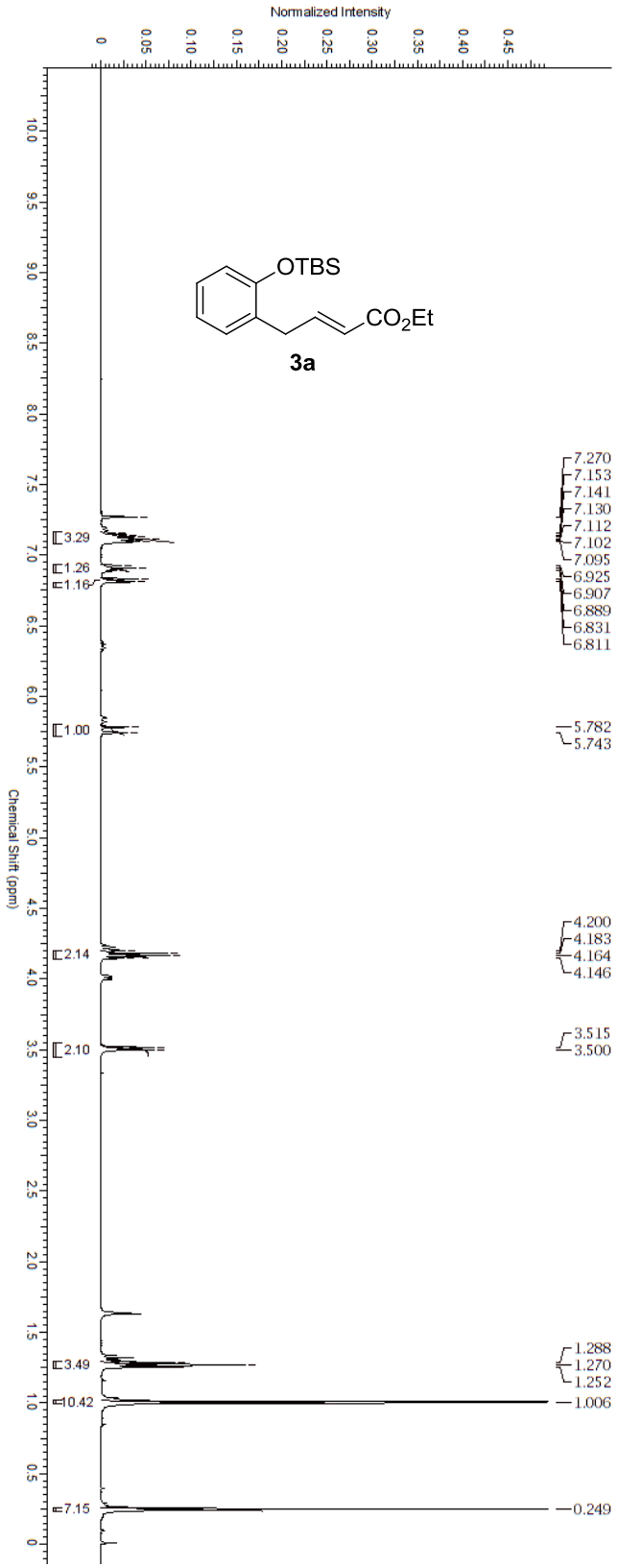


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 2b

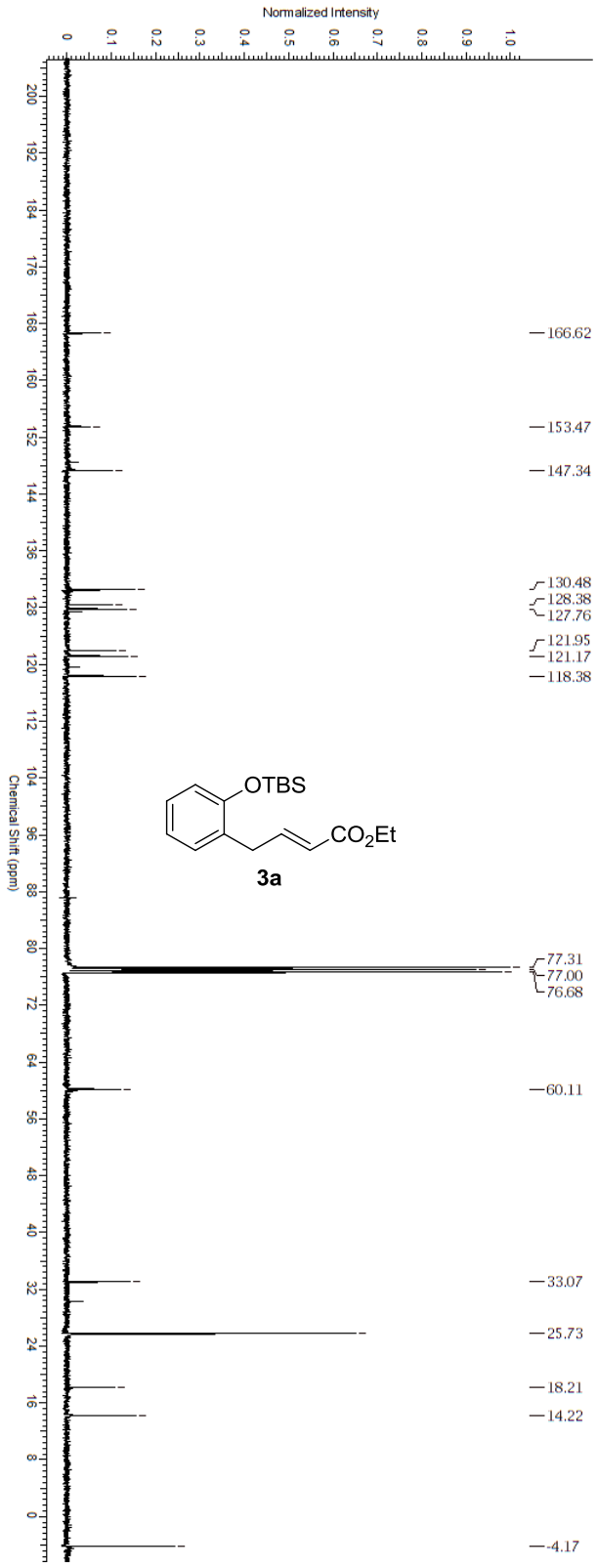


2b

^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 2b



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3a (major) and its *cis* isomer (minor); only δ values corresponding to the peaks of the *trans* isomer are reported



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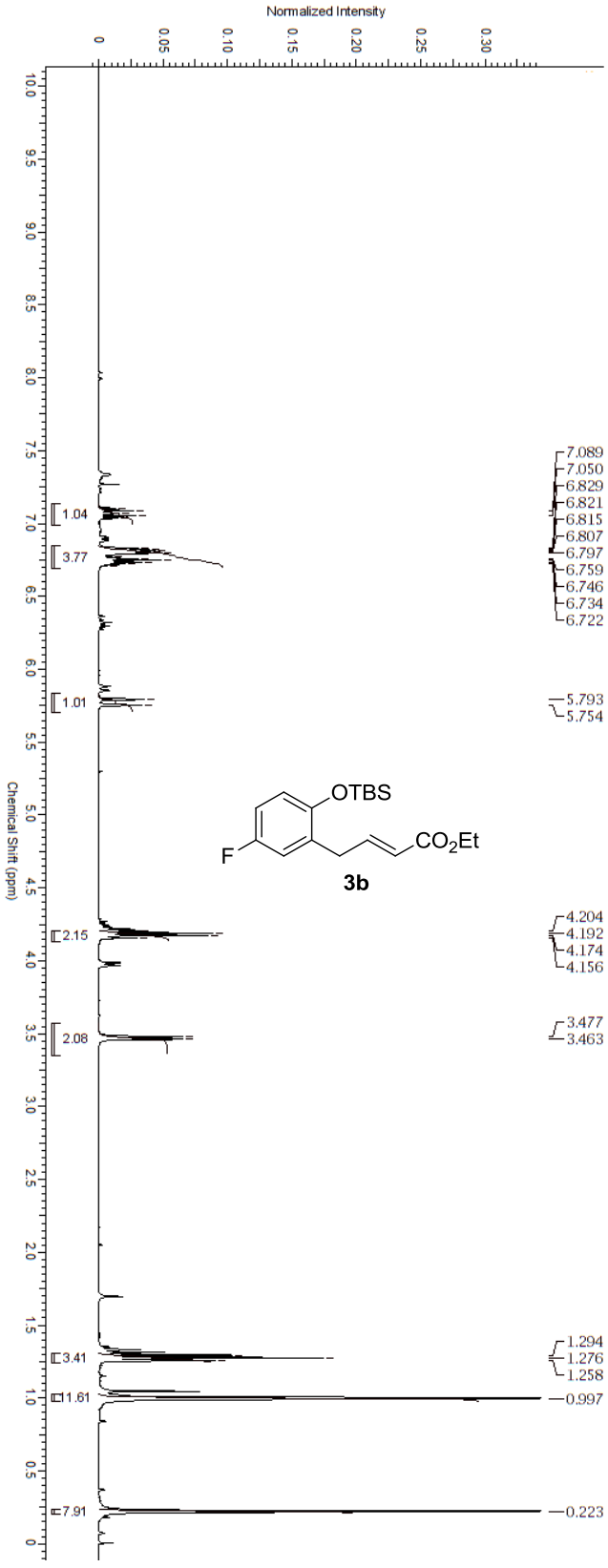

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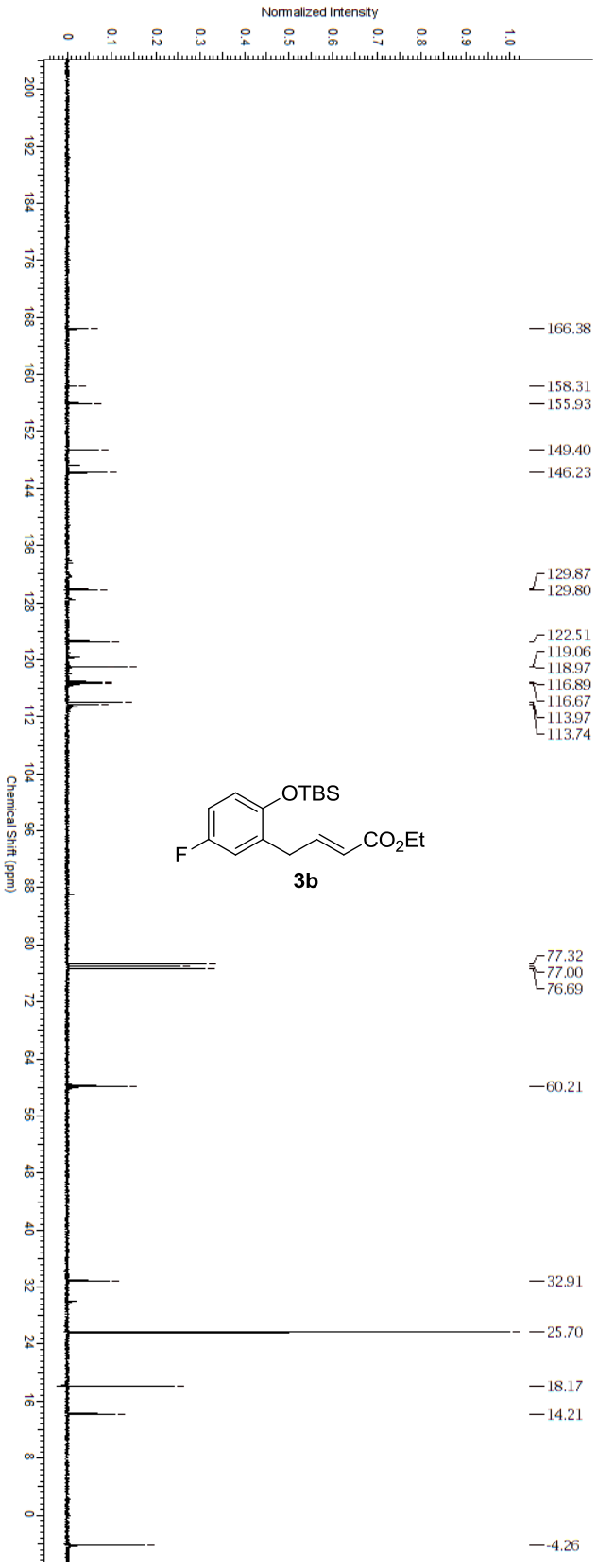
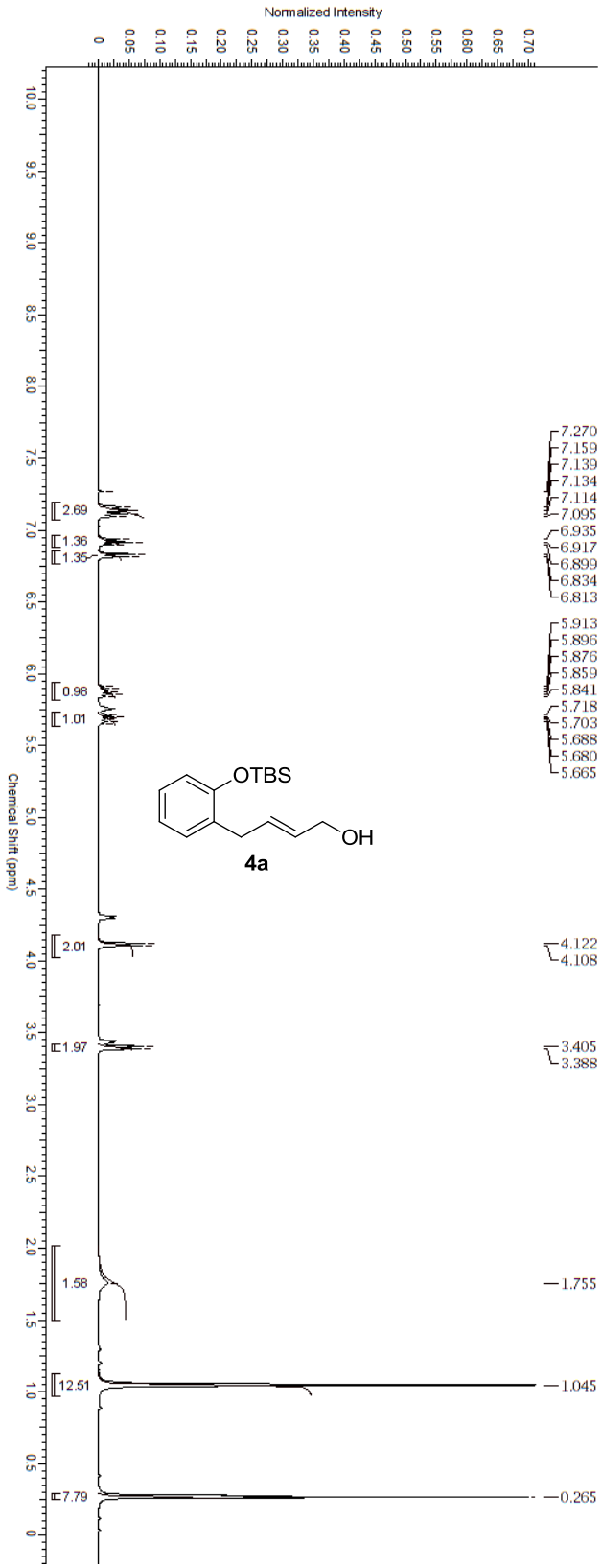


^{13}C NMR (400 MHz, $CDCl_3$) spectrum of 3b (major) and its *cis* isomer (minor); only δ values corresponding to the peaks of the *trans* isomer are reported



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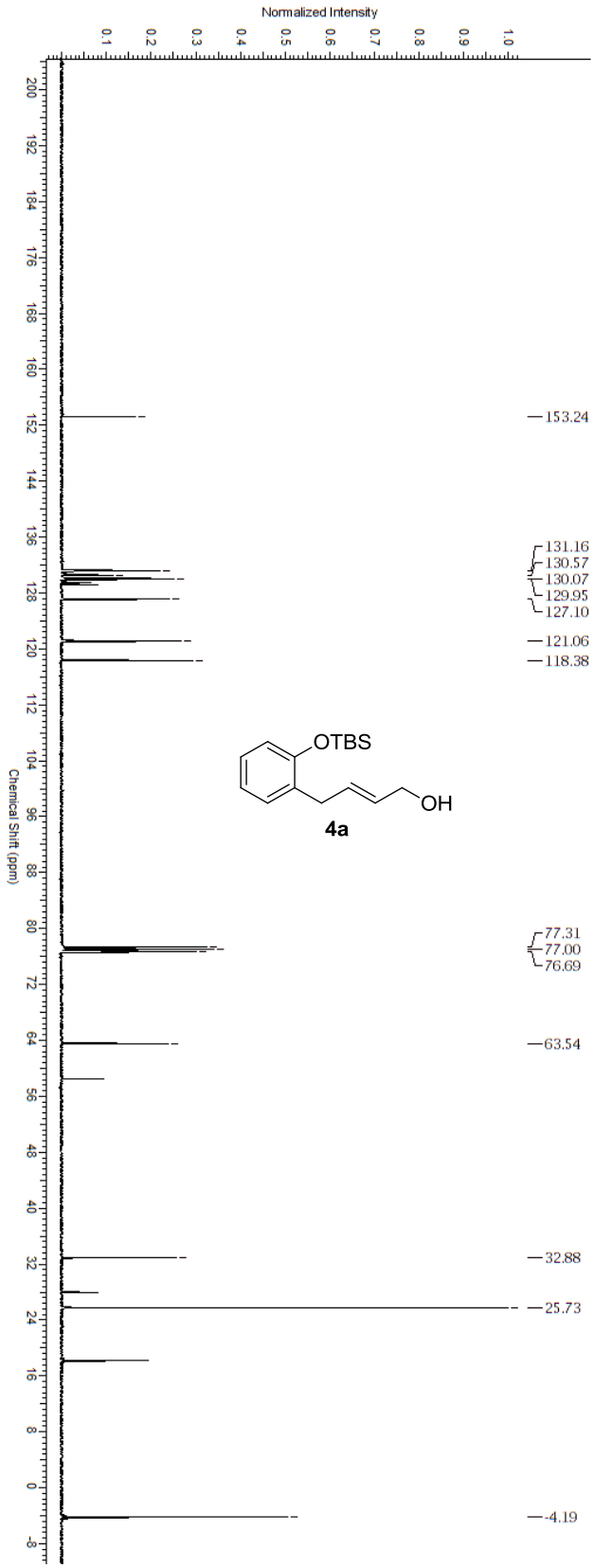

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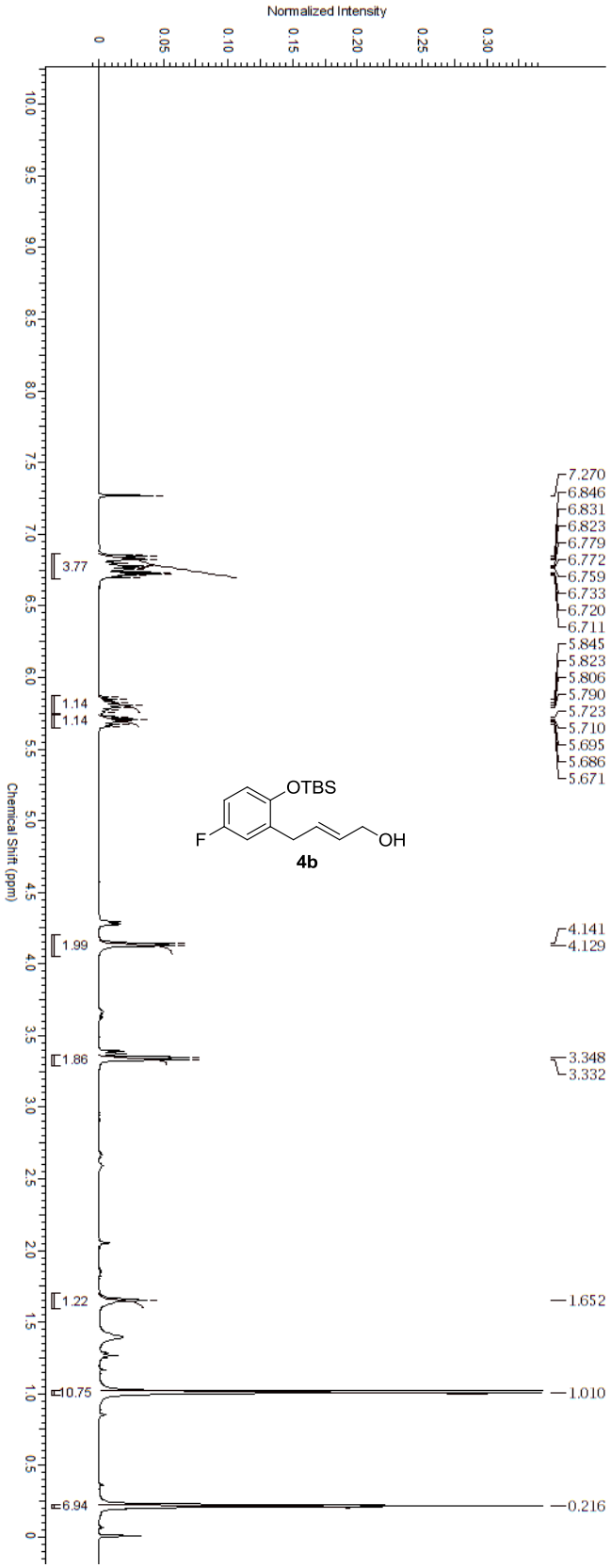

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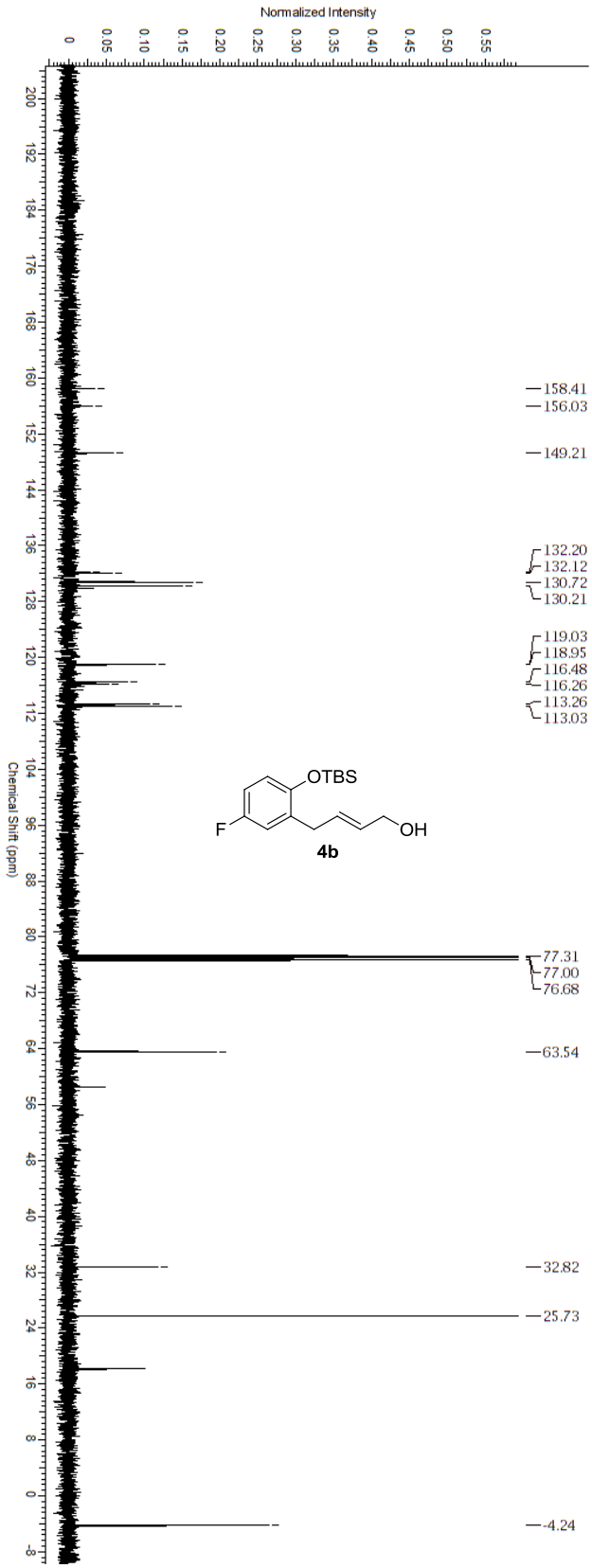
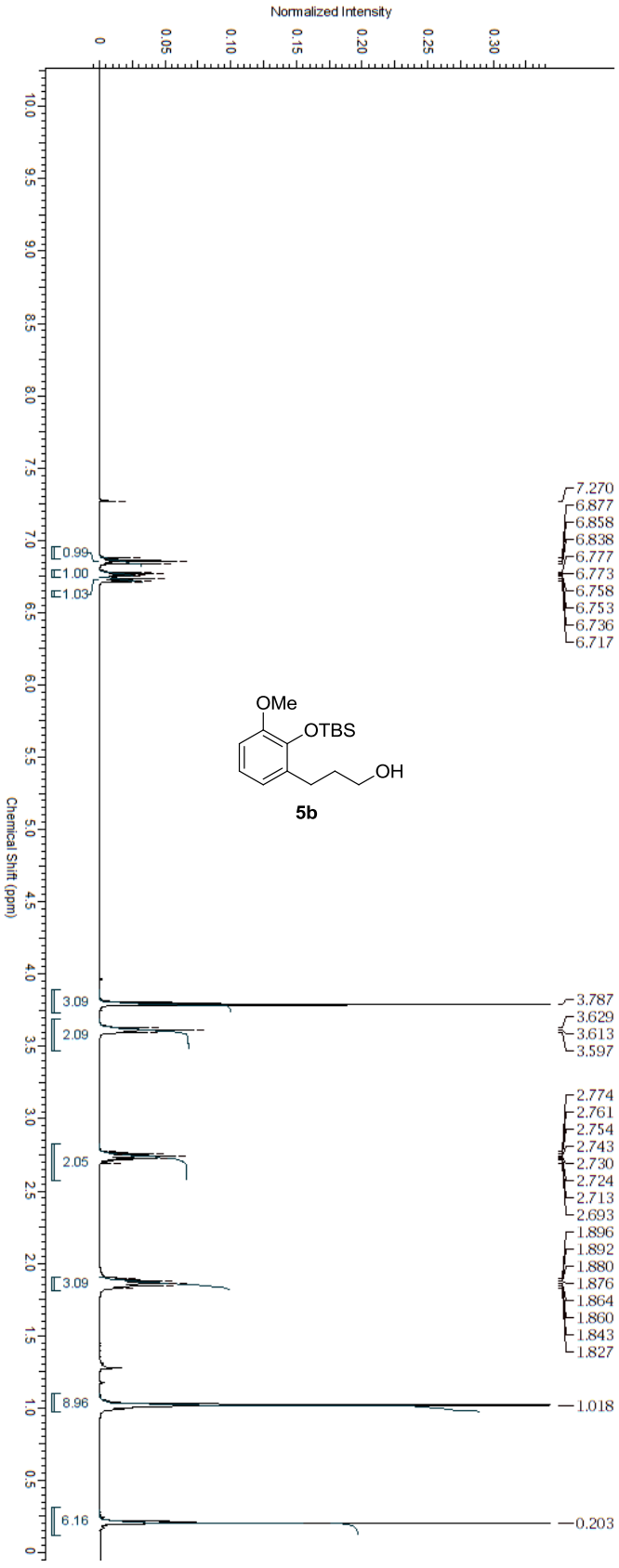


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 4b (major) and its *cis* isomer (minor); only δ values corresponding to the peaks of the *trans* isomer are reported



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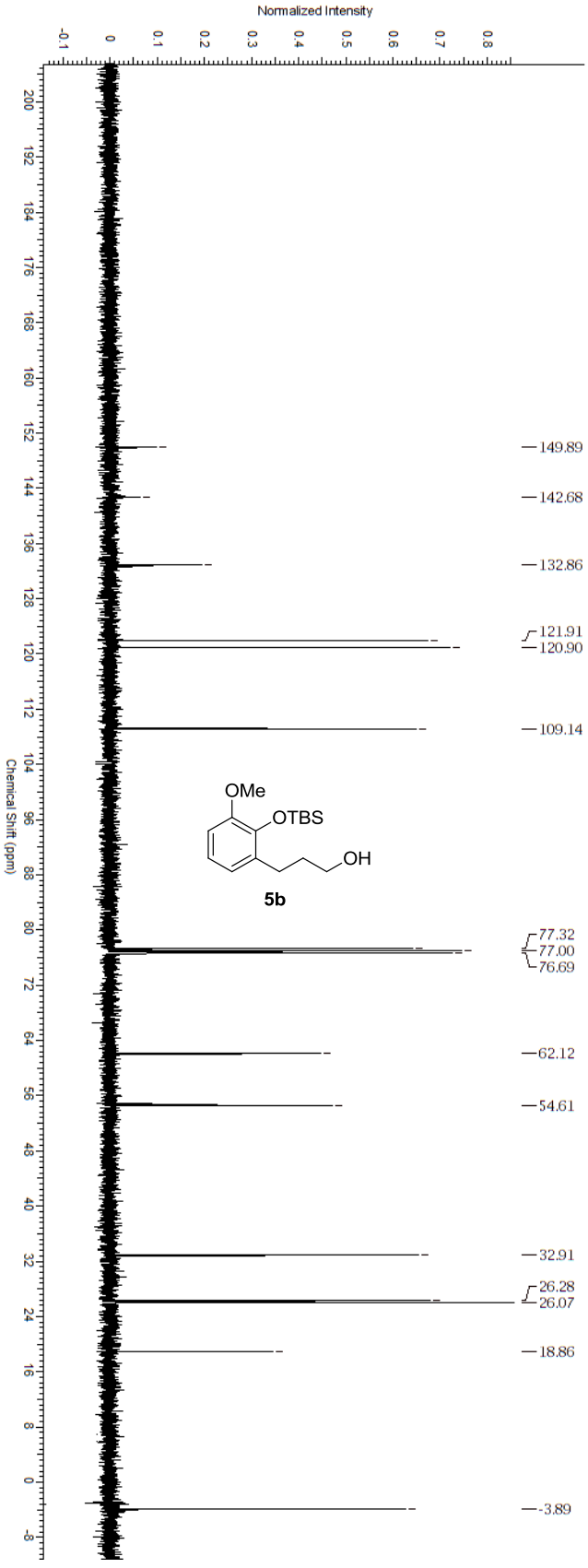
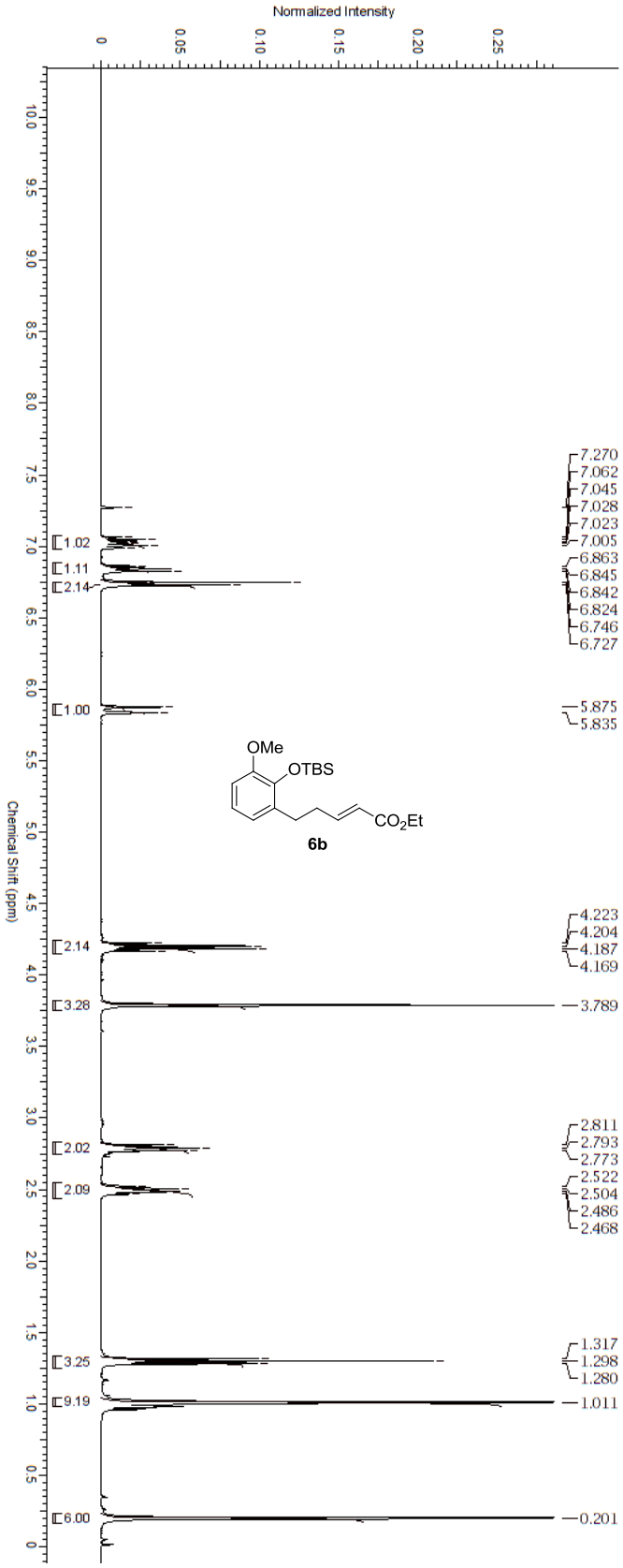
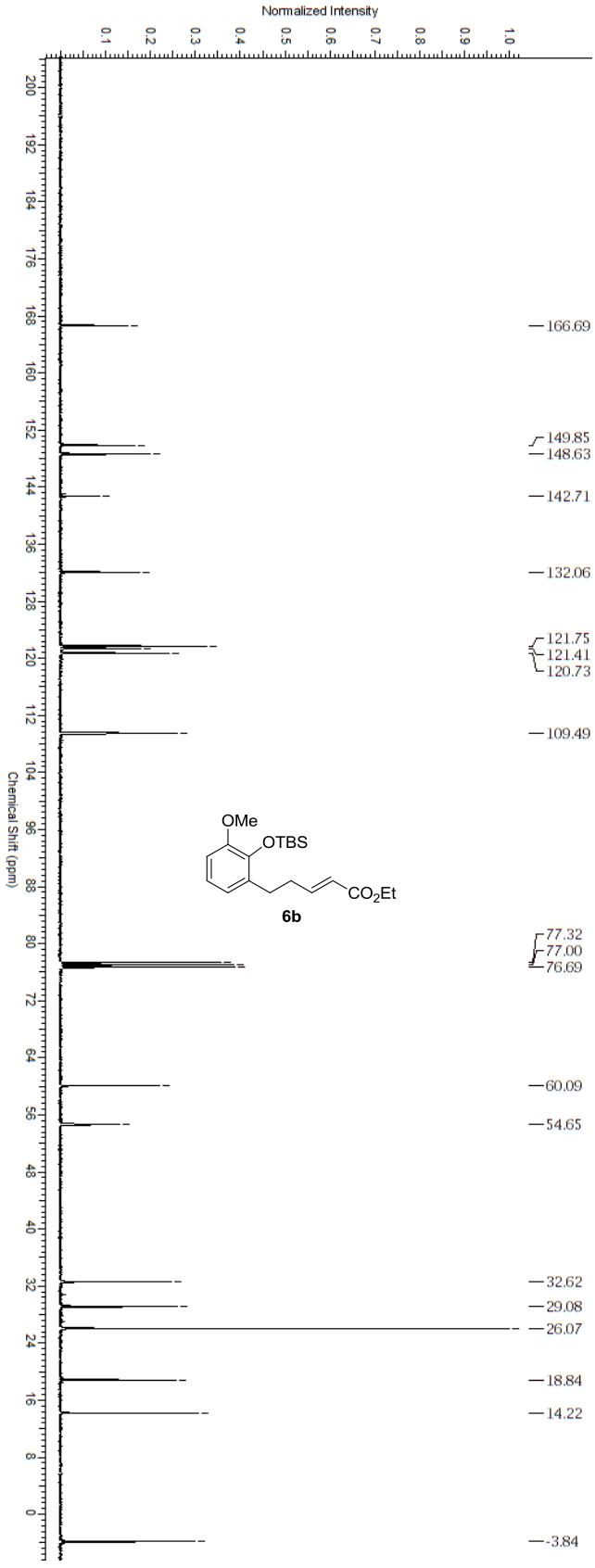


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 5b



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



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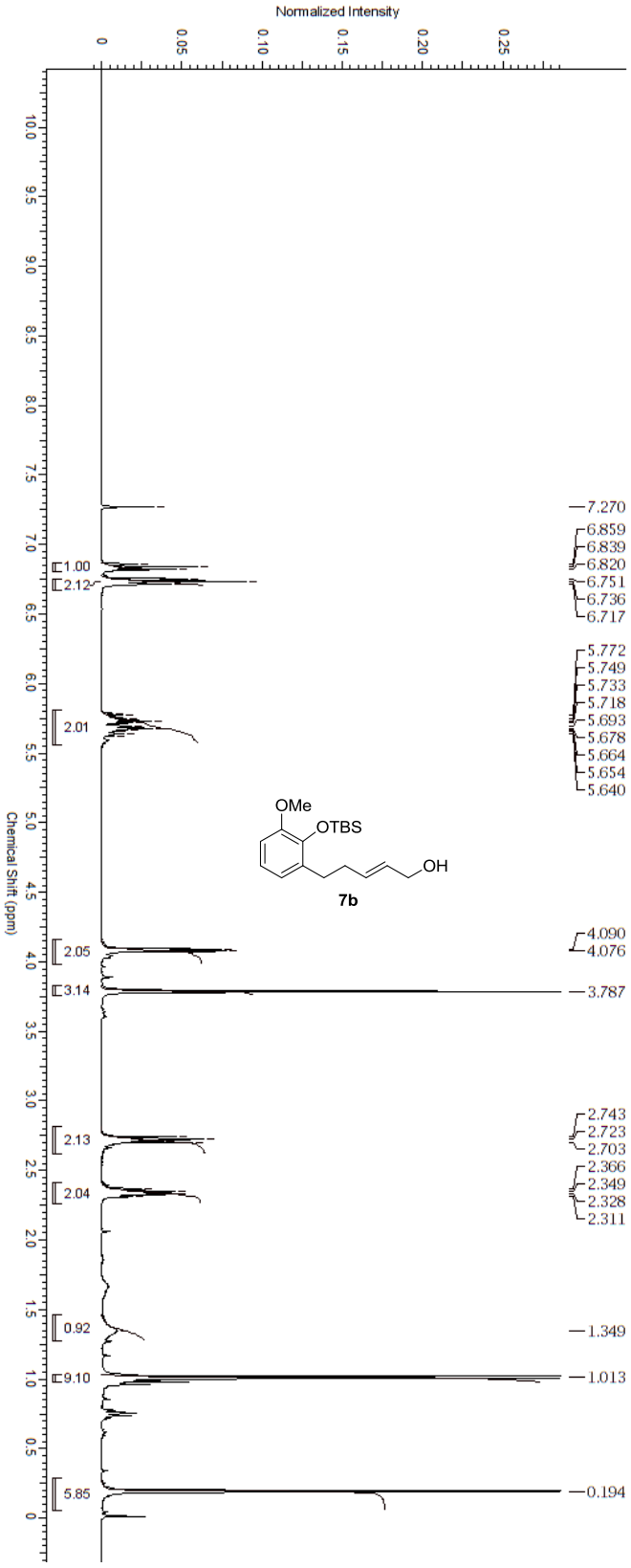

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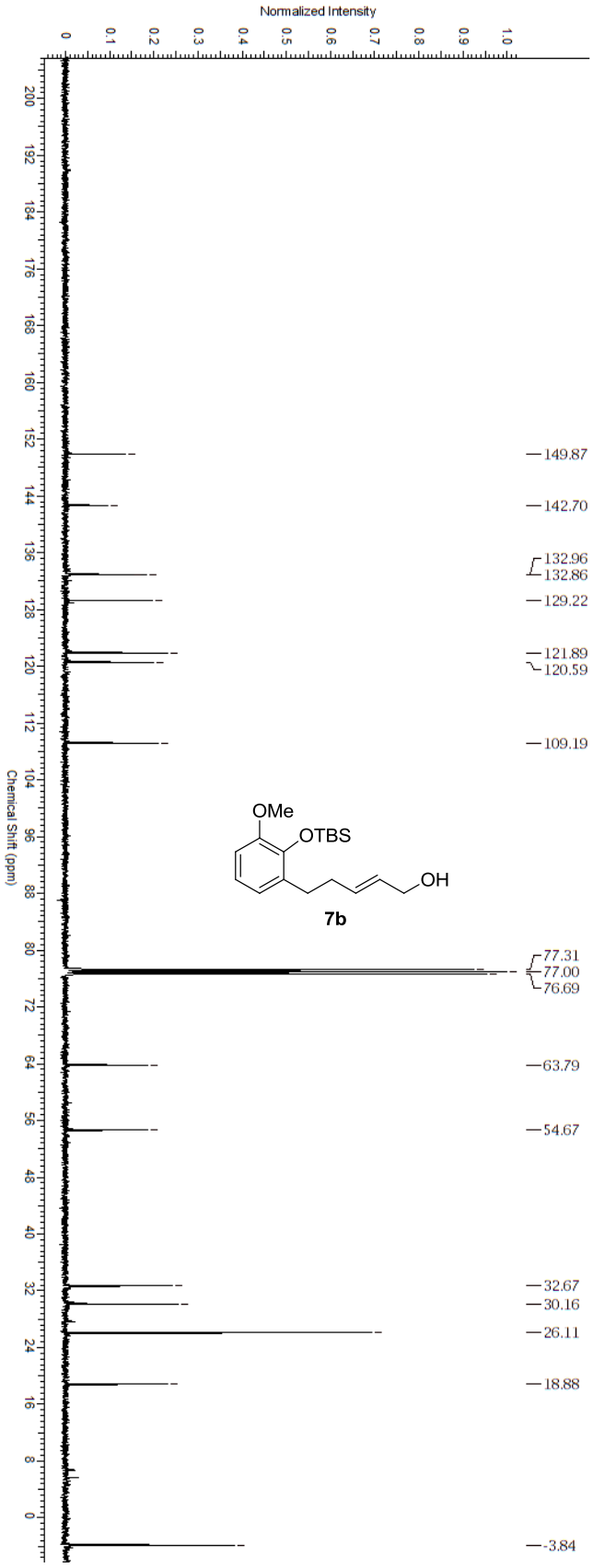

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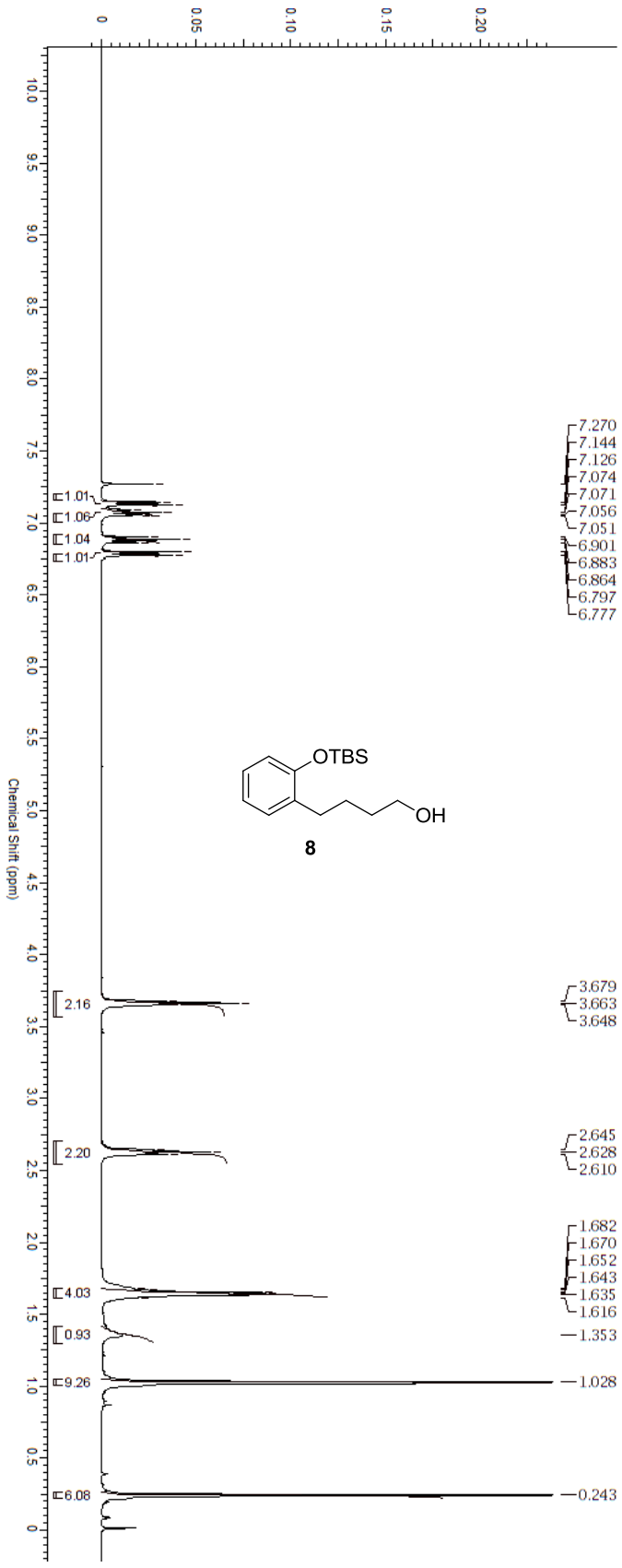

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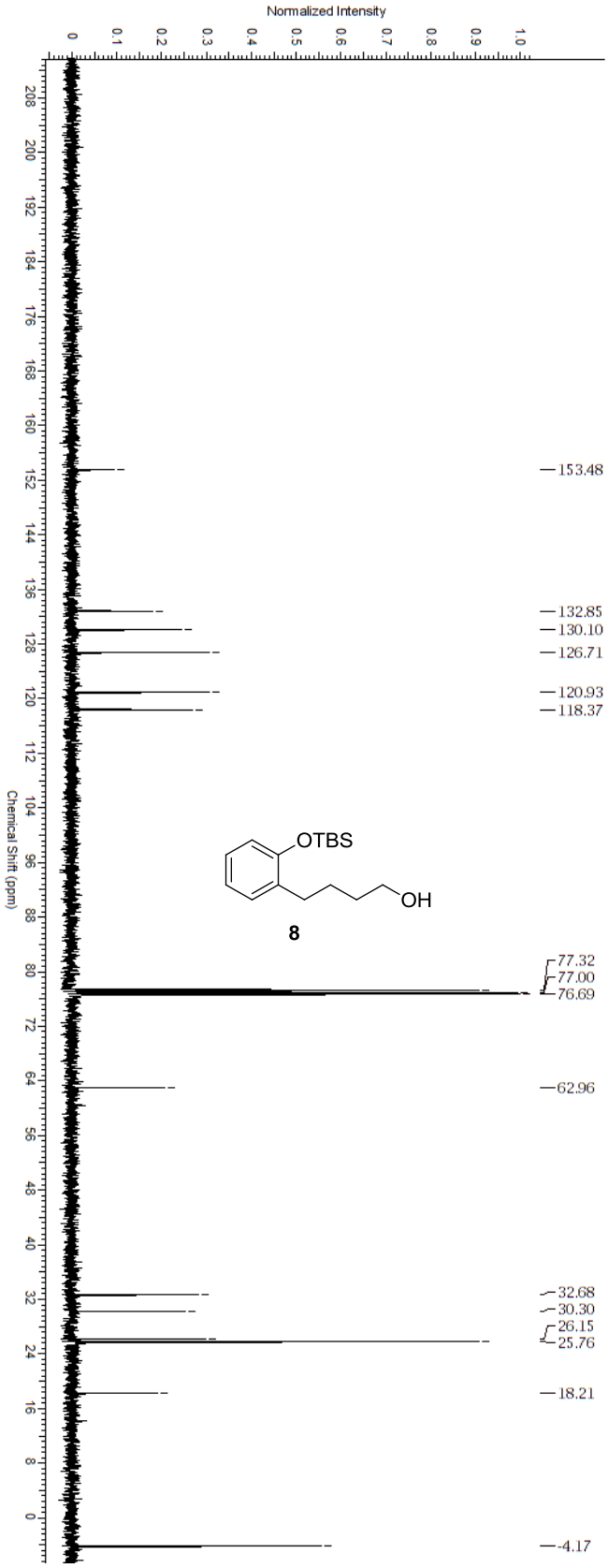
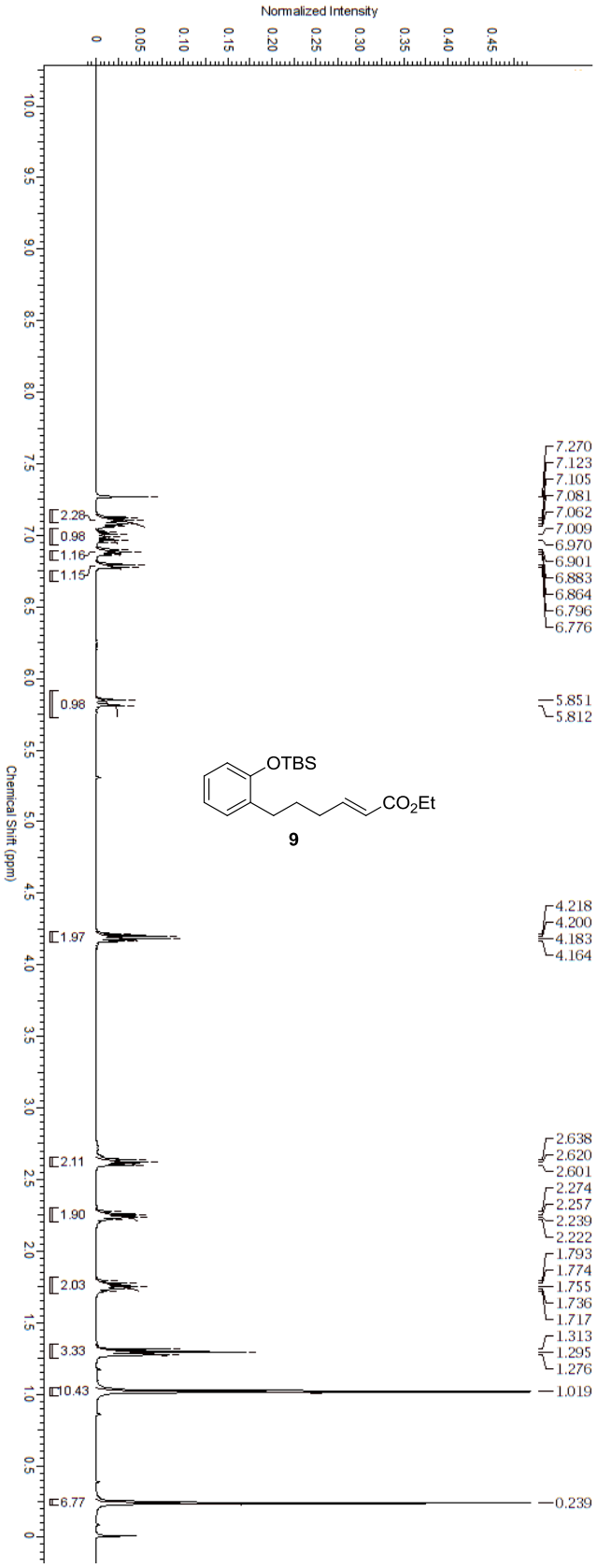
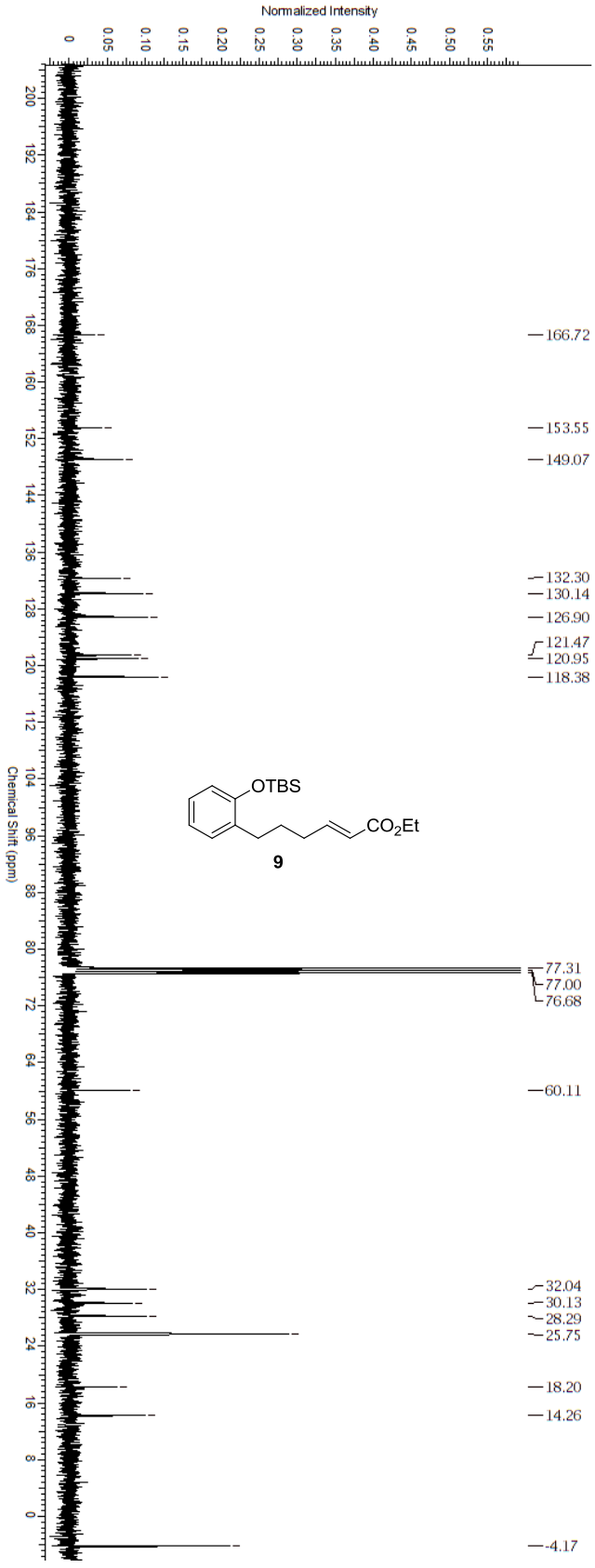


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 8



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9



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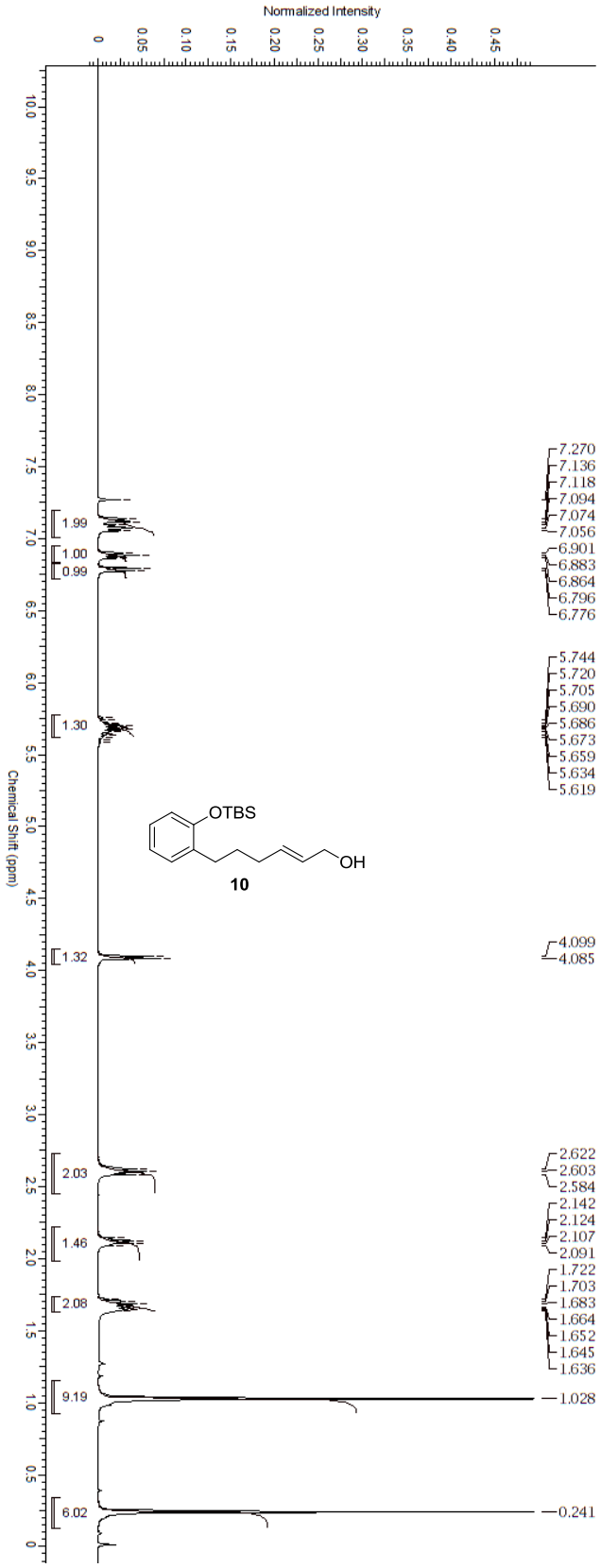

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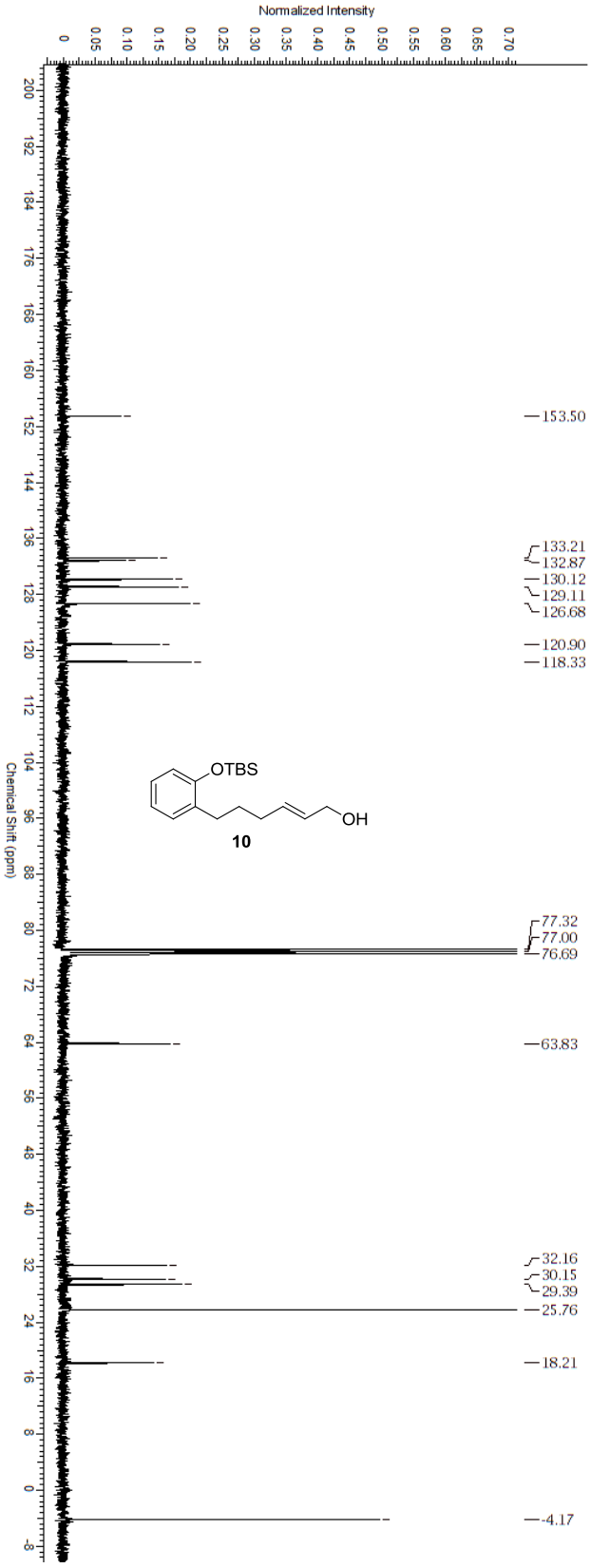

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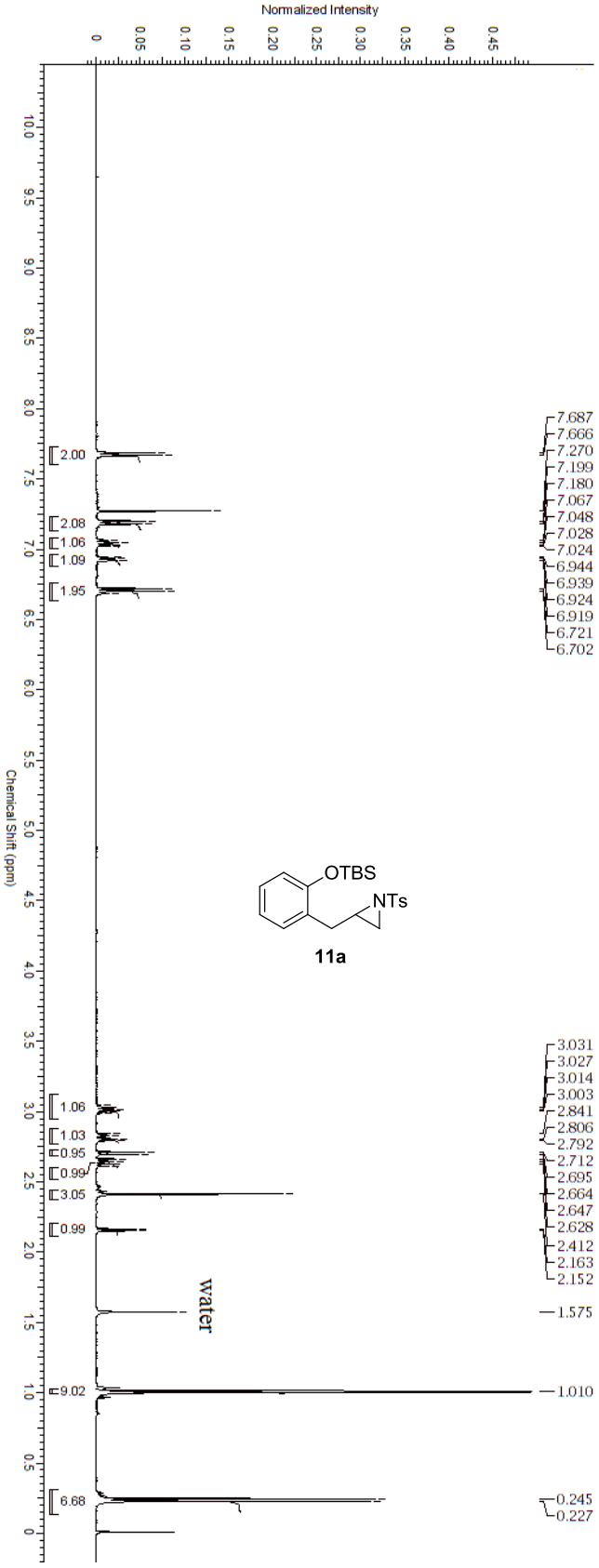

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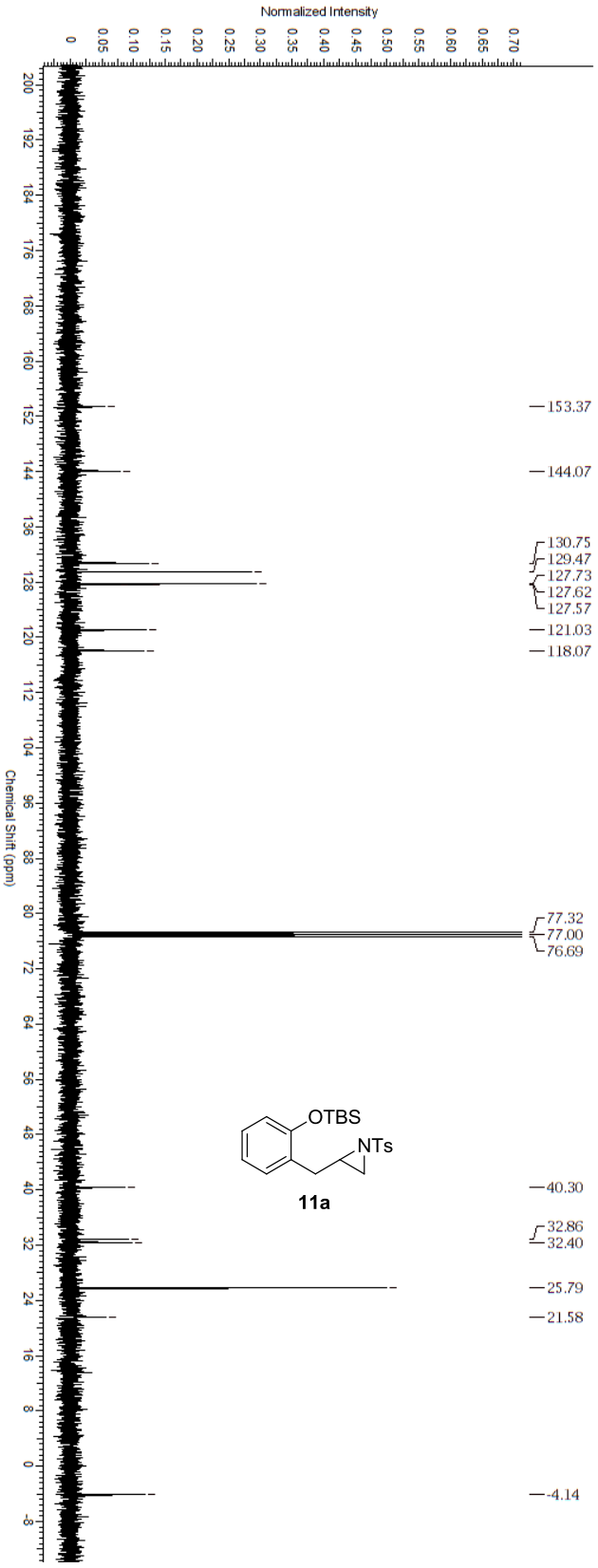

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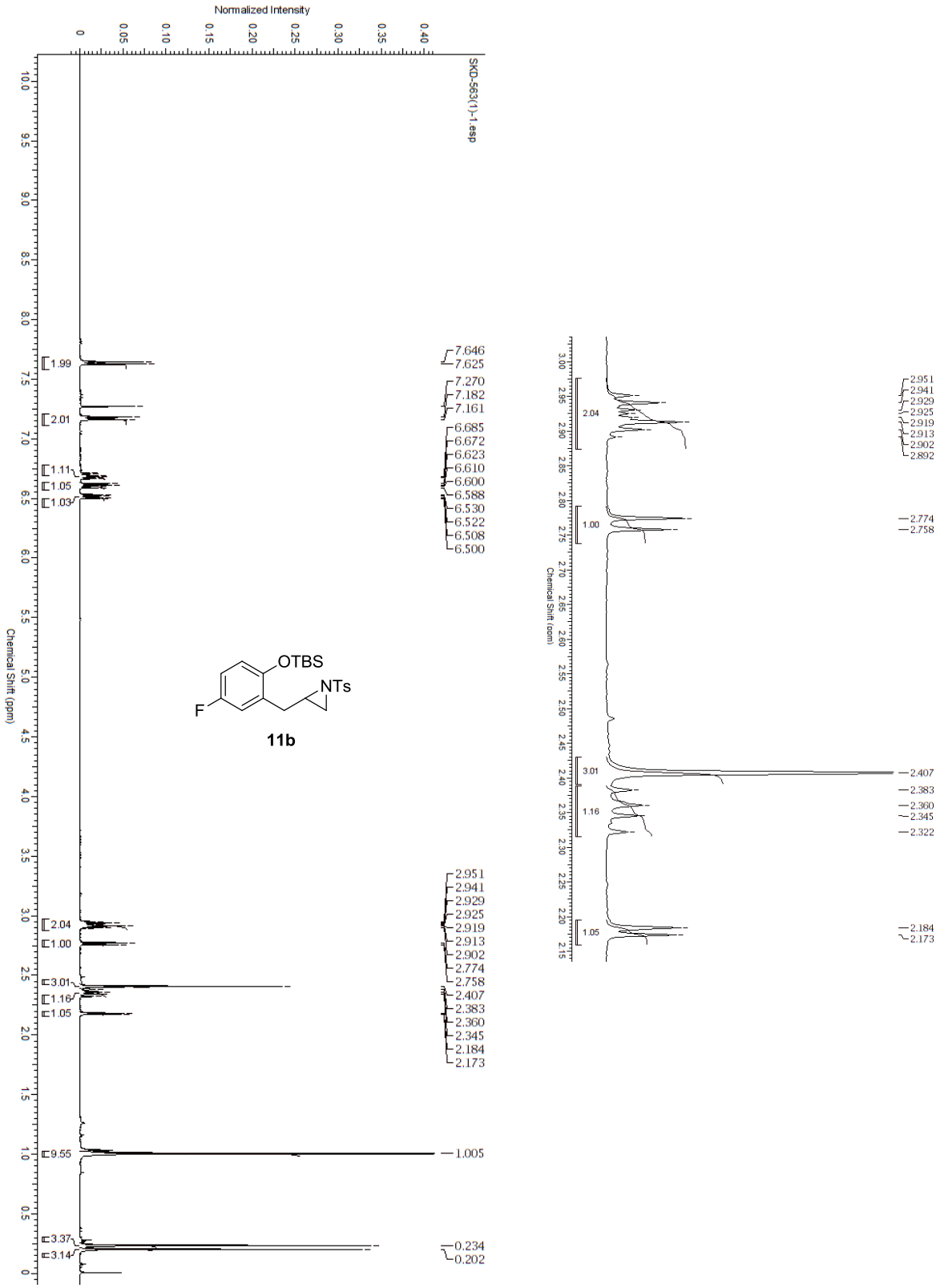

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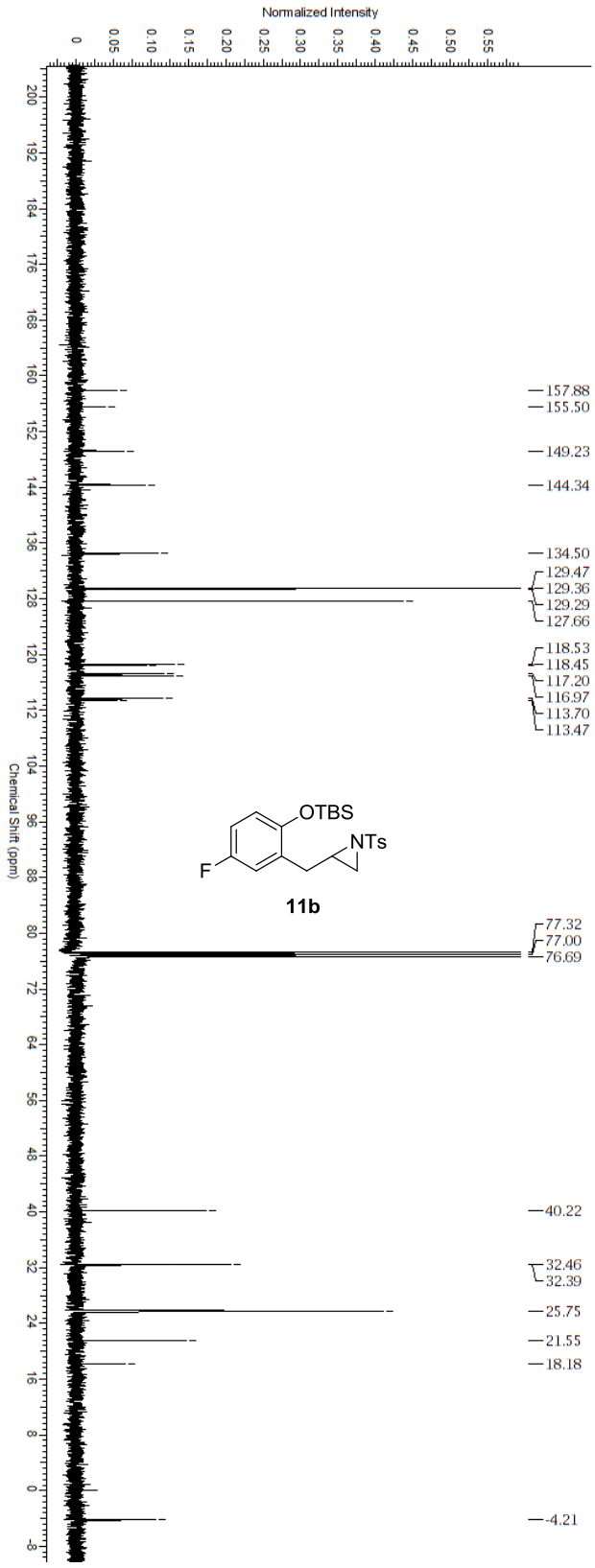

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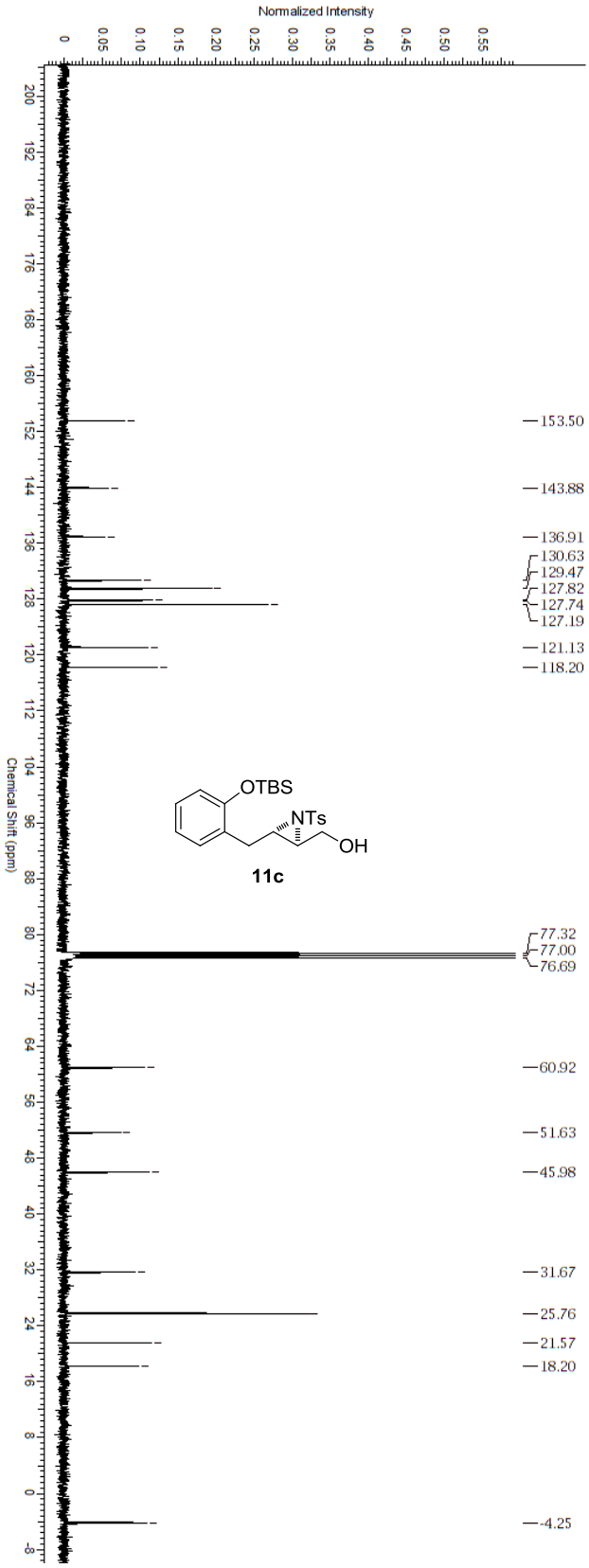
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 11c



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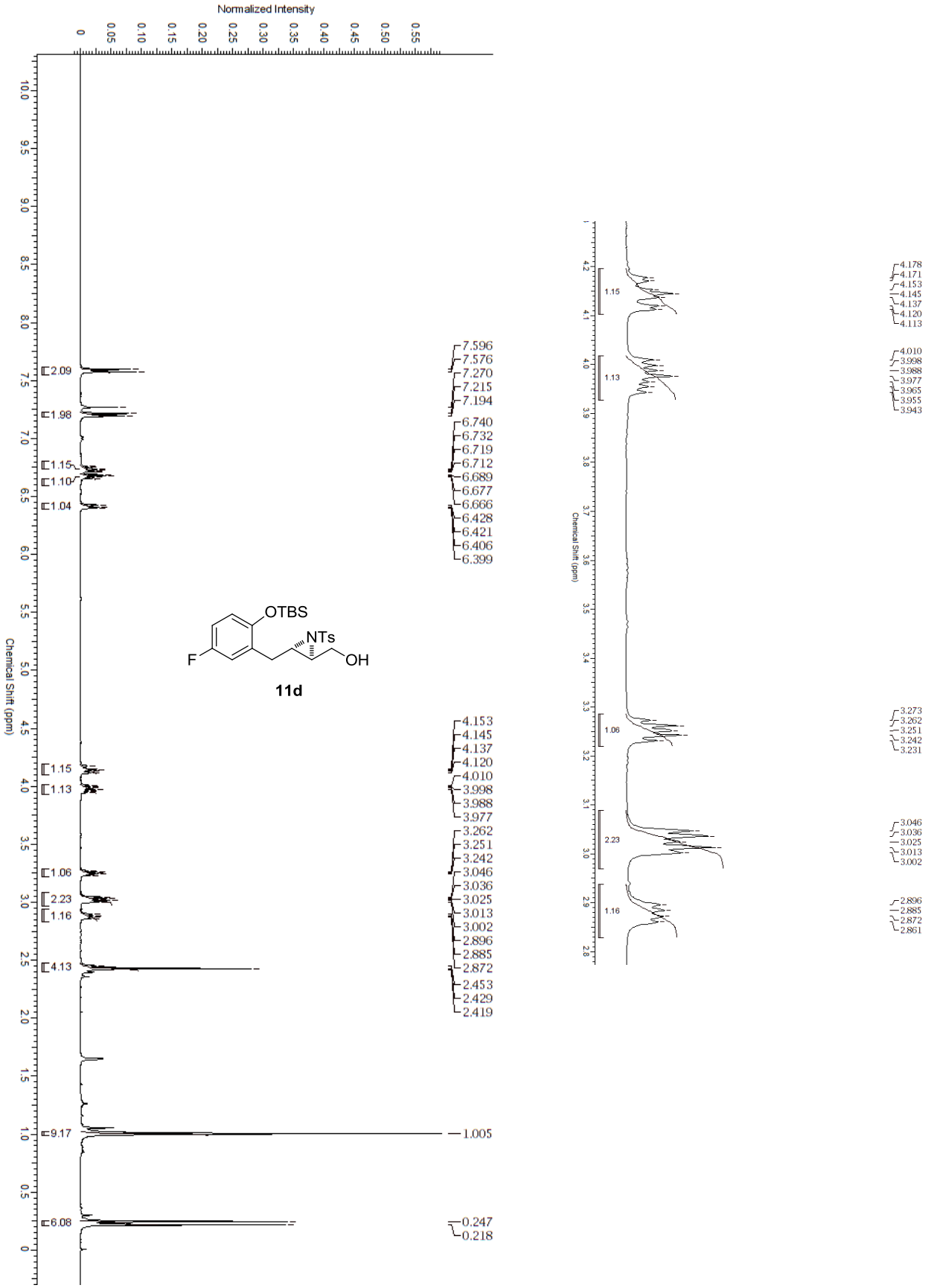

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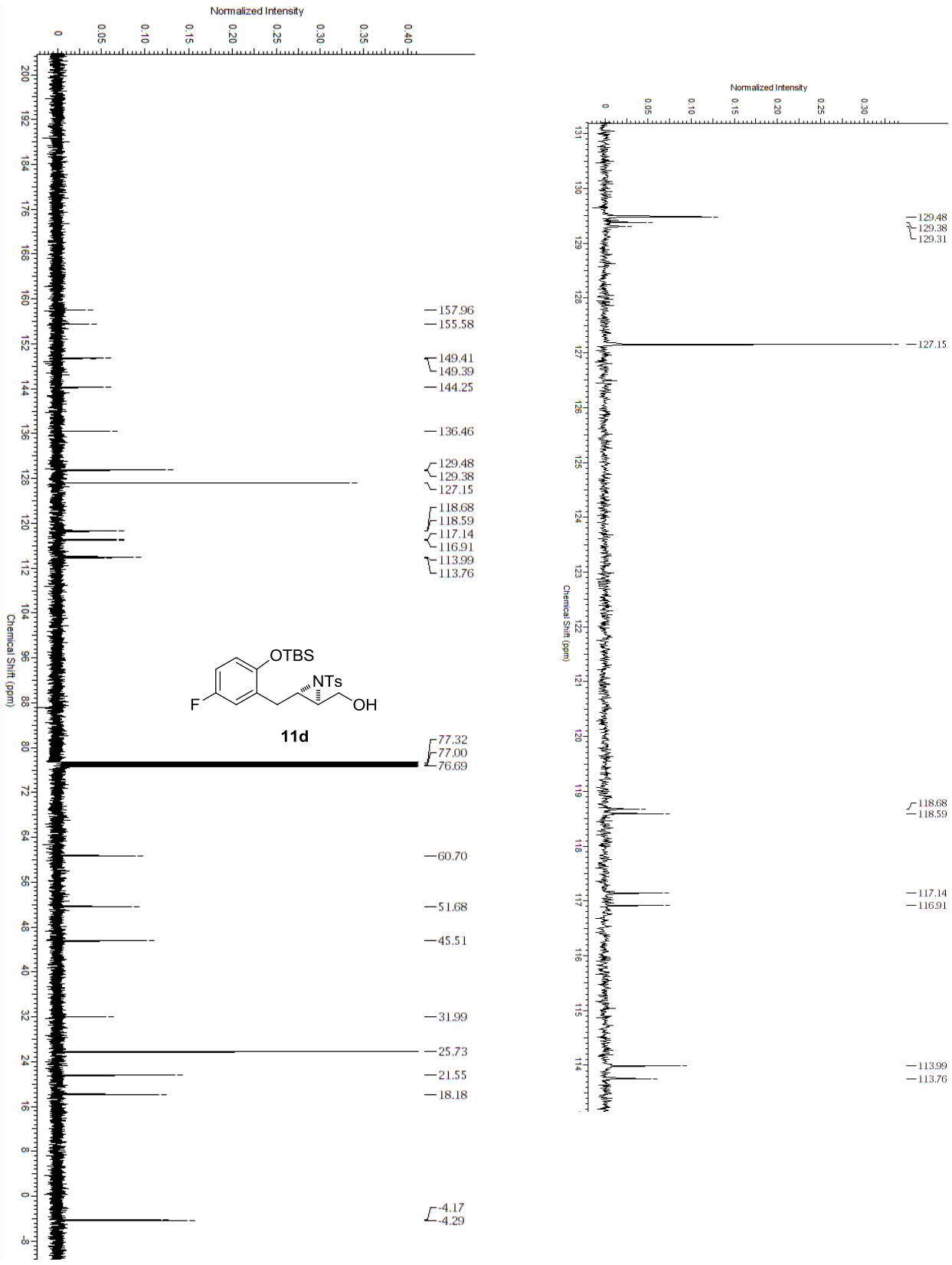

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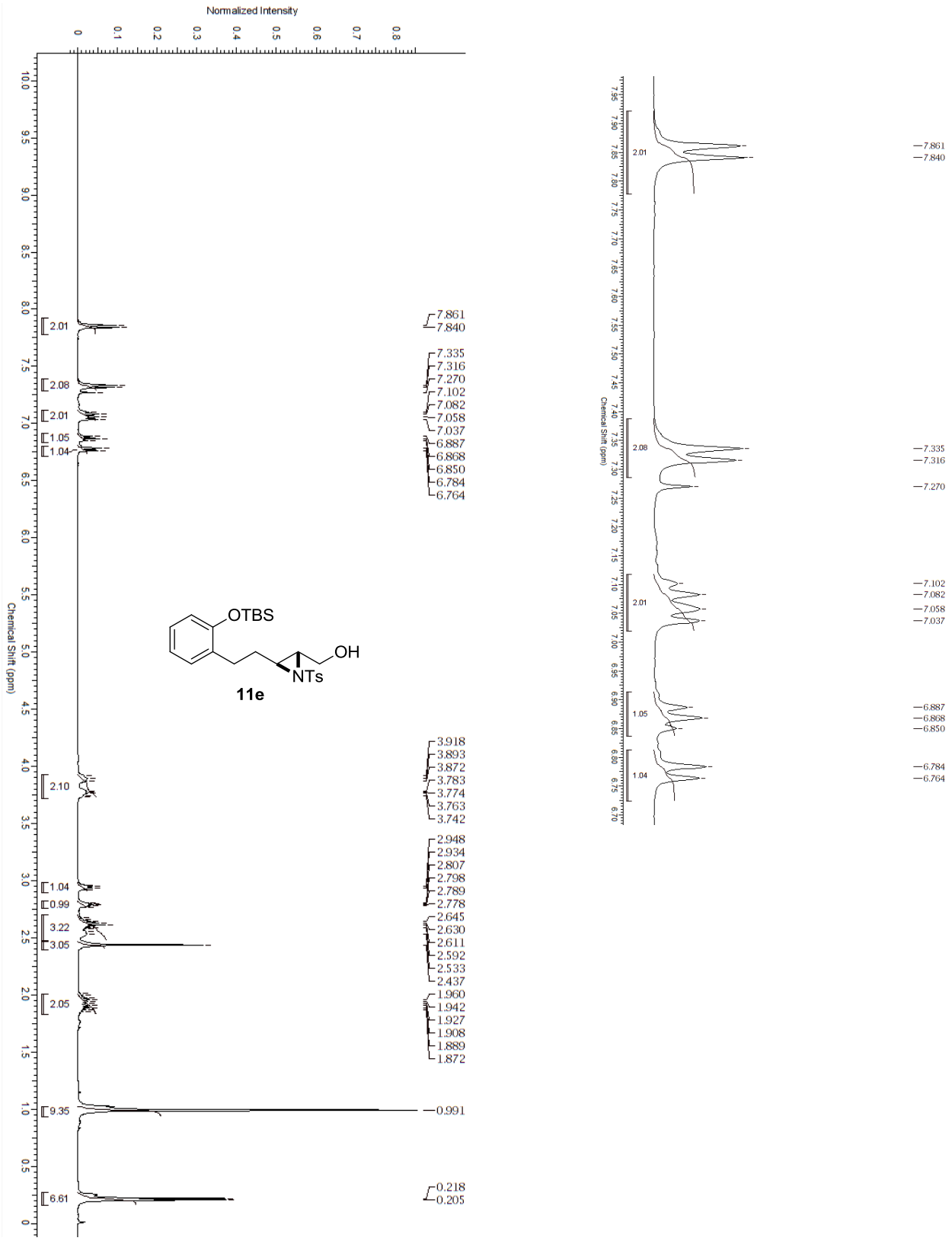

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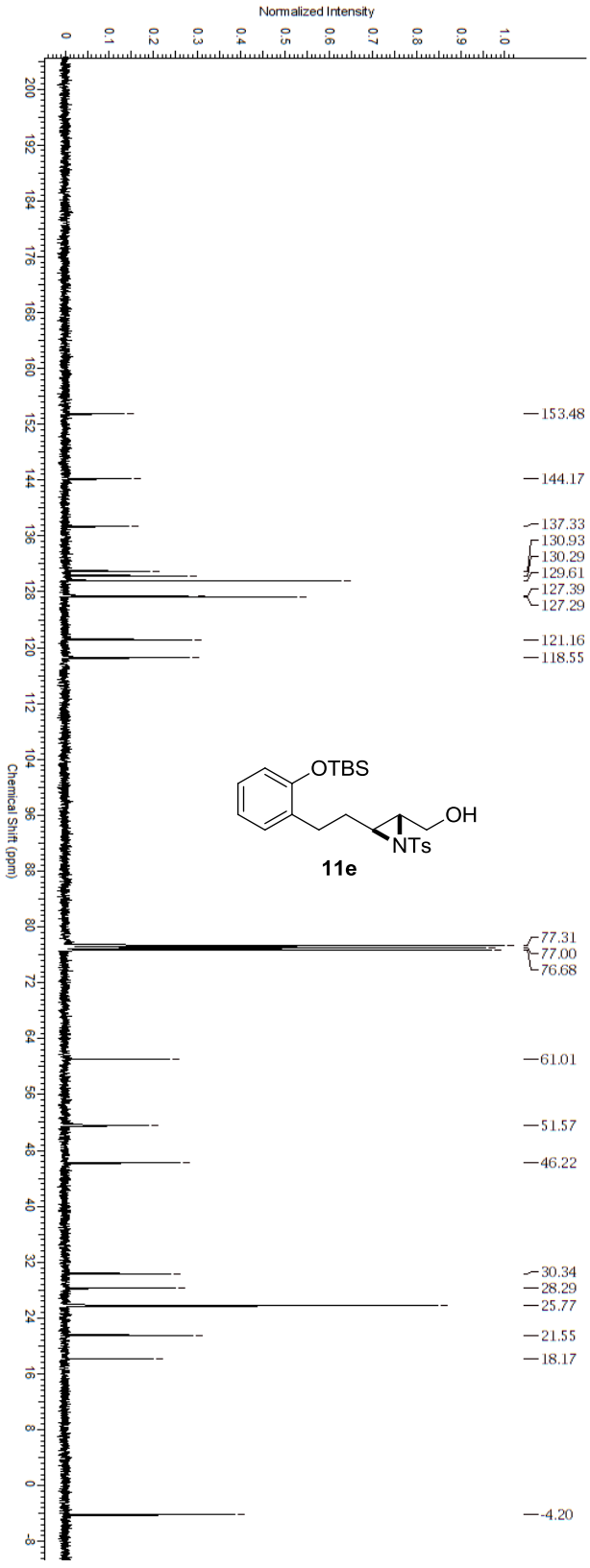

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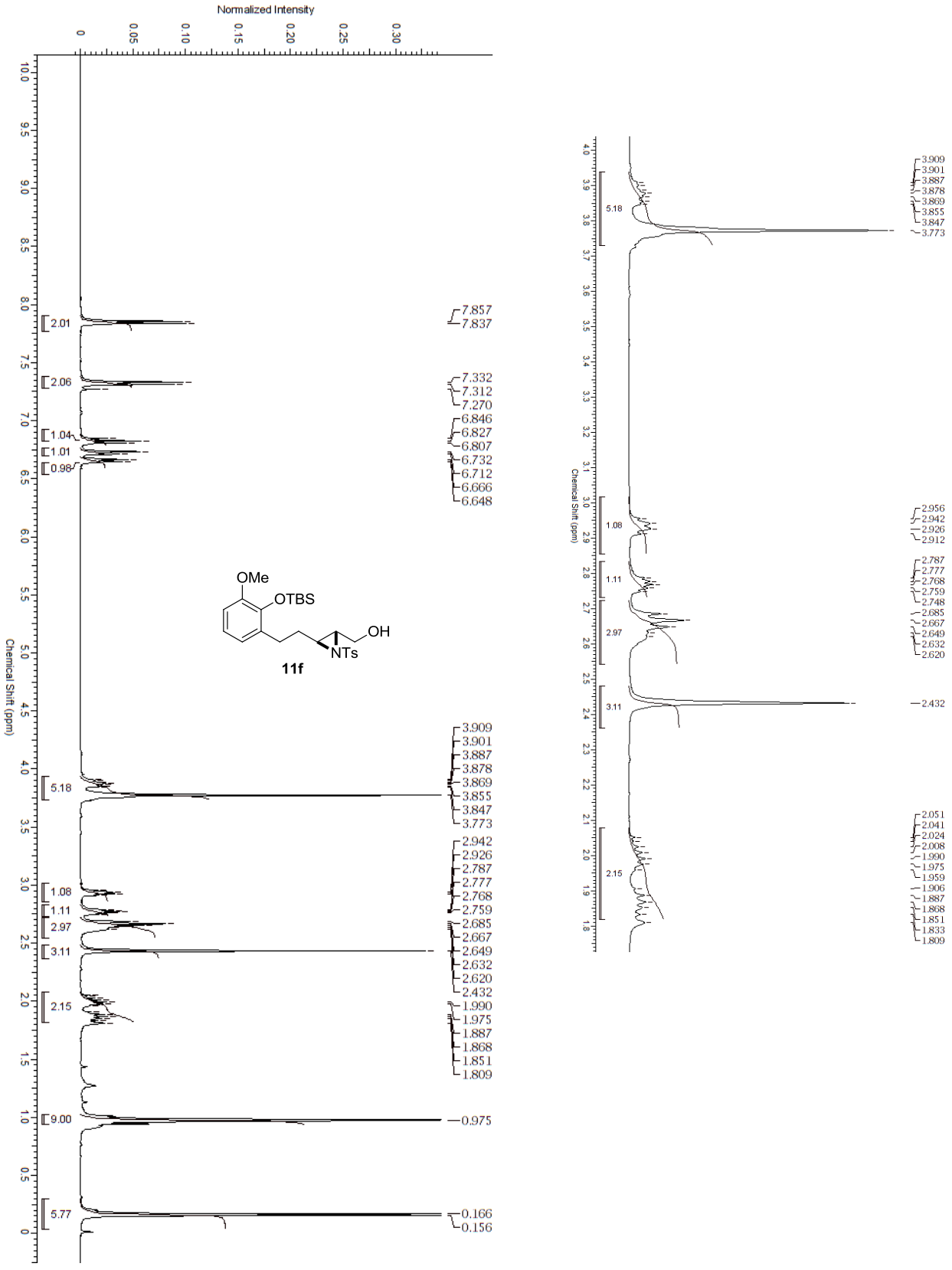

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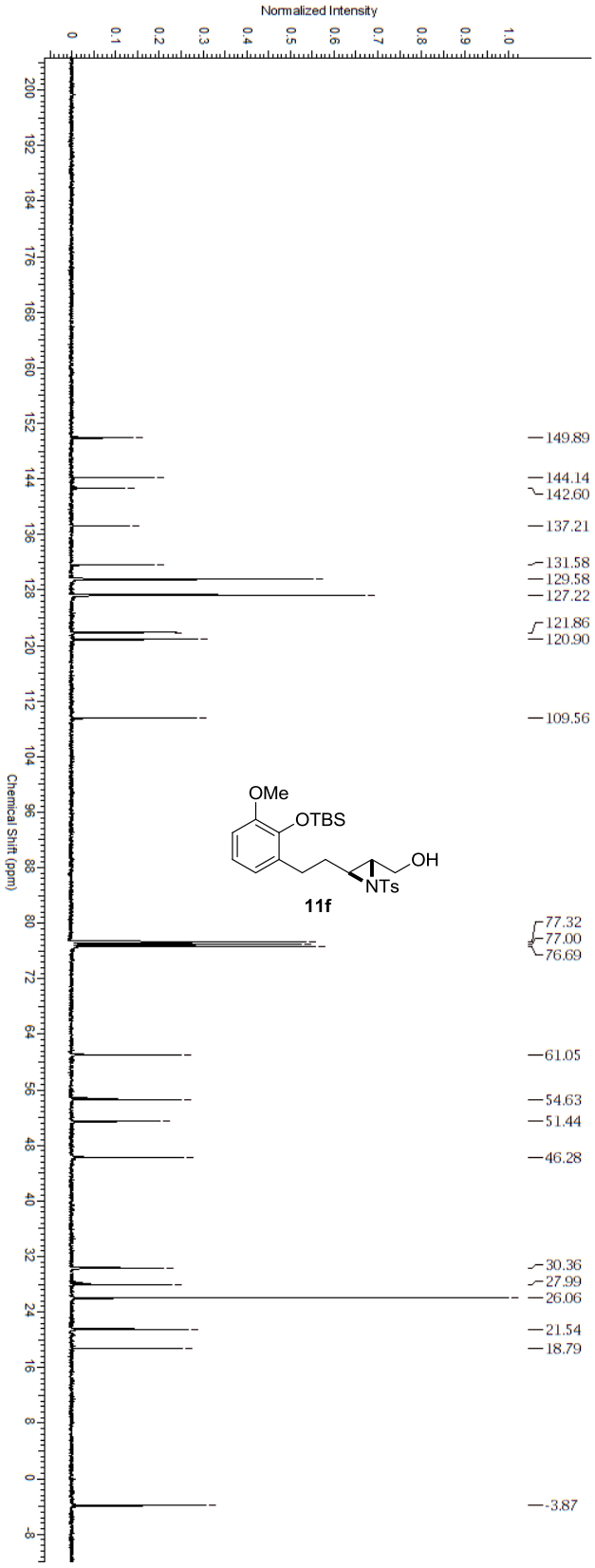

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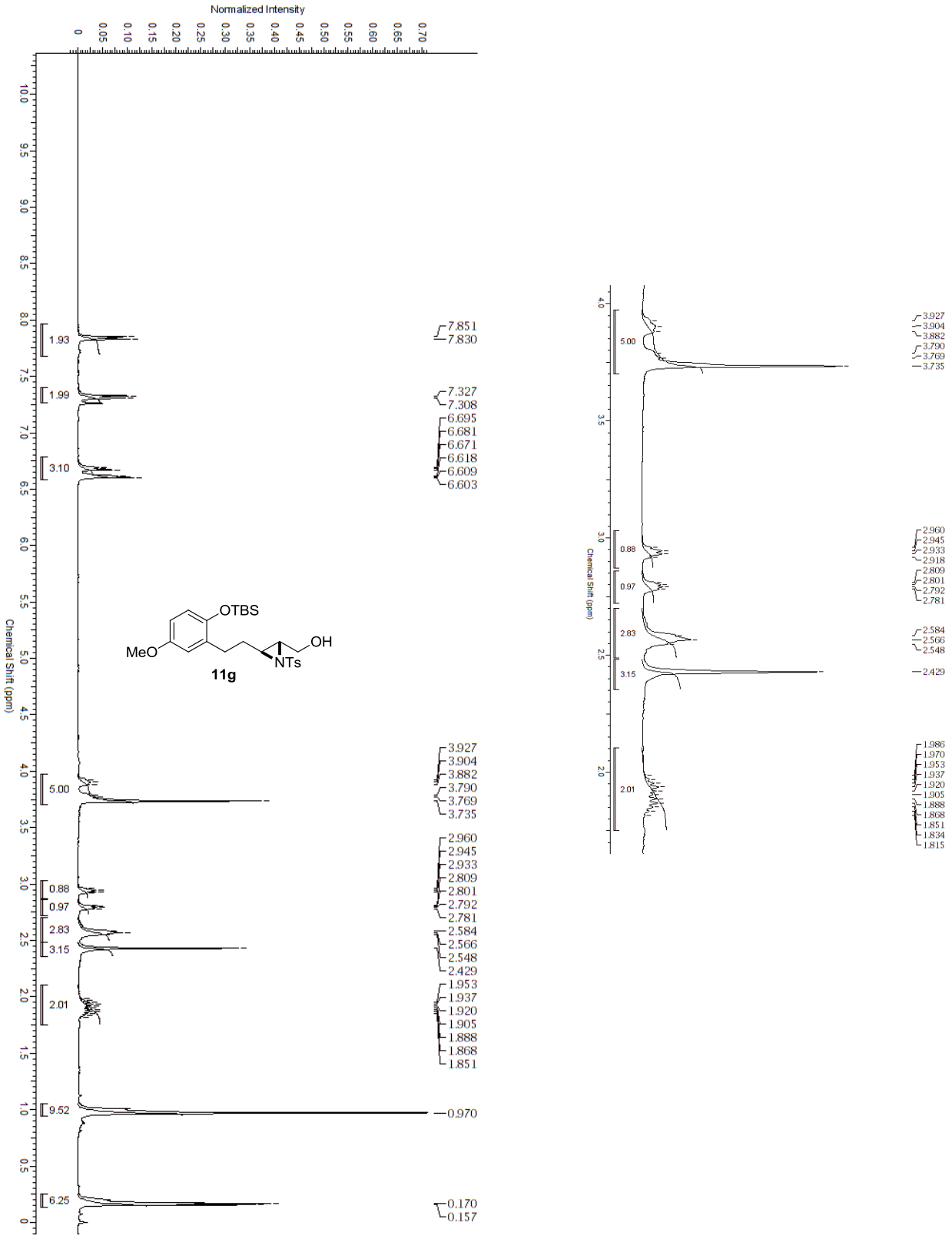

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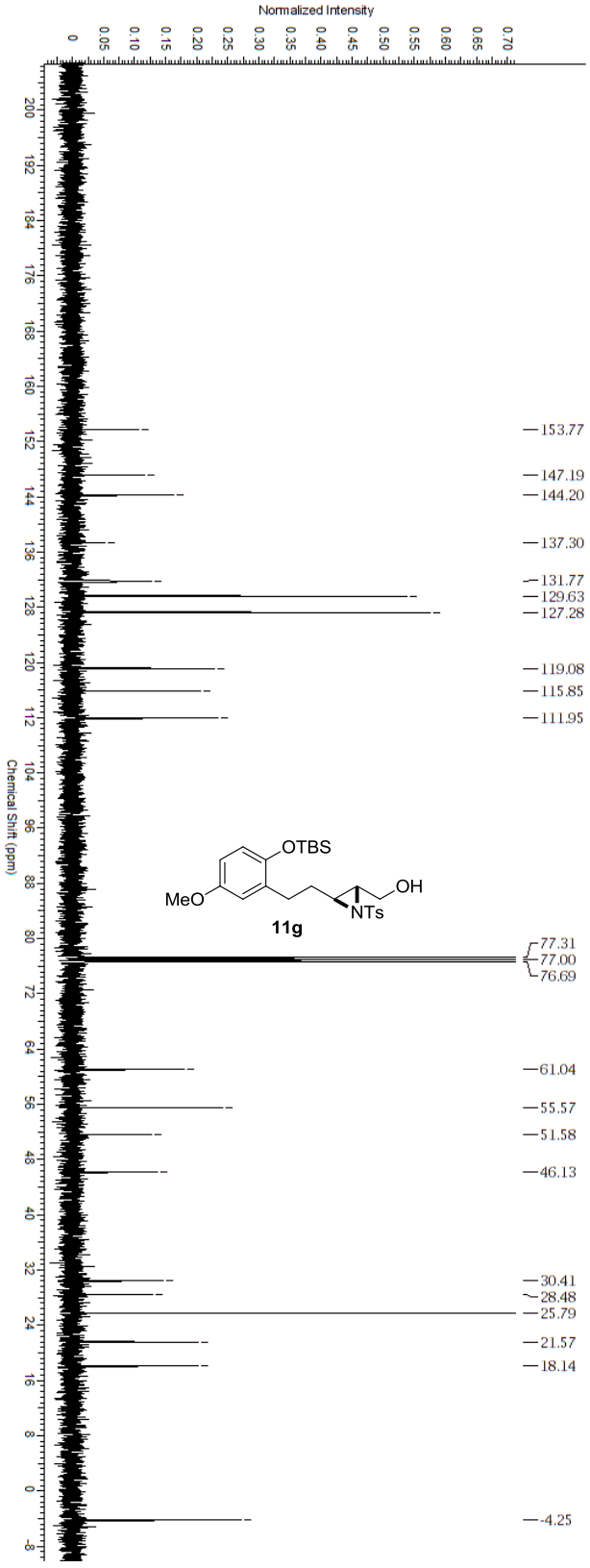

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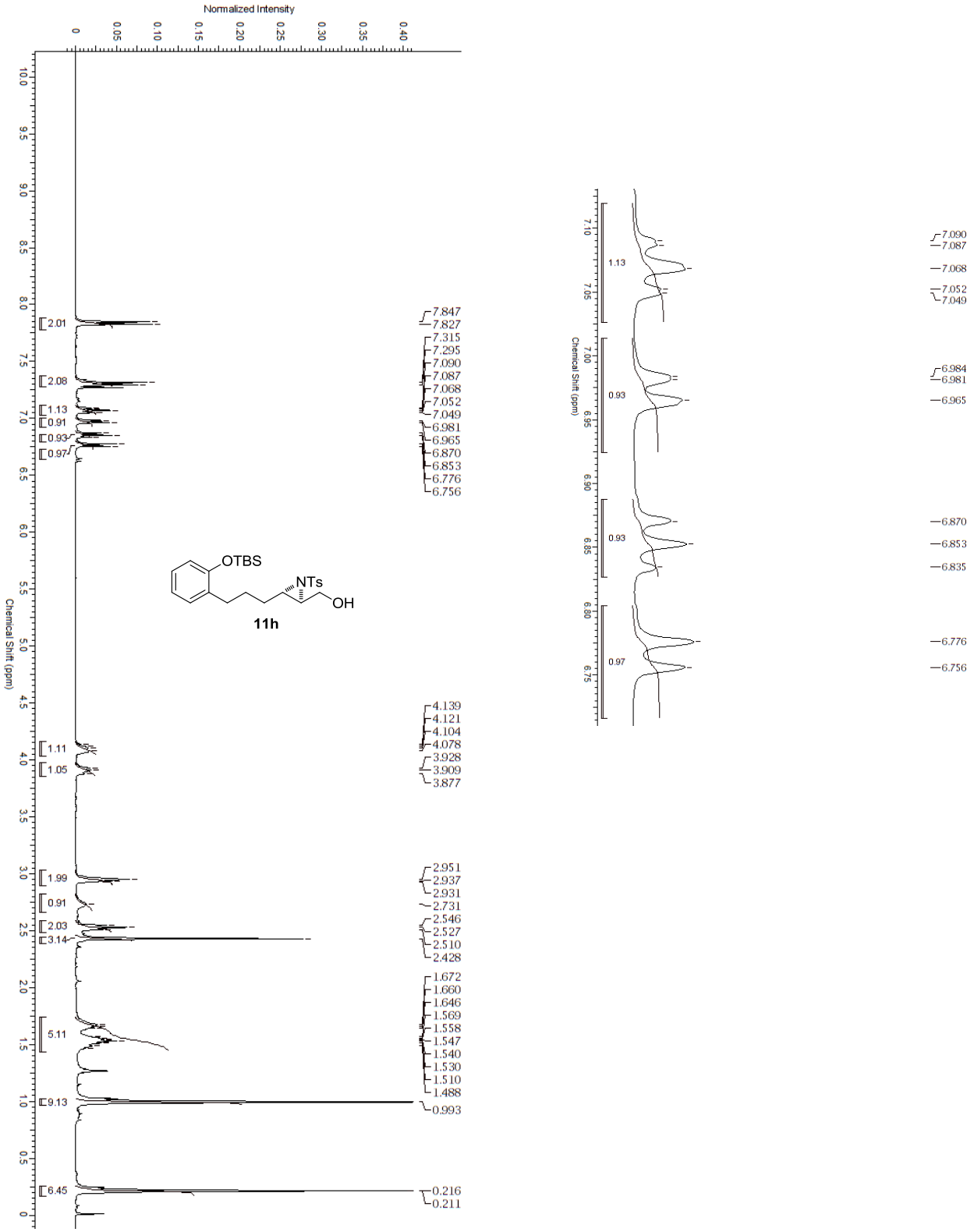

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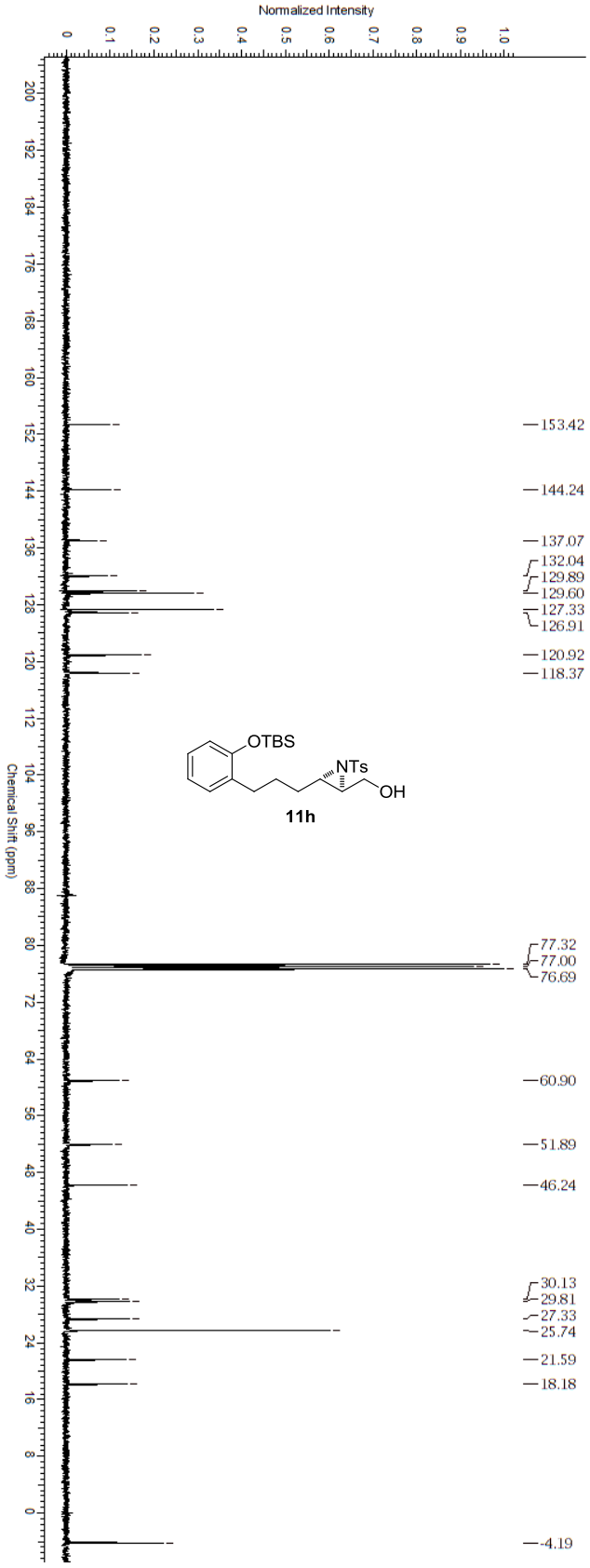

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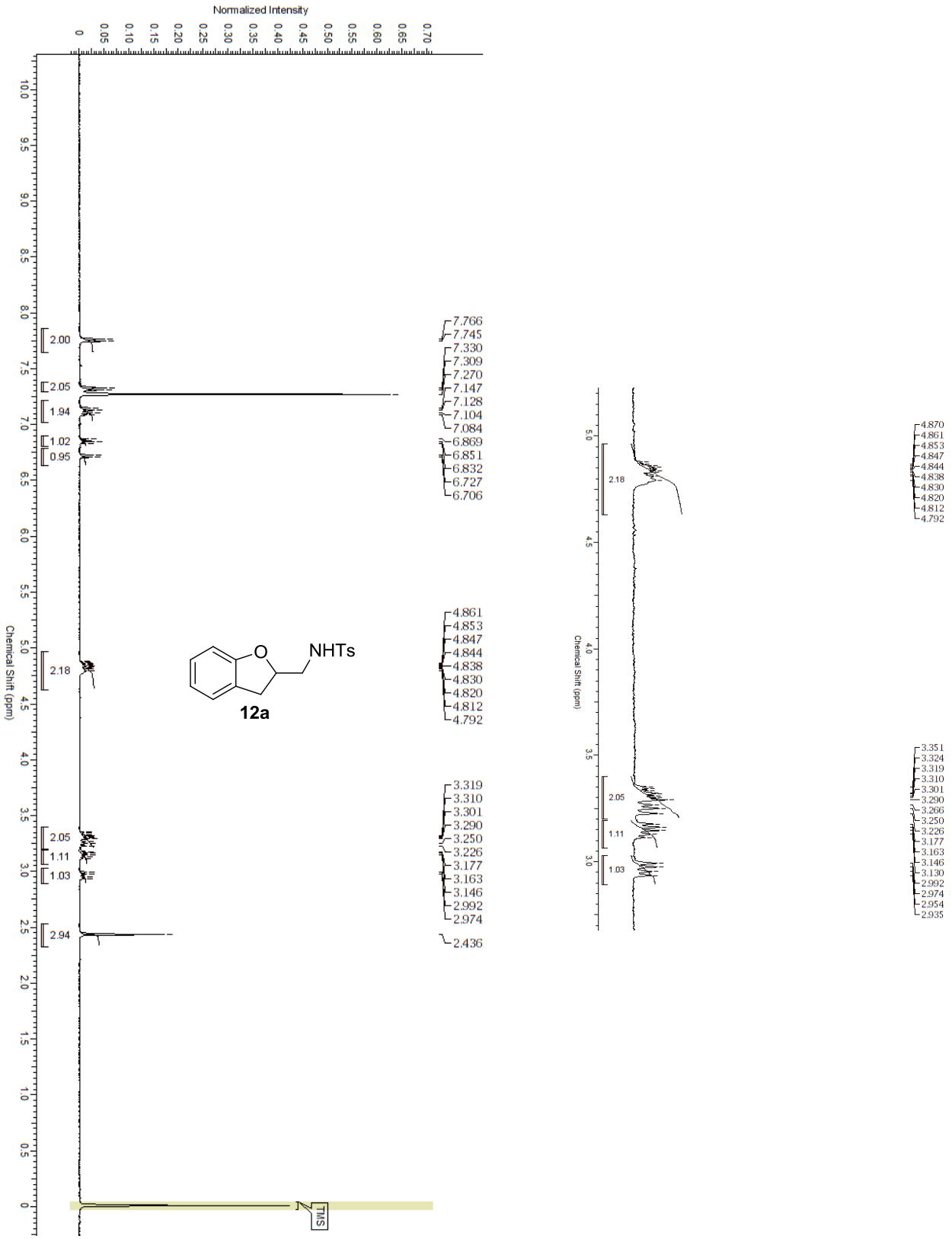

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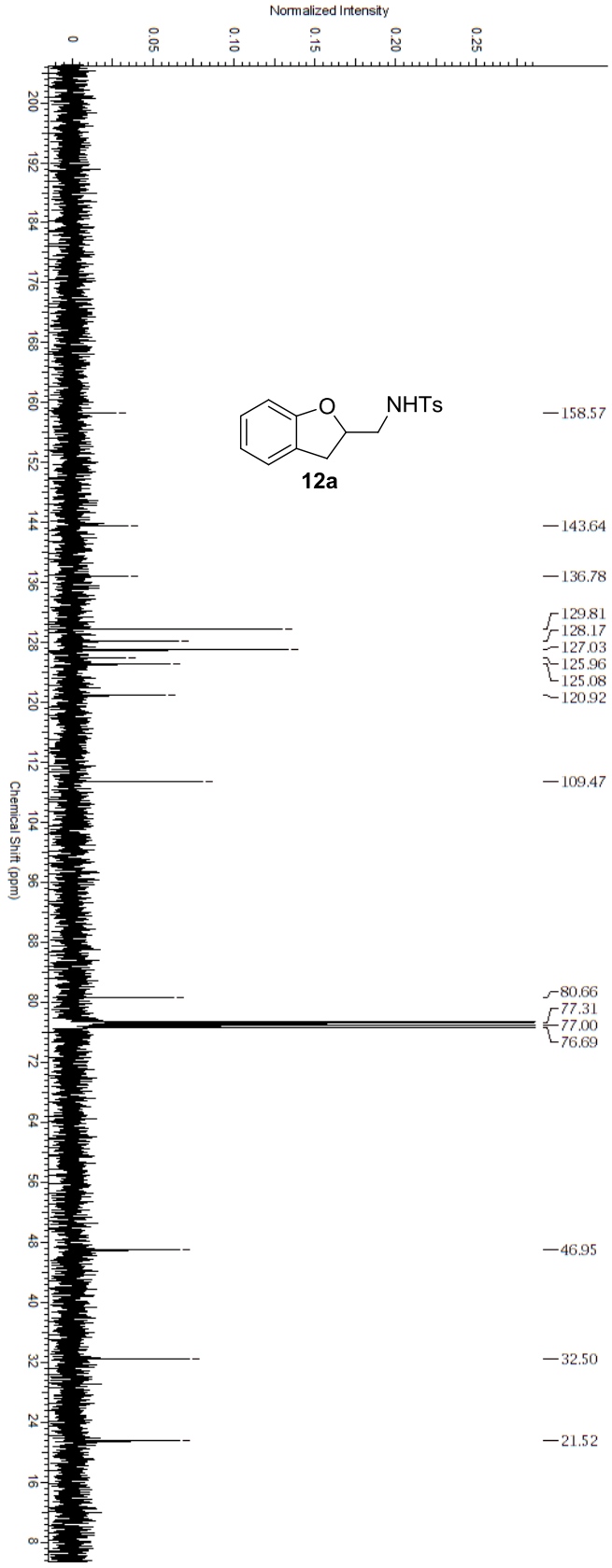
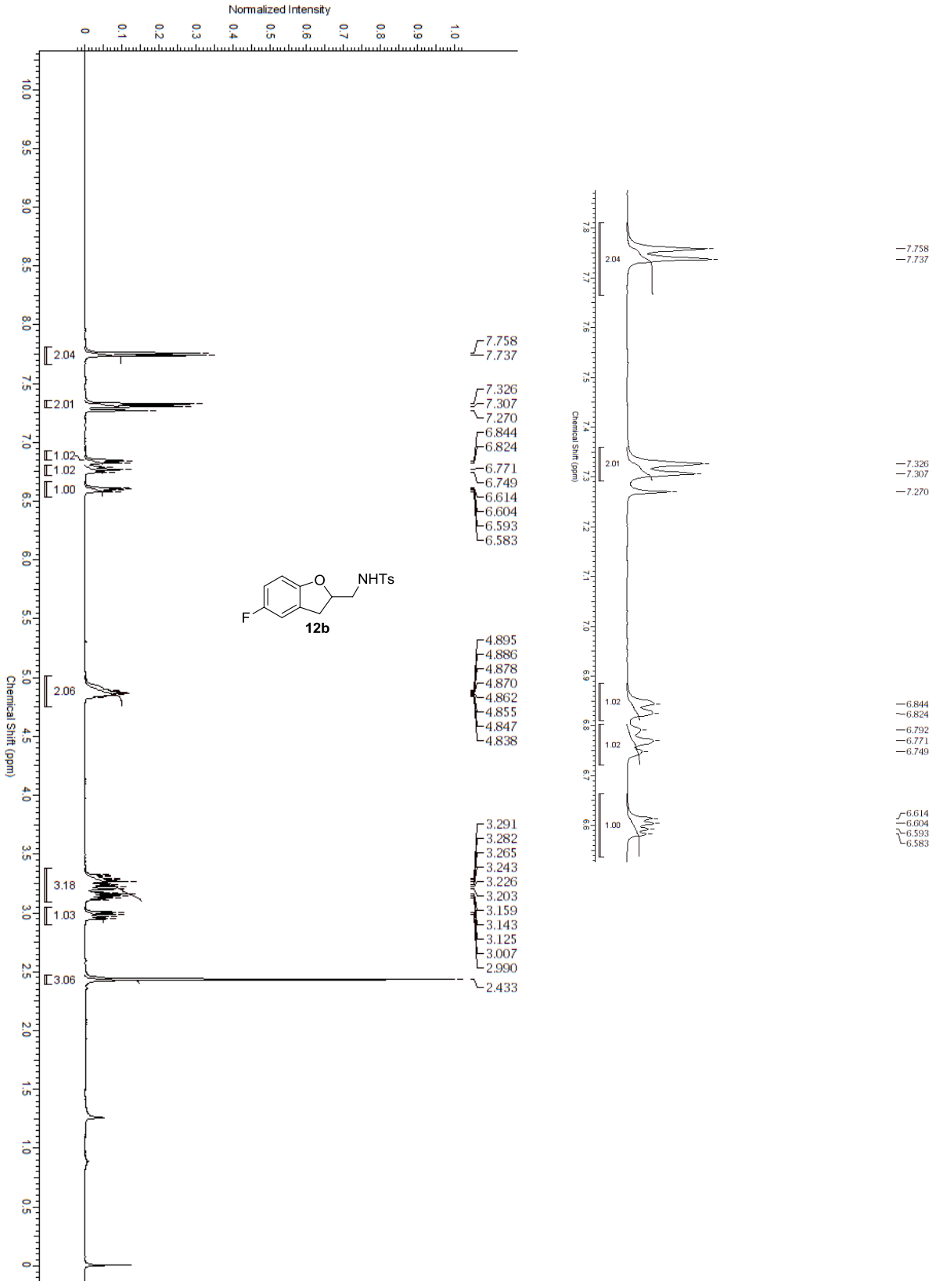
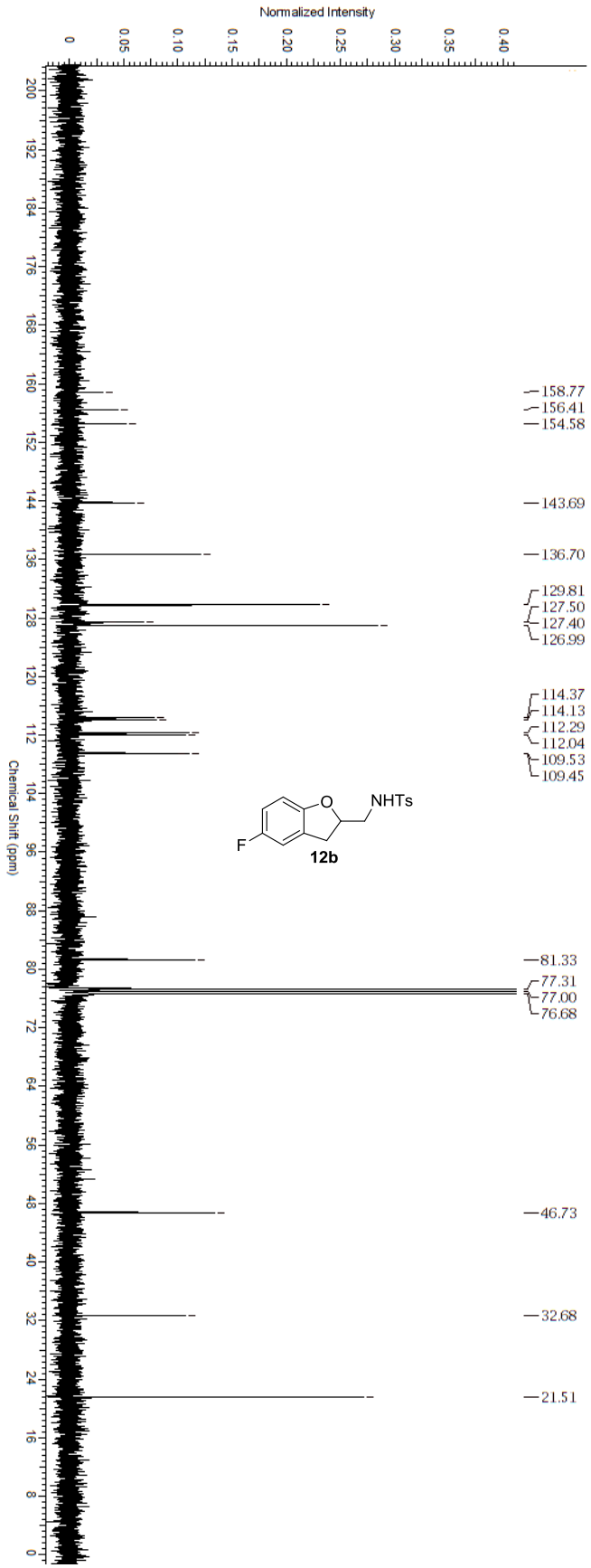


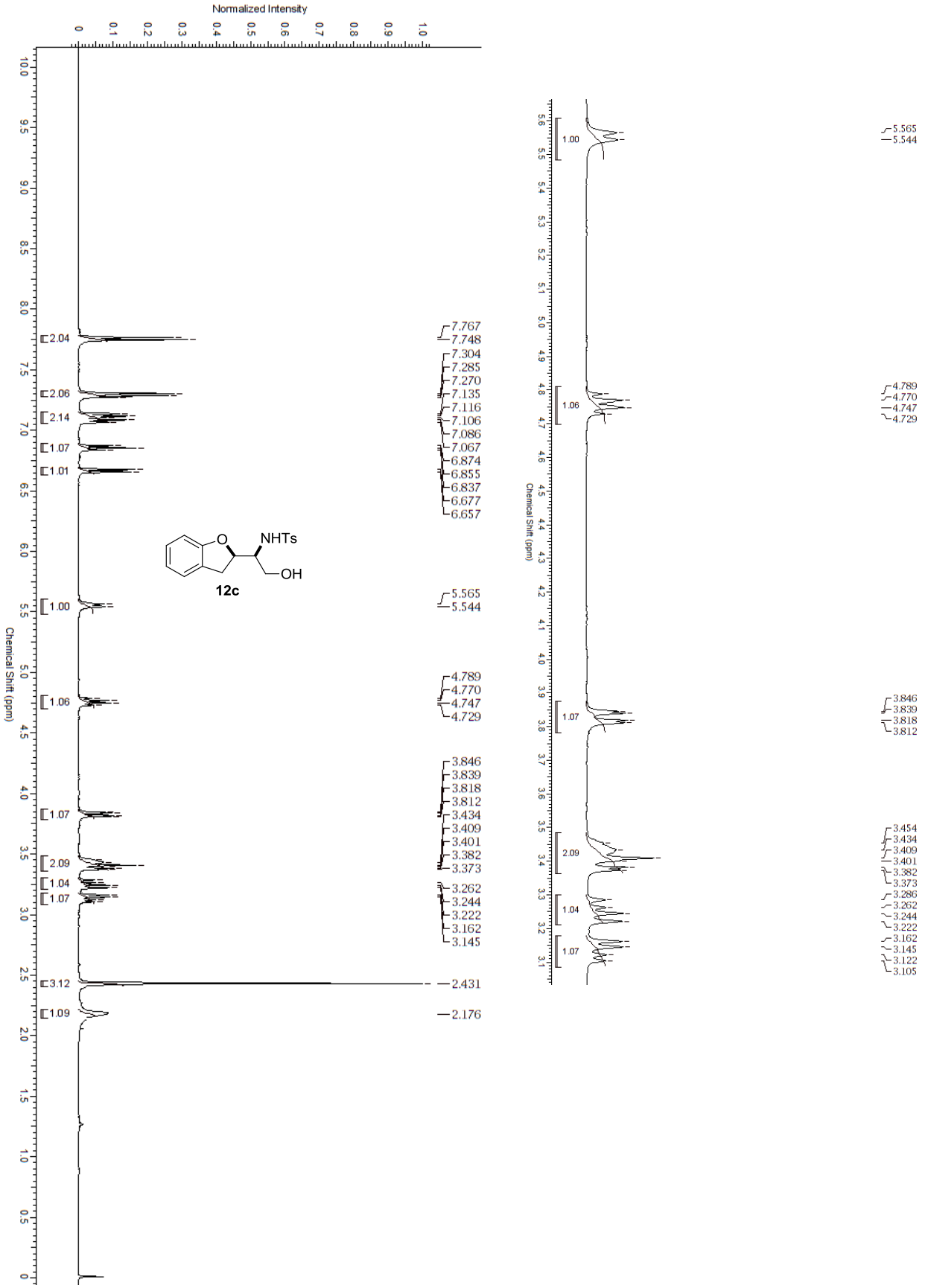
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 12a



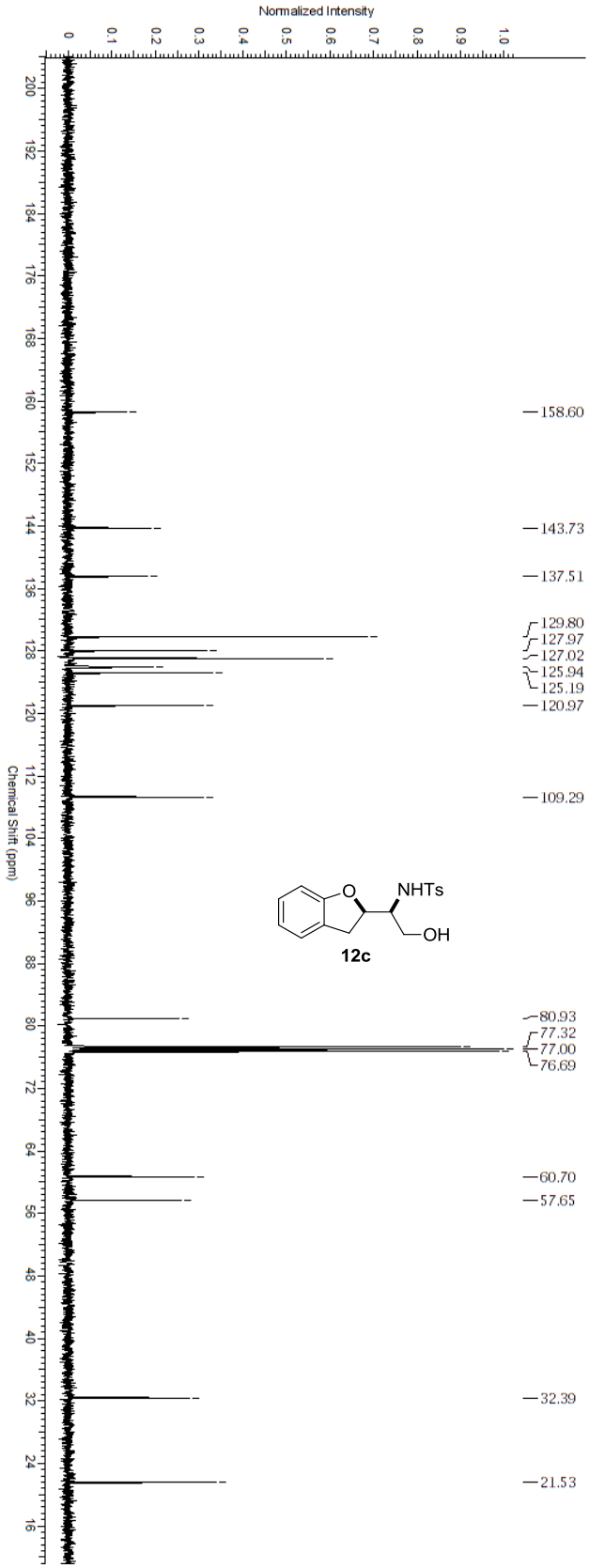
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 12b



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 12b

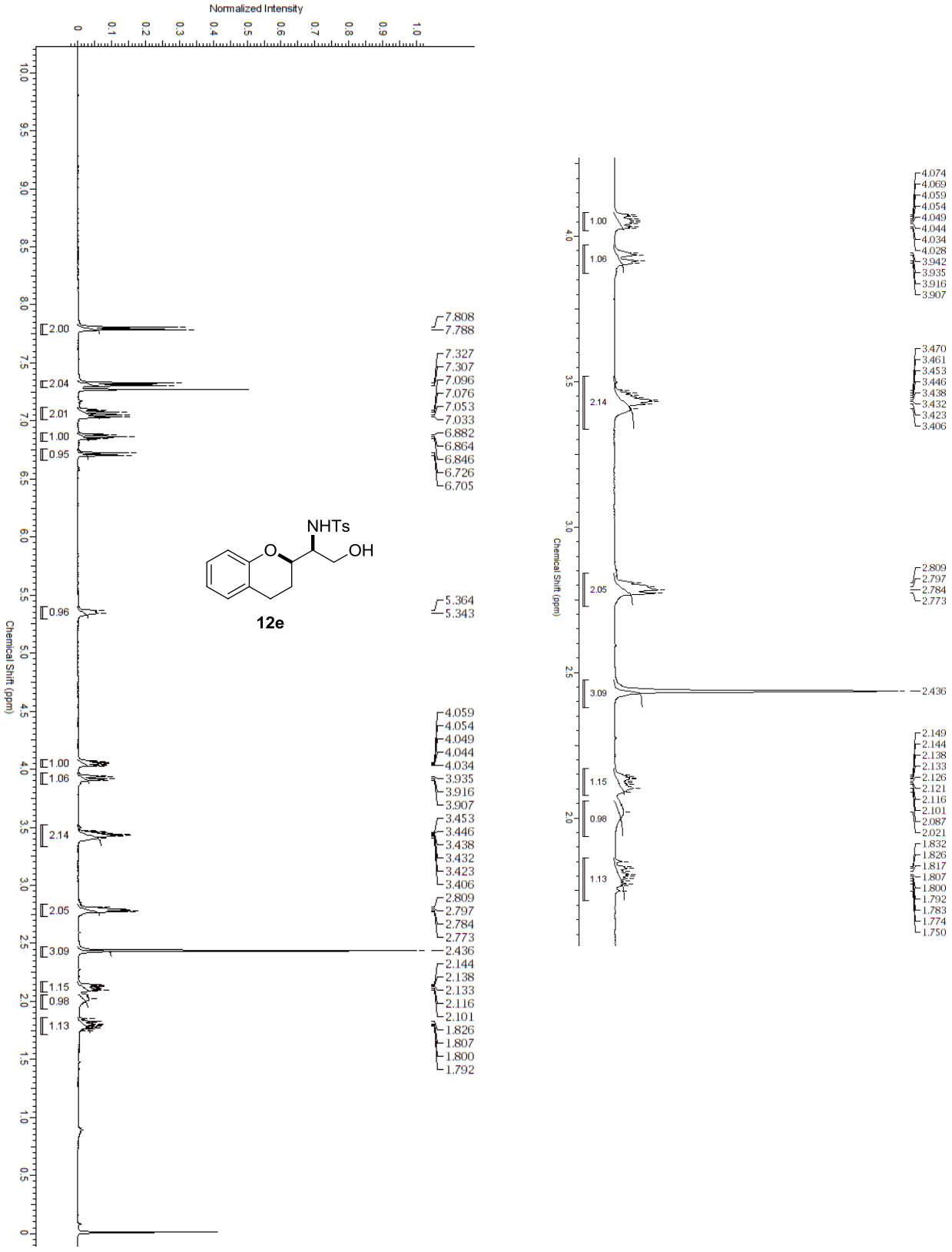


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 12c

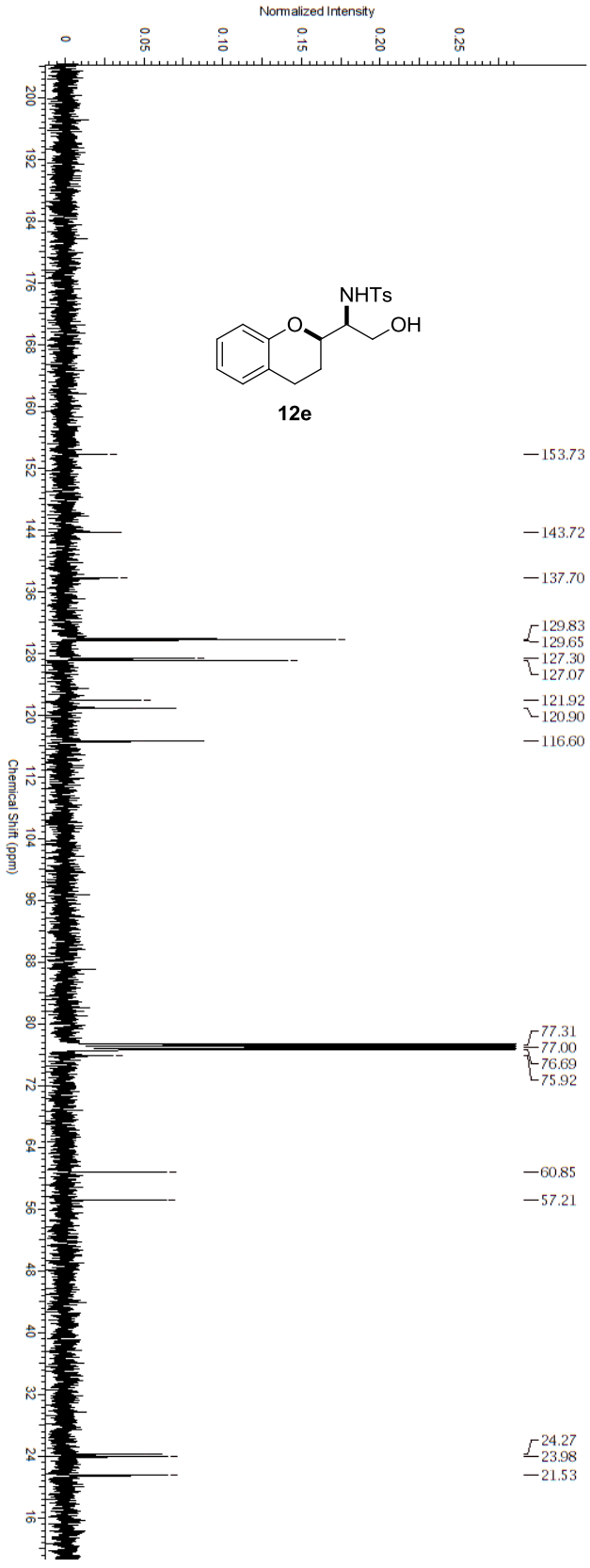


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 12c

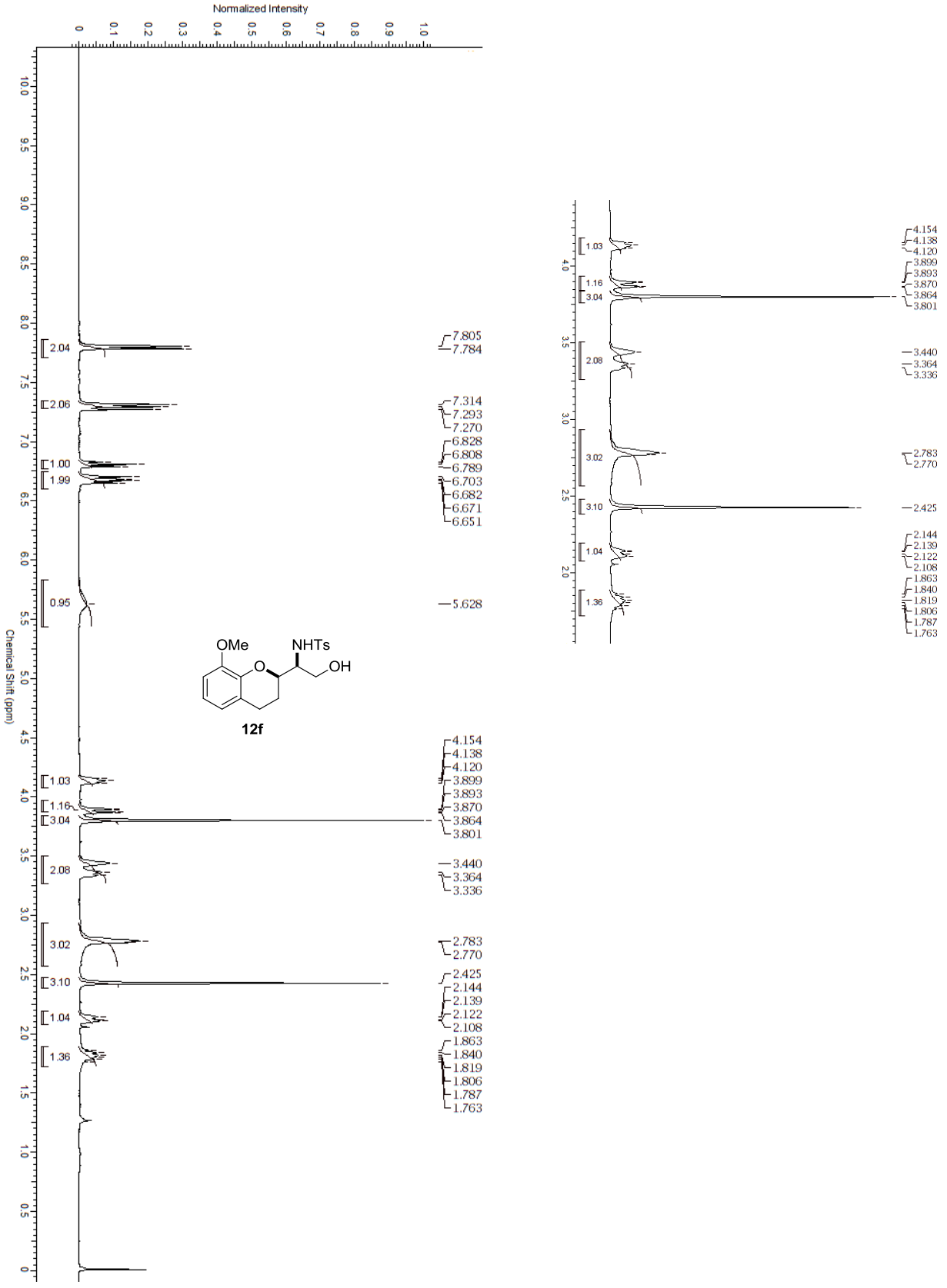
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 12d



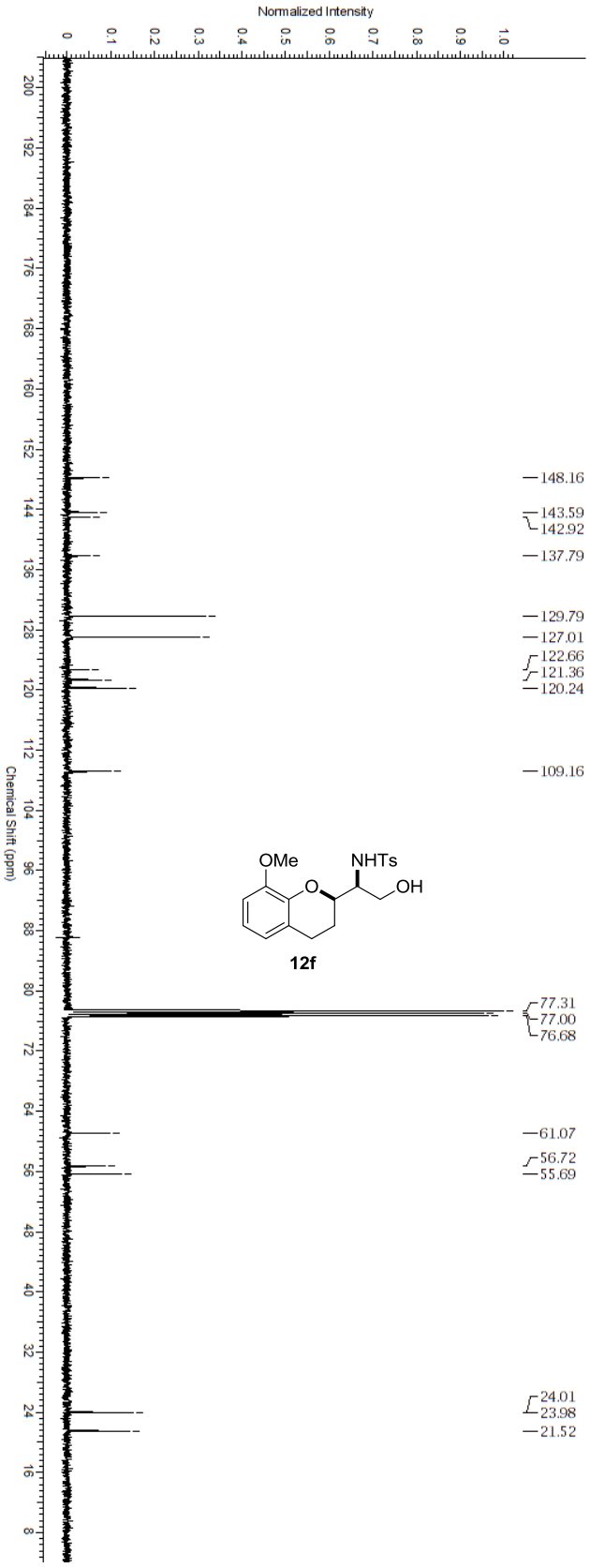
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 12e



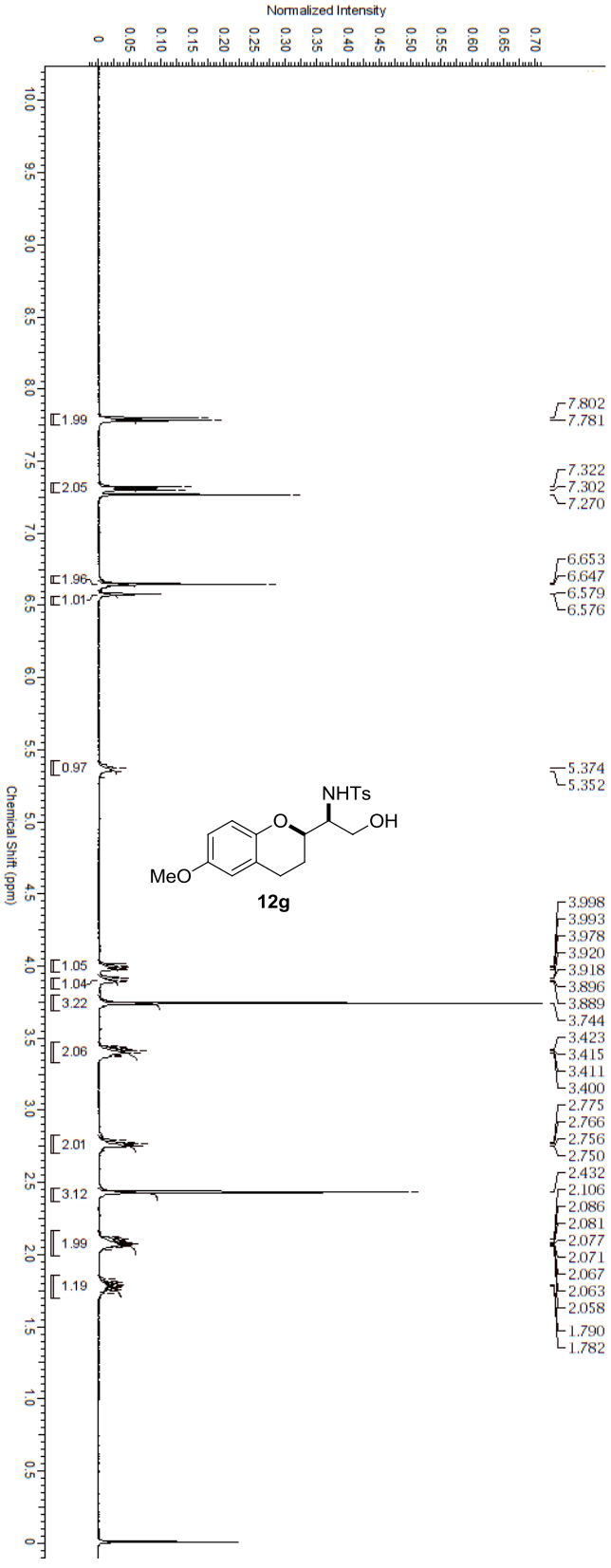
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 12e



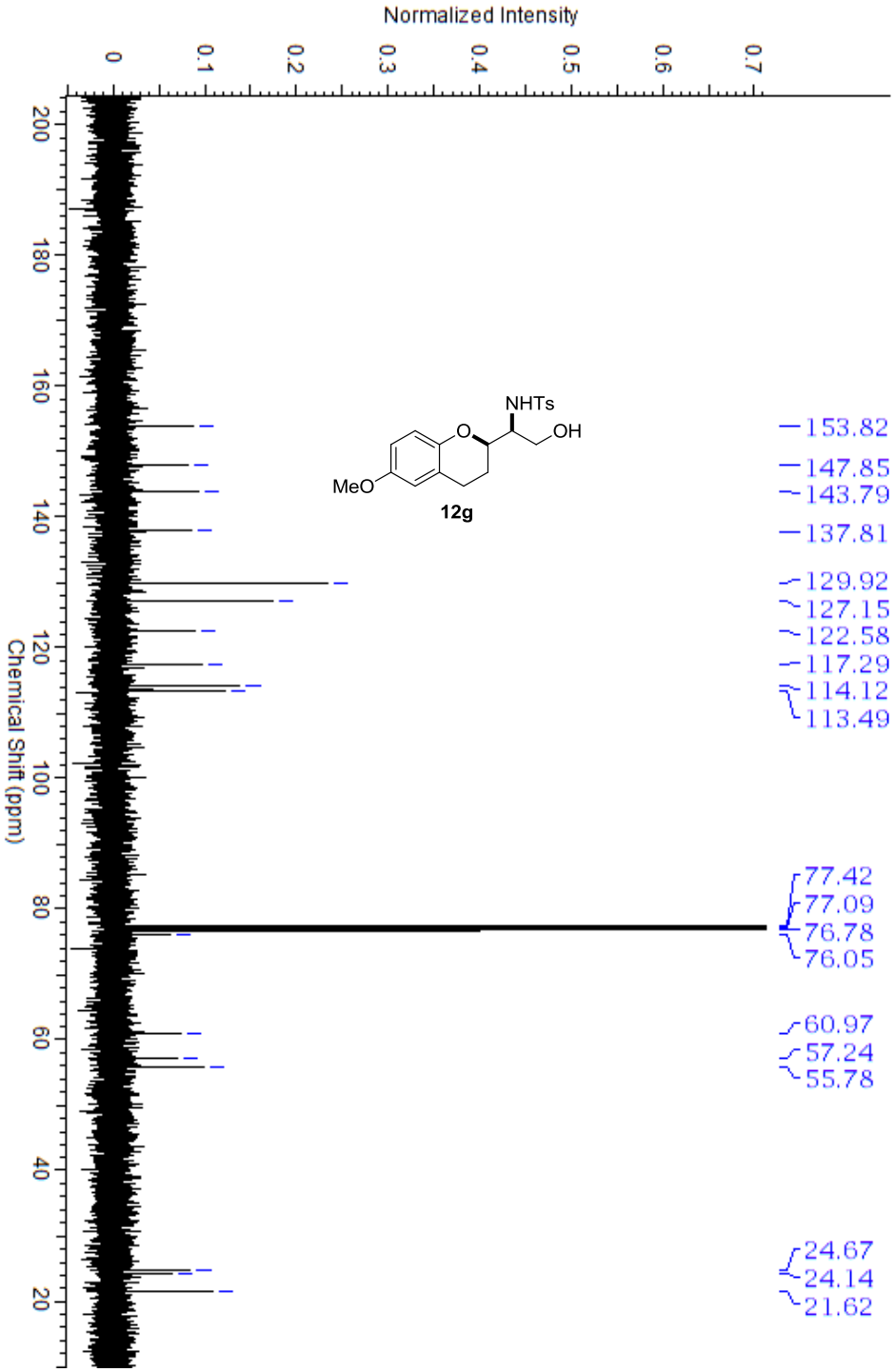
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 12f



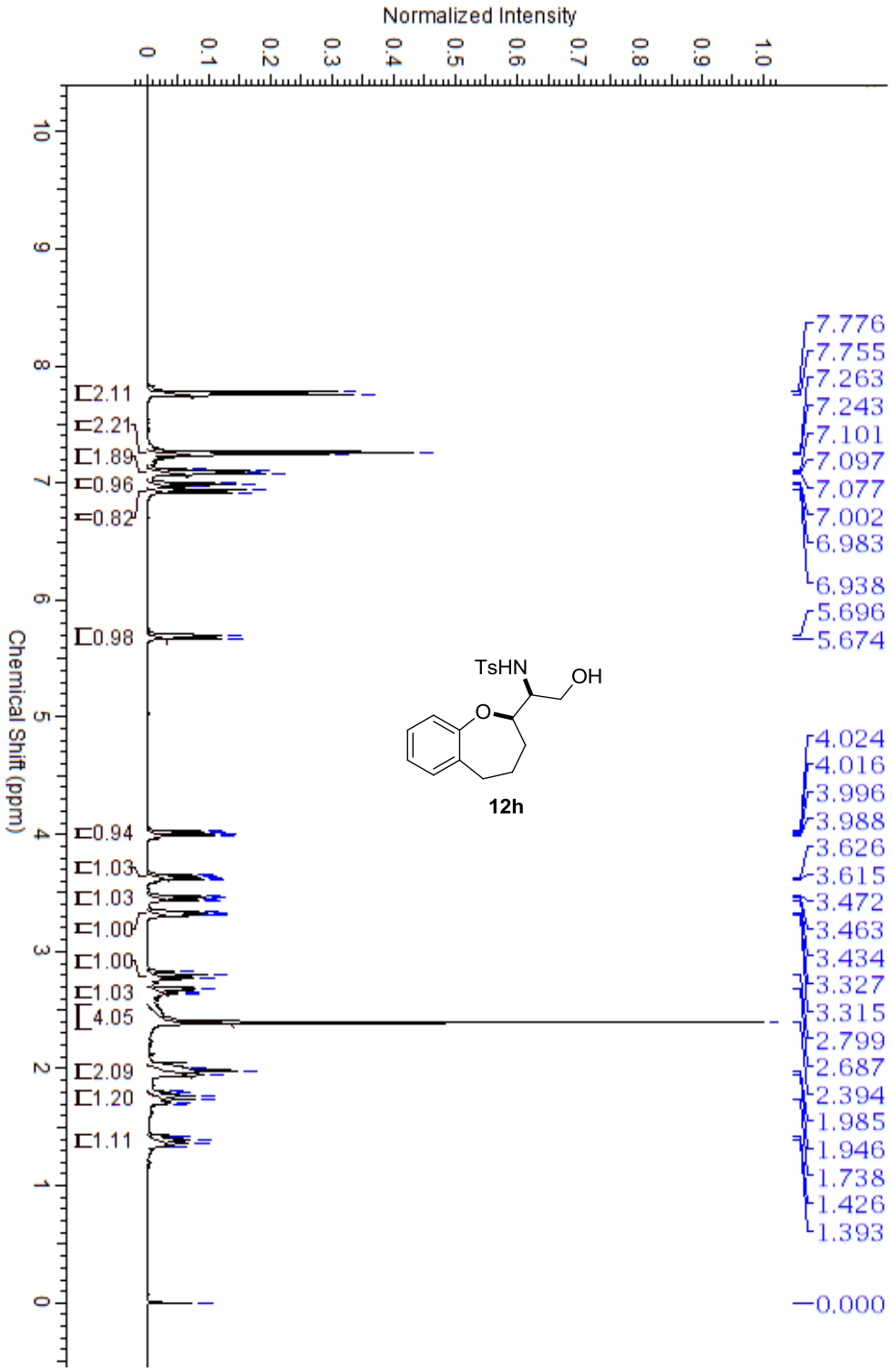
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 12f



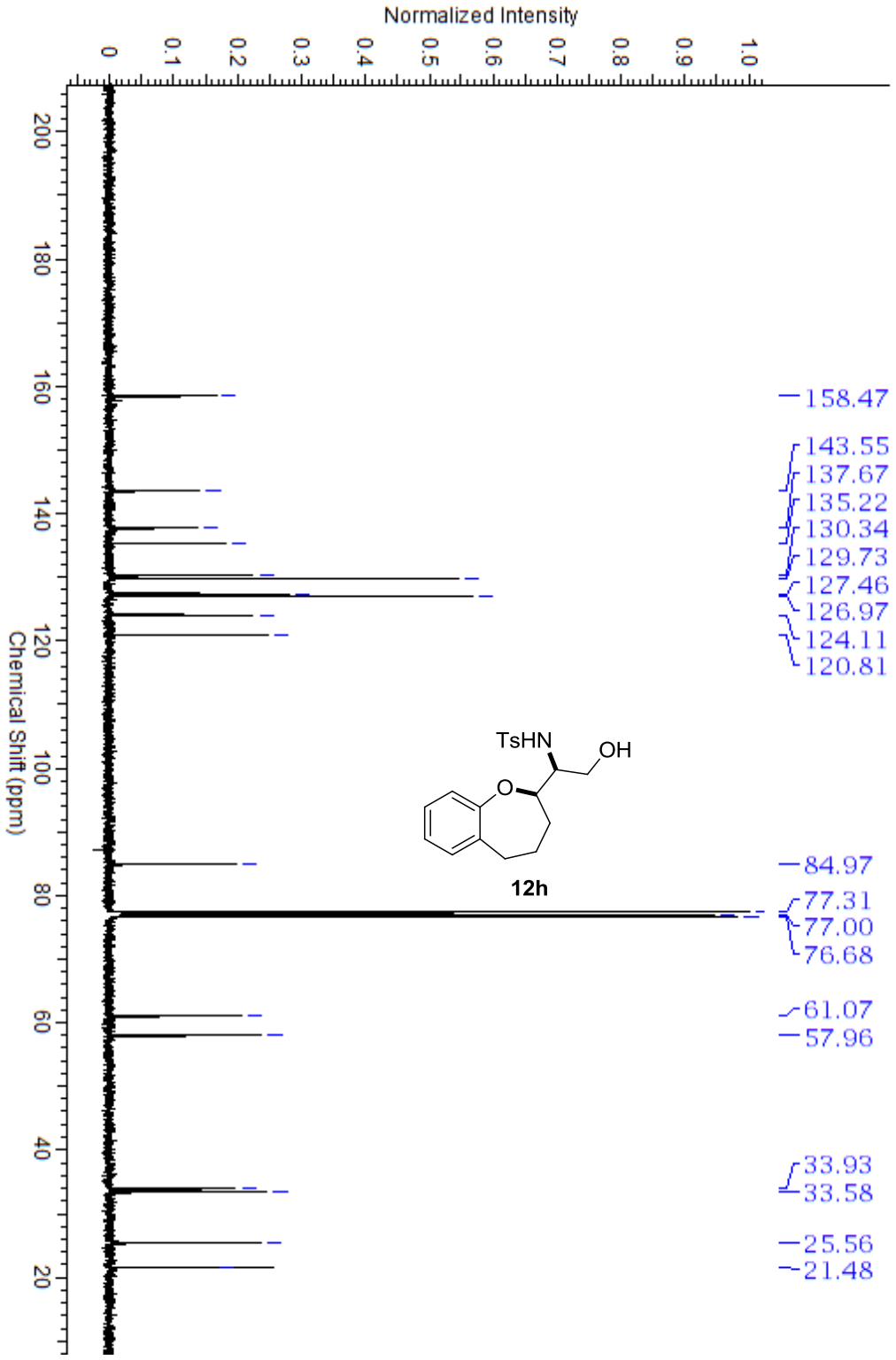
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 12g



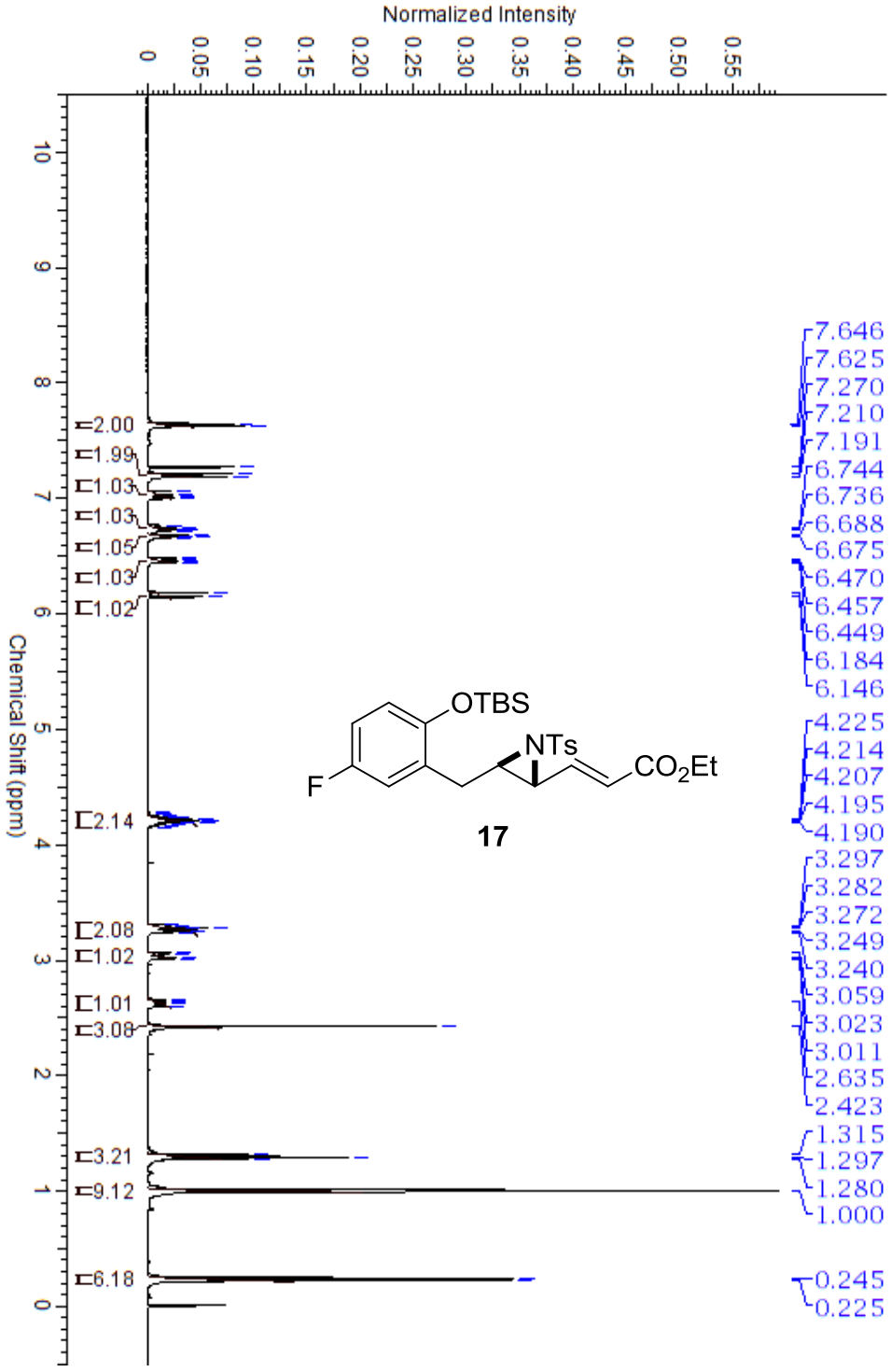
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 12g



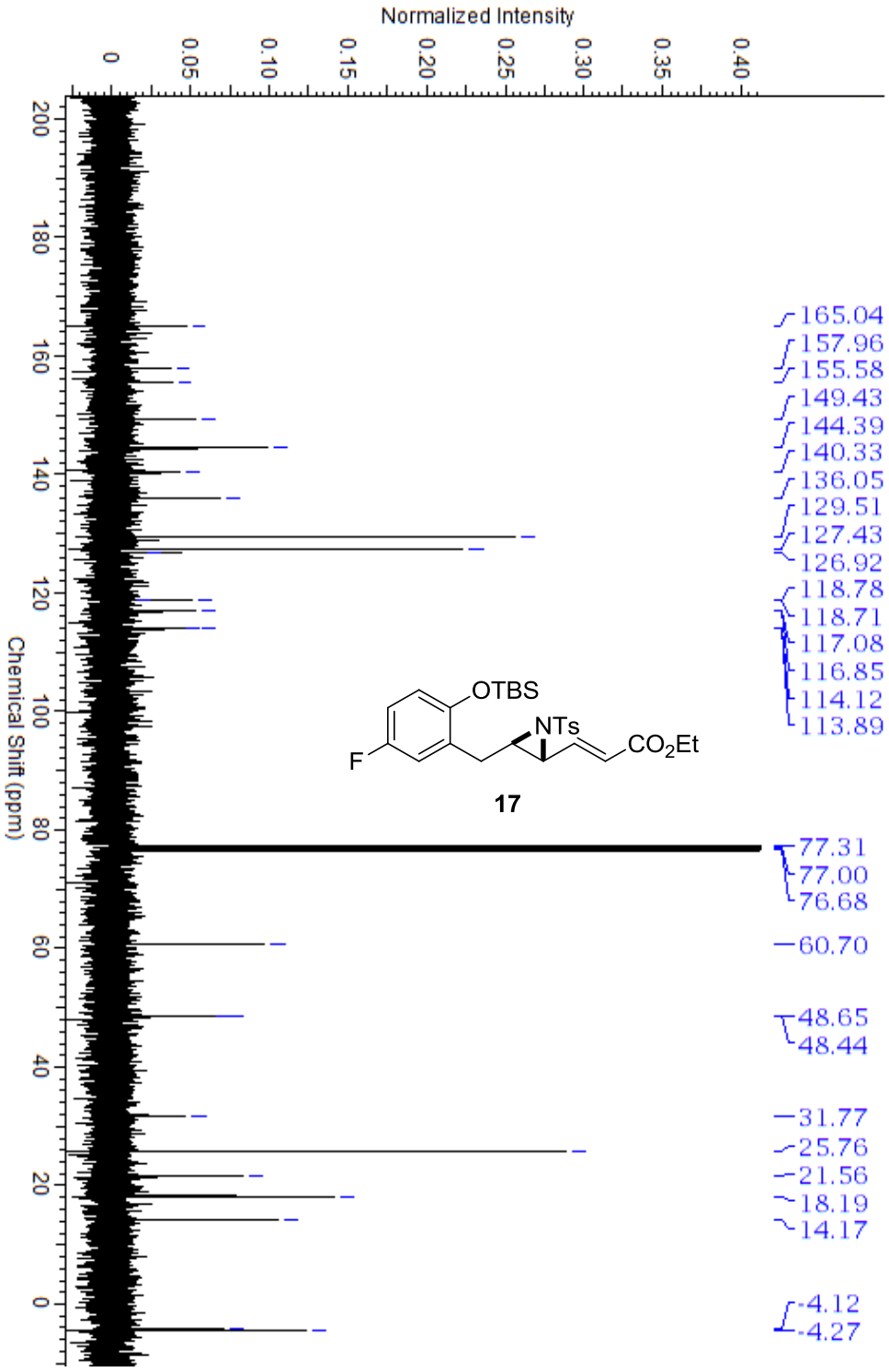
^{1}H NMR (400 MHz, $CDCl_3$) of 12h



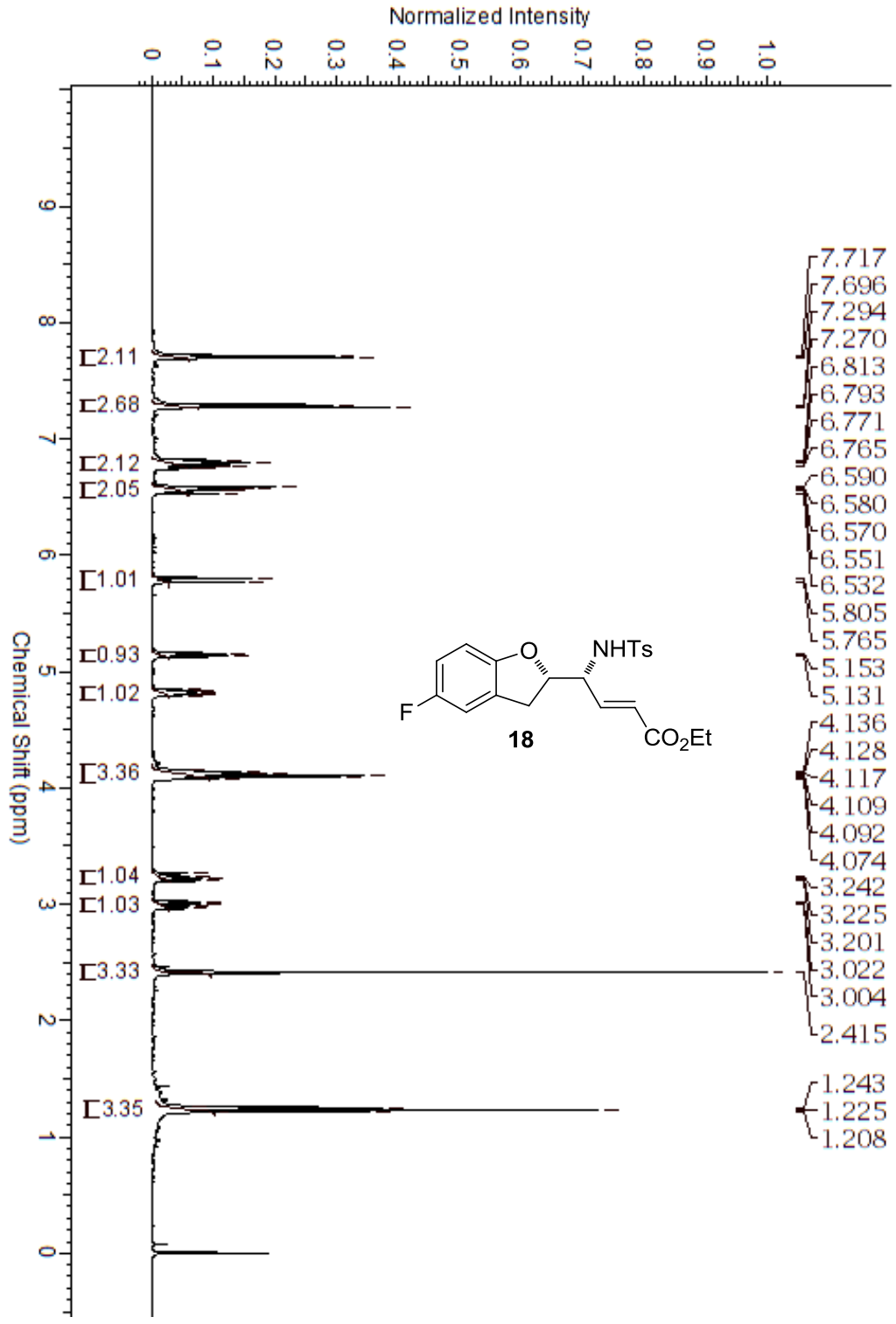
^{13}C NMR (100 MHz, $CDCl_3$) of 12h



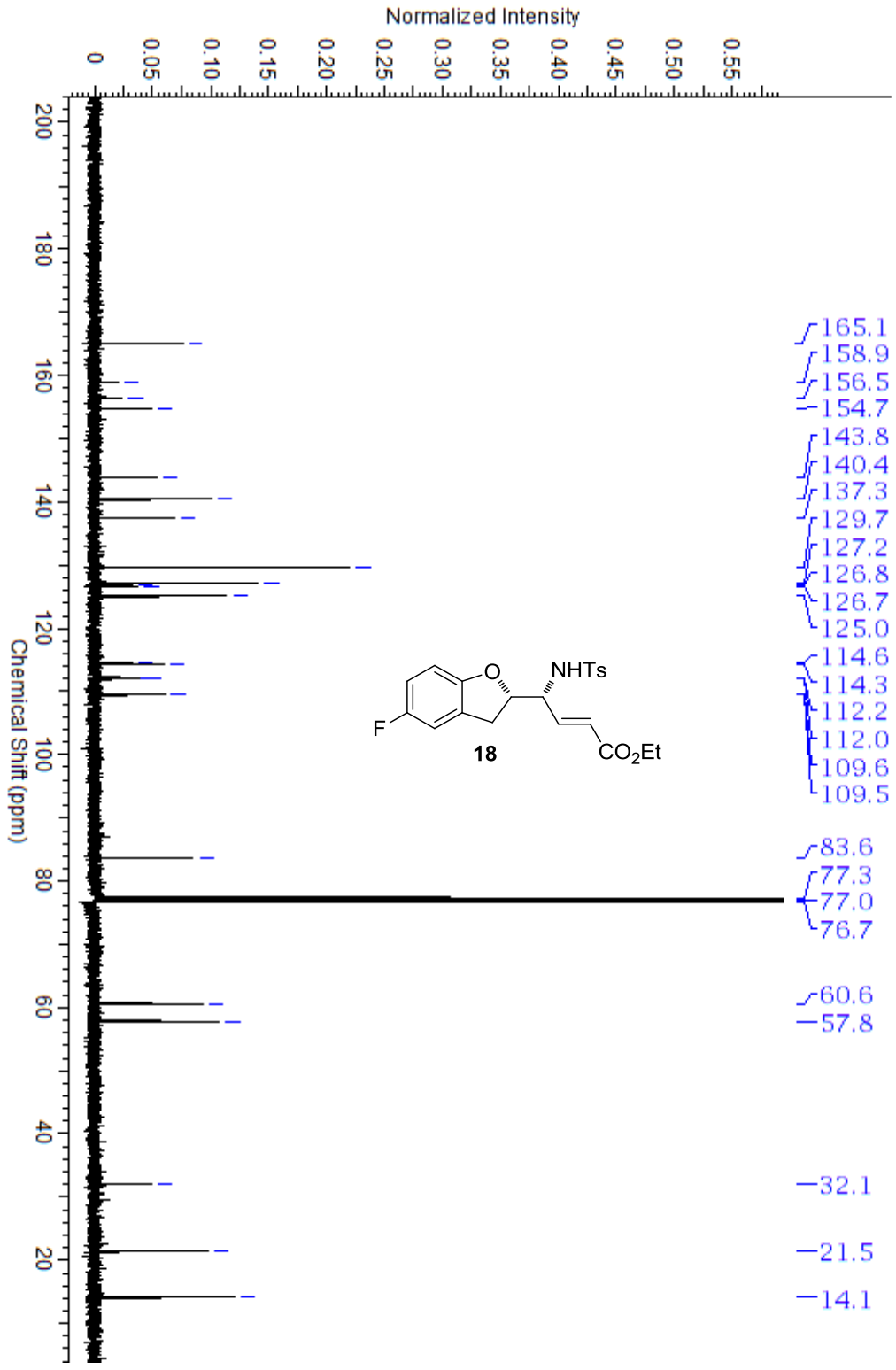
^{1}H NMR (400 MHz, $CDCl_3$) of 17



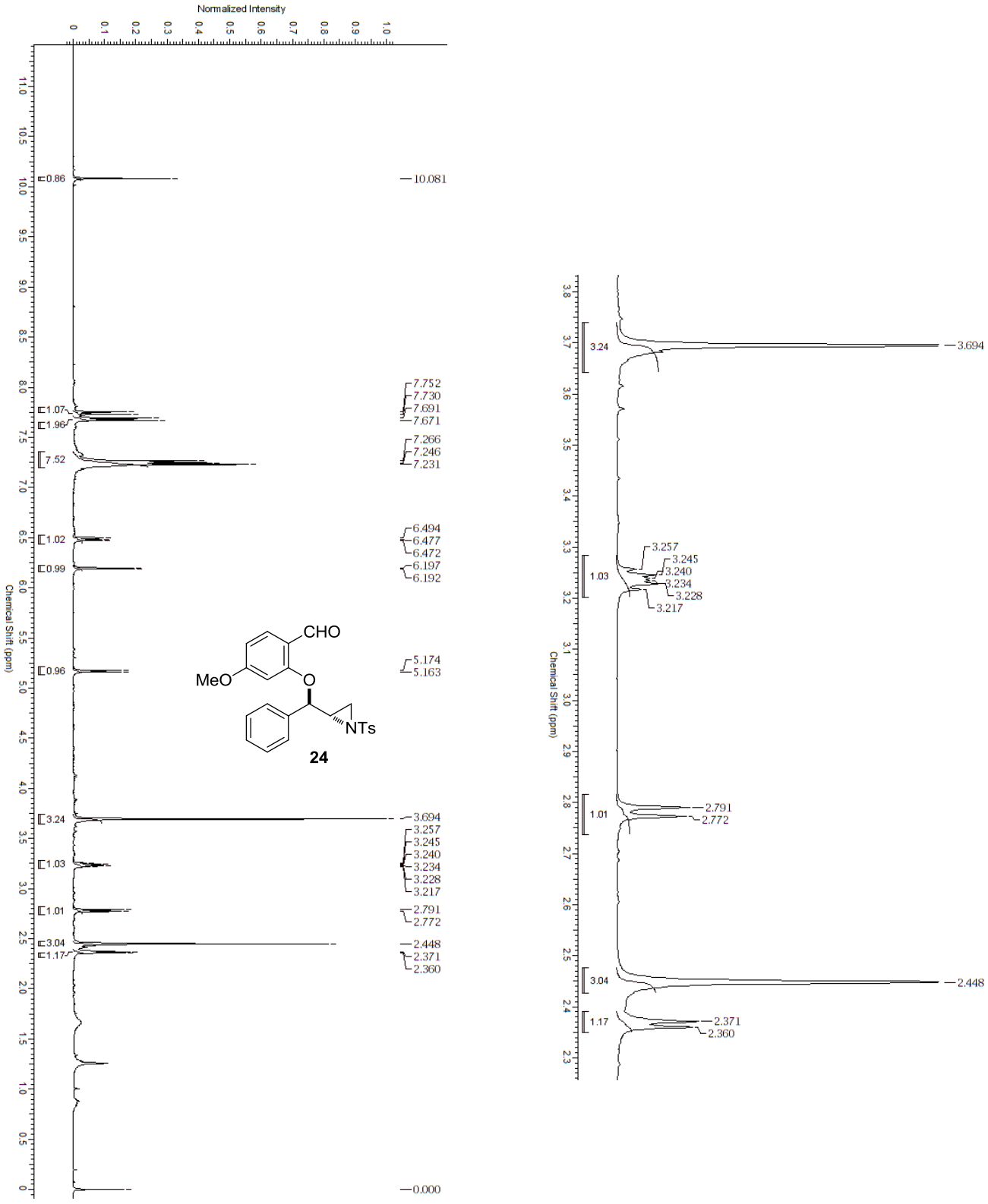
^{13}C NMR (100 MHz, $CDCl_3$) of 17



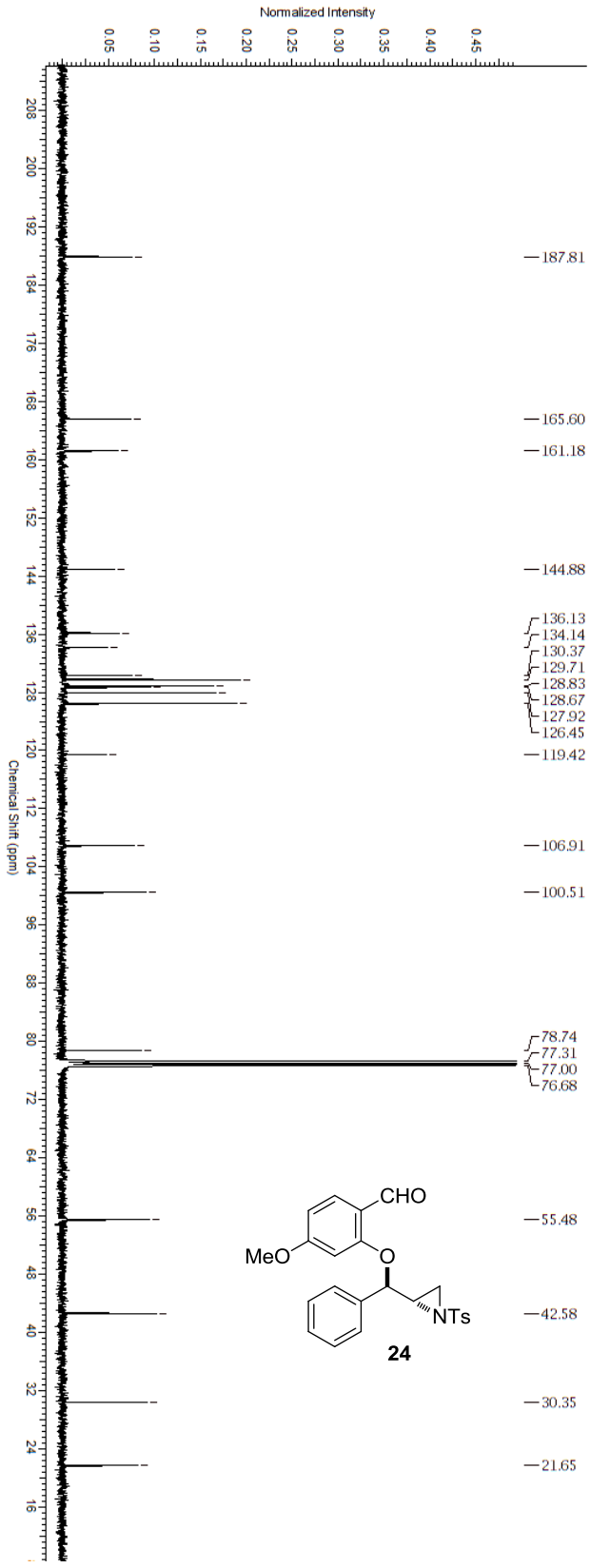
^{1}H NMR (400 MHz, $CDCl_3$) of 18



^{13}C NMR (100 MHz, $CDCl_3$) of 18

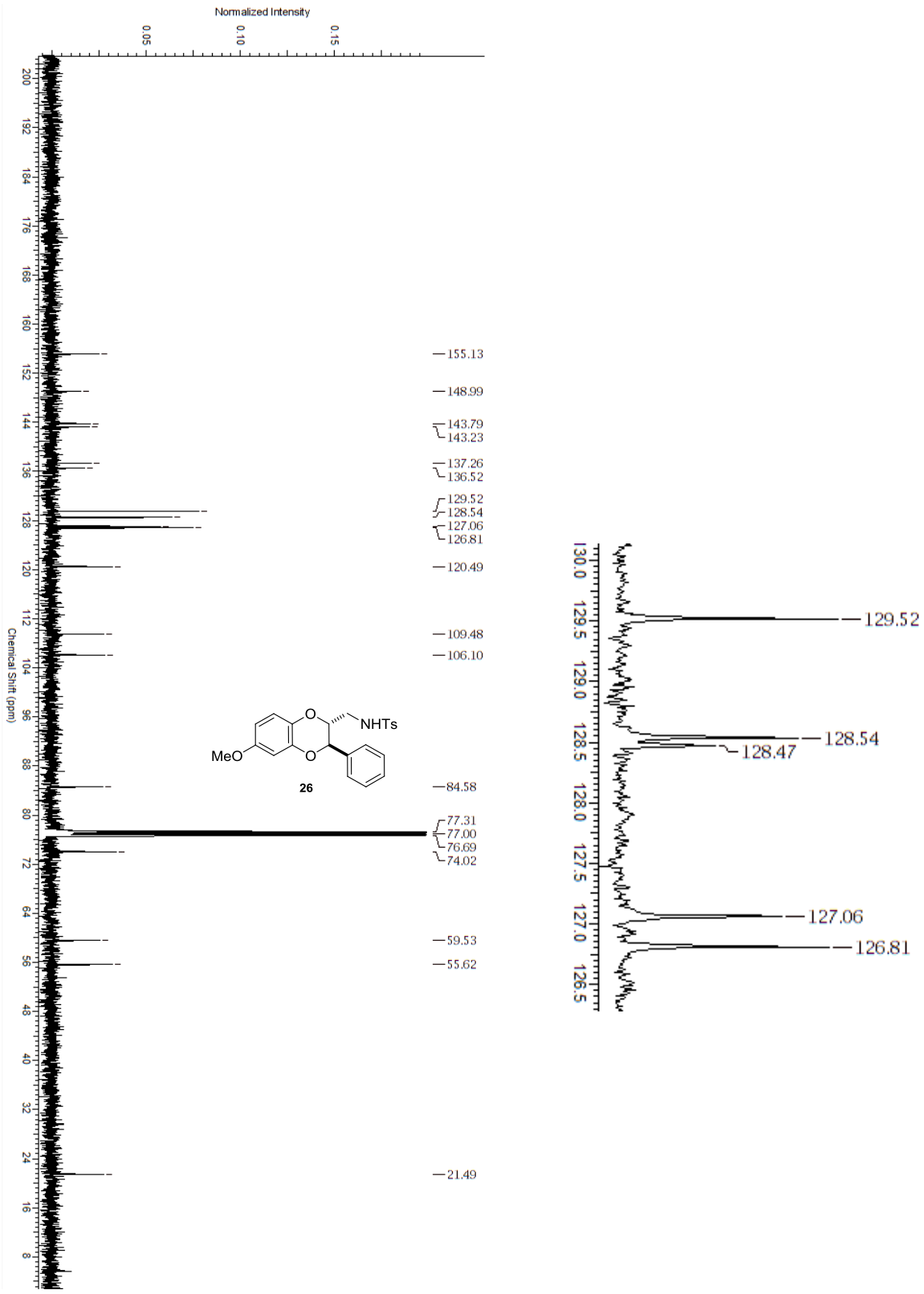


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 24



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 24

^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 26



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of 26