Supporting Information for

Metal carbonyl mediated rearrangement of ethyl 3-oxo-2-(1,2,4-oxadiazol-5-yl)propanoates: Synthesis of fully substituted pyrimidines

Ekaterina E. Galenko, Timur O. Zanakhov, Mikhail S. Novikov, and Alexander F. Khlebnikov*

Saint Petersburg State University, Institute of Chemistry, 7/9 Universitetskaya Naberezhnaya, St. Petersburg 199034, Russia

e-mail: a.khlebnikov@spbu.ru

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X-RAY DIFFRACTION EXPERIMENTS

Crystal structures of **3e** and **7** were determined by single crystal X-ray diffraction analysis. Suitable crystals were selected and fixed on micro-amounts and the diffraction data were collected on diffractometer. The crystals **3e** and **7** were measured at temperature 100 K, using monochromated CuKα radiation. The unit cell parameters and refinement characteristics of the crystal structures of **3e** and **7** are given below. Using Olex2[1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimization.

References

1. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J .A. K.; Puschmann, H. J. Appl. Cryst. 2009,

42, 339.

2. Sheldrick, G. M. Acta Cryst. 2015, A71, 3.

3. Sheldrick, G. M. Acta Cryst. 2015, C71, 3.

Ethyl 4-(4-fluorophenyl)-2-(4-methoxyphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate 3e

Single crystals of **3e** were obtained by slow recrystallization from methanol at room temperature (CCDC 2236696)

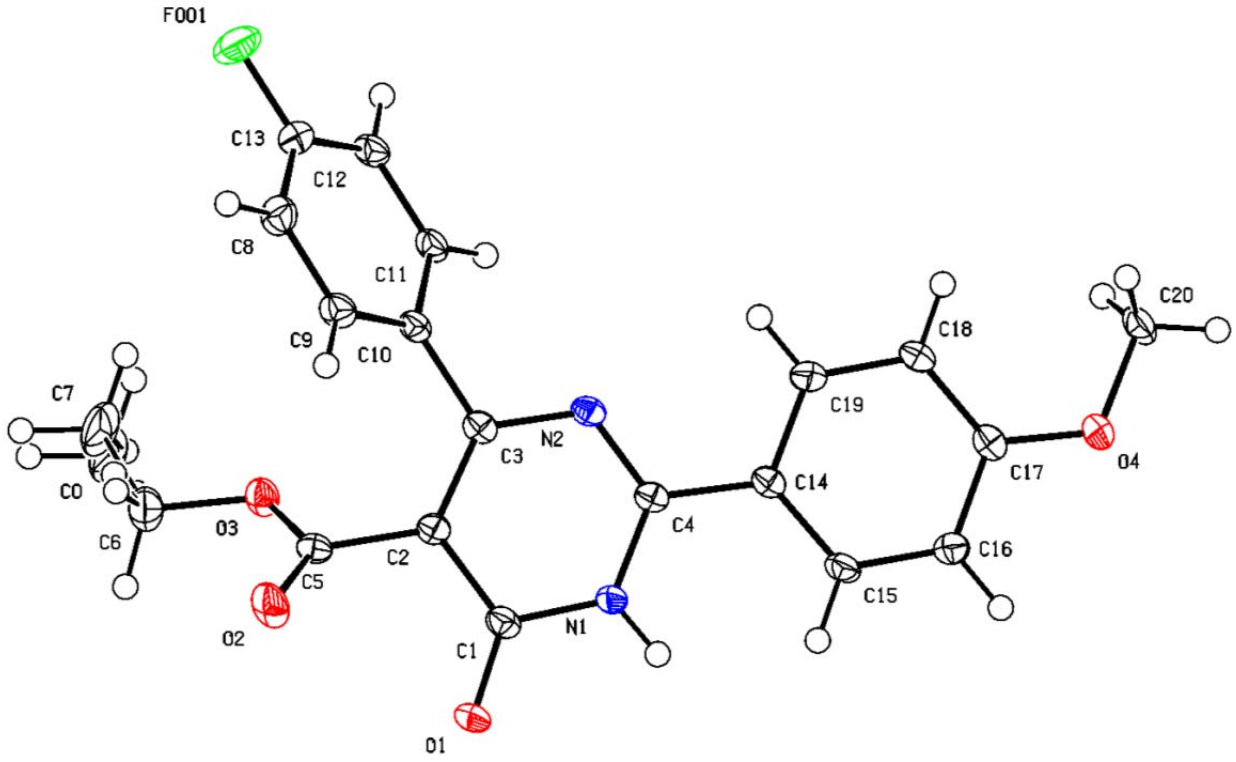


Figure S1. Molecular structure of compound **3e**, displacement parameters are drawn at 50% probability level.

Table S1. Crystal data and structure refinement for 3e.

Identification code	**3e** (176)
Empirical formula	$C_{20}H_{17}FN_2O_4$
Formula weight	368.35
Temperature/K	100.00(17)
Crystal system	triclinic
Space group	P-1
a/Å	7.0037(5)
b/Å	8.0678(4)
c/Å	16.6349(10)
α/°	96.374(5)
β/°	91.813(6)
γ/°	107.232(6)
Volume/Å^3	890.14(10)
Z	2
ρ_{calc}g/cm^3	1.374
μ/mm^{-1}	0.869
F(000)	384.0
Crystal size/mm^3	0.16 × 0.07 × 0.04
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.358 to 144.976
Index ranges	$-7 \le h \le 8$, $-9 \le k \le 6$, $-18 \le l \le 20$
Reflections collected	6796
Independent reflections	3509 [R_{int} = 0.0504, R_{sigma} = 0.0493]
Data/restraints/parameters	3509/0/250
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0525, wR_2 = 0.1404
Final R indexes [all data]	R_1 = 0.0628, wR_2 = 0.1527
Largest diff. peak/hole / e Å^{-3}	0.33/-0.30

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3e. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F001	10837.7(19)	8211.4(14)	9909.0(7)	33.4(3)
O3	5410.1(18)	2113.0(14)	8156.8(7)	20.4(3)
O4	8183.9(19)	7945.2(15)	2903.5(8)	21.1(3)
O2	6713(2)	3.7(16)	7673.8(8)	28.4(3)
O1	5221(2)	-205.2(15)	5964.2(8)	24.4(3)
N2	7973(2)	5034.1(17)	6304.9(9)	16.1(3)
N1	6407(2)	2399.0(17)	5478.4(9)	15.8(3)
C5	6333(2)	1351(2)	7607.4(11)	17.3(3)
C14	7511(2)	5128(2)	4874.8(10)	15.6(3)
C2	6774(2)	2340(2)	6895.3(10)	15.6(3)
C16	7089(2)	5296(2)	3442.1(11)	19.3(4)
C1	6086(2)	1391(2)	6105.1(11)	17.6(4)
C11	8167(2)	6773(2)	7941.1(11)	17.8(4)
C13	10092(3)	7215(2)	9190.2(11)	22.2(4)
C17	8002(2)	7109(2)	3571.7(11)	17.2(3)
C18	8668(3)	7919(2)	4352.6(12)	22.9(4)

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3e. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C12	8915(3)	7794(2)	8674.2(11)	20.6(4)
C3	7724(2)	4123(2)	6954.8(10)	15.6(3)
C10	8570(2)	5188(2)	7739.6(10)	16.2(3)
C9	9770(3)	4651(2)	8277.7(11)	20.3(4)
C15	6838(2)	4328(2)	4082.7(11)	18.6(4)
C4	7293(2)	4167(2)	5583.7(10)	14.7(3)
C19	8418(3)	6938(2)	4992.4(11)	22.5(4)
C8	10555(3)	5674(2)	9003.4(11)	23.0(4)
C6	4958(3)	1271(2)	8880.1(12)	26.9(4)
C20	8932(3)	9826(2)	3017.5(12)	23.2(4)
C0	3820(40)	2230(30)	9349(14)	40(2)
C7	4200(40)	2520(30)	9493(14)	40(2)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3e. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F001	46.6(7)	28.3(6)	23.2(6)	-8.0(5)	-8.1(5)	13.1(5)
O3	25.9(6)	18.4(6)	20.5(6)	5.1(5)	5.1(5)	10.8(5)
O4	27.3(6)	16.0(6)	19.9(6)	6.1(5)	2.0(5)	5.1(5)
O2	45.4(8)	18.7(6)	29.3(7)	8.9(5)	10.5(6)	19.2(6)
O1	36.5(7)	10.7(6)	21.9(7)	0.8(5)	3.5(5)	0.8(5)
N2	17.8(6)	11.4(6)	19.7(7)	0.9(5)	2.1(5)	5.9(5)
N1	19.8(6)	11.4(6)	15.3(7)	0.5(5)	2.6(5)	3.7(5)
C5	19.8(7)	12.4(7)	20.0(9)	0.6(6)	1.2(6)	5.8(6)
C14	14.5(7)	13.5(8)	19.7(9)	2.4(6)	3.3(6)	5.1(6)
C2	18.1(7)	12.8(7)	17.6(8)	0.9(6)	1.6(6)	7.8(6)
C16	20.9(8)	16.7(8)	18.8(9)	-0.3(6)	1.1(7)	4.3(6)
C1	18.7(7)	13.4(7)	20.9(9)	2.3(6)	4.7(7)	4.8(6)
C11	22.1(8)	12.2(7)	20.6(9)	5.1(6)	2.5(7)	6.2(6)
C13	27.8(9)	18.9(8)	17.8(9)	-0.1(7)	0.0(7)	5.0(7)
C17	15.6(7)	16.4(8)	21.9(9)	5.4(6)	3.8(6)	7.0(6)
C18	32.1(9)	11.2(7)	23.4(9)	2.9(6)	1.1(7)	3.2(6)
C12	28.6(8)	11.6(7)	22.6(9)	2.2(6)	4.8(7)	7.2(6)
C3	16.0(7)	13.5(7)	19.9(9)	2.3(6)	3.3(6)	8.1(6)
C10	18.0(7)	12.5(7)	18.9(8)	3.3(6)	3.8(6)	5.2(6)
C9	24.0(8)	15.2(8)	23.7(9)	2.9(6)	2.8(7)	8.7(6)
C15	22.0(8)	10.9(7)	21.7(9)	1.5(6)	2.8(7)	3.3(6)
C4	13.5(7)	12.9(7)	18.8(8)	0.9(6)	2.8(6)	5.7(5)
C19	30.6(9)	13.8(8)	20.6(9)	-0.1(6)	-0.7(7)	4.0(6)
C8	27.3(9)	22.9(8)	21.3(9)	4.7(7)	-0.9(7)	10.8(7)
C6	32.8(9)	28.2(9)	21.9(9)	7.7(7)	6.3(8)	10.7(7)
C20	29.9(9)	15.6(8)	25.8(9)	9.0(7)	6.5(7)	6.5(7)
C0	64(7)	44(7)	18(7)	2(5)	15(4)	24(5)
C7	64(7)	44(7)	18(7)	2(5)	15(4)	24(5)

Table S4. Bond Lengths for 3e.

Atom	Atom	Length/Å
F001	C13	1.359(2)
O3	C5	1.334(2)
O3	C6	1.445(2)
O4	C17	1.354(2)
O4	C20	1.4390(19)
O2	C5	1.209(2)
O1	C1	1.242(2)
N2	C3	1.361(2)
N2	C4	1.318(2)
N1	C1	1.376(2)
N1	C4	1.365(2)
C5	C2	1.491(2)
C14	C15	1.402(2)
C14	C4	1.469(2)
C14	C19	1.398(2)
C2	C1	1.437(2)
C2	C3	1.385(2)
C16	C17	1.400(2)
C16	C15	1.375(2)
C11	C12	1.386(2)
C11	C10	1.397(2)
C13	C12	1.381(3)
C13	C8	1.381(3)
C17	C18	1.387(3)
C18	C19	1.380(3)
C3	C10	1.481(2)
C10	C9	1.396(2)
C9	C8	1.382(3)
C6	C0	1.46(3)
C6	C7	1.57(3)

Table S5. Bond Angles for 3e.

Atom	Atom	Atom	Angle/°
C5	O3	C6	115.68(13)
C17	O4	C20	117.80(14)
C4	N2	C3	118.06(14)
C4	N1	C1	123.64(14)
O3	C5	C2	111.50(13)
O2	C5	O3	123.87(16)
O2	C5	C2	124.60(15)
C15	C14	C4	123.50(14)
C19	C14	C15	117.87(16)
C19	C14	C4	118.63(15)
C1	C2	C5	117.57(14)
C3	C2	C5	123.90(15)
C3	C2	C1	118.46(15)
C15	C16	C17	120.40(16)
O1	C1	N1	119.97(15)
O1	C1	C2	125.19(16)
N1	C1	C2	114.82(14)
C12	C11	C10	120.61(16)
F001	C13	C12	118.57(15)
F001	C13	C8	118.69(16)
C12	C13	C8	122.73(17)
O4	C17	C16	116.02(15)
O4	C17	C18	124.62(15)
C18	C17	C16	119.35(16)
C19	C18	C17	119.92(16)
C13	C12	C11	118.20(15)
N2	C3	C2	123.27(15)
N2	C3	C10	114.63(13)
C2	C3	C10	122.10(15)
C11	C10	C3	119.05(15)
C9	C10	C11	119.41(16)
C9	C10	C3	121.54(14)
C8	C9	C10	120.48(15)
C16	C15	C14	120.89(15)
N2	C4	N1	121.67(15)
N2	C4	C14	119.05(14)
N1	C4	C14	119.28(15)
C18	C19	C14	121.55(17)
C13	C8	C9	118.55(16)
O3	C6	C0	105.8(12)
O3	C6	C7	107.1(11)

Table S6. Torsion Angles for 3e.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
F001	C13	C12	C11	179.77(15)	C12	C13	C8	C9	-1.5(3)
F001	C13	C8	C9	179.01(15)	C3	N2	C4	N1	-1.7(2)
O3	C5	C2	C1	-126.50(15)	C3	N2	C4	C14	178.89(13)
O3	C5	C2	C3	50.6(2)	C3	C2	C1	O1	179.73(16)
O4	C17	C18	C19	-179.59(16)	C3	C2	C1	N1	-1.8(2)
O2	C5	C2	C1	51.8(2)	C3	C10	C9	C8	179.47(16)
O2	C5	C2	C3	-131.17(19)	C10	C11	C12	C13	1.1(3)
N2	C3	C10	C11	47.4(2)	C10	C9	C8	C13	1.3(3)
N2	C3	C10	C9	-132.12(16)	C15	C14	C4	N2	-179.99(14)
C5	O3	C6	C0	-175.2(7)	C15	C14	C4	N1	0.5(2)
C5	O3	C6	C7	171.4(8)	C15	C14	C19	C18	-0.6(3)
C5	C2	C1	O1	-3.0(2)	C15	C16	C17	O4	179.88(14)
C5	C2	C1	N1	175.39(13)	C15	C16	C17	C18	0.5(3)
C5	C2	C3	N2	-174.48(14)	C4	N2	C3	C2	-0.8(2)
C5	C2	C3	C10	6.0(2)	C4	N2	C3	C10	178.73(13)
C2	C3	C10	C11	-133.13(17)	C4	N1	C1	O1	178.06(14)
C2	C3	C10	C9	47.4(2)	C4	N1	C1	C2	-0.5(2)
C16	C17	C18	C19	-0.3(3)	C4	C14	C15	C16	-179.84(14)
C1	N1	C4	N2	2.3(2)	C4	C14	C19	C18	-179.97(15)
C1	N1	C4	C14	-178.23(13)	C19	C14	C15	C16	0.8(2)
C1	C2	C3	N2	2.6(2)	C19	C14	C4	N2	-0.7(2)
C1	C2	C3	C10	-176.92(13)	C19	C14	C4	N1	179.88(14)
C11	C10	C9	C8	0.0(3)	C8	C13	C12	C11	0.2(3)
C17	C16	C15	C14	-0.8(3)	C6	O3	C5	O2	3.1(2)
C17	C18	C19	C14	0.4(3)	C6	O3	C5	C2	-178.65(14)
C12	C11	C10	C3	179.27(15)	C20	O4	C17	C16	174.00(14)
C12	C11	C10	C9	-1.2(2)	C20	O4	C17	C18	-6.7(2)

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3e.

Atom	*x*	*y*	*z*	U(eq)
H1	6018.97	1874.7	4982.16	19
H16	6639.49	4731.51	2908.3	23
H11	7372.86	7154.69	7572.12	21
H18	9295.58	9146.85	4447	28
H12	8624.84	8862.08	8817.87	25
H9	10048.76	3573.98	8143.76	24
H15	6201.02	3101.97	3987.29	22
H19	8872.44	7507.1	5525.04	27
H8	11395.31	5324.81	9365.94	28
H6BC	6207.78	1327.35	9192.38	32
H6BD	4160.59	28.68	8738.44	32
H6AA	6172.6	1071.43	9118.2	32
H6AB	3911.5	128.14	8749.72	32
H20A	8890	10265.72	2493.35	35
H20B	10316.55	10197.26	3251.7	35

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3e.

Atom	*x*	*y*	*z*	U(eq)
H20C	8097.39	10294.37	3385.06	35
H0A	4589.06	3471.12	9450.08	61
H0B	3543.03	1764.49	9867.36	61
H0C	2546.67	2097.95	9045.48	61
H7A	5204.96	3677.98	9585.82	61
H7B	3971.1	2036.96	10008.44	61
H7C	2938.83	2639.63	9268	61

Table S8. Atomic Occupancy for 3e.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
H6BC	0.5	H6BD	0.5	H6AA	0.5
H6AB	0.5	C0	0.5	H0A	0.5
H0B	0.5	H0C	0.5	C7	0.5
H7A	0.5	H7B	0.5	H7C	0.5

Ethyl 2-phenyl-4-(phenyl(pyridin-2-yl)amino)-6-(p-tolyl)pyrimidine-5-carboxylate 8

Single crystals of **8** were obtained by slow recrystallization from methanol at room temperature (CCDC 2236697)

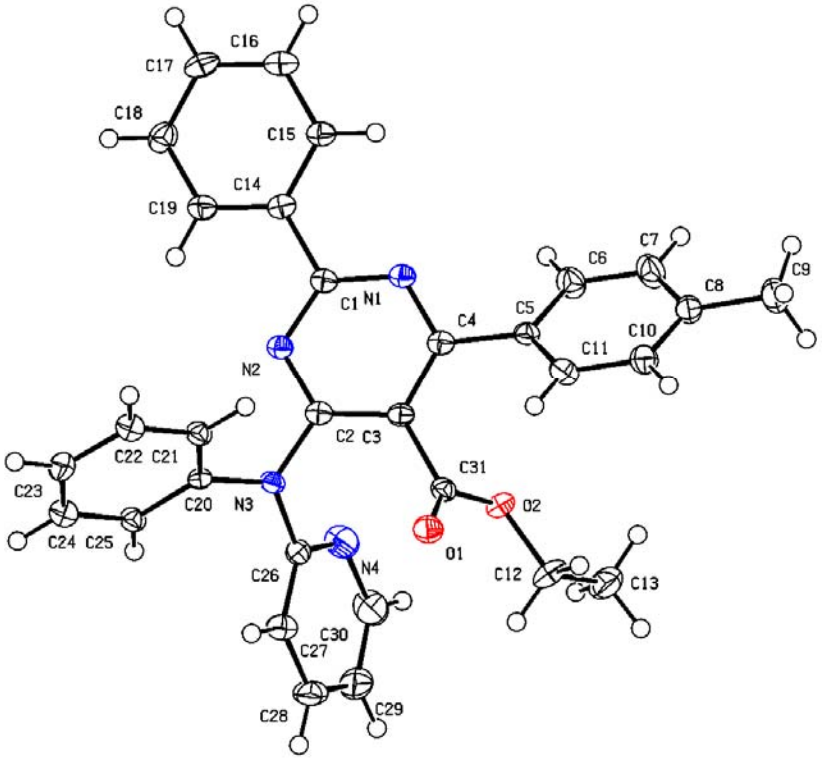


Figure S2. Molecular structure of compound **8**, displacement parameters are drawn at 50% probability level.

Table S9. Crystal data and structure refinement for 8.

Identification code	22-172
Empirical formula	$C_{31}H_{26}N_4O_2$
Formula weight	486.56
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.0365(3)
b/Å	7.74810(10)
c/Å	20.9647(4)
α/°	90
β/°	107.459(2)
γ/°	90
Volume/Å^3	2484.91(8)
Z	4
ρ_{calc}g/cm^3	1.301
μ/mm^{-1}	0.661
F(000)	1024.0
Crystal size/mm^3	0.04 × 0.02 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.778 to 144.97
Index ranges	-19 ≤ h ≤ 19, -9 ≤ k ≤ 5, -25 ≤ l ≤ 25

Reflections collected	16192
Independent reflections	4865 [R_{int} = 0.0417, R_{sigma} = 0.0393]
Data/restraints/parameters	4865/0/324
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0485, wR_2 = 0.1155
Final R indexes [all data]	R_1 = 0.0568, wR_2 = 0.1201
Largest diff. peak/hole / e $Å^{-3}$	0.45/-0.36

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 8. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O2	5785.9(7)	3344.3(15)	1154.6(5)	20.6(3)
O1	6520.8(8)	5092.4(16)	650.2(6)	23.9(3)
N3	8278.0(9)	4320.7(17)	1752.8(7)	17.4(3)
N1	6802.4(9)	6462.1(17)	2864.6(7)	18.1(3)
N2	8169.3(9)	5656.4(17)	2717.7(7)	17.9(3)
C21	9007.5(11)	6975(2)	1728.1(8)	19.1(2)
C20	9048.2(10)	5222(2)	1747.9(7)	16.5(3)
C1	7672.0(10)	6317(2)	3072.4(8)	17.1(3)
C3	6839.9(10)	5154(2)	1840.5(8)	17.1(3)
N4	7594.1(11)	1610(2)	1697.9(9)	32.4(4)
C26	8035.1(10)	2724(2)	1418.5(8)	18.5(3)
C4	6382.3(11)	5913(2)	2244.5(8)	17.5(3)
C14	8131.3(11)	6930(2)	3758.8(8)	18.3(3)
C31	6376.6(10)	4546(2)	1146.3(8)	18.1(3)
C2	7749.0(10)	5057.0(19)	2109.5(8)	16.6(3)
C5	5425.7(10)	6209(2)	2019.9(8)	18.4(3)
C15	7673.7(11)	7883(2)	4112.3(8)	20.6(3)
C25	9815.3(10)	4349(2)	1765.0(8)	19.1(2)
C19	9018.4(11)	6597(2)	4057.1(8)	22.5(4)
C8	3616.0(11)	6830(2)	1642.6(9)	24.6(4)
C16	8105.9(12)	8528(2)	4744.2(8)	24.6(4)
C11	4986.6(11)	6800(2)	1380.2(9)	23.9(4)
C22	9736.7(11)	7898(2)	1732.6(9)	25.8(3)
C17	8991.2(12)	8228(2)	5027.4(8)	25.6(4)
C27	8218.4(12)	2346(2)	824.2(8)	23.9(4)
C23	10513.7(11)	7091(2)	1750.6(9)	26.6(4)
C18	9445.4(12)	7246(2)	4686.7(9)	25.9(4)
C24	10547.4(12)	5306(2)	1763.9(9)	25.8(3)
C10	4093.3(11)	7109(2)	1195.9(9)	25.6(4)
C6	4952.1(12)	5936(3)	2469.9(9)	27.3(4)
C28	7943.0(13)	777(2)	515.0(9)	30.4(4)
C12	5251.0(12)	2732(2)	505.2(9)	28.2(4)
C7	4061.3(12)	6248(3)	2279.2(10)	31.1(4)
C29	7479.5(13)	-362(3)	786.8(11)	35.3(5)
C9	2650.8(12)	7187(3)	1444.6(11)	34.9(4)
C13	4677.6(14)	1338(3)	632.0(10)	36.9(5)
C30	7315.2(14)	93(3)	1374.1(12)	38.0(5)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 8. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	23.7(6)	20.0(6)	16.3(5)	-2.7(4)	3.2(4)	-3.4(5)
O1	25.9(6)	29.2(7)	17.5(6)	1.7(5)	8.0(5)	0.1(5)
N3	18.4(6)	16.0(6)	19.7(6)	-3.3(5)	8.6(5)	-0.1(5)
N1	21.1(7)	16.2(6)	17.9(6)	-1.4(5)	7.3(5)	-0.2(5)
N2	20.0(7)	16.6(6)	17.9(6)	-1.3(5)	7.1(5)	-0.6(5)
C21	19.6(5)	18.5(6)	19.5(5)	-1.0(4)	6.2(4)	2.9(5)
C20	17.3(7)	20.7(8)	11.6(7)	-1.8(6)	4.4(6)	-0.2(6)
C1	21.8(8)	12.8(7)	17.8(8)	0.9(6)	7.7(6)	-0.4(6)
C3	21.4(8)	14.1(7)	16.5(7)	-0.2(6)	6.7(6)	0.1(6)
N4	35.2(9)	26.3(8)	40.0(9)	-2.2(7)	17.7(7)	-2.8(7)
C26	18.0(7)	15.9(8)	20.2(8)	-0.6(6)	3.4(6)	3.3(6)
C4	22.2(8)	13.2(7)	18.2(7)	0.5(6)	7.8(6)	-1.5(6)
C14	24.5(8)	14.8(7)	16.2(7)	0.7(6)	7.2(6)	-2.9(6)
C31	18.3(7)	17.4(8)	18.9(8)	-0.7(6)	6.1(6)	3.0(6)
C2	22.1(8)	11.7(7)	17.0(7)	1.4(6)	7.4(6)	-0.3(6)
C5	19.7(8)	16.7(8)	19.7(8)	-3.7(6)	7.3(6)	-0.6(6)
C15	25.6(8)	17.8(8)	19.5(8)	-1.3(6)	8.6(6)	-1.2(7)
C25	19.6(5)	18.5(6)	19.5(5)	-1.0(4)	6.2(4)	2.9(5)
C19	26.0(9)	23.4(8)	19.1(8)	-2.0(7)	8.4(7)	-0.4(7)
C8	20.0(8)	20.6(8)	33.1(9)	-6.4(7)	7.6(7)	-0.9(7)
C16	36.4(10)	19.5(8)	20.0(8)	-2.3(6)	11.9(7)	-1.4(7)
C11	24.6(9)	25.5(9)	23.3(8)	0.9(7)	9.7(7)	4.4(7)
C22	24.6(6)	26.0(7)	27.3(6)	-4.1(5)	8.4(5)	1.0(5)
C17	37.5(10)	23.3(9)	14.5(7)	-1.7(6)	5.6(7)	-5.2(7)
C27	29.2(9)	22.0(8)	20.9(8)	-1.5(7)	8.0(7)	3.0(7)
C23	21.5(8)	30.4(10)	28.1(9)	-7.0(7)	7.8(7)	-6.7(7)
C18	25.4(9)	30.1(9)	20.0(8)	1.3(7)	3.2(7)	-1.7(7)
C24	24.6(6)	26.0(7)	27.3(6)	-4.1(5)	8.4(5)	1.0(5)
C10	22.8(8)	27.6(9)	24.8(9)	0.0(7)	4.7(7)	4.8(7)
C6	24.7(9)	35.3(10)	23.8(8)	3.3(7)	10.0(7)	1.4(8)
C28	35.7(10)	27.7(9)	26.0(9)	-7.8(7)	6.4(8)	7.6(8)
C12	33.5(10)	27.7(9)	18.2(8)	-4.7(7)	-0.2(7)	-7.6(8)
C7	25.0(9)	39.7(11)	32.8(10)	1.7(8)	15.3(8)	-0.6(8)
C29	33.0(10)	22.6(9)	47.5(12)	-12.1(8)	7.7(9)	-0.2(8)
C9	22.1(9)	32.8(10)	49.7(12)	-7.9(9)	10.6(8)	0.4(8)
C13	35.5(11)	40.6(12)	33.3(10)	-10.8(9)	8.4(8)	-13.3(9)
C30	38.1(11)	26.4(10)	55.6(13)	-7.0(9)	23.1(10)	-7.1(8)

Table S12. Bond Lengths for 8.

Atom	Atom	Length/Å
O2	C31	1.332(2)
O2	C12	1.4538(19)
O1	C31	1.208(2)
N3	C20	1.422(2)
N3	C26	1.417(2)
N3	C2	1.409(2)
N1	C1	1.335(2)
N1	C4	1.341(2)
N2	C1	1.344(2)
N2	C2	1.334(2)
C21	C20	1.359(2)
C21	C22	1.368(2)
C20	C25	1.395(2)
C1	C14	1.484(2)
C3	C4	1.405(2)
C3	C31	1.498(2)
C3	C2	1.399(2)
N4	C26	1.356(2)
N4	C30	1.364(3)
C26	C27	1.395(2)
C4	C5	1.481(2)
C14	C15	1.400(2)
C14	C19	1.396(2)
C5	C11	1.392(2)
C5	C6	1.393(2)
C15	C16	1.391(2)
C25	C24	1.390(2)
C19	C18	1.386(2)
C8	C10	1.393(3)
C8	C7	1.387(3)
C8	C9	1.503(2)
C16	C17	1.384(3)
C11	C10	1.388(2)
C22	C23	1.384(2)
C17	C18	1.390(3)
C27	C28	1.386(3)
C23	C24	1.384(3)
C6	C7	1.384(3)
C28	C29	1.382(3)
C12	C13	1.493(3)
C29	C30	1.380(3)

Table S13. Bond Angles for 8.

Atom	Atom	Atom	Angle/°
C31	O2	C12	115.96(13)
C26	N3	C20	122.38(13)
C2	N3	C20	117.88(13)
C2	N3	C26	119.73(13)
C1	N1	C4	117.45(13)
C2	N2	C1	116.60(14)
C20	C21	C22	119.26(16)
C21	C20	N3	117.20(14)
C21	C20	C25	121.28(15)
C25	C20	N3	121.52(14)
N1	C1	N2	125.92(14)
N1	C1	C14	117.07(14)
N2	C1	C14	117.00(14)
C4	C3	C31	121.40(14)
C2	C3	C4	116.70(14)
C2	C3	C31	121.86(14)
C26	N4	C30	118.00(17)
N4	C26	N3	116.35(14)
N4	C26	C27	121.95(16)
C27	C26	N3	121.68(15)
N1	C4	C3	121.05(15)
N1	C4	C5	115.46(14)
O1	C31	C3	123.98(15)
N2	C2	N3	115.87(14)
N2	C2	C3	122.22(14)
C3	C2	N3	121.92(14)
C11	C5	C4	122.25(14)
C11	C5	C6	118.78(15)
C6	C5	C4	118.95(15)
C16	C15	C14	120.21(16)
C24	C25	C20	118.68(16)
C18	C19	C14	120.37(16)
C10	C8	C9	120.93(17)
C7	C8	C10	117.99(16)
C7	C8	C9	121.07(17)
C17	C16	C15	120.15(16)
C10	C11	C5	120.43(16)
C21	C22	C23	121.65(17)
C16	C17	C18	119.96(16)
C28	C27	C26	118.65(17)
C24	C23	C22	118.76(17)
C19	C18	C17	120.17(17)
C23	C24	C25	120.37(16)
C11	C10	C8	121.04(16)

Table S13. Bond Angles for 8.

Atom	Atom	Atom	Angle/°
C3	C4	C5	123.47(14)
C15	C14	C1	119.72(15)
C19	C14	C1	121.19(14)
C19	C14	C15	119.09(15)
O2	C31	C3	110.77(13)
O1	C31	O2	125.24(15)
C7	C6	C5	120.19(17)
C29	C28	C27	120.17(17)
O2	C12	C13	106.92(15)
C6	C7	C8	121.57(17)
C30	C29	C28	118.36(18)
N4	C30	C29	122.85(19)

Table S14. Torsion Angles for 8.

A	B	C	D	Angle/°
N3	C20	C25	C24	-179.55(14)
N3	C26	C27	C28	-178.41(15)
N1	C1	C14	C15	-10.8(2)
N1	C1	C14	C19	170.20(15)
N1	C4	C5	C11	137.36(16)
N1	C4	C5	C6	-40.7(2)
N2	C1	C14	C15	169.56(14)
N2	C1	C14	C19	-9.4(2)
C21	C20	C25	C24	0.2(2)
C21	C22	C23	C24	0.0(3)
C20	N3	C26	N4	148.53(15)
C20	N3	C26	C27	-33.3(2)
C20	N3	C2	N2	-45.35(19)
C20	N3	C2	C3	134.53(15)
C20	C21	C22	C23	0.6(3)
C20	C25	C24	C23	0.4(3)
C1	N1	C4	C3	2.4(2)
C1	N1	C4	C5	-176.01(14)
C1	N2	C2	N3	-178.10(13)
C1	N2	C2	C3	2.0(2)
C1	C14	C15	C16	-177.21(15)
C1	C14	C19	C18	177.10(15)
C3	C4	C5	C11	-41.0(2)
C3	C4	C5	C6	140.97(17)
N4	C26	C27	C28	-0.3(3)
C26	N3	C20	C21	144.07(15)
C26	N3	C20	C25	-36.2(2)
C26	N3	C2	N2	134.23(15)
C26	N3	C2	C3	-45.9(2)
C26	N4	C30	C29	1.4(3)
C26	C27	C28	C29	1.4(3)
C4	N1	C1	N2	-0.5(2)
C4	N1	C1	C14	179.93(14)
C4	C3	C31	O2	-59.71(19)
C4	C3	C31	O1	119.70(18)
C4	C3	C2	N3	179.84(14)
C4	C3	C2	N2	-0.3(2)
C14	C15	C16	C17	-0.1(3)
C14	C19	C18	C17	0.3(3)
C31	O2	C12	C13	176.84(15)
C31	C3	C4	N1	-179.68(14)
C31	C3	C4	C5	-1.5(2)
C31	C3	C2	N3	-2.5(2)
C31	C3	C2	N2	177.39(14)
C2	N3	C20	C21	-36.4(2)
C2	N3	C20	C25	143.41(15)
C2	N3	C26	N4	-31.0(2)
C2	N3	C26	C27	147.16(16)
C2	N2	C1	N1	-1.7(2)
C2	N2	C1	C14	177.89(13)
C2	C3	C4	N1	-2.0(2)
C2	C3	C4	C5	176.23(14)
C2	C3	C31	O2	122.73(16)
C2	C3	C31	O1	-57.9(2)
C5	C11	C10	C8	-0.3(3)
C5	C6	C7	C8	0.1(3)
C15	C14	C19	C18	-1.9(2)
C15	C16	C17	C18	-1.5(3)
C19	C14	C15	C16	1.8(2)
C16	C17	C18	C19	1.4(3)
C11	C5	C6	C7	0.1(3)
C22	C21	C20	N3	179.04(14)
C22	C21	C20	C25	-0.7(2)
C22	C23	C24	C25	-0.6(3)
C27	C28	C29	C30	-1.1(3)
C10	C8	C7	C6	-0.4(3)
C6	C5	C11	C10	0.0(3)
C28	C29	C30	N4	-0.4(3)
C12	O2	C31	O1	-3.4(2)
C12	O2	C31	C3	176.05(14)
C7	C8	C10	C11	0.5(3)
C9	C8	C10	C11	179.21(17)
C9	C8	C7	C6	-179.14(18)
C30	N4	C26	N3	177.10(17)

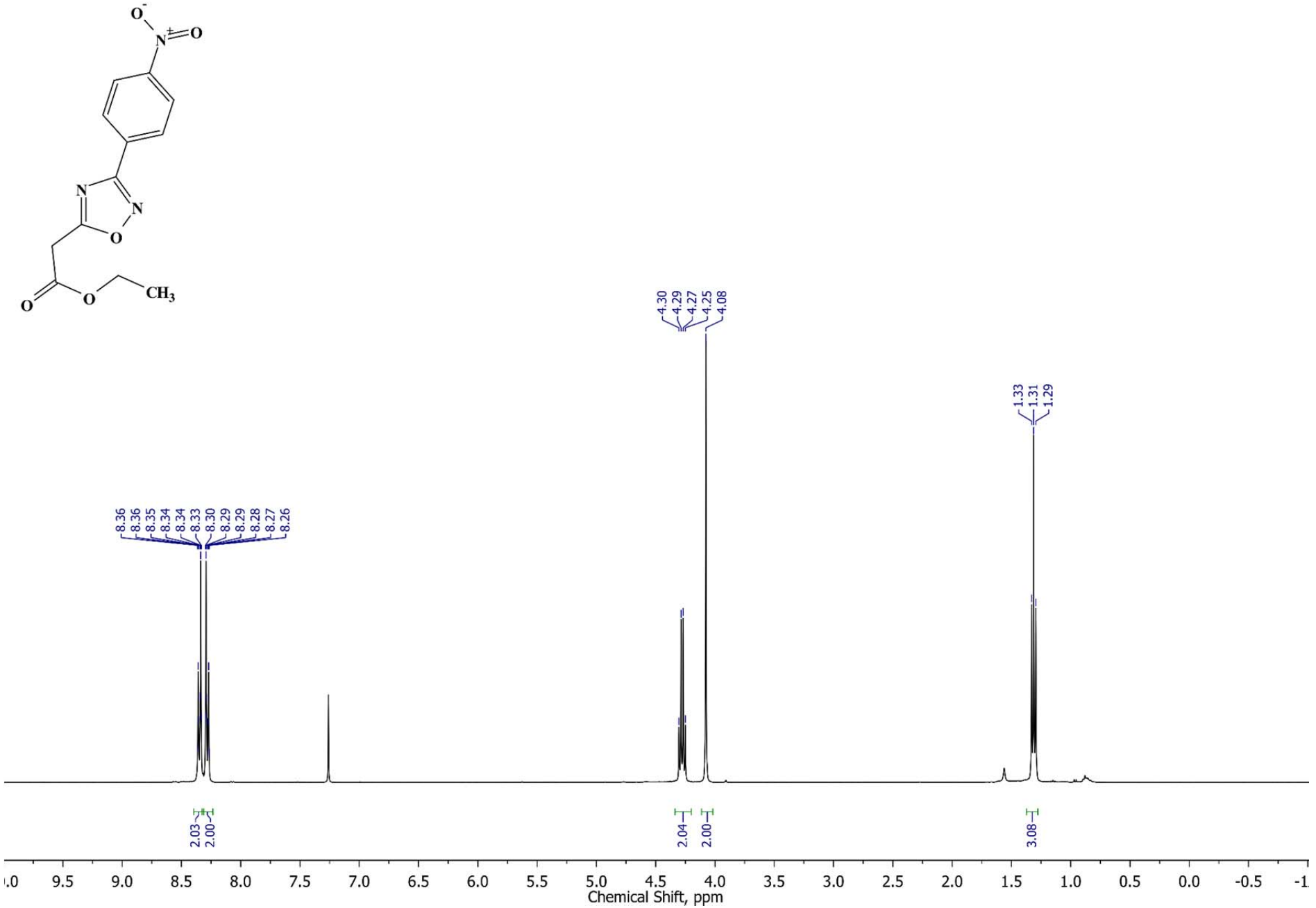
Table S14. Torsion Angles for 8.

A	B	C	D	Angle/°
C4	C5	C11	C10	-178.11(16)
C4	C5	C6	C7	178.25(17)
C30	N4	C26	C27	-1.1(3)

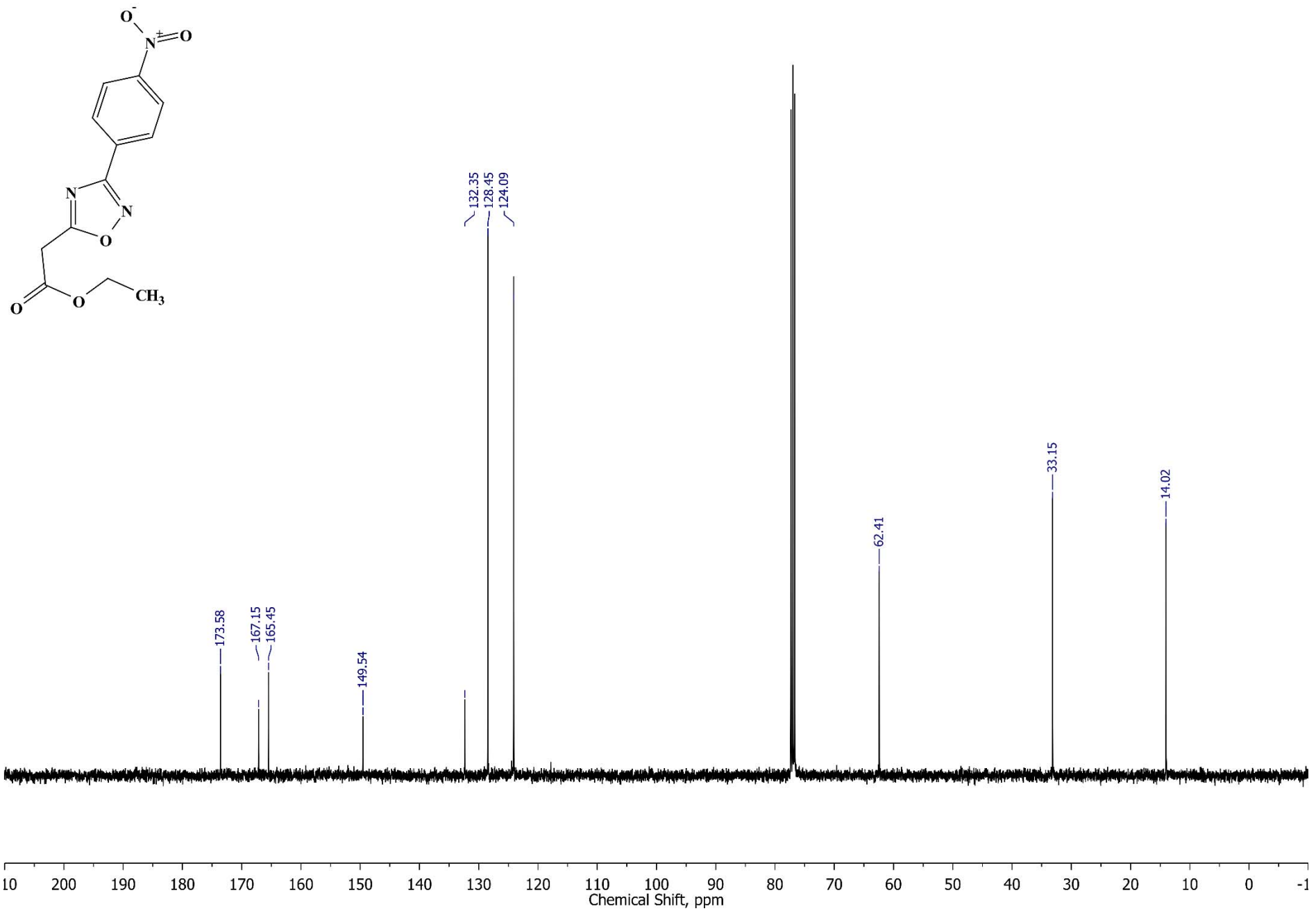
Table S15. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 8.

Atom	*x*	*y*	*z*	U(eq)
H21	8478.78	7552.13	1711.35	23
H15	7065.86	8089.8	3919.91	25
H25	9836.74	3123.63	1777.32	23
H19	9331.4	5921.97	3827.4	27
H16	7792.84	9175.25	4982.04	29
H11	5300.29	6993.03	1067.69	29
H22	9709.07	9122.62	1723.28	31
H17	9288.19	8693.8	5454.44	31
H27	8525.76	3146.5	635.09	29
H23	11014.31	7750.7	1753.65	32
H18	10049.99	7018.87	4885.87	31
H24	11074.17	4732.72	1772.24	31
H10	3802.94	7517.05	758.21	31
H6	5241.45	5534.64	2908.86	33
H28	8073.17	484.07	115.23	36
H12A	5625.54	2275.84	244.96	34
H12B	4892.08	3686.39	249.4	34
H7	3747.56	6057.81	2591.95	37
H29	7279	-1431.58	574.51	42
H9A	2520.46	8224.57	1164.59	52
H9B	2470.91	7368.43	1846.95	52
H9C	2331.68	6202.37	1193.18	52
H13A	4297.82	902.35	204.61	55
H13B	4317.75	1802.63	896.04	55
H13C	5040.75	394.61	878.7	55
H30	6993.82	-683.78	1560.84	46

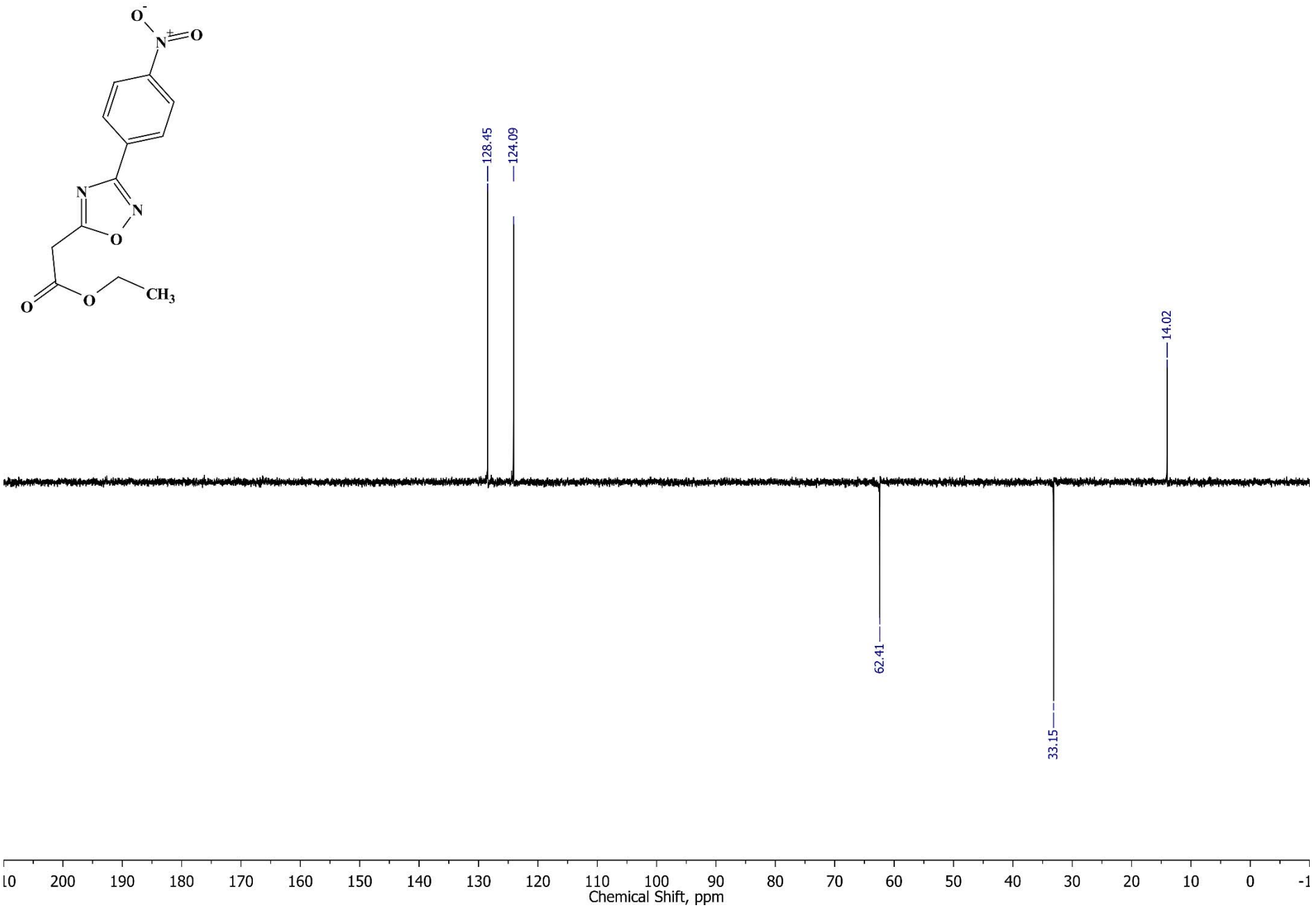
Ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)acetate (4g), ^{1}H NMR, $CDCl_3$, 400 MHz



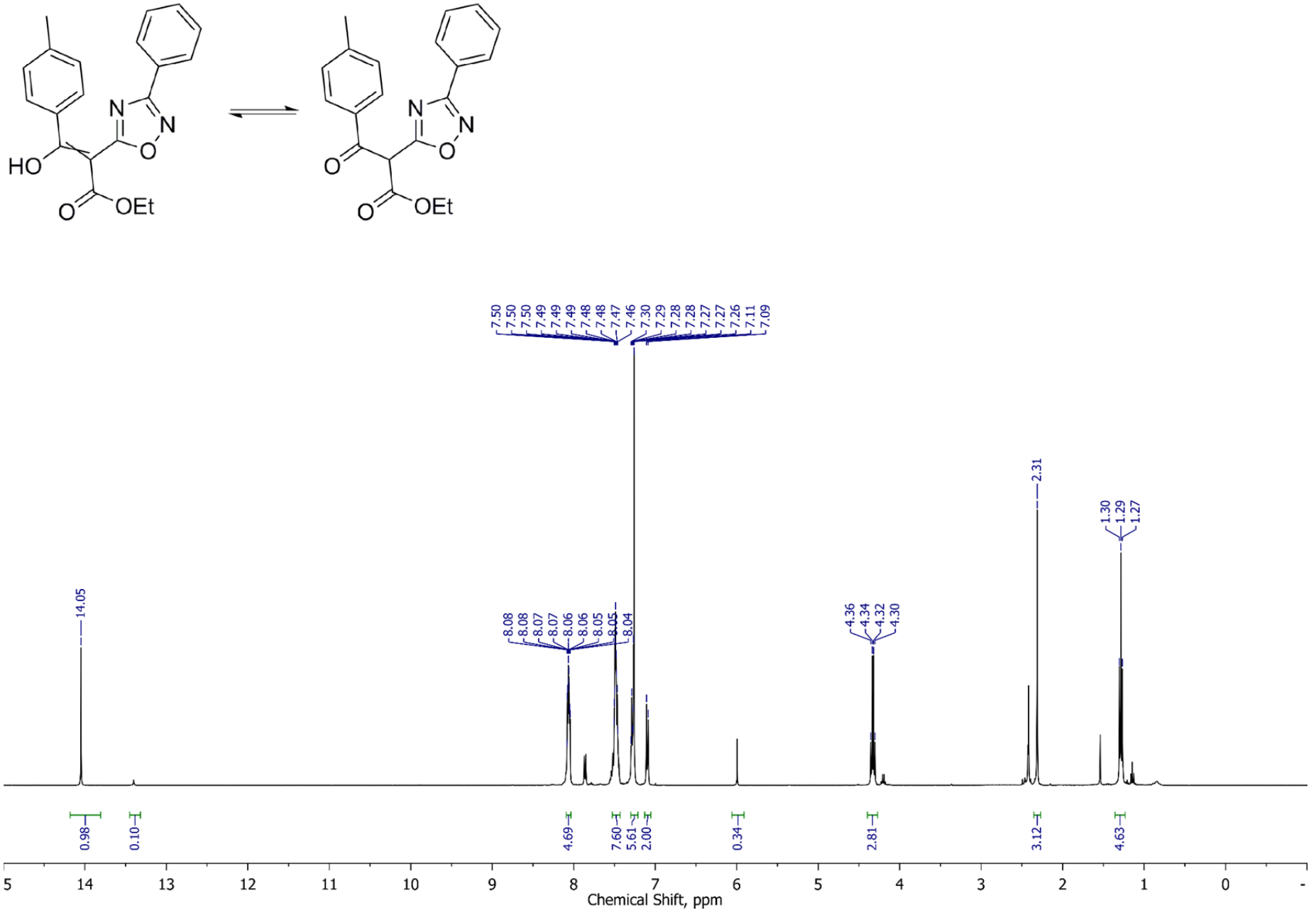
Ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)acetate (4g), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



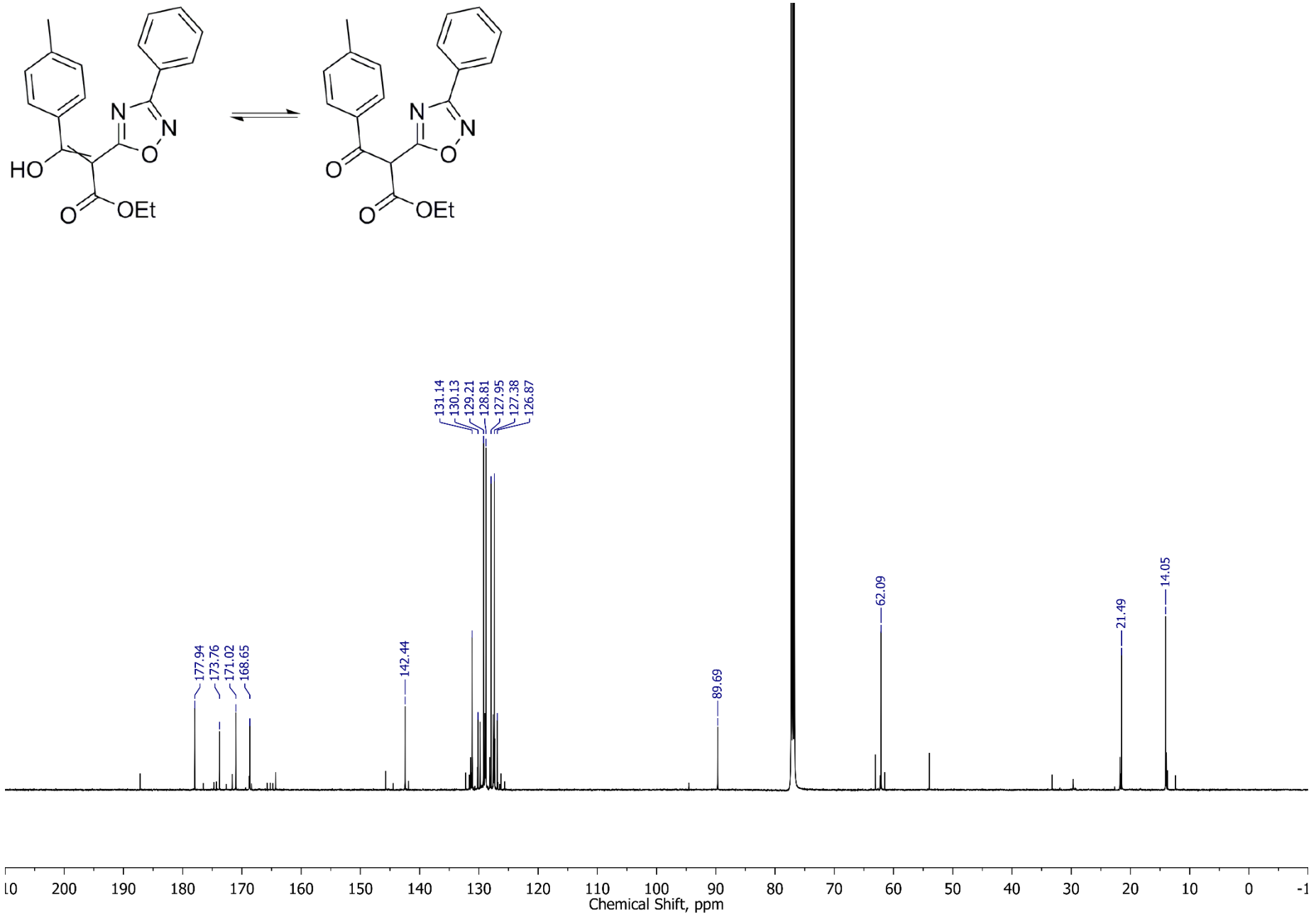
Ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)acetate (4g), DEPT, $CDCl_3$, 101 MHz



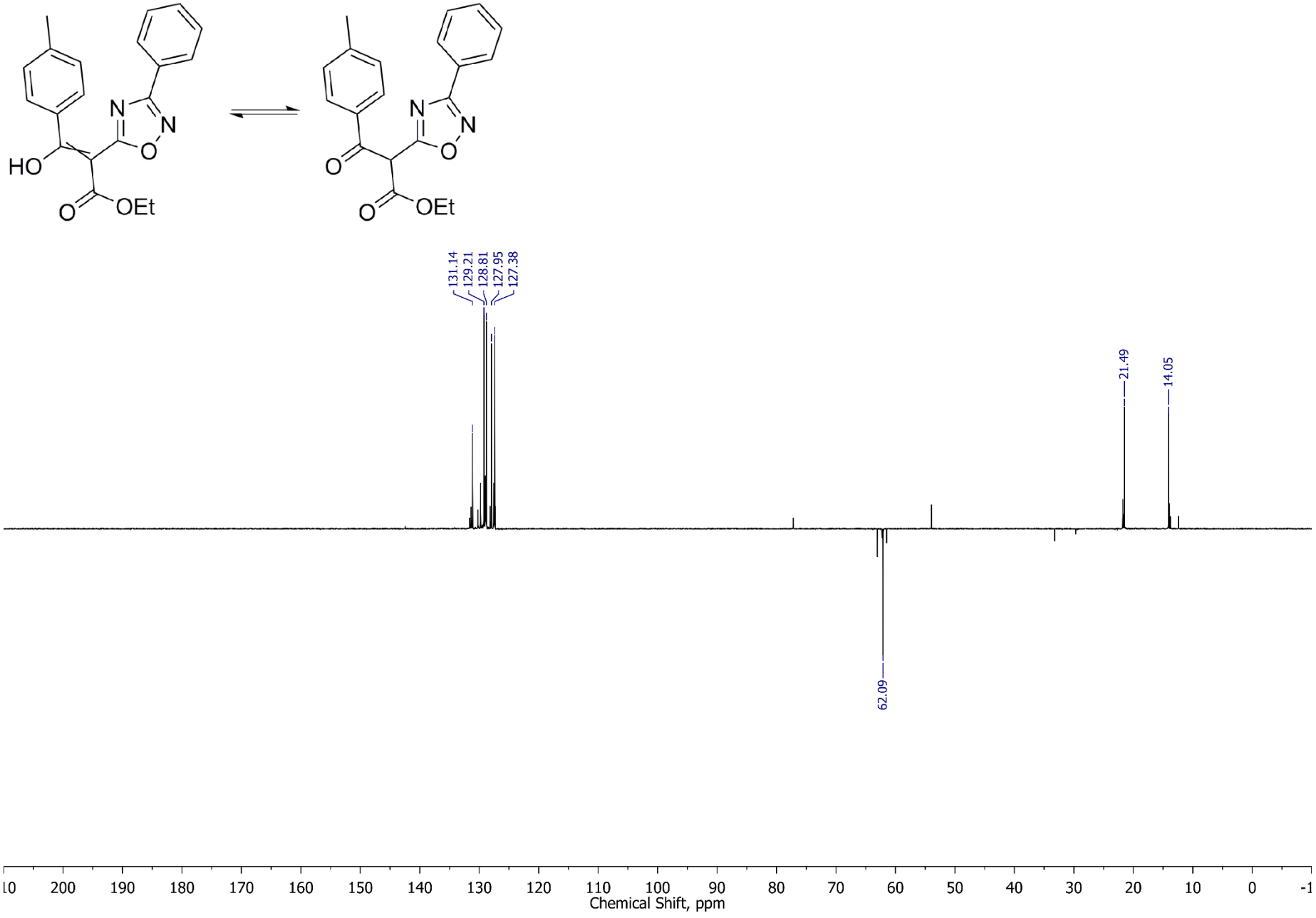
Ethyl 3-hydroxy-2-(3-phenyl-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)acrylate/ ethyl 3-oxo-2-(3-phenyl-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)propanoate (1a), ^{1}H NMR, $CDCl_3$, 400 MHz



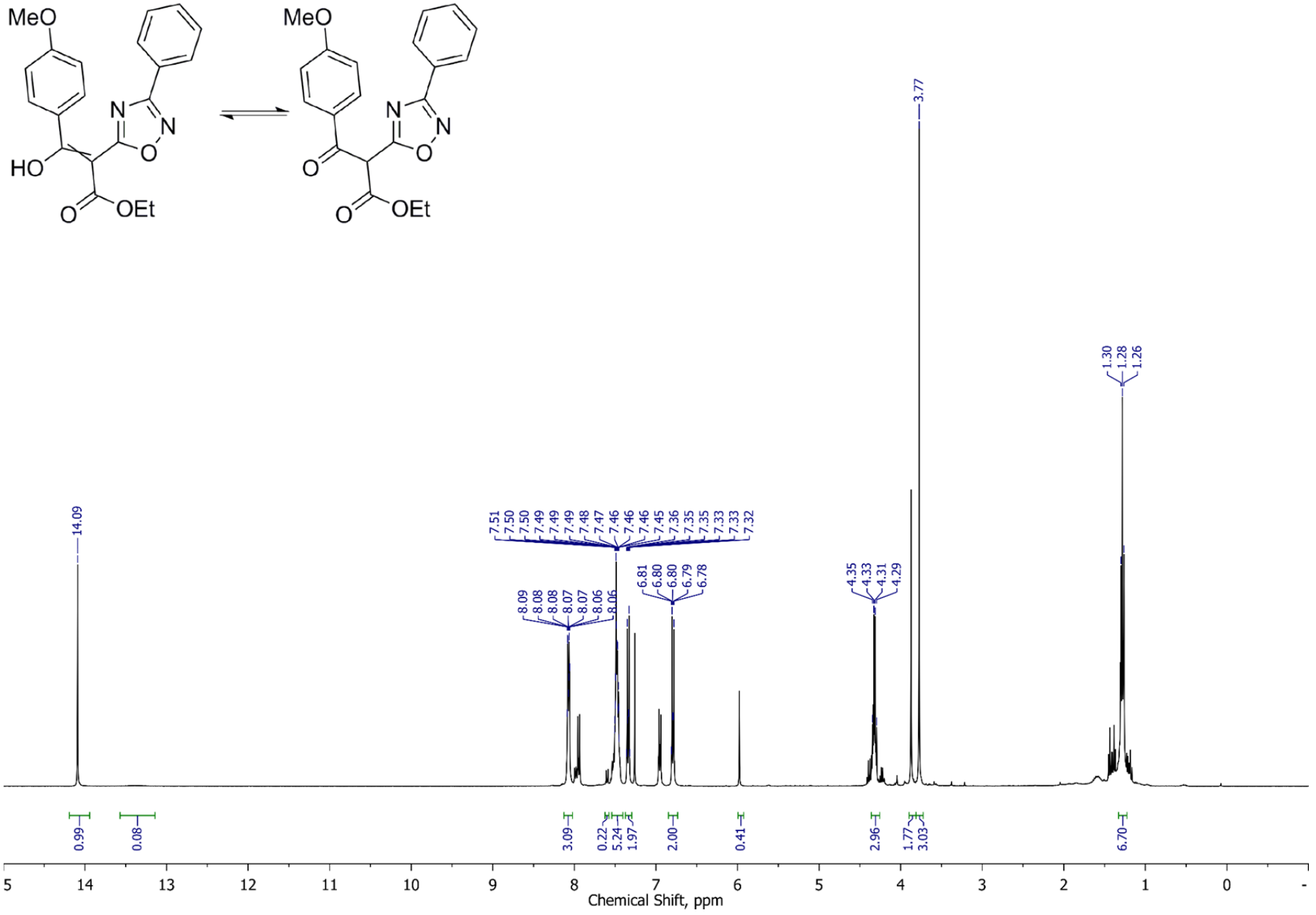
Ethyl 3-hydroxy-2-(3-phenyl-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)acrylate/ ethyl 3-oxo-2-(3-phenyl-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)propanoate (1a), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



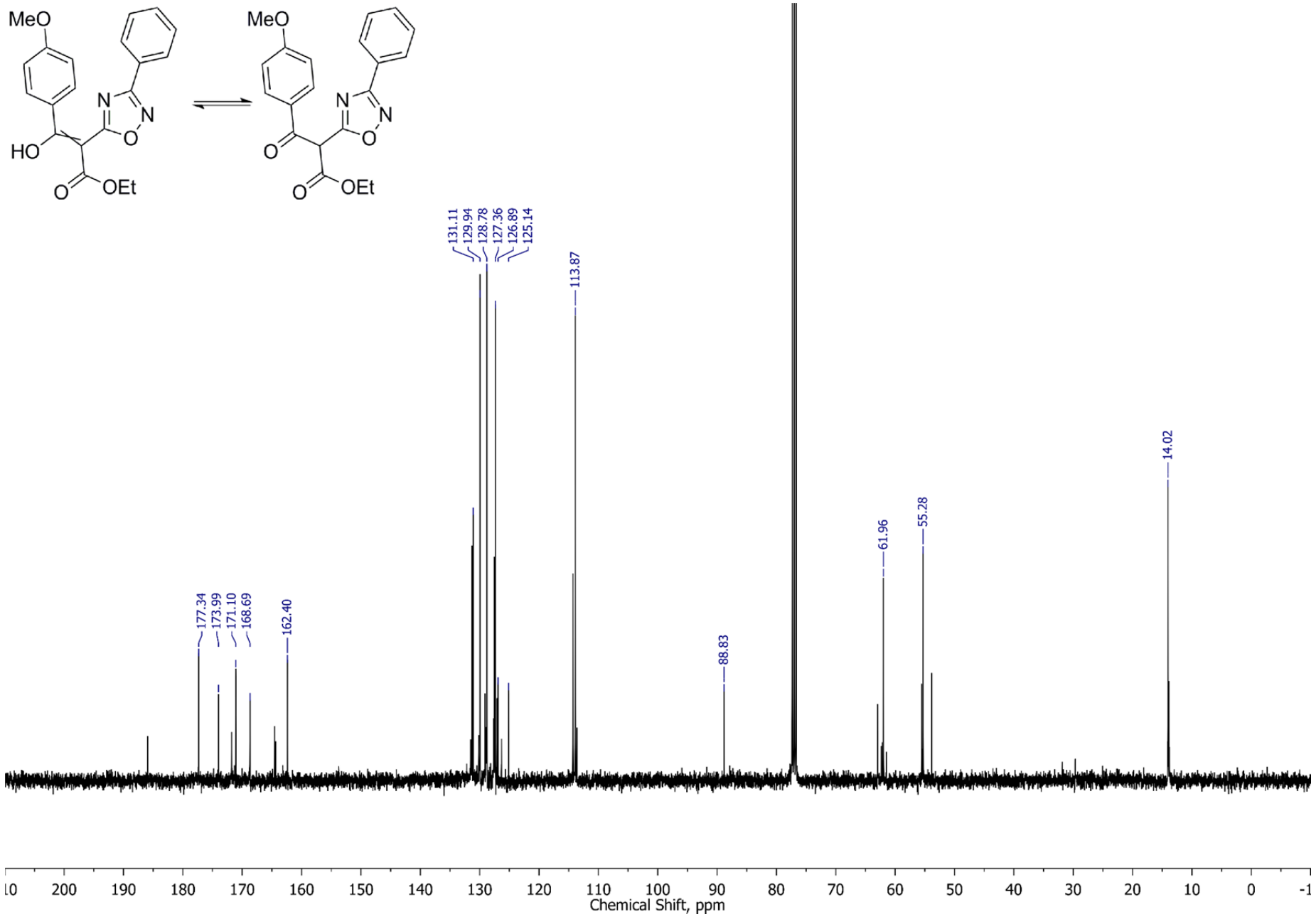
Ethyl 3-hydroxy-2-(3-phenyl-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)acrylate/ ethyl 3-oxo-2-(3-phenyl-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)propanoate (1a), DEPT, $CDCl_3$, 101 MHz



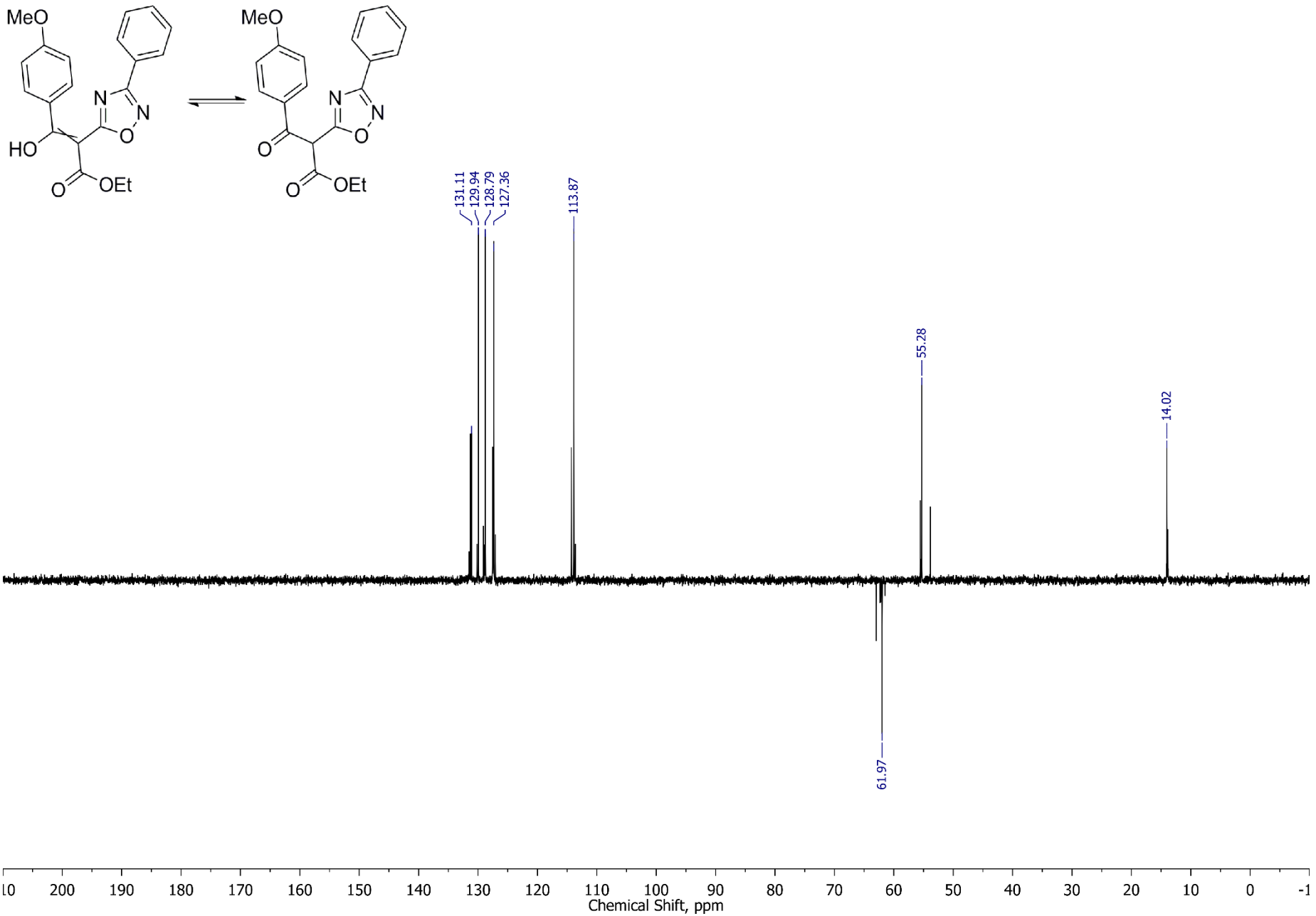
Ethyl 3-hydroxy-3-(4-methoxyphenyl)-2-(3-phenyl-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-methoxyphenyl)-3-oxo-2-(3-phenyl-1,2,4-oxadiazol-5-yl)propanoate (1b), ^{1}H NMR, $CDCl_3$, 400 MHz



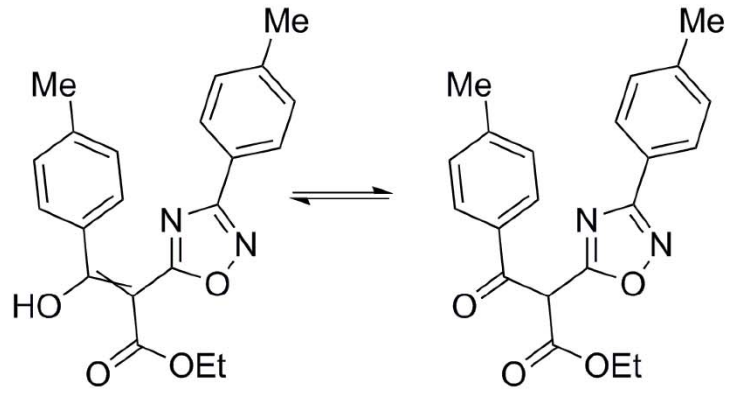
Ethyl 3-hydroxy-3-(4-methoxyphenyl)-2-(3-phenyl-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-methoxyphenyl)-3-oxo-2-(3-phenyl-1,2,4-oxadiazol-5-yl)propanoate (1b), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz

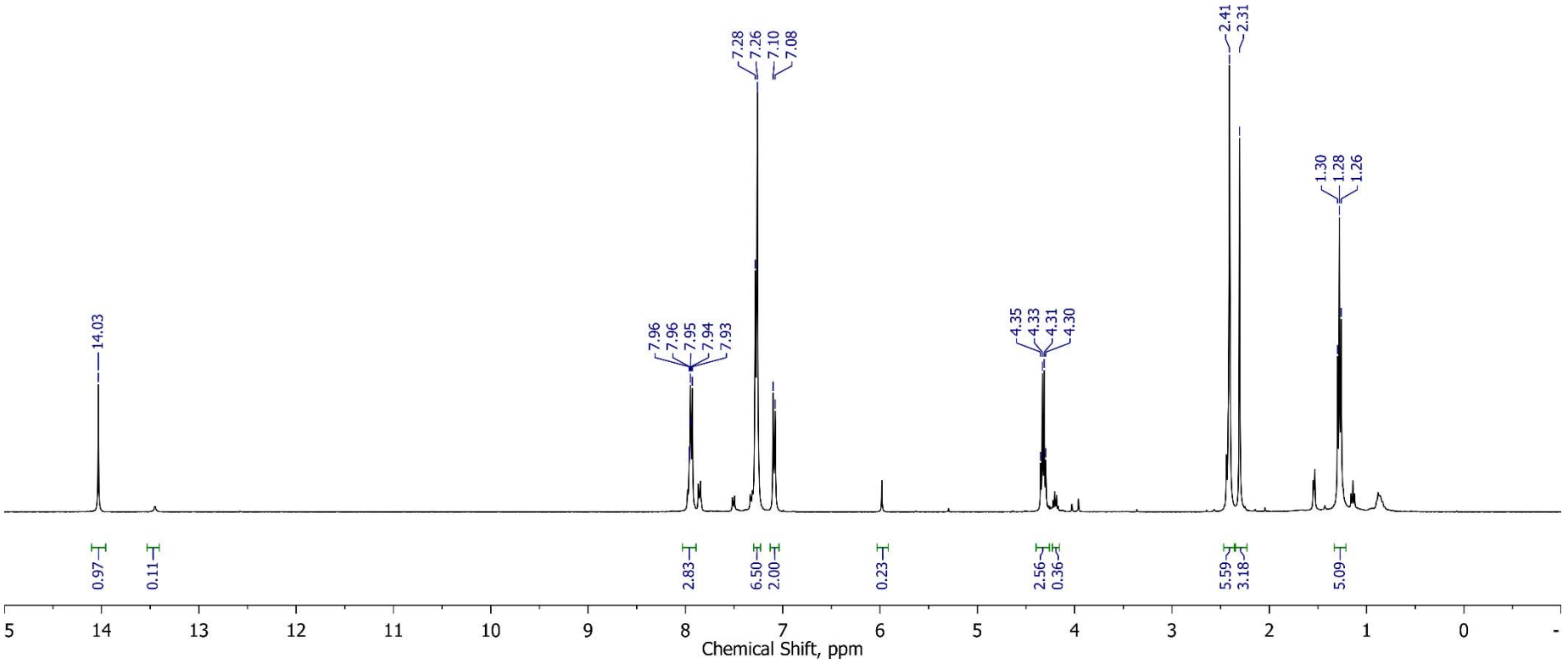


Ethyl 3-hydroxy-3-(4-methoxyphenyl)-2-(3-phenyl-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-methoxyphenyl)-3-oxo-2-(3-phenyl-1,2,4-oxadiazol-5-yl)propanoate (1b), DEPT, $CDCl_3$, 101 MHz

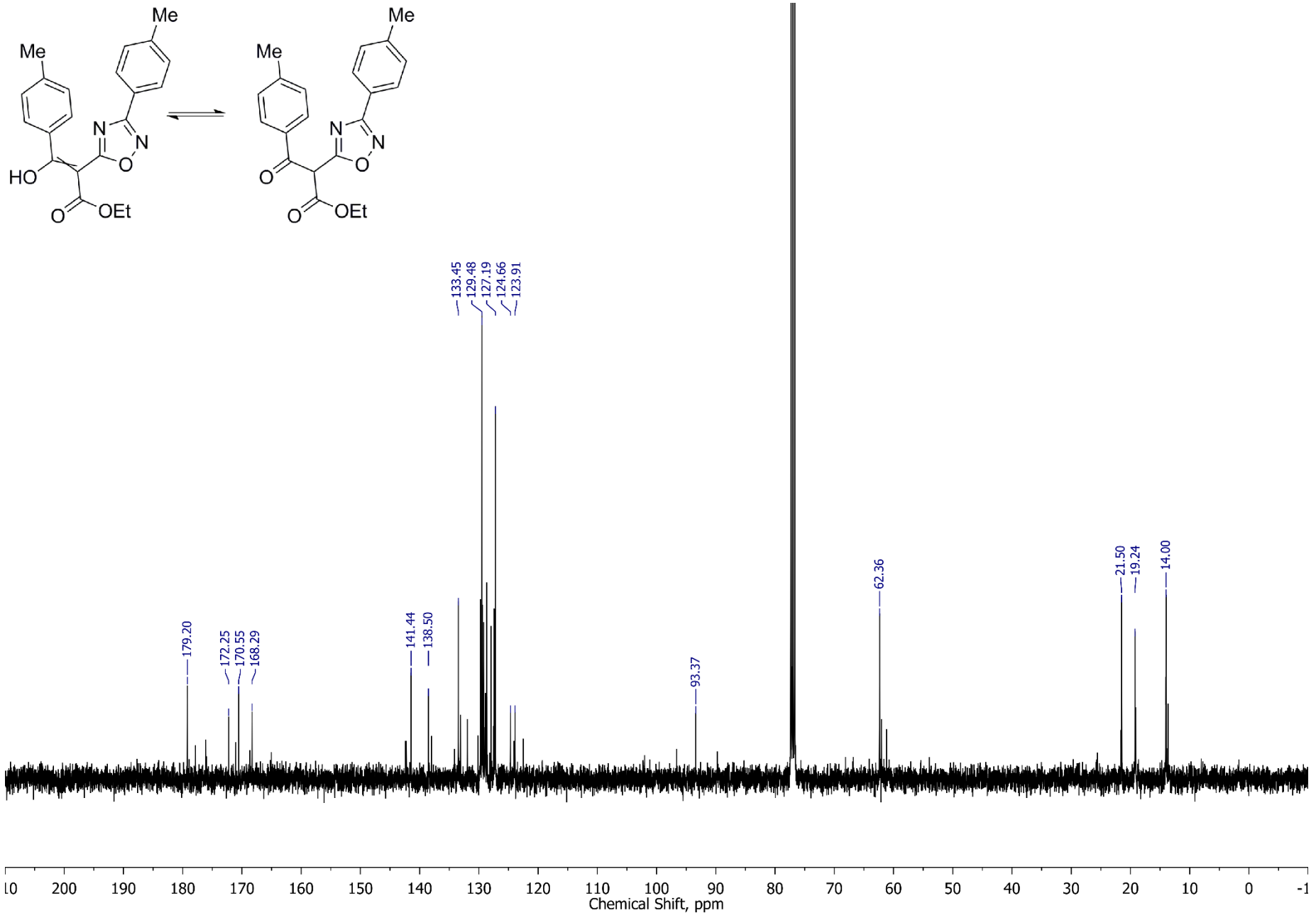


Ethyl 3-hydroxy-3-(*p*-tolyl)-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-oxo-3-(*p*-tolyl)-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)propanoate (1c), ^{1}H NMR, $CDCl_3$, 400 MHz

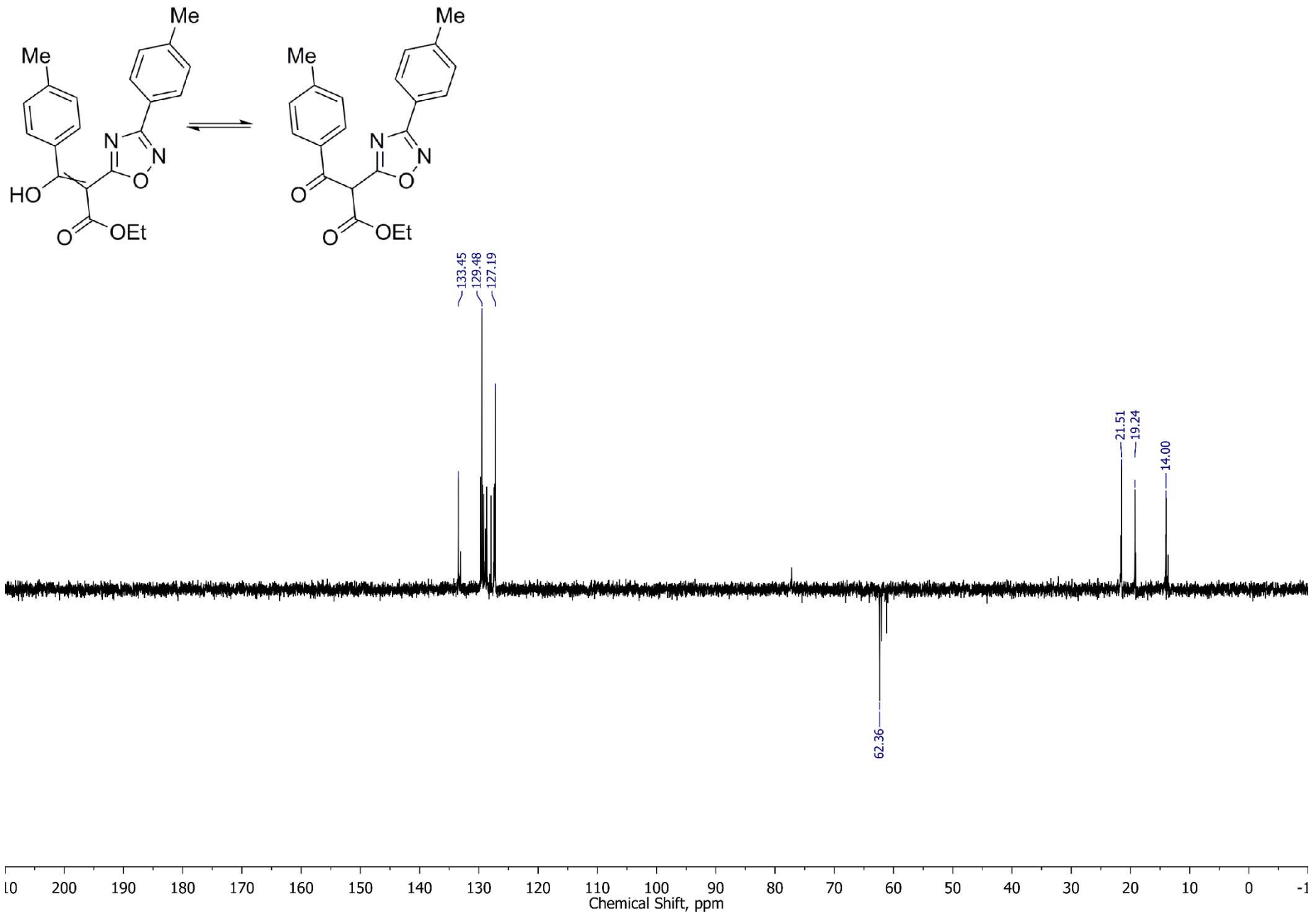




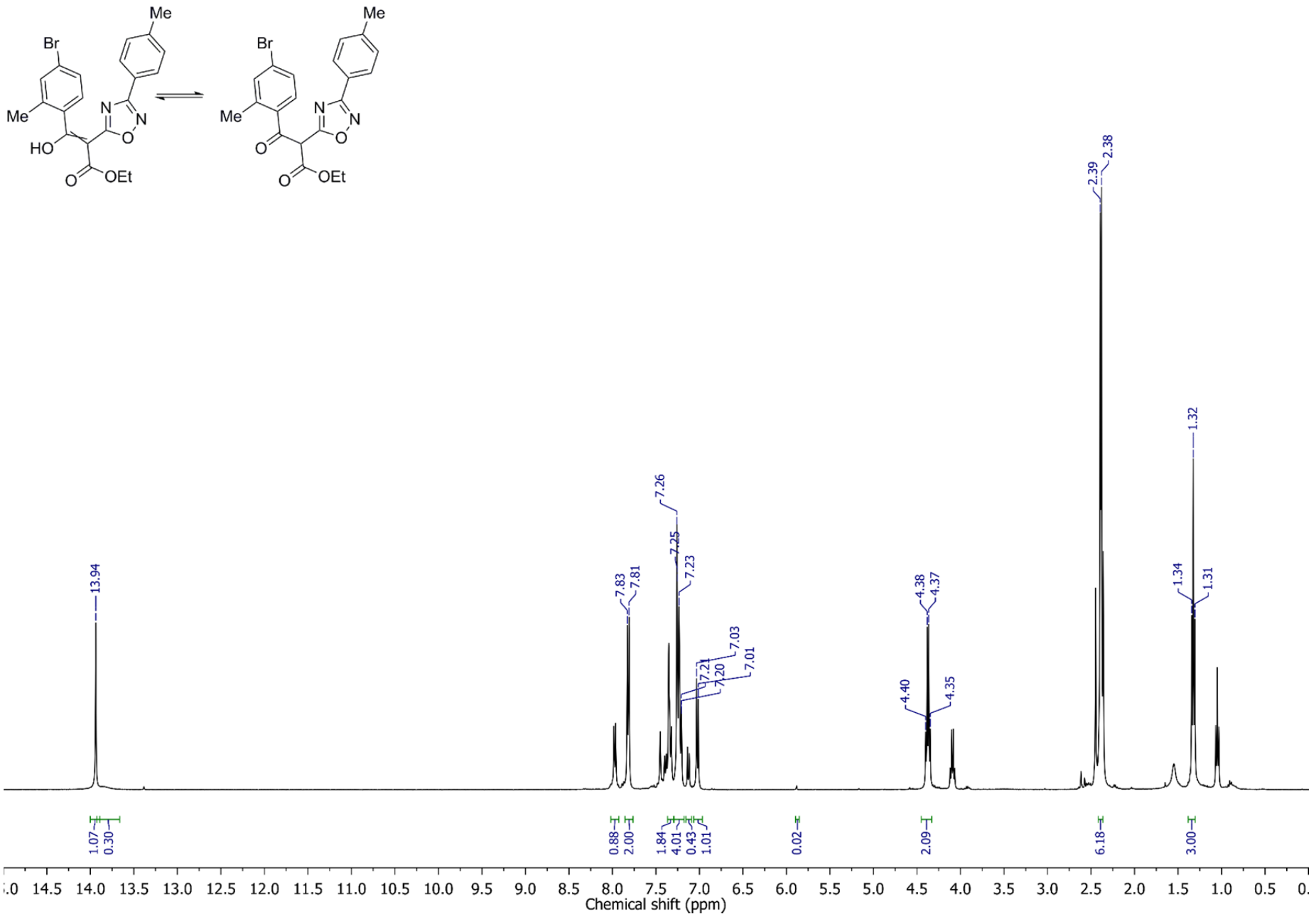
Ethyl 3-hydroxy-3-(*p*-tolyl)-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-oxo-3-(*p*-tolyl)-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)propanoate (1c), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



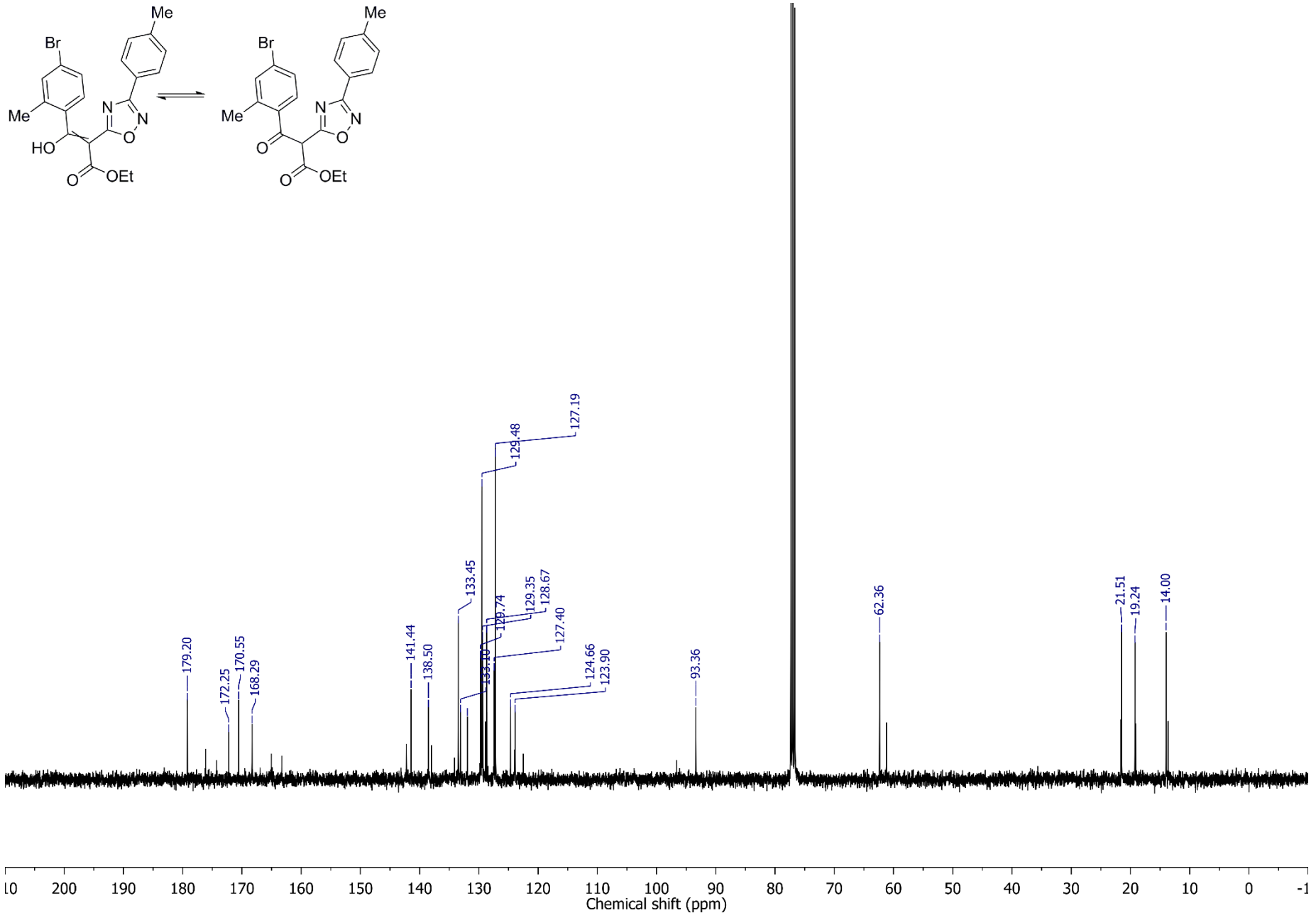
Ethyl 3-hydroxy-3-(*p*-tolyl)-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-oxo-3-(*p*-tolyl)-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)propanoate (1c), DEPT, $CDCl_3$, 101 MHz



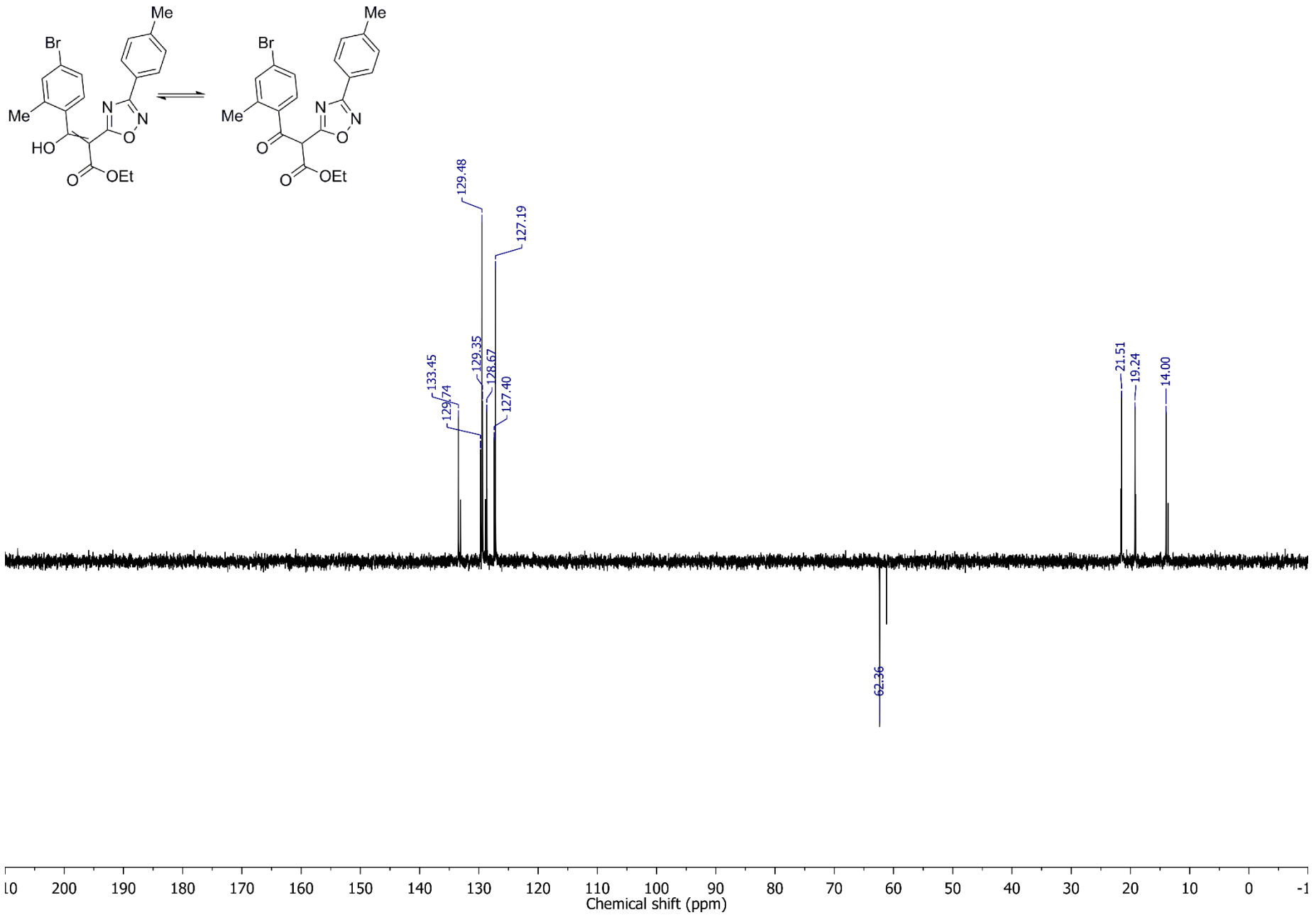
Ethyl 3-(4-bromo-2-methylphenyl)-3-hydroxy-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-bromo-2-methylphenyl)-3-oxo-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)propanoate (1d), ^{1}H NMR, $CDCl_3$, 400 MHz



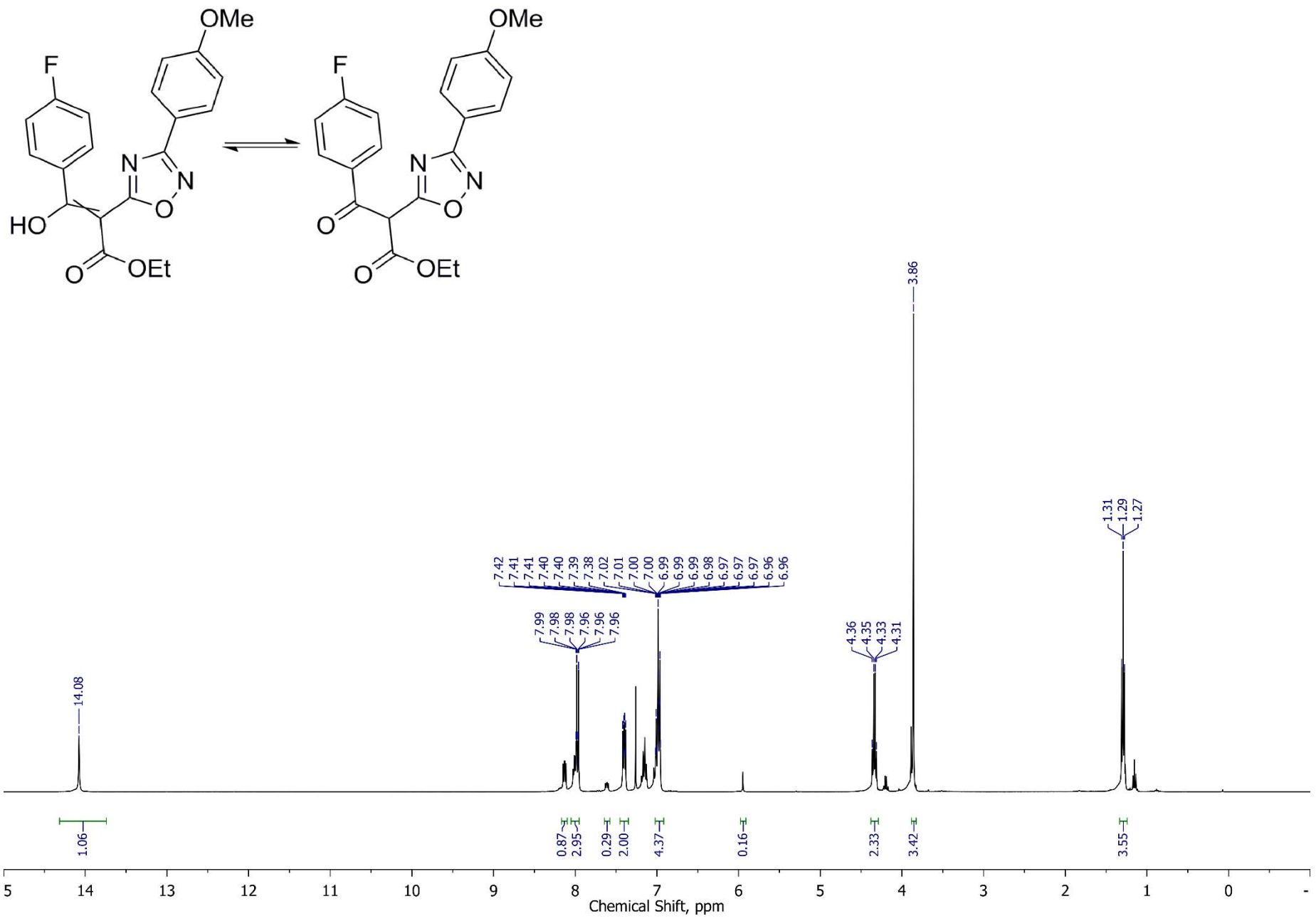
Ethyl 3-(4-bromo-2-methylphenyl)-3-hydroxy-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-bromo-2-methylphenyl)-3-oxo-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)propanoate (1d), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



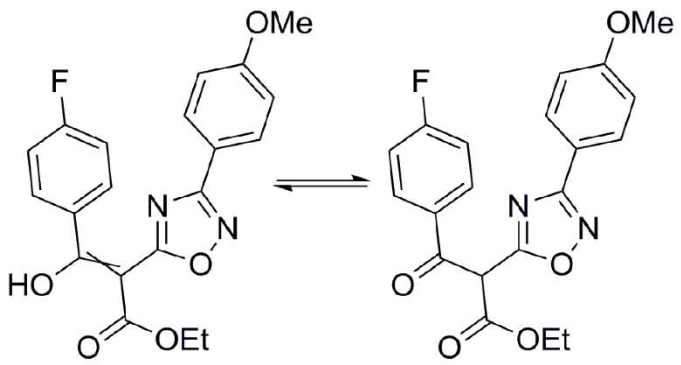
Ethyl 3-(4-bromo-2-methylphenyl)-3-hydroxy-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-bromo-2-methylphenyl)-3-oxo-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)propanoate (1d), DEPT, $CDCl_3$, 101 MHz

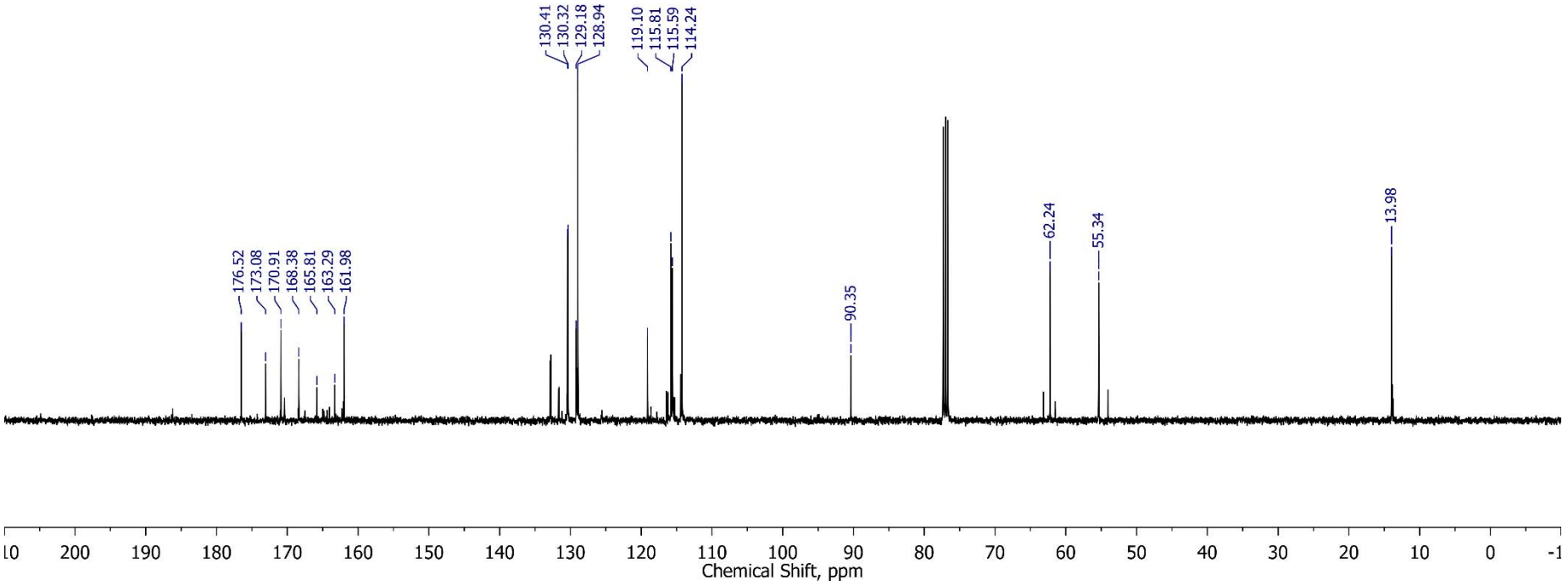


Ethyl 3-(4-fluorophenyl)-3-hydroxy-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-fluorophenyl)-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)-3-oxopropanoate (1e), ^{1}H NMR, $CDCl_3$, 400 MHz

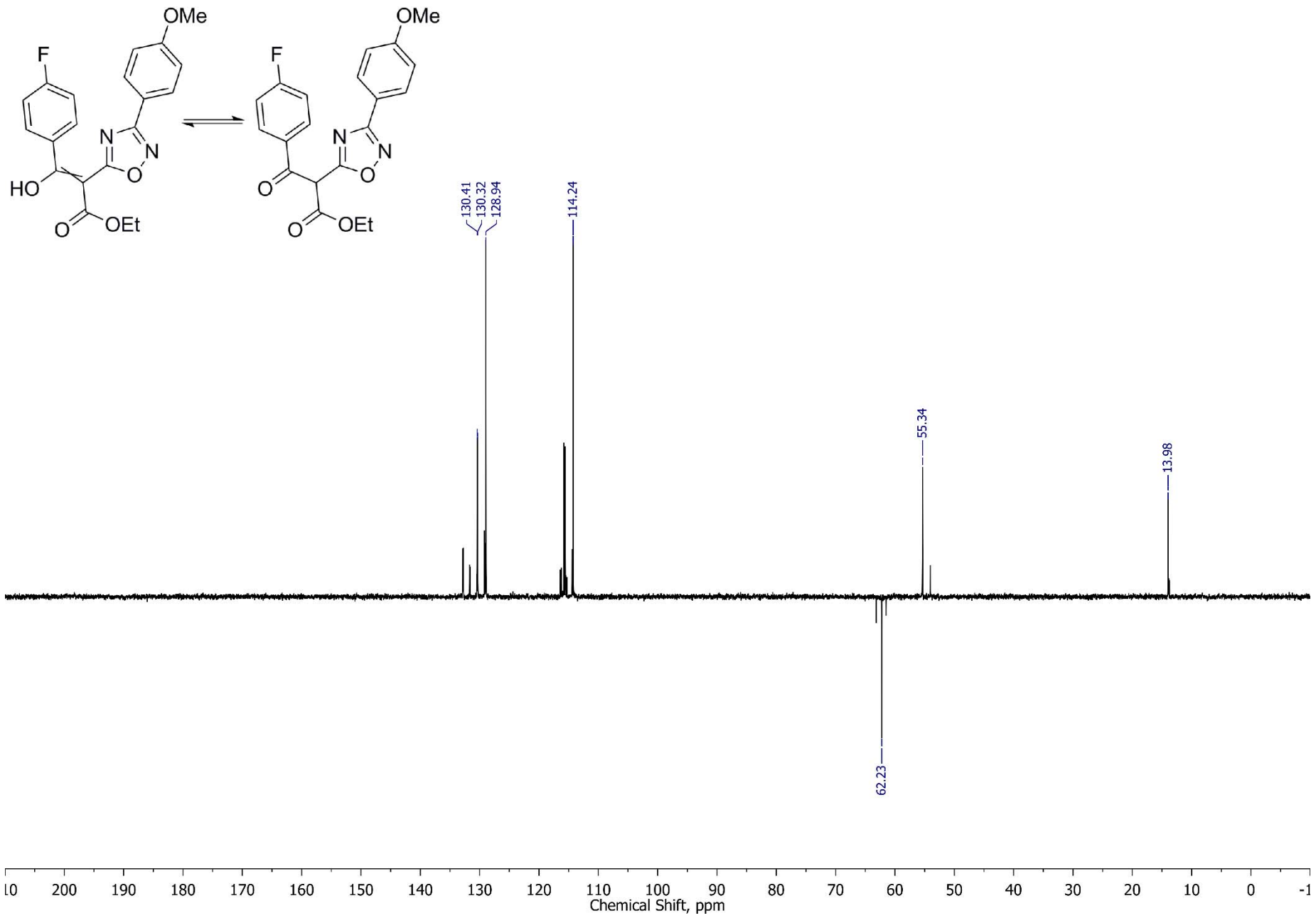


Ethyl 3-(4-fluorophenyl)-3-hydroxy-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-fluorophenyl)-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)-3-oxopropanoate (1e), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz

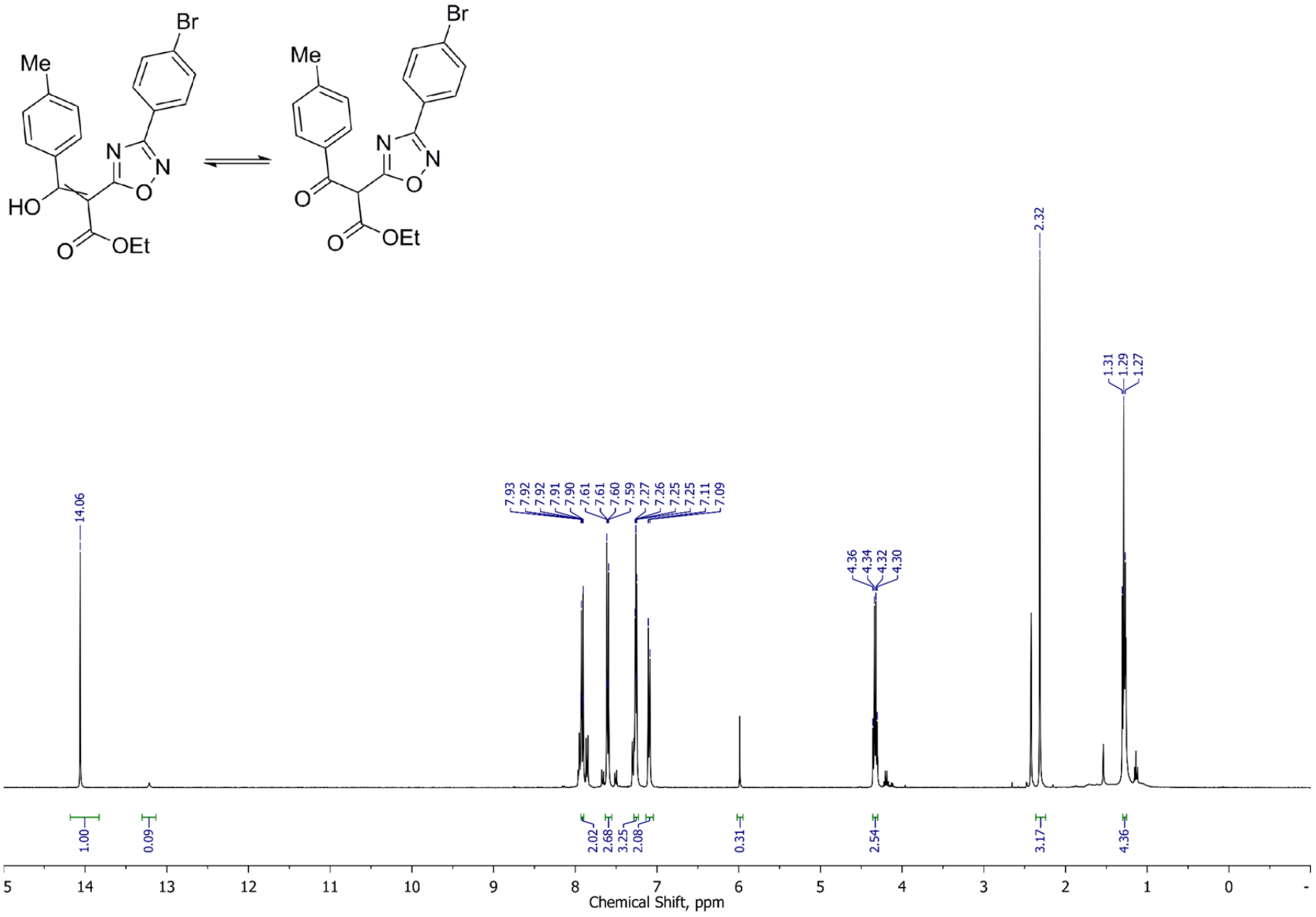




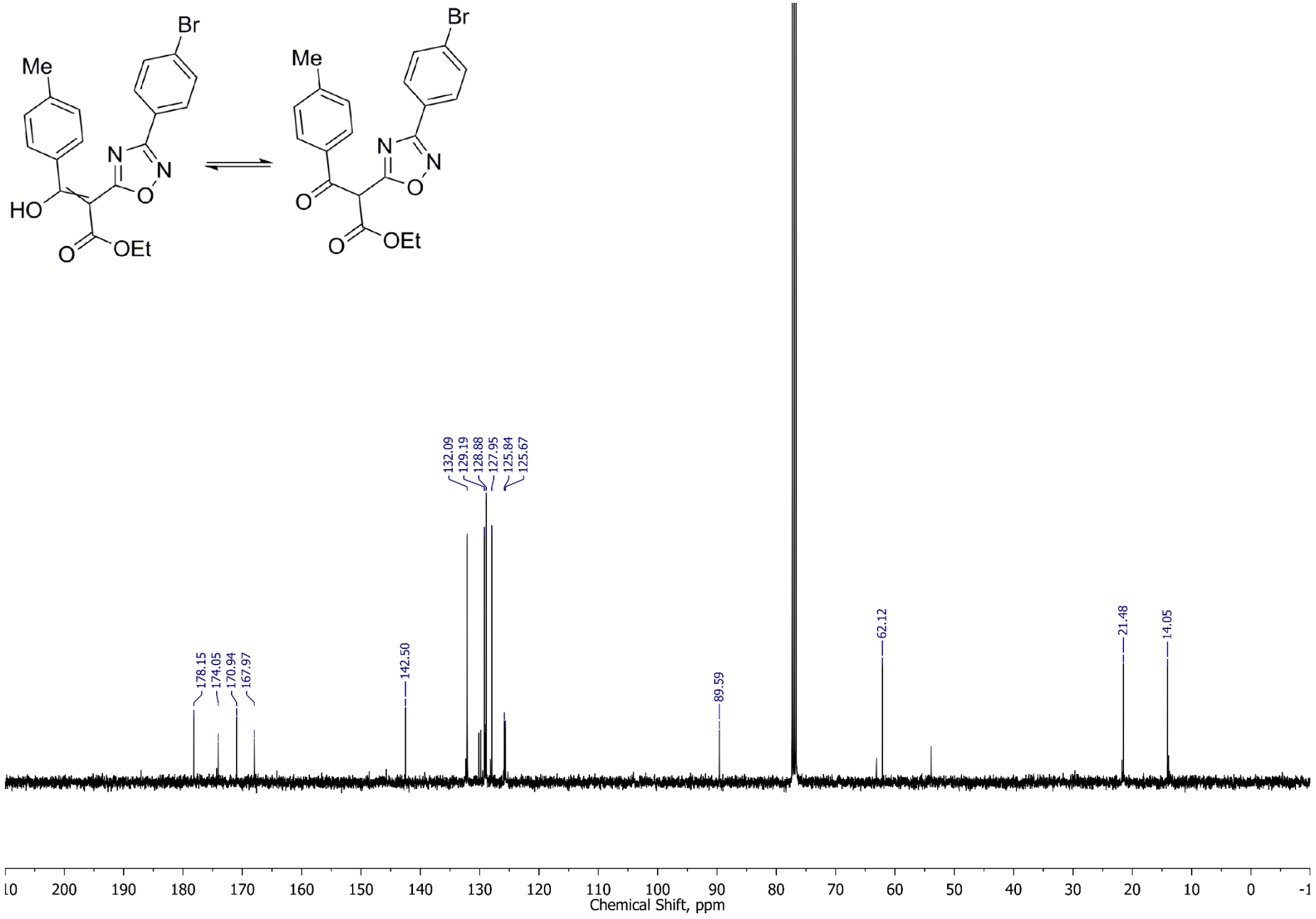
Ethyl 3-(4-fluorophenyl)-3-hydroxy-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)acrylate/ ethyl 3-(4-fluorophenyl)-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)-3-oxopropanoate (1e), DEPT, $CDCl_3$, 101 MHz



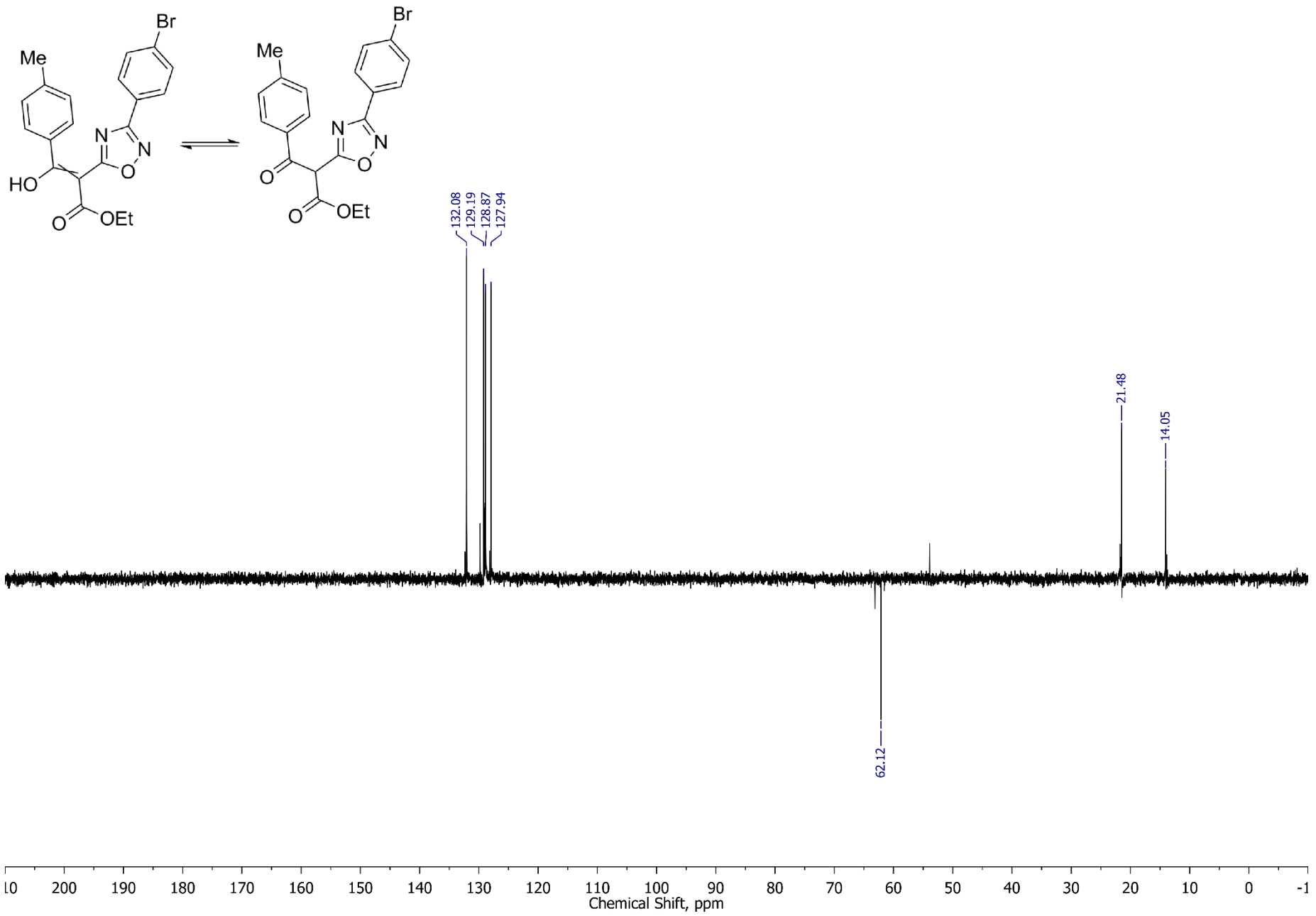
Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-hydroxy-3-(*p*-tolyl)acrylate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-3-(*p*-tolyl)propanoate (1f), ^{1}H NMR, $CDCl_3$, 400 MHz



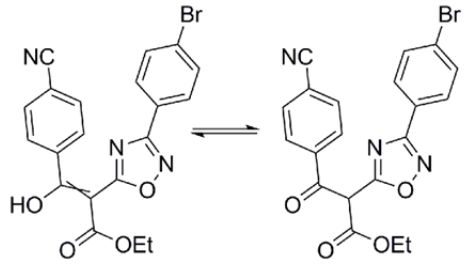
Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-hydroxy-3-(*p*-tolyl)acrylate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-3-(*p*-tolyl)propanoate (1f), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz

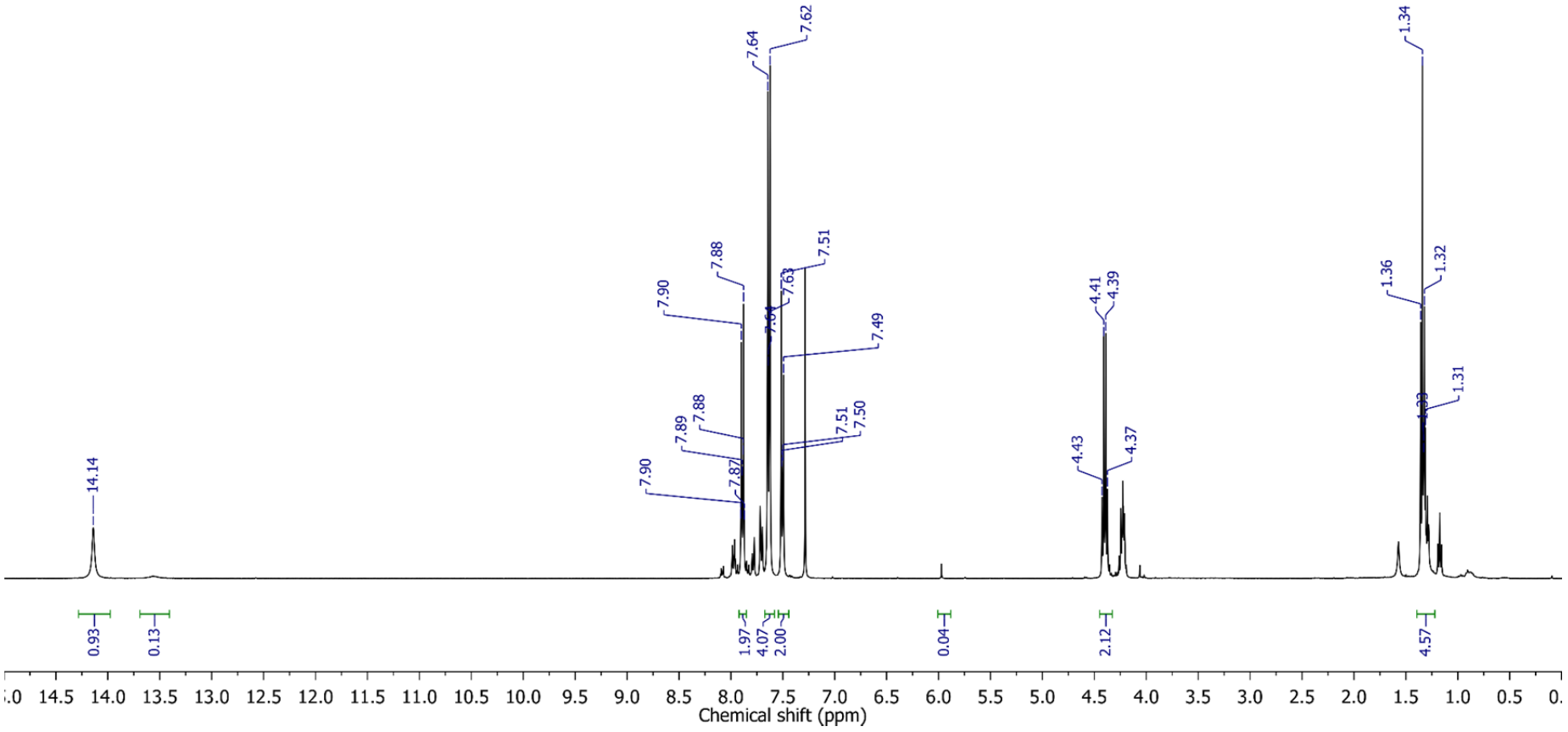


Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-hydroxy-3-(*p*-tolyl)acrylate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-3-(*p*-tolyl)propanoate (1f), DEPT, $CDCl_3$, 101 MHz

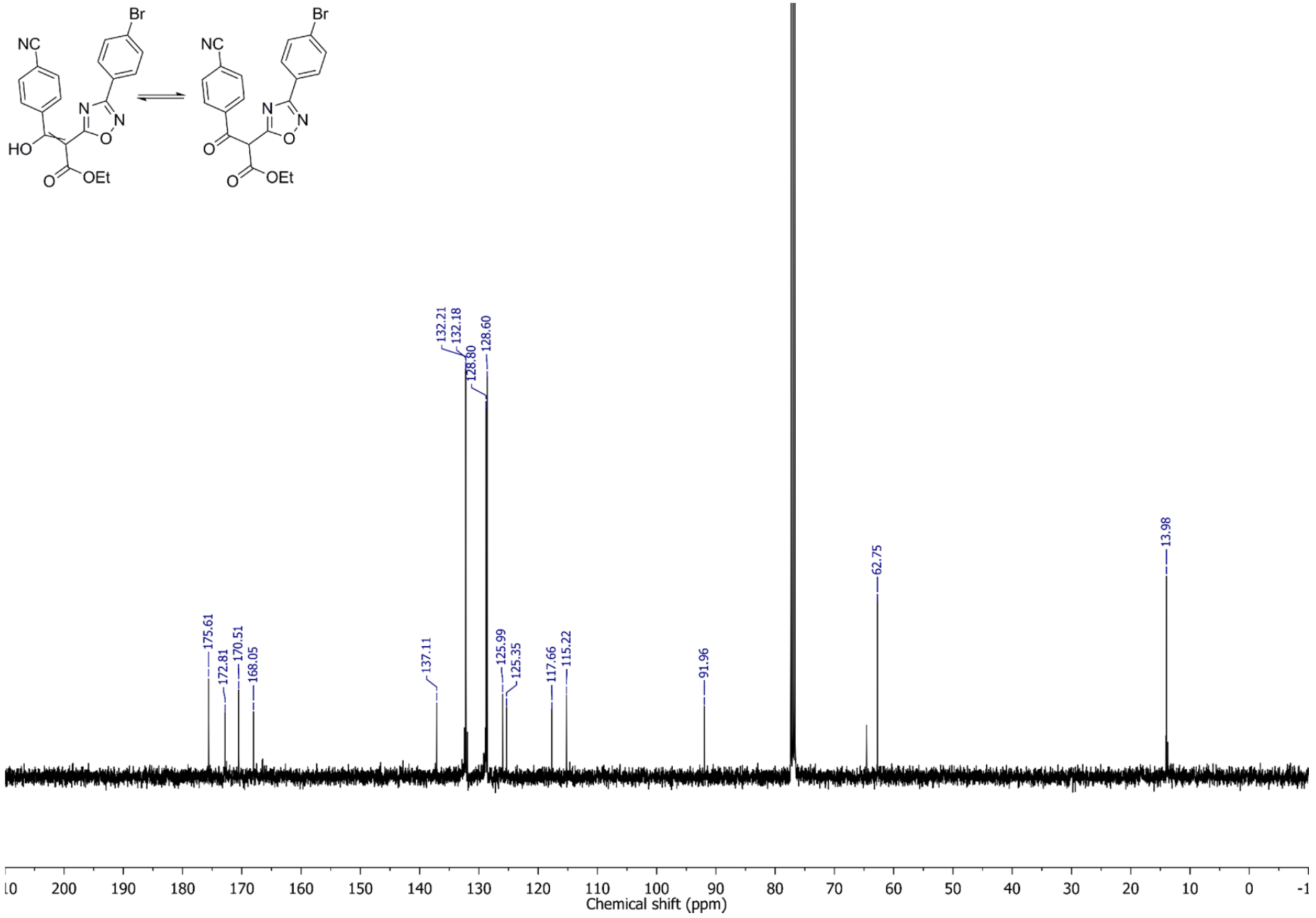


Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-(4-cyanophenyl)-3-hydroxyacrylate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-(4-cyanophenyl)-3-oxopropanoate (1g), ^{1}H NMR, $CDCl_3$, 400 MHz

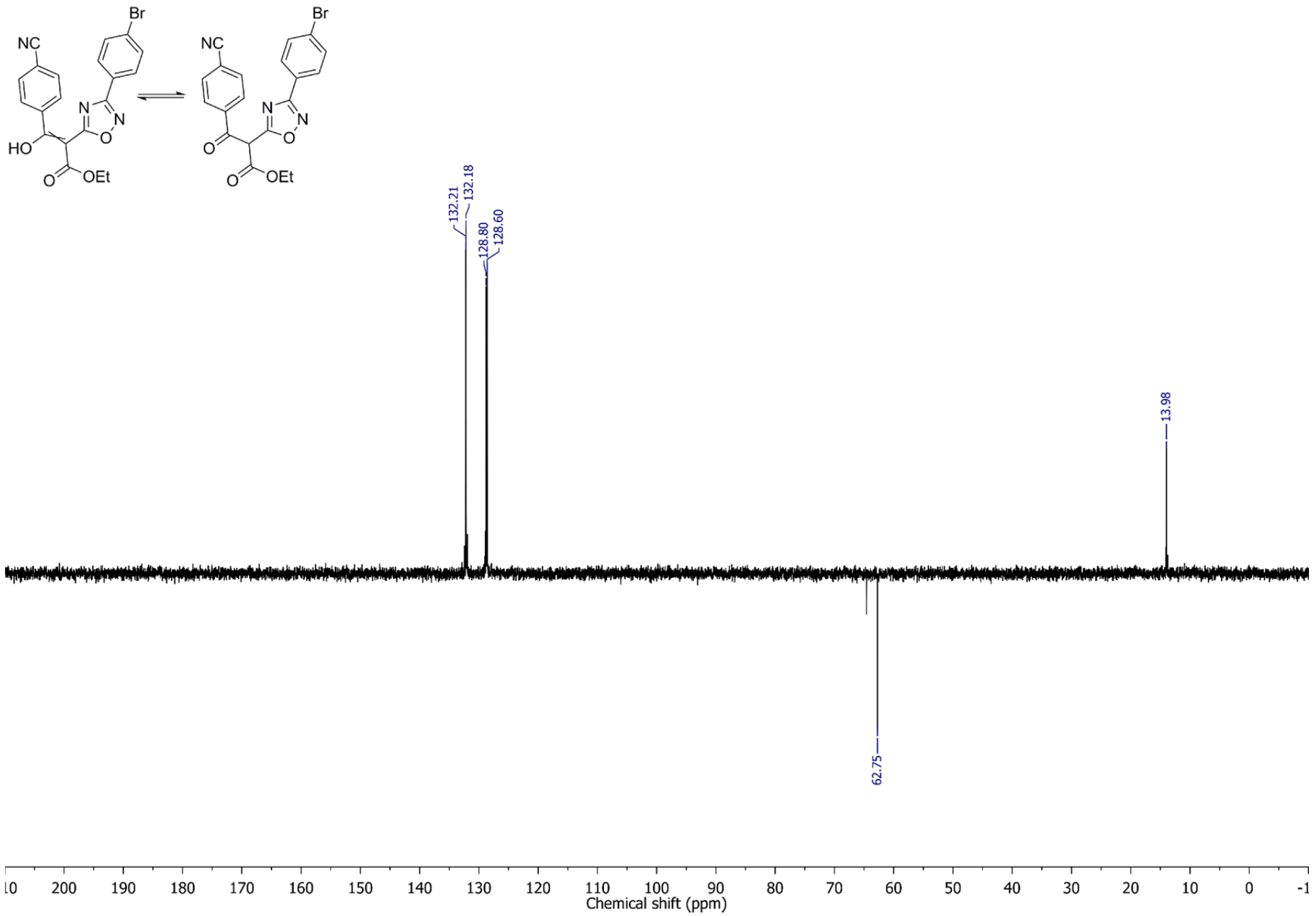




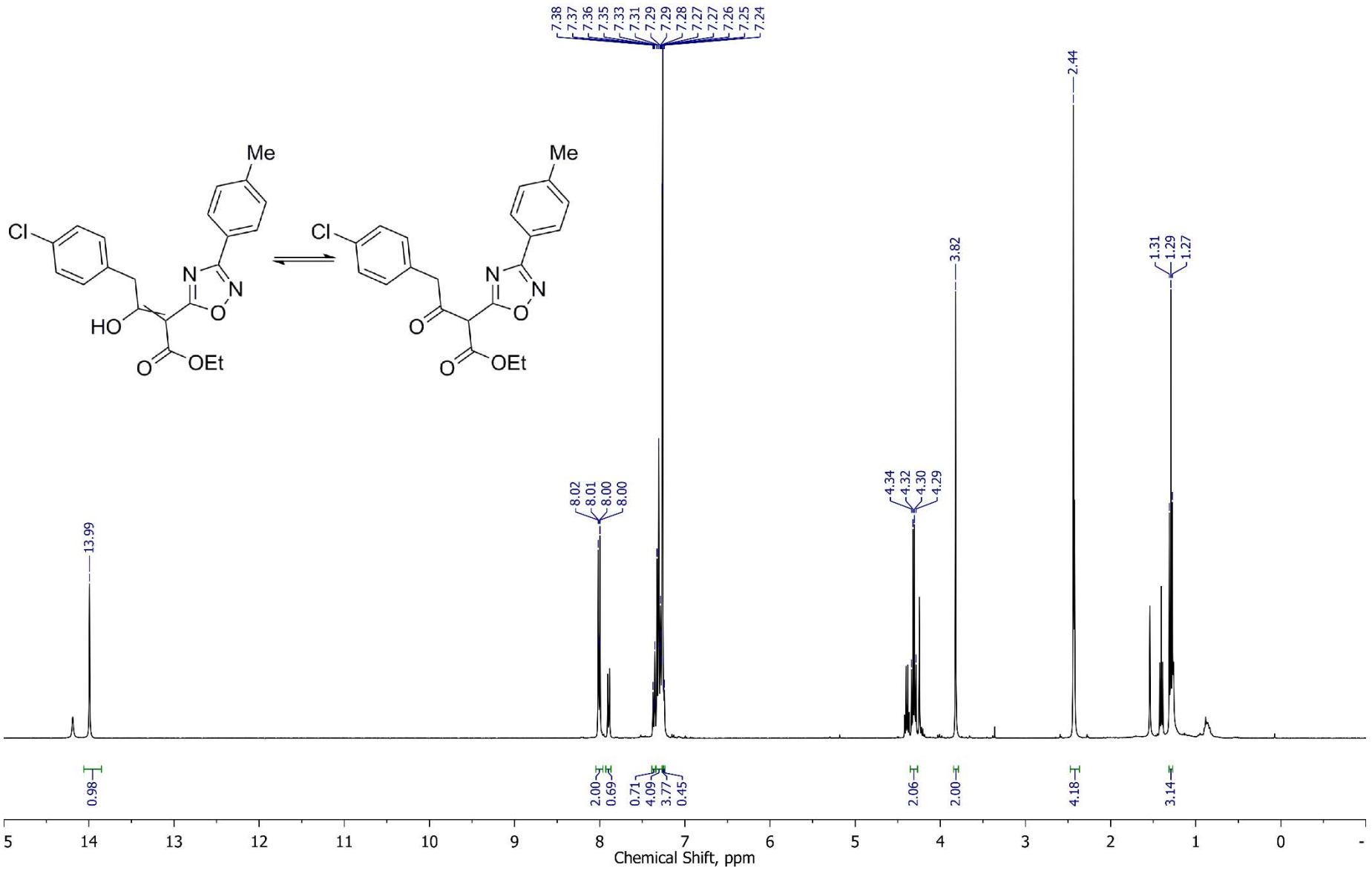
Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-(4-cyanophenyl)-3-hydroxyacrylate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-(4-cyanophenyl)-3-oxopropanoate (1g), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



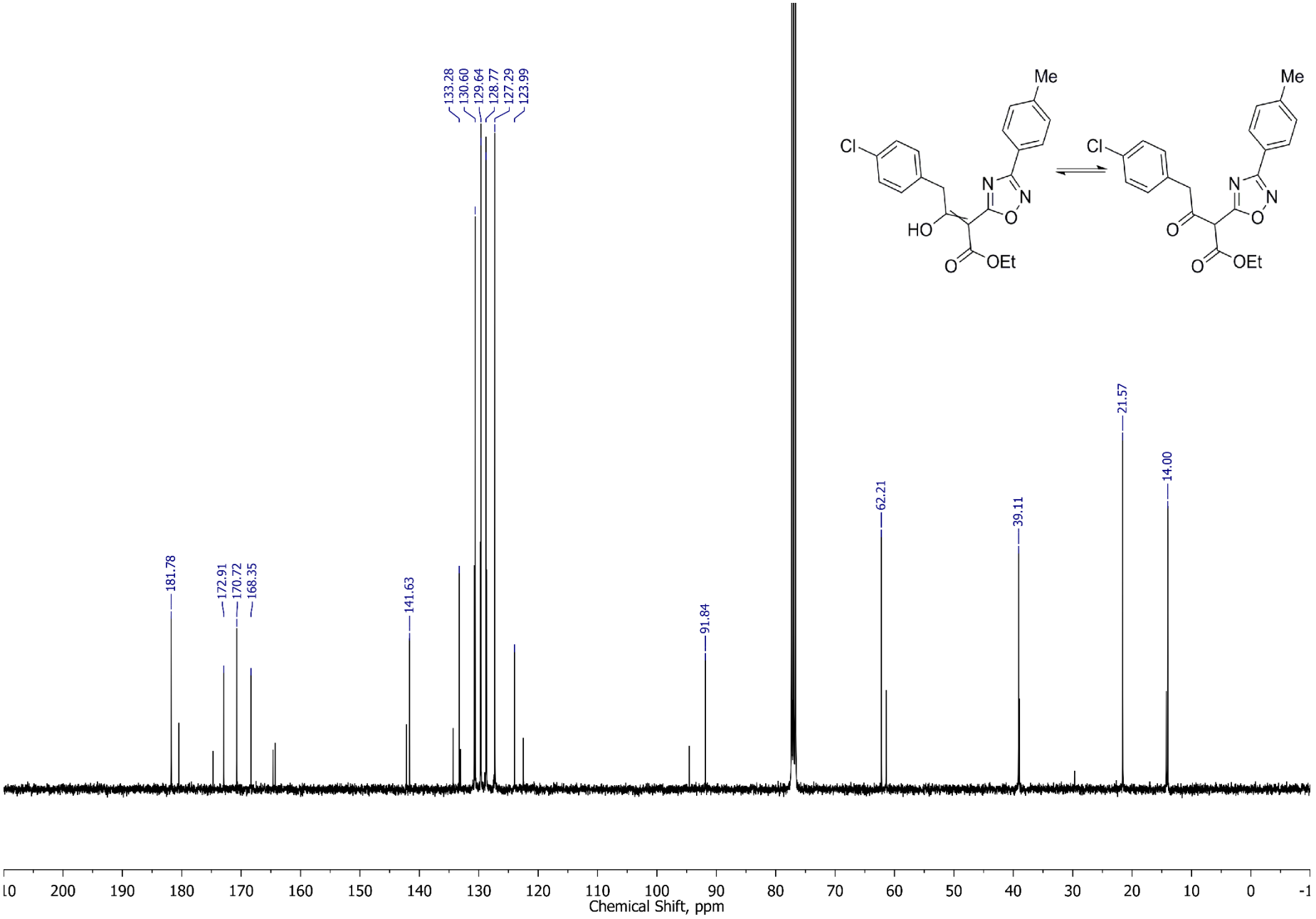
Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-(4-cyanophenyl)-3-hydroxyacrylate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-(4-cyanophenyl)-3-oxopropanoate (1g), DEPT, $CDCl_3$, 101 MHz



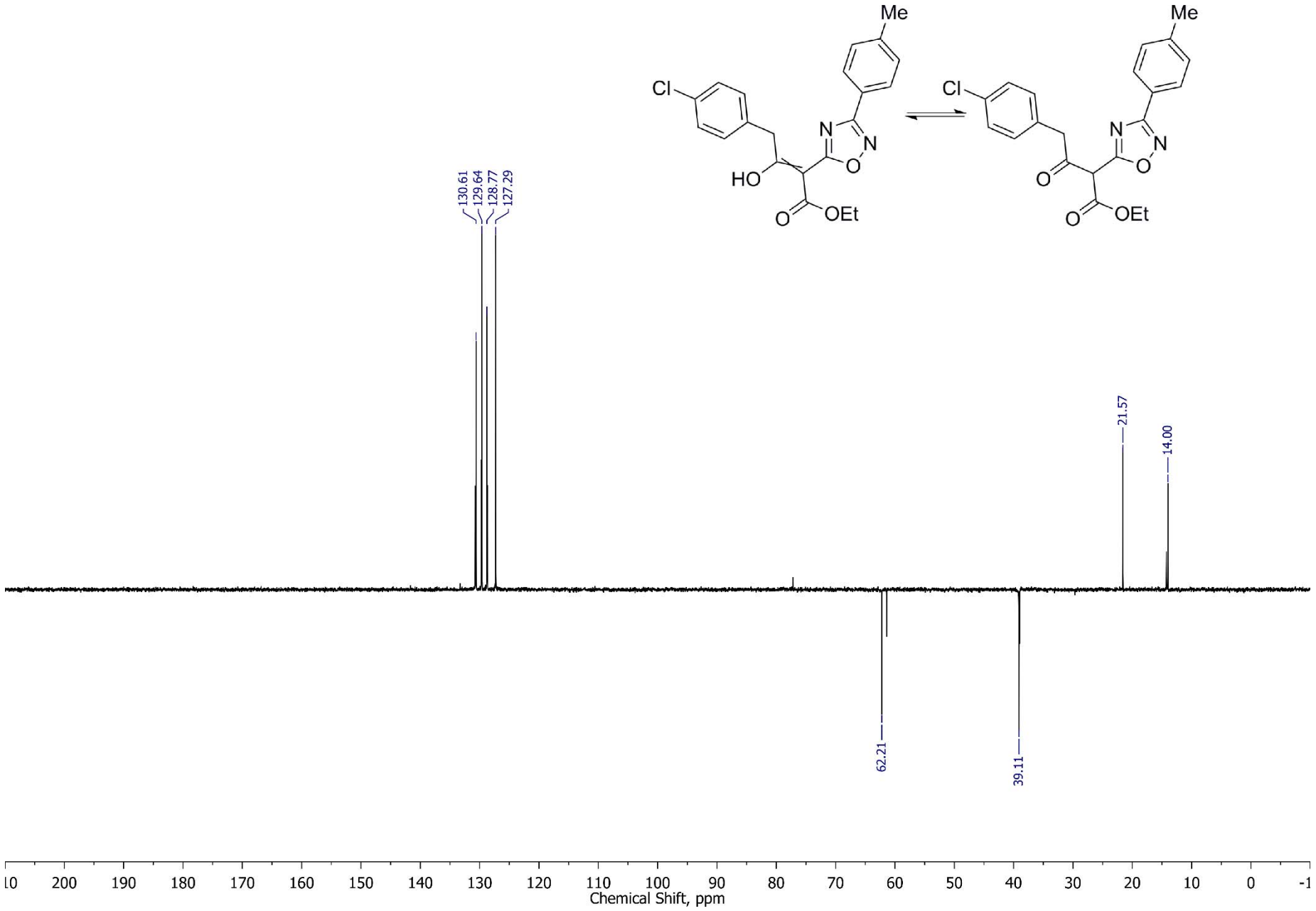
Ethyl 4-(4-chlorophenyl)-3-hydroxy-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)but-2-enoate/ ethyl 4-(4-chlorophenyl)-3-oxo-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)butanoate (1h), ^{1}H NMR, $CDCl_3$, 400 MHz



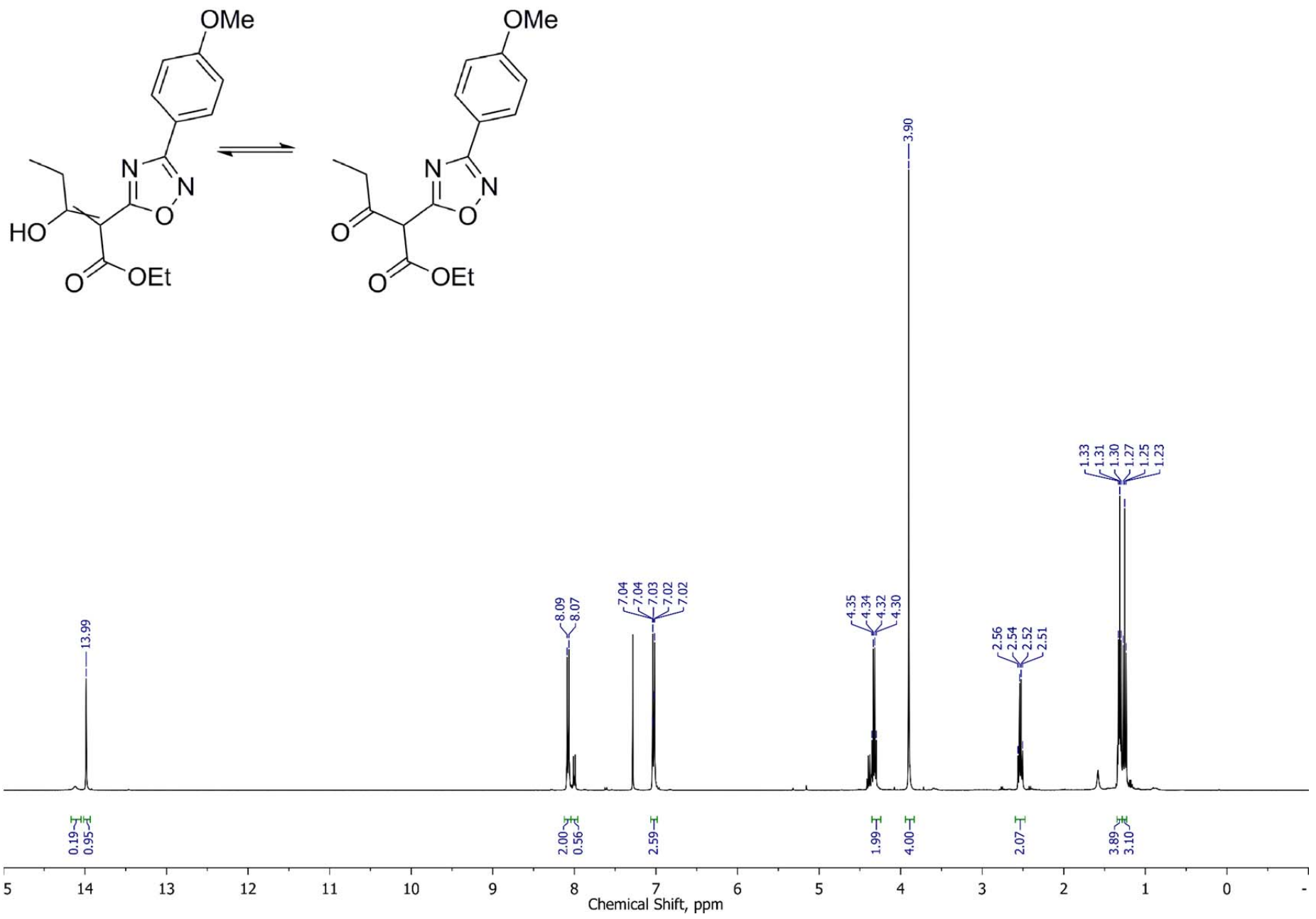
Ethyl 4-(4-chlorophenyl)-3-hydroxy-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)but-2-enoate/ ethyl 4-(4-chlorophenyl)-3-oxo-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)butanoate (1h), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



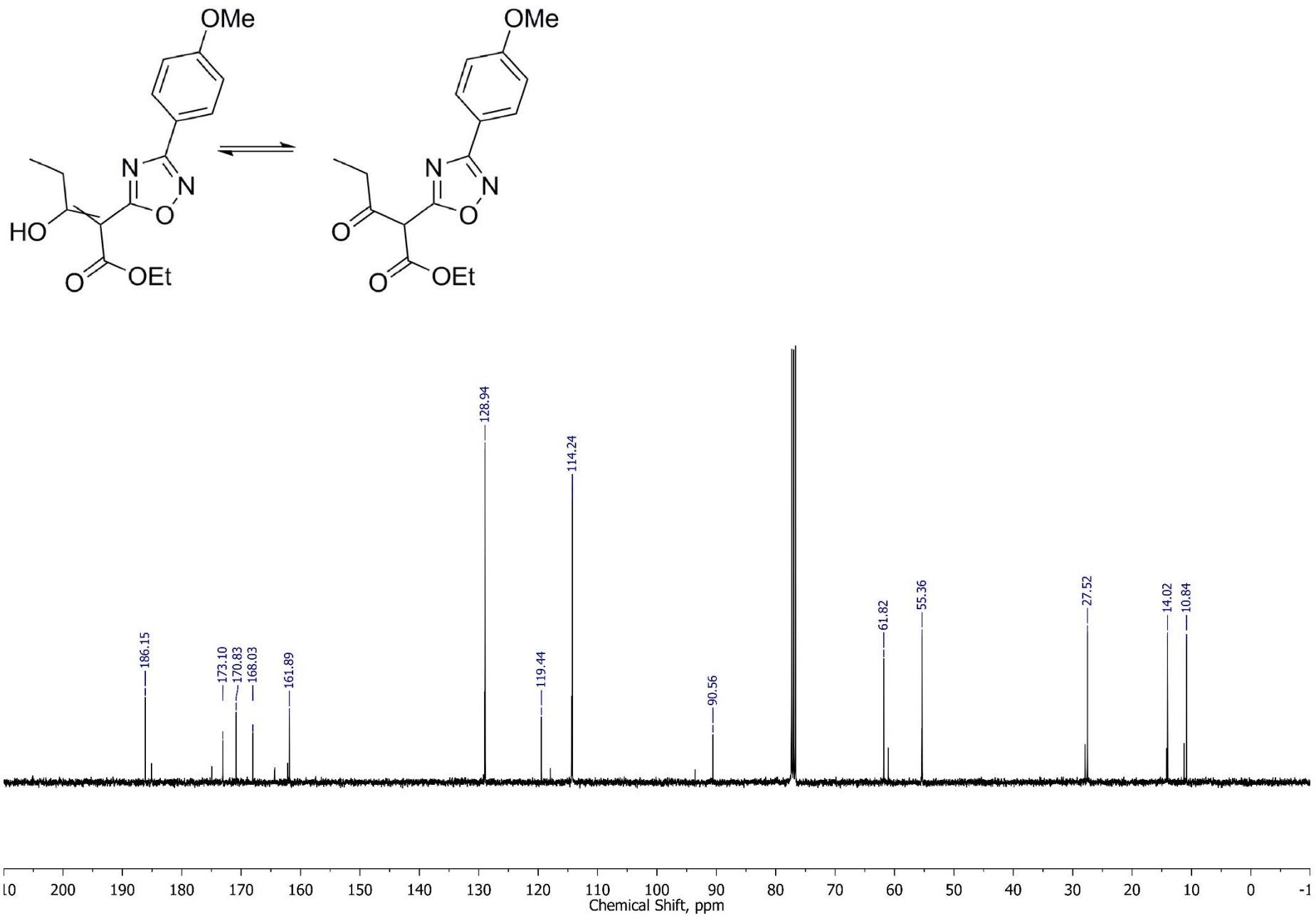
Ethyl 4-(4-chlorophenyl)-3-hydroxy-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)but-2-enoate/ ethyl 4-(4-chlorophenyl)-3-oxo-2-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)butanoate (1h), DEPT, $CDCl_3$, 101 MHz



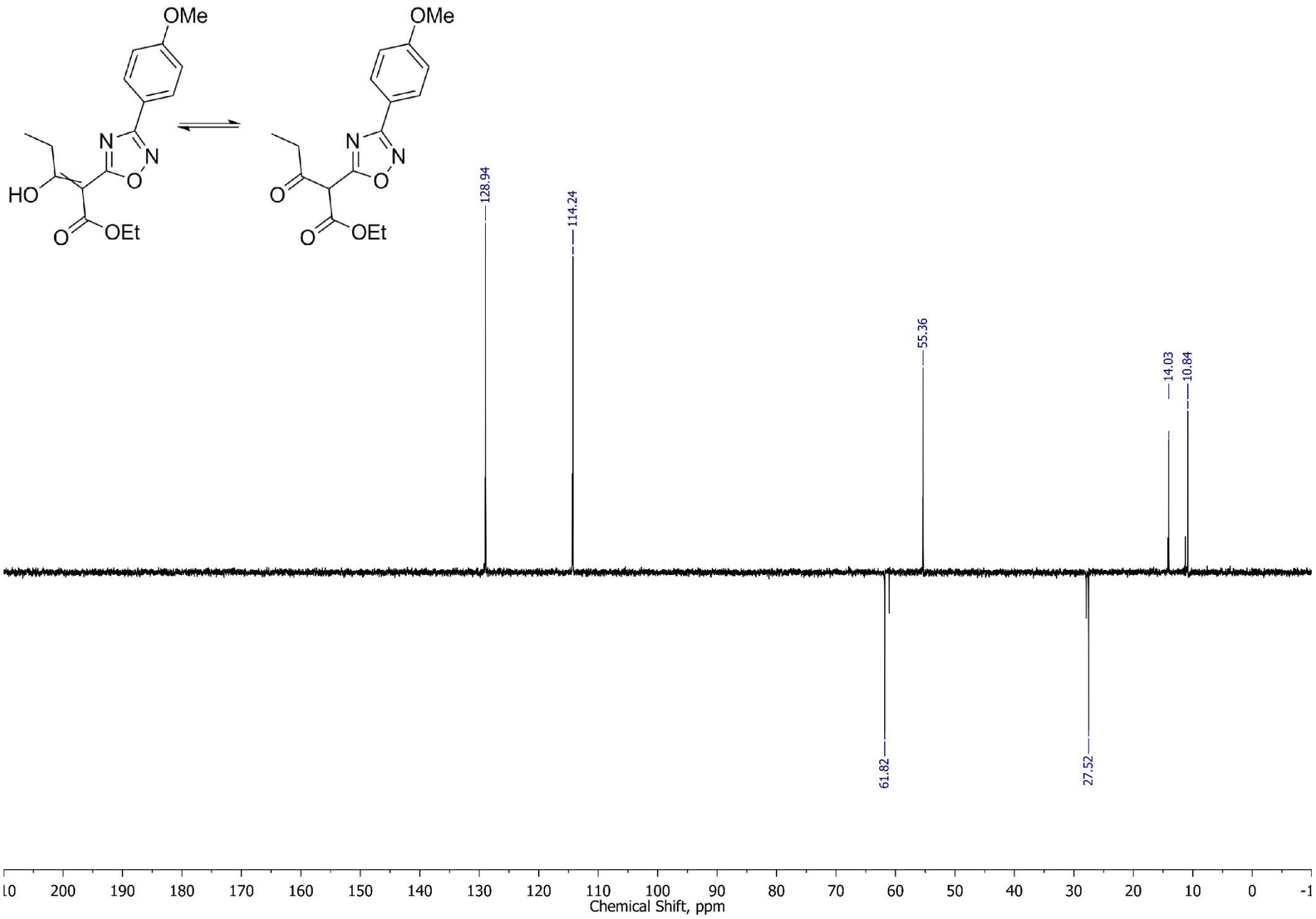
Ethyl 3-hydroxy-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)pent-2-enoate/ ethyl 2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)-3-oxopentanoate (1i), ^{1}H NMR, $CDCl_3$, 400 MHz



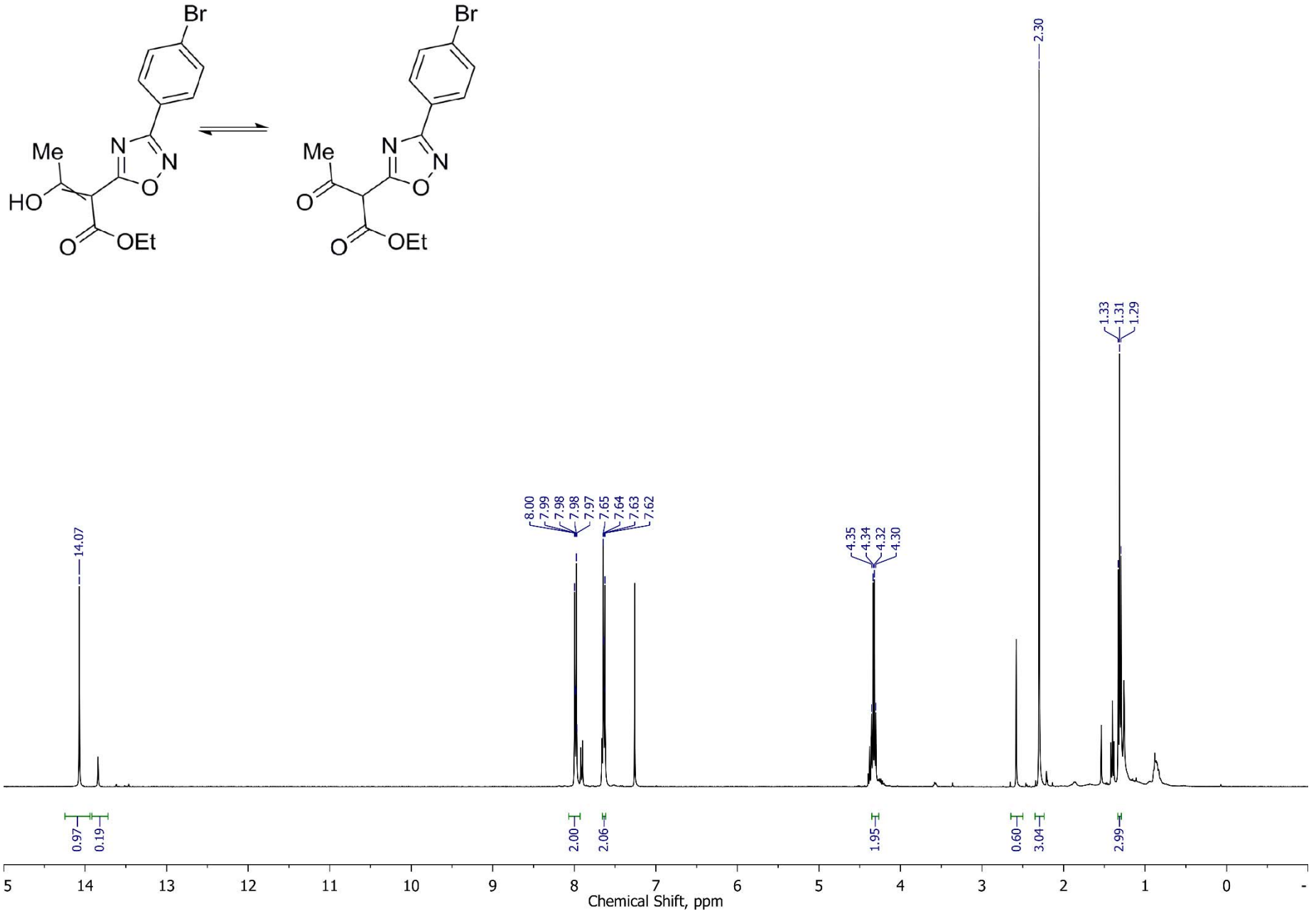
Ethyl 3-hydroxy-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)pent-2-enoate/ ethyl 2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)-3-oxopentanoate (1i), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



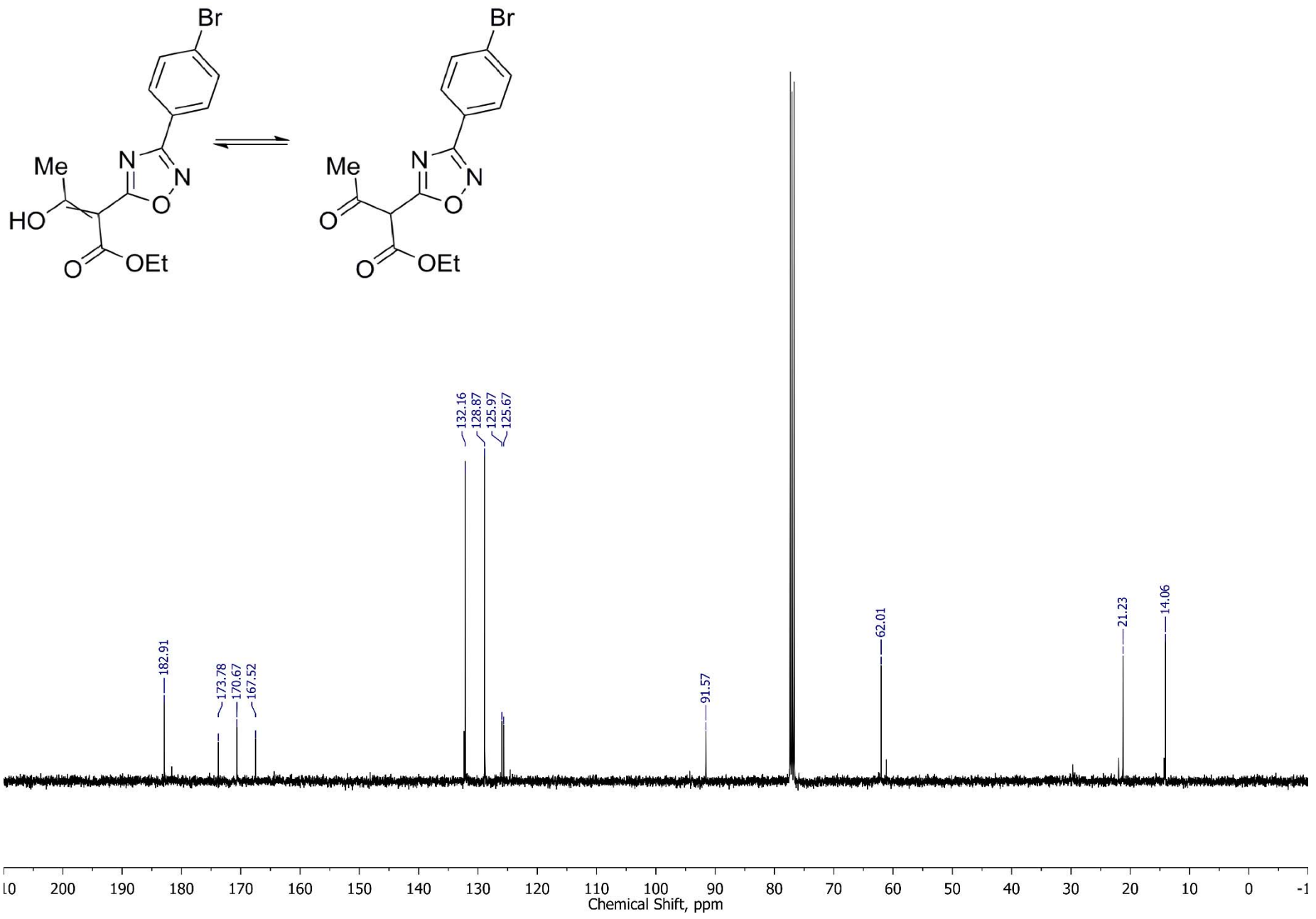
Ethyl 3-hydroxy-2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)pent-2-enoate/ ethyl 2-(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)-3-oxopentanoate (1i), DEPT, $CDCl_3$, 101 MHz



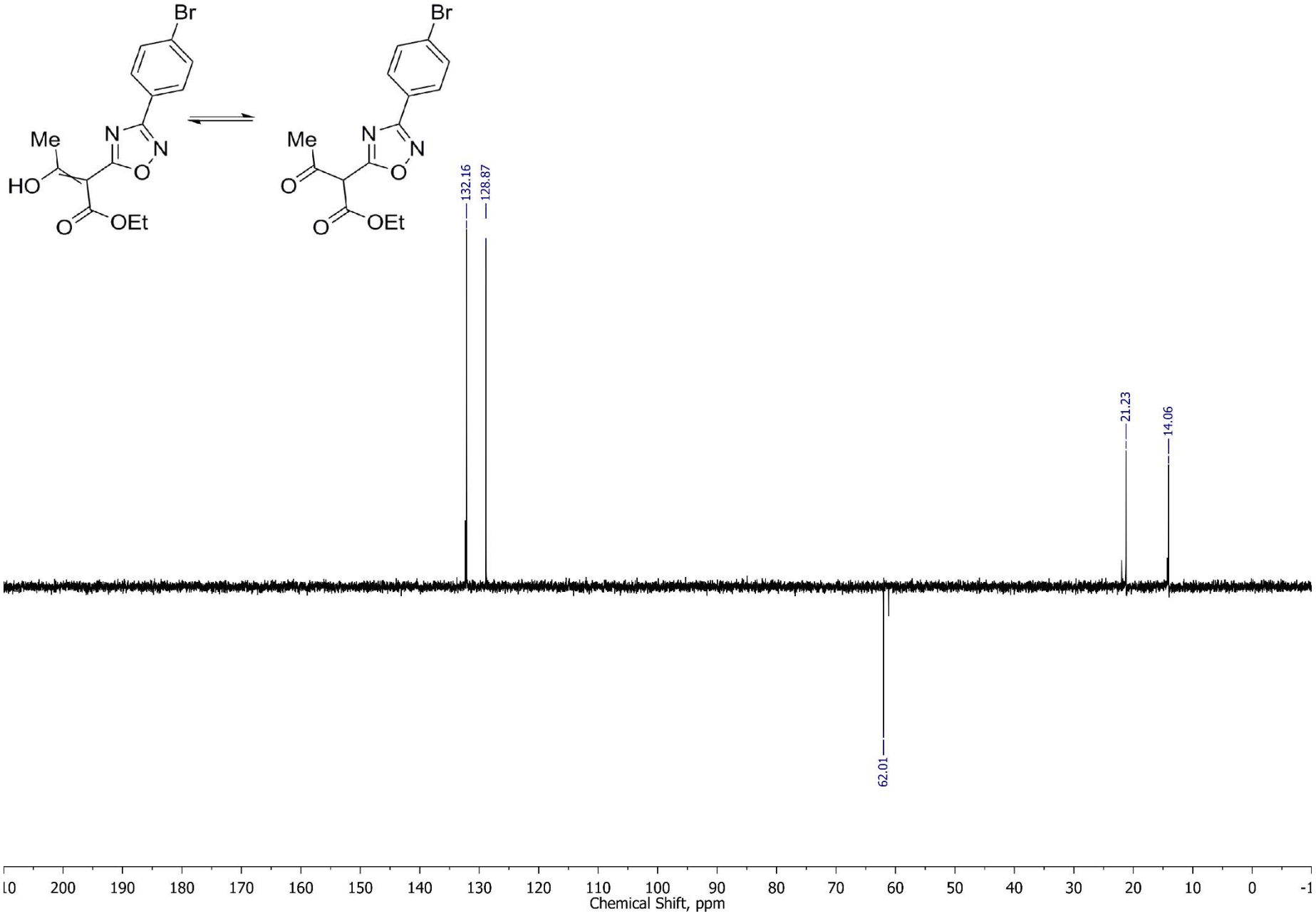
Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-hydroxybut-2-enoate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-oxobutanoate (1j), ^{1}H NMR, $CDCl_3$, 400 MHz



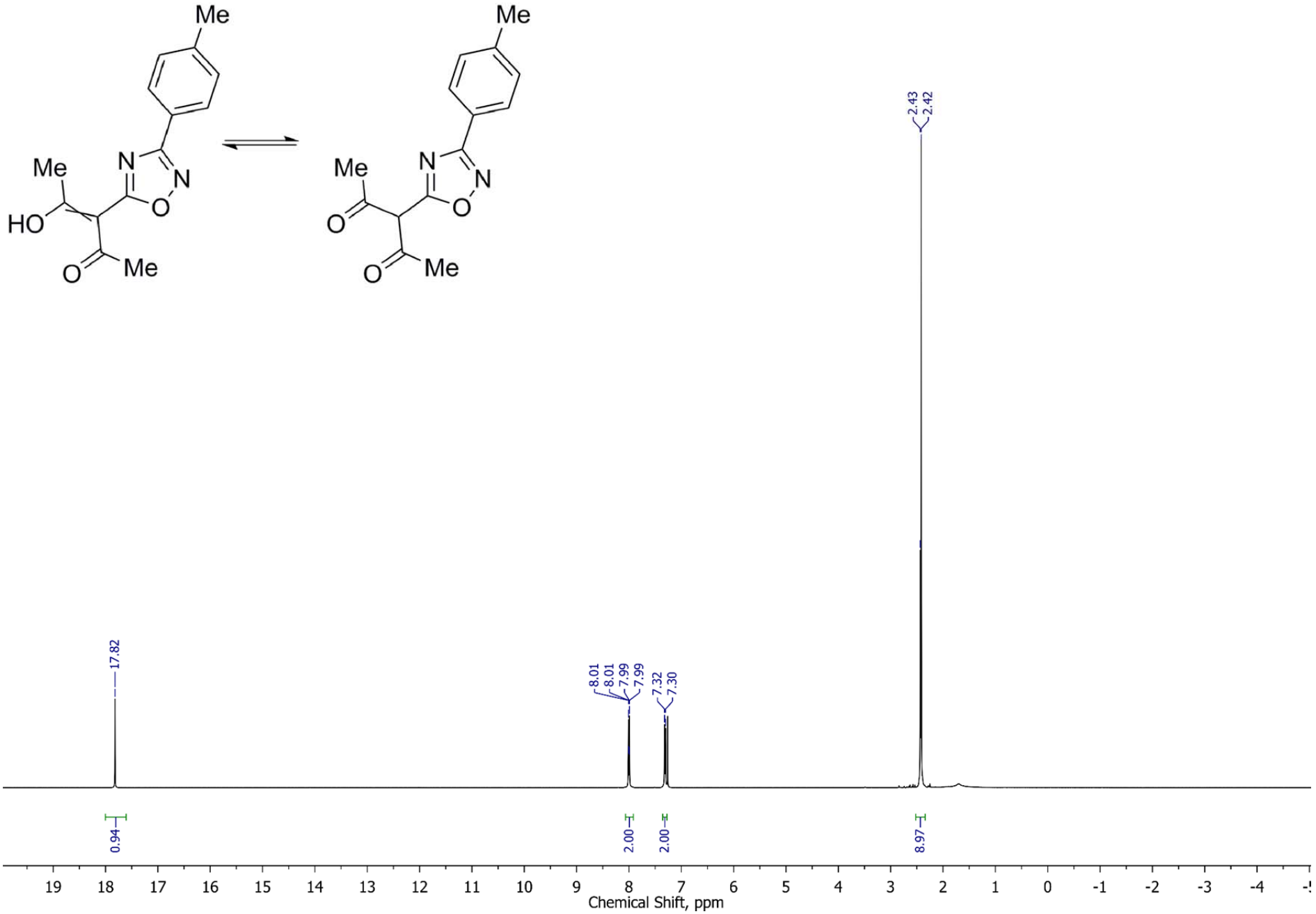
Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-hydroxybut-2-enoate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-oxobutanoate (1j), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



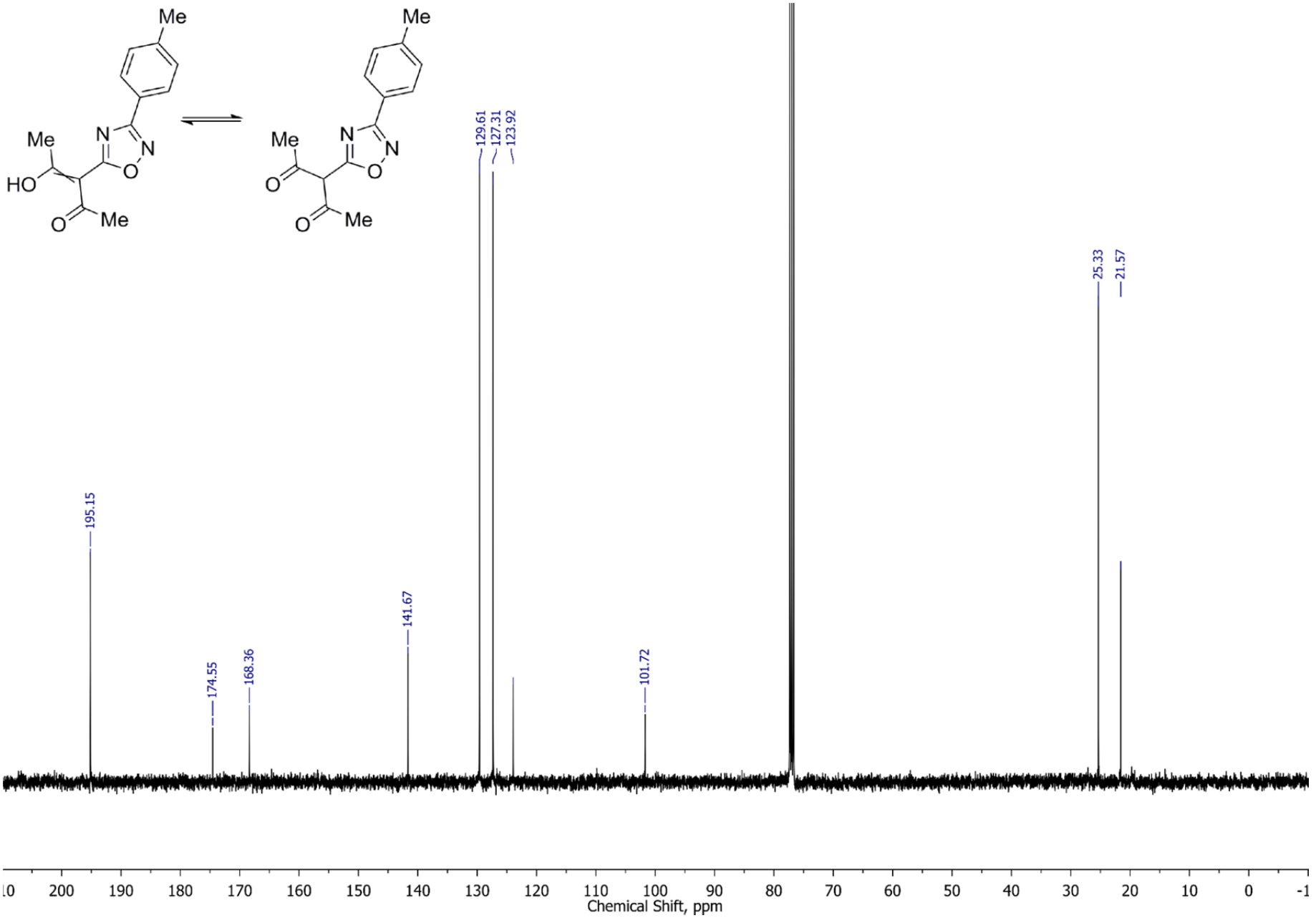
Ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-hydroxybut-2-enoate/ ethyl 2-(3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl)-3-oxobutanoate (1j), DEPT, $CDCl_3$, 101 MHz



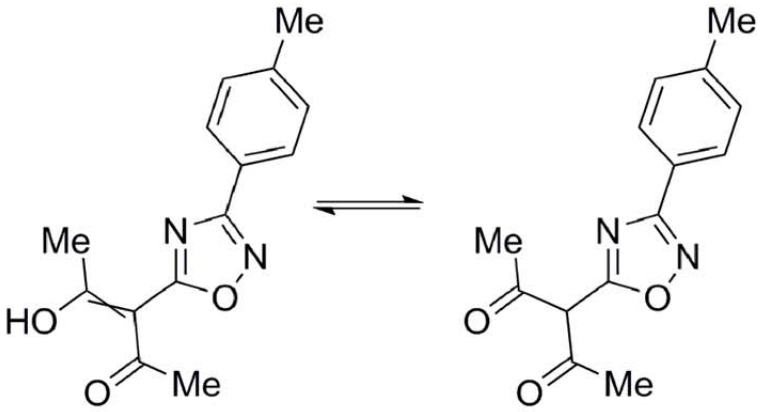
4-Hydroxy-3-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)pent-3-en-2-one/3-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)pentane-2,4-dione (1k), ^{1}H NMR, $CDCl_3$, 400 MHz

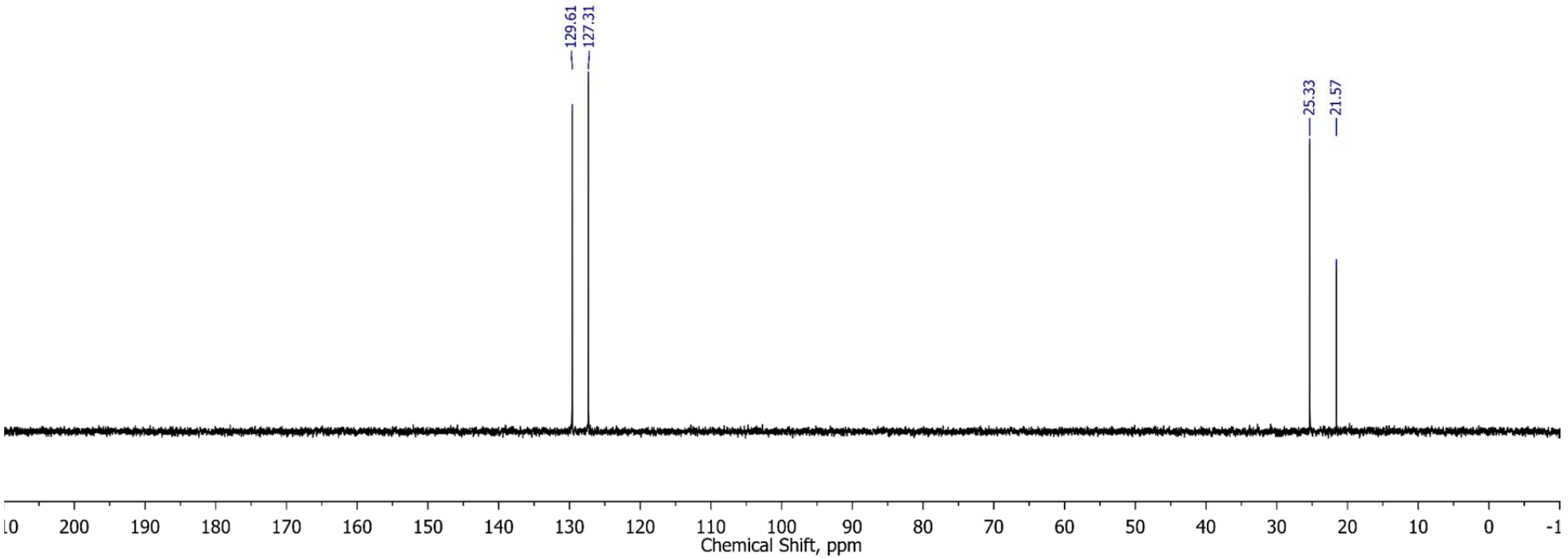


4-Hydroxy-3-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)pent-3-en-2-one/3-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)pentane-2,4-dione (1k), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz

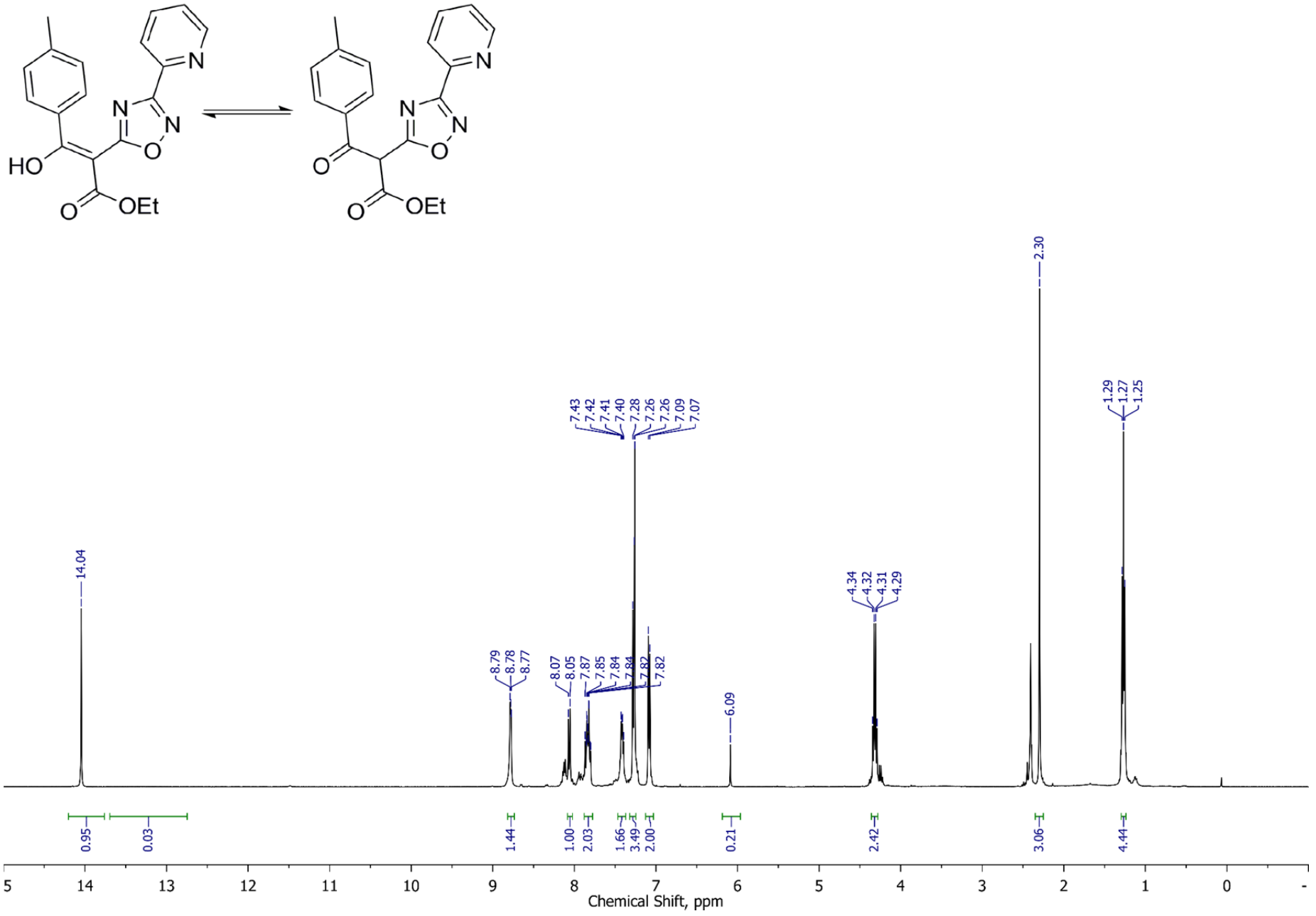


4-Hydroxy-3-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)pent-3-en-2-one/3-(3-(*p*-tolyl)-1,2,4-oxadiazol-5-yl)pentane-2,4-dione (1k), DEPT, $CDCl_3$, 101 MHz

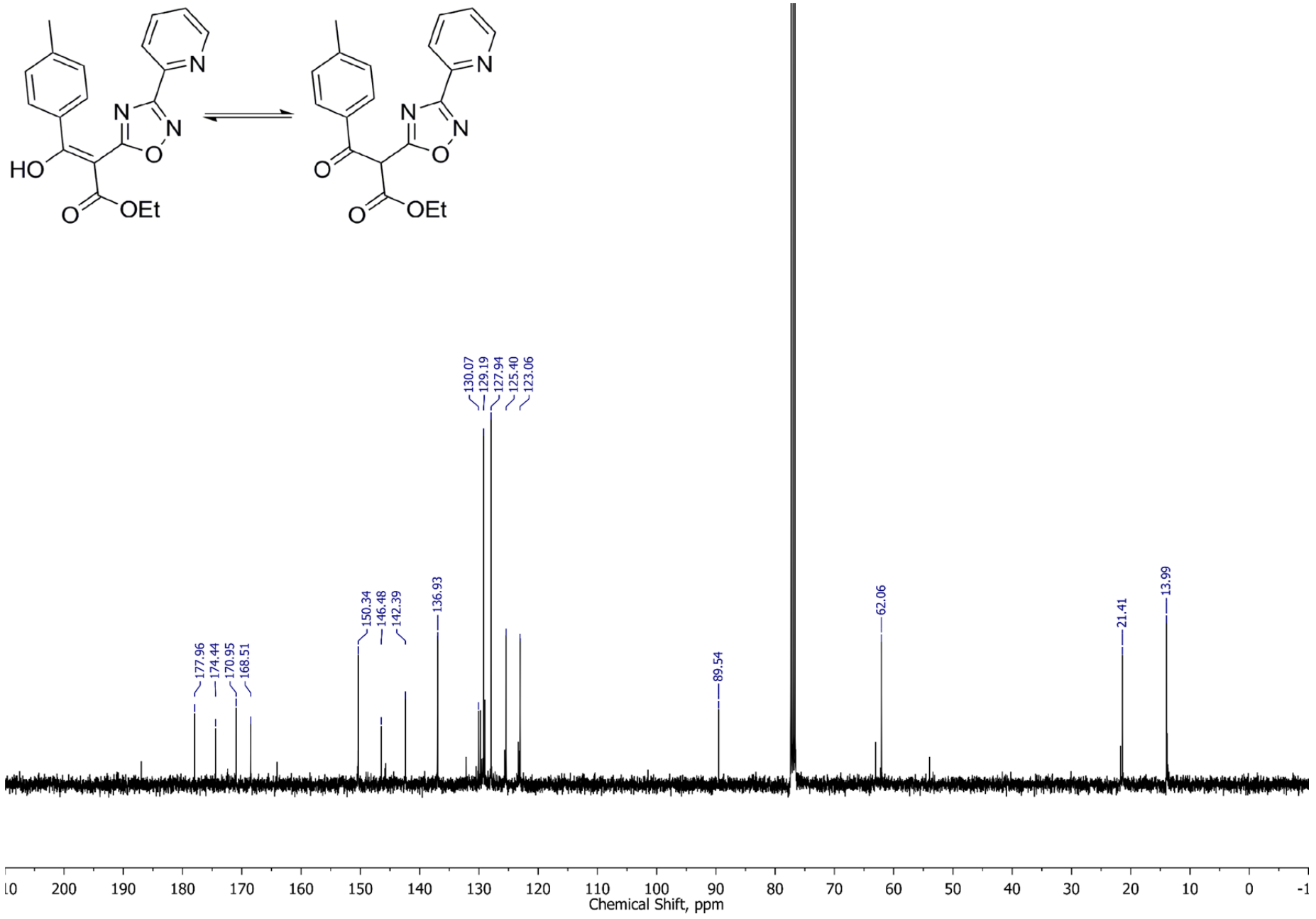




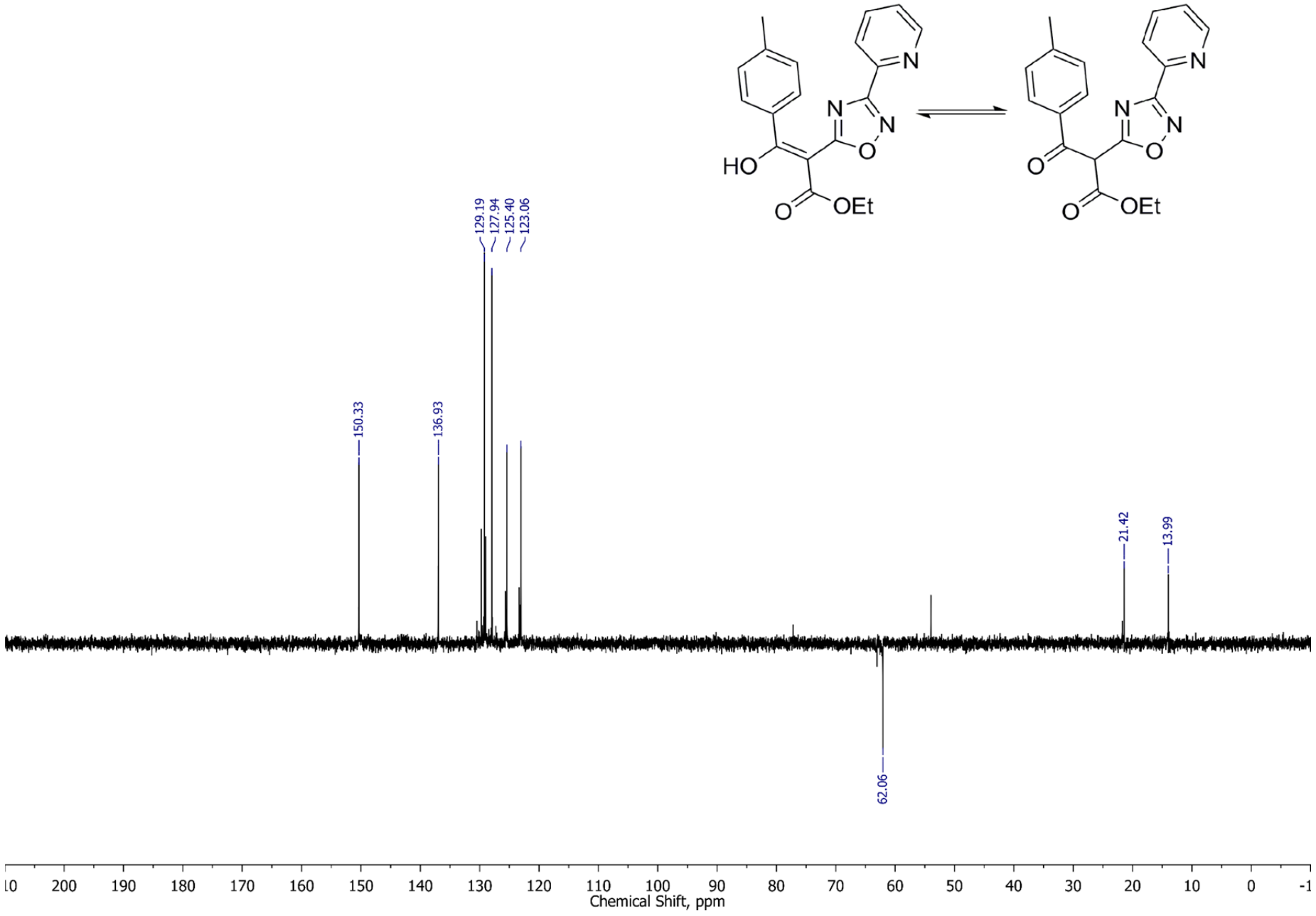
Ethyl 3-hydroxy-2-(3-(pyridin-2-yl)-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)acrylate / ethyl 3-oxo-2-(3-(pyridin-2-yl)-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)propanoate (1l), ^{1}H NMR, $CDCl_3$, 400 MHz



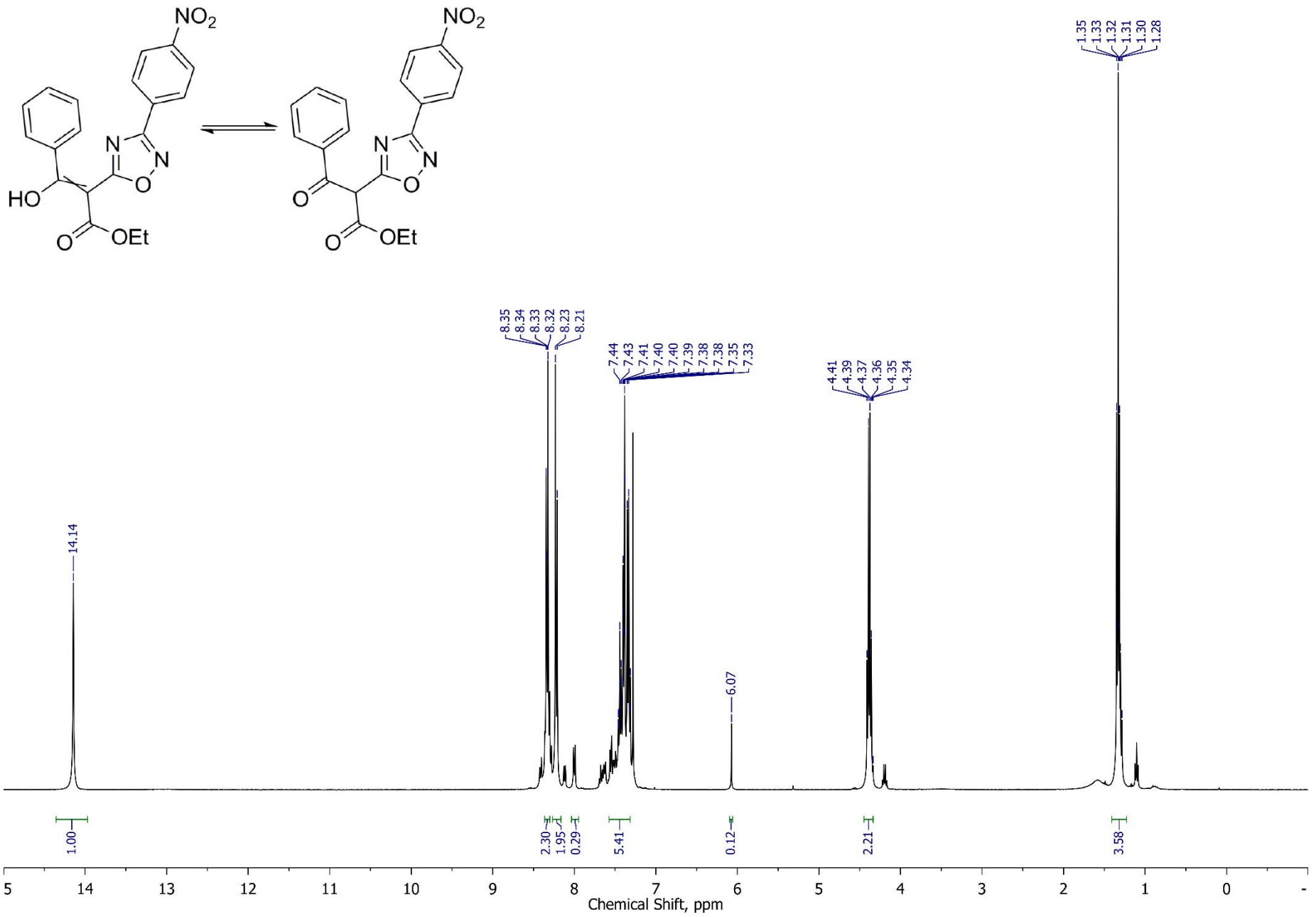
Ethyl 3-hydroxy-2-(3-(pyridin-2-yl)-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)acrylate / ethyl 3-oxo-2-(3-(pyridin-2-yl)-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)propanoate (1l), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



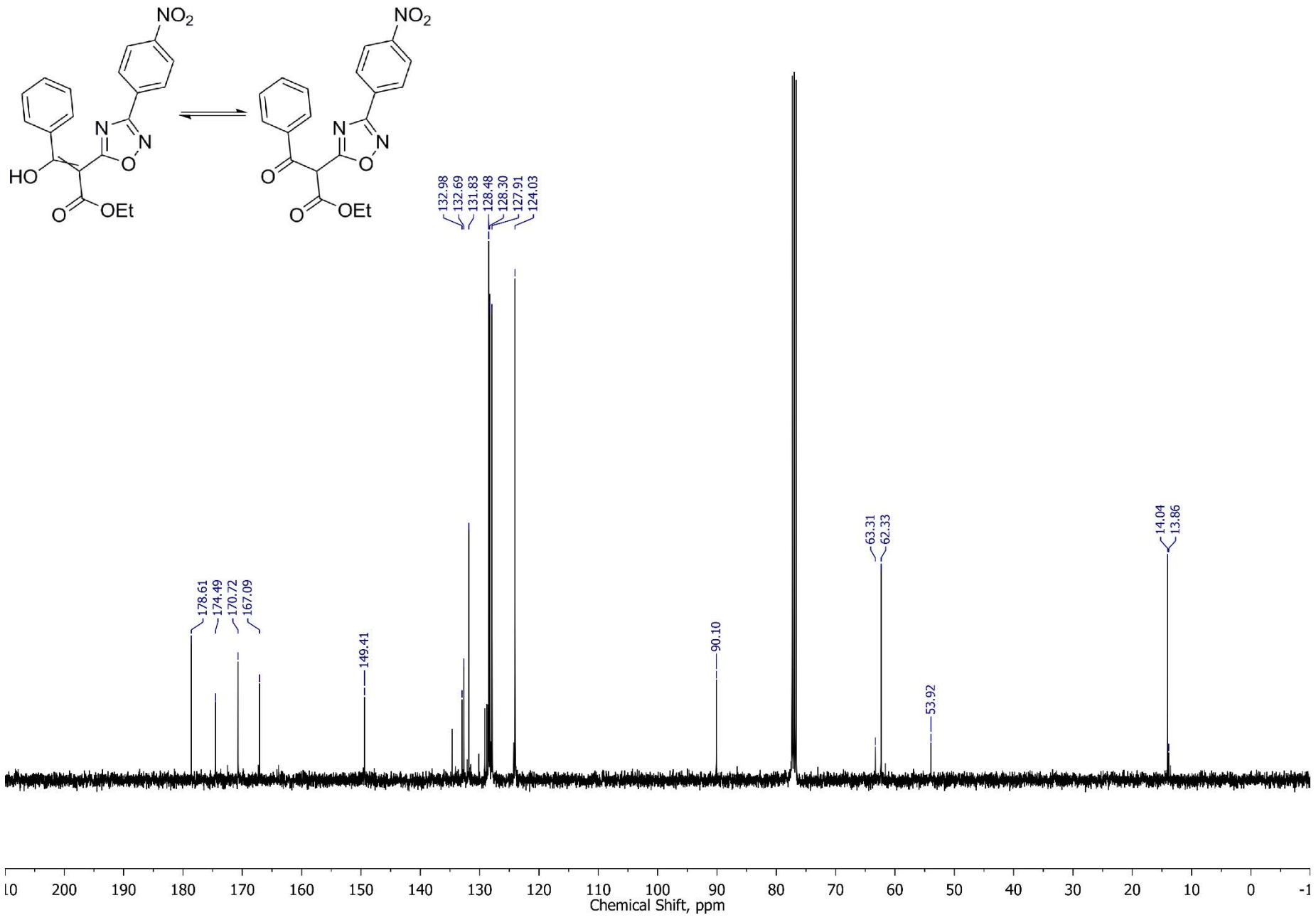
Ethyl 3-hydroxy-2-(3-(pyridin-2-yl)-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)acrylate / ethyl 3-oxo-2-(3-(pyridin-2-yl)-1,2,4-oxadiazol-5-yl)-3-(*p*-tolyl)propanoate (1l), DEPT, $CDCl_3$, 101 MHz



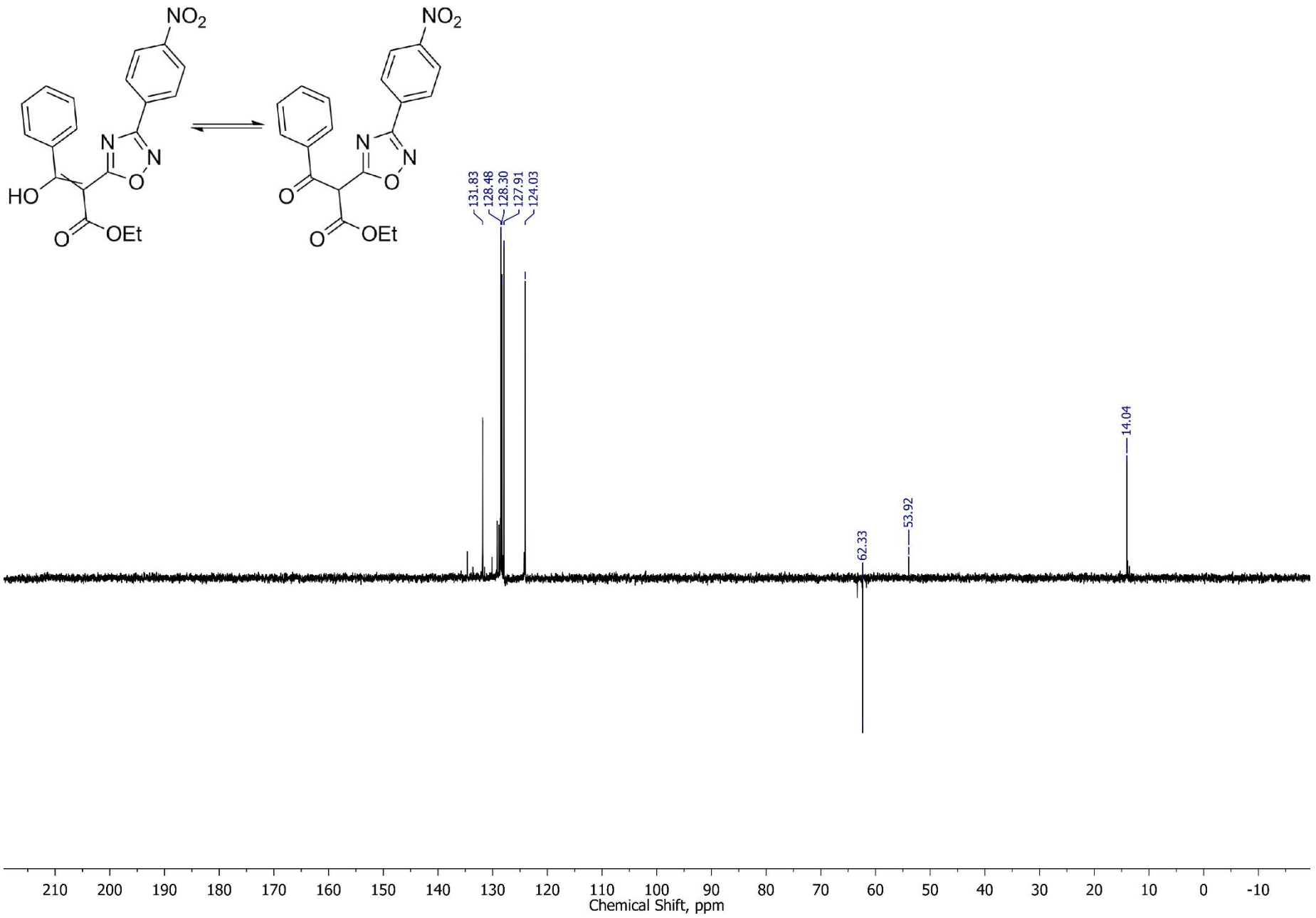
Ethyl 3-hydroxy-2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-phenylacrylate/ ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-3-phenylpropanoate (1m), ^{1}H NMR, $CDCl_3$, 400 MHz



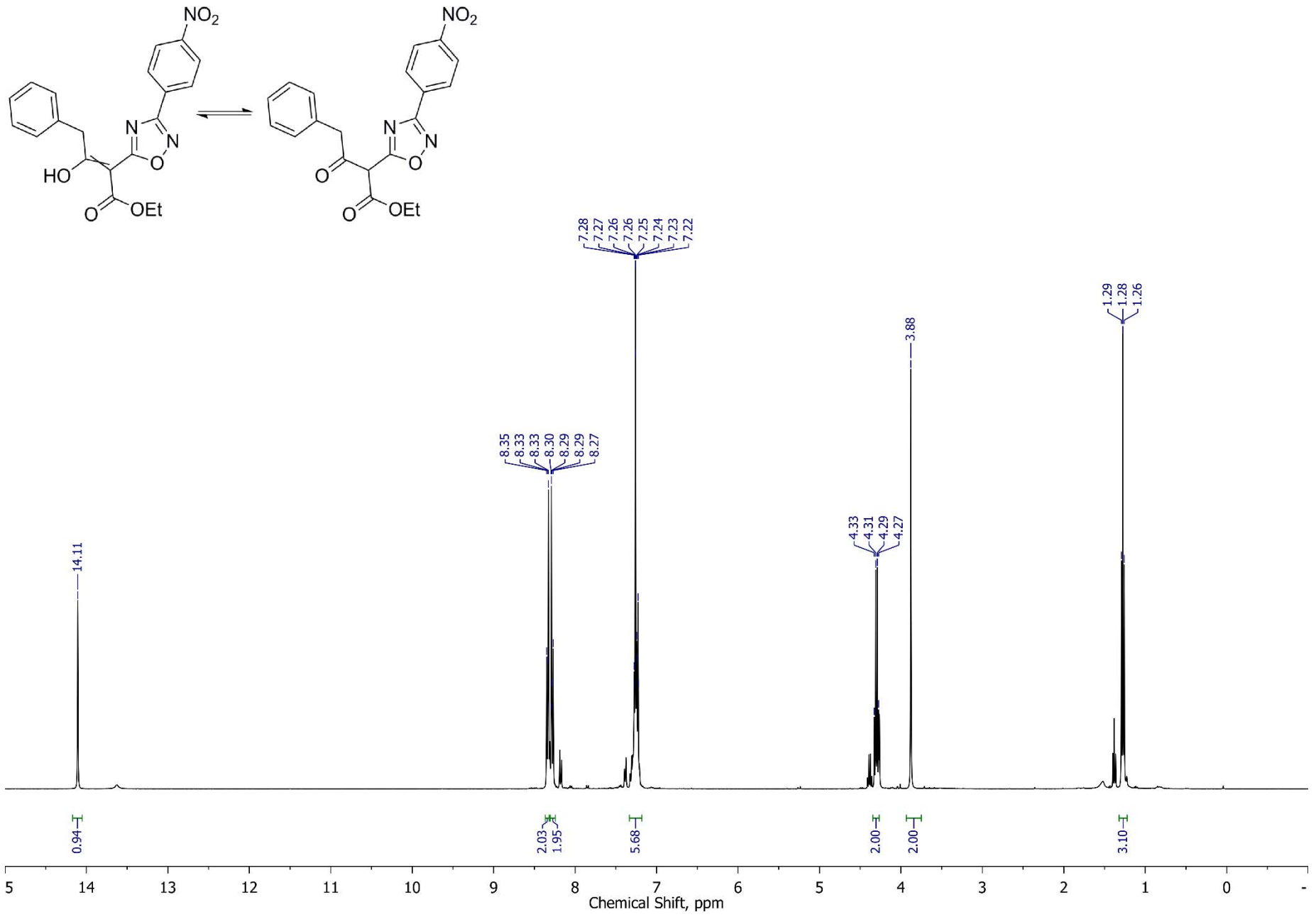
Ethyl 3-hydroxy-2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-phenylacrylate/ ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-3-phenylpropanoate (1m), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



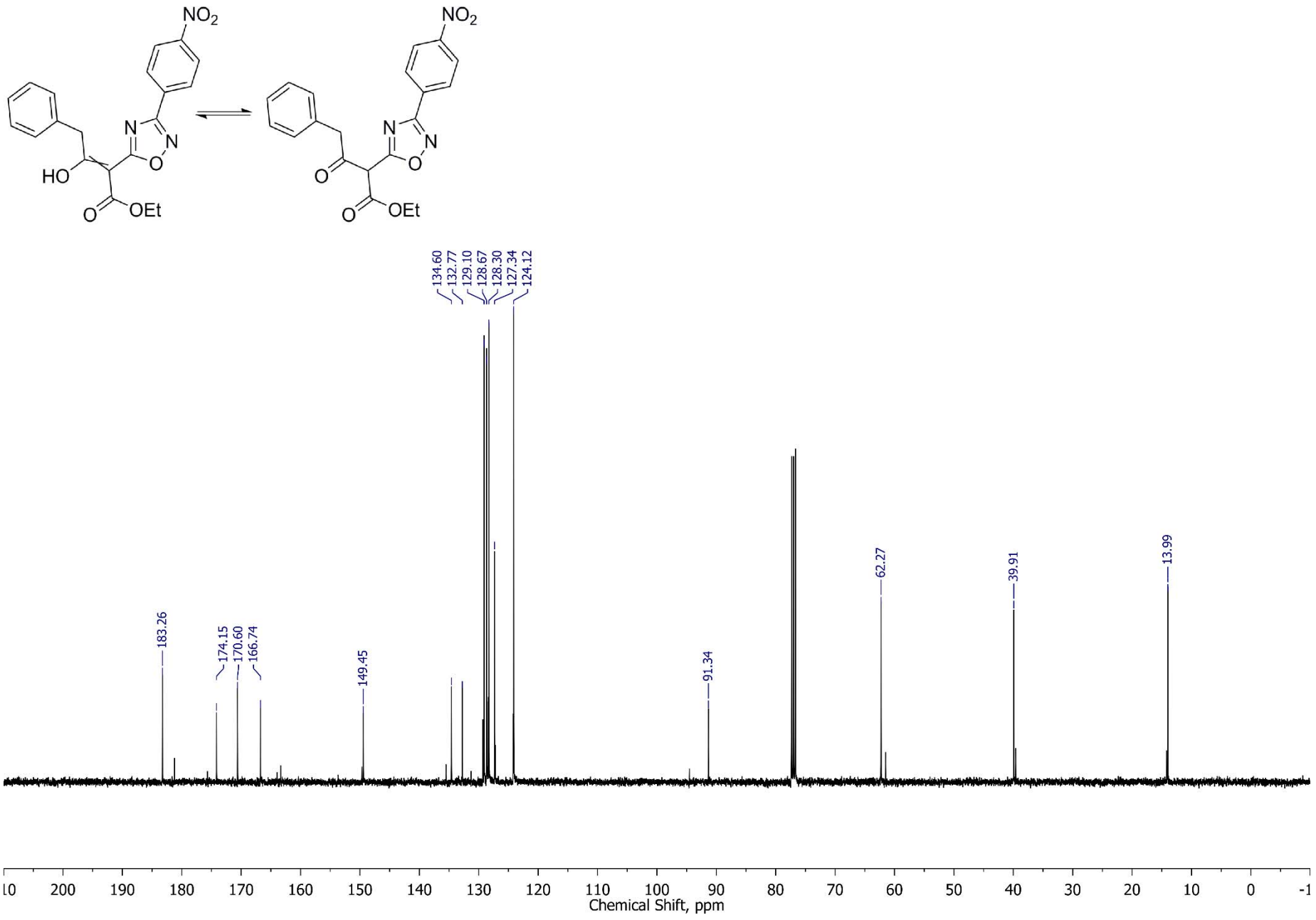
Ethyl 3-hydroxy-2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-phenylacrylate/ ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-3-phenylpropanoate (1m), DEPT, $CDCl_3$, 101 MHz



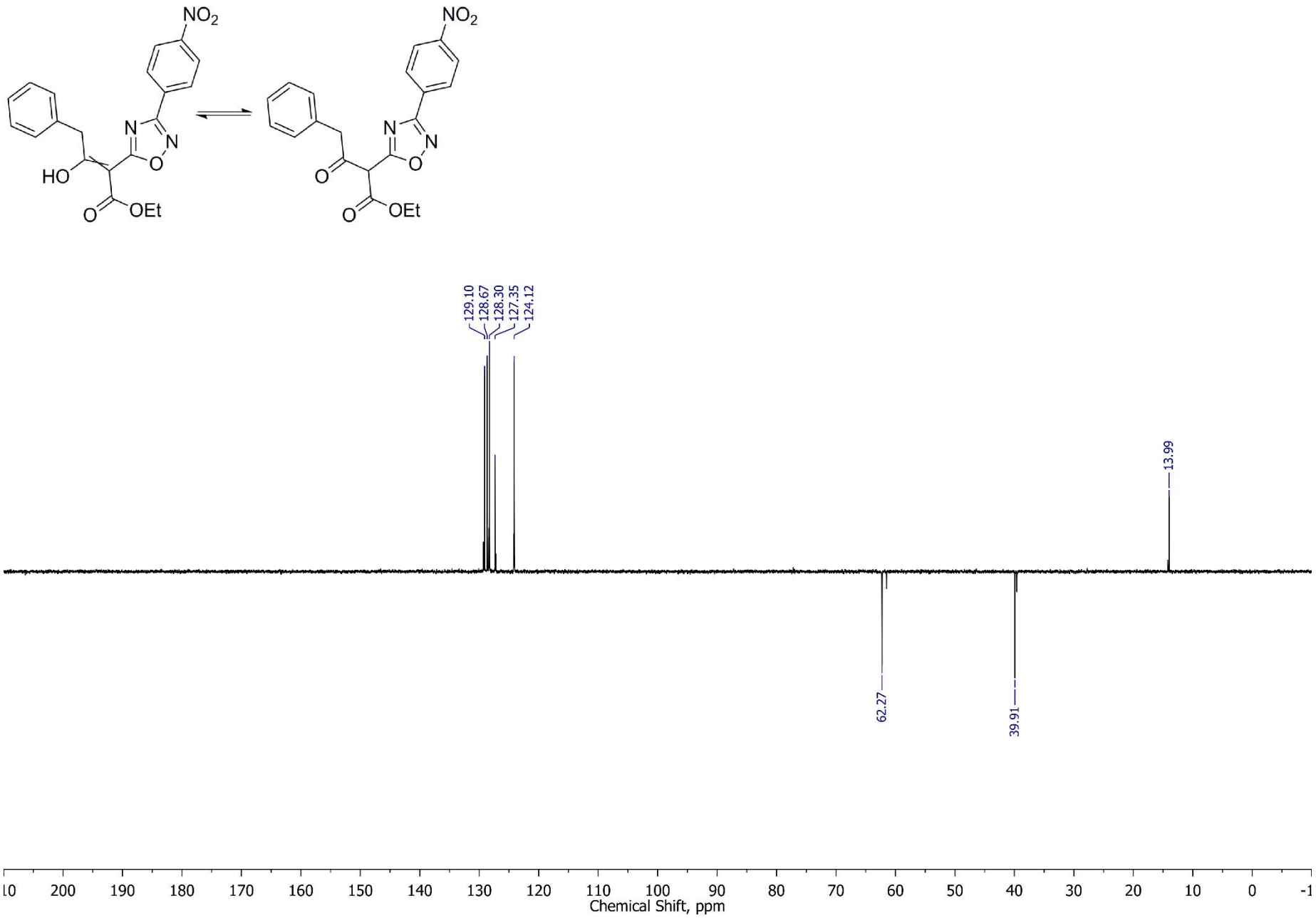
Ethyl 3-hydroxy-2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-4-phenylbut-2-enoate/ ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-4-phenylbutanoate (1n), ^{1}H NMR, $CDCl_3$, 400 MHz



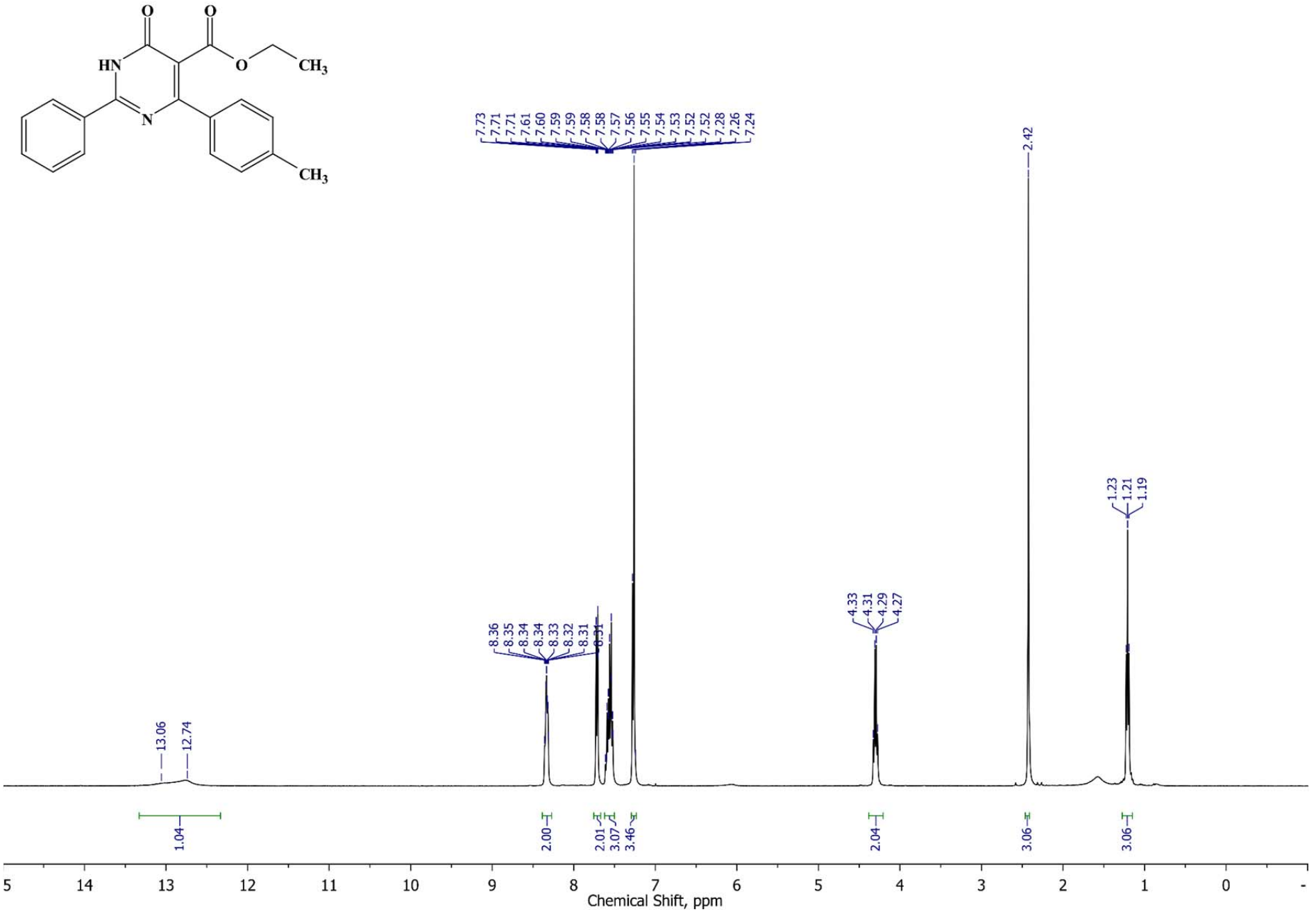
Ethyl 3-hydroxy-2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-4-phenylbut-2-enoate/ ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-4-phenylbutanoate (1n), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



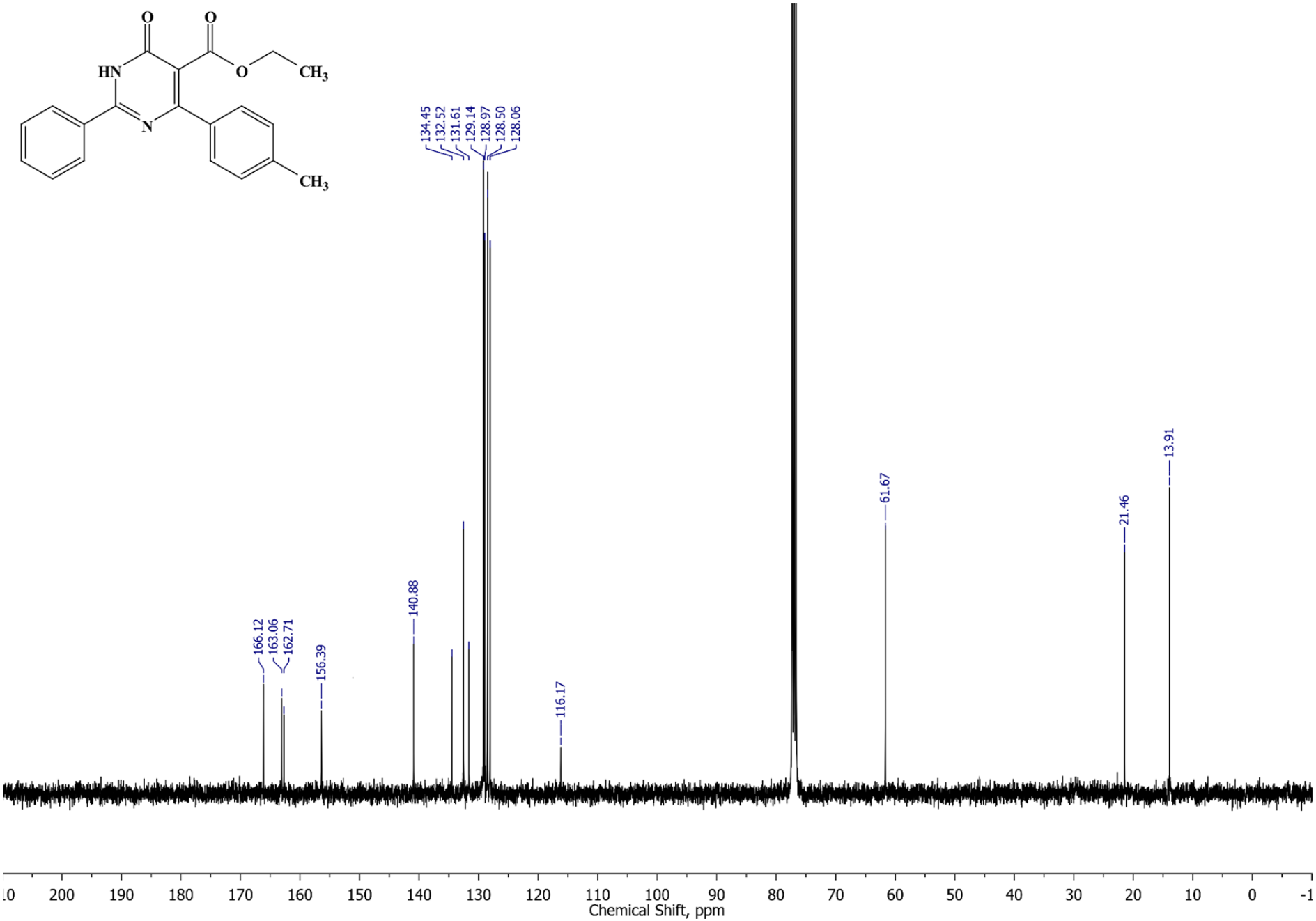
Ethyl 3-hydroxy-2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-4-phenylbut-2-enoate/ ethyl 2-(3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)-3-oxo-4-phenylbutanoate (1n), DEPT, $CDCl_3$, 101 MHz



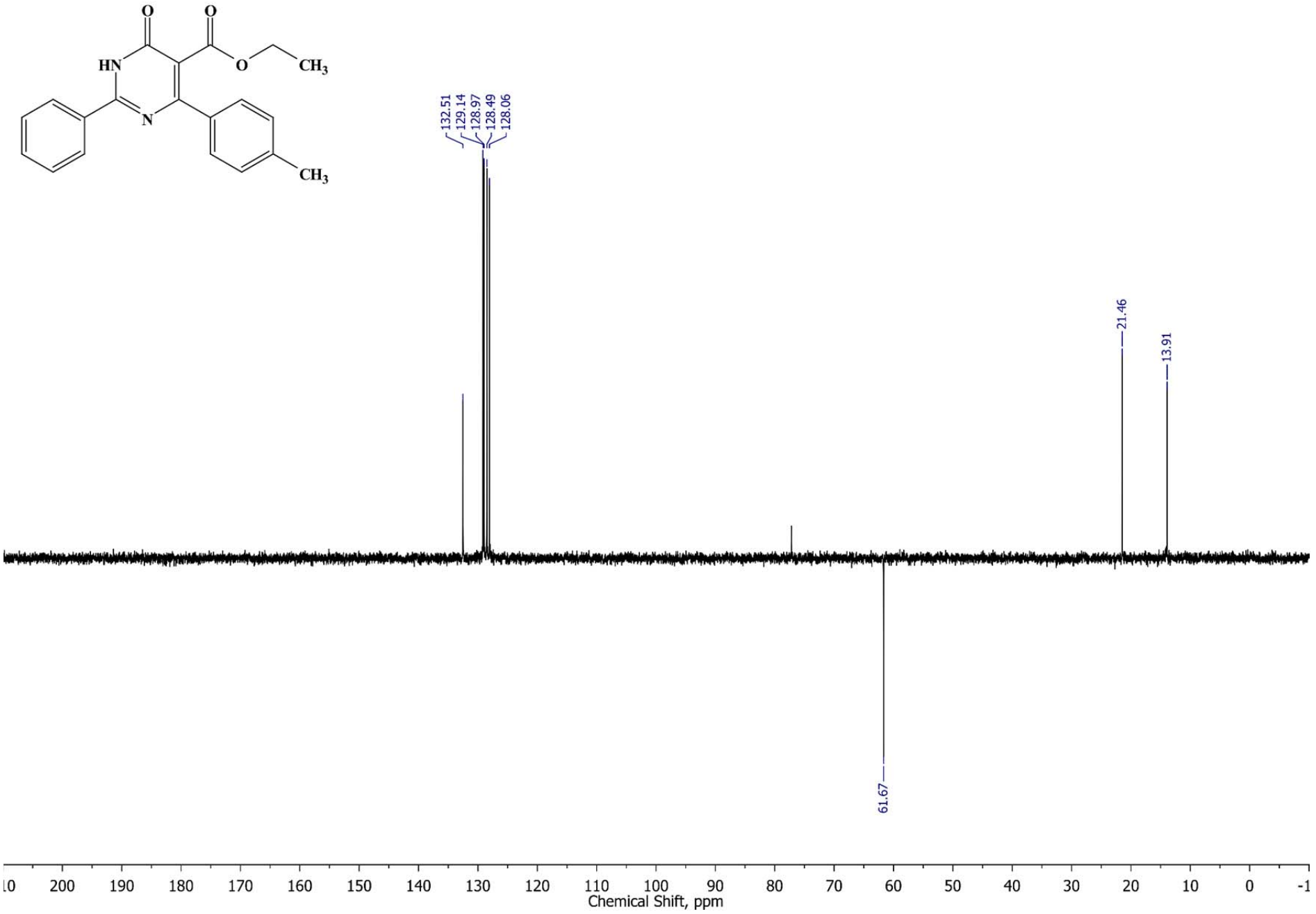
Ethyl 6-oxo-2-phenyl-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3a), ^{1}H NMR, $CDCl_3$, 400 MHz



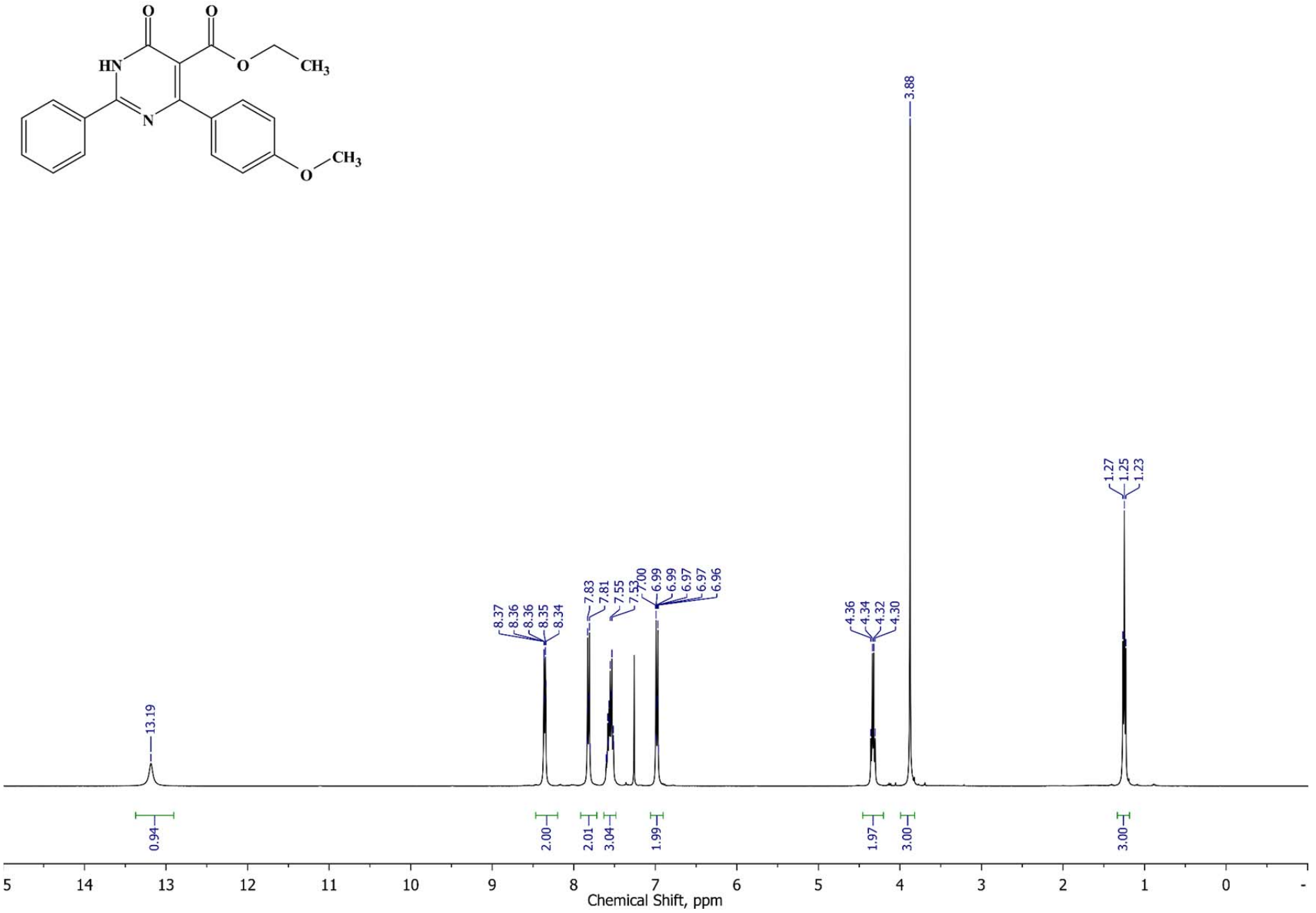
Ethyl 6-oxo-2-phenyl-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3a), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



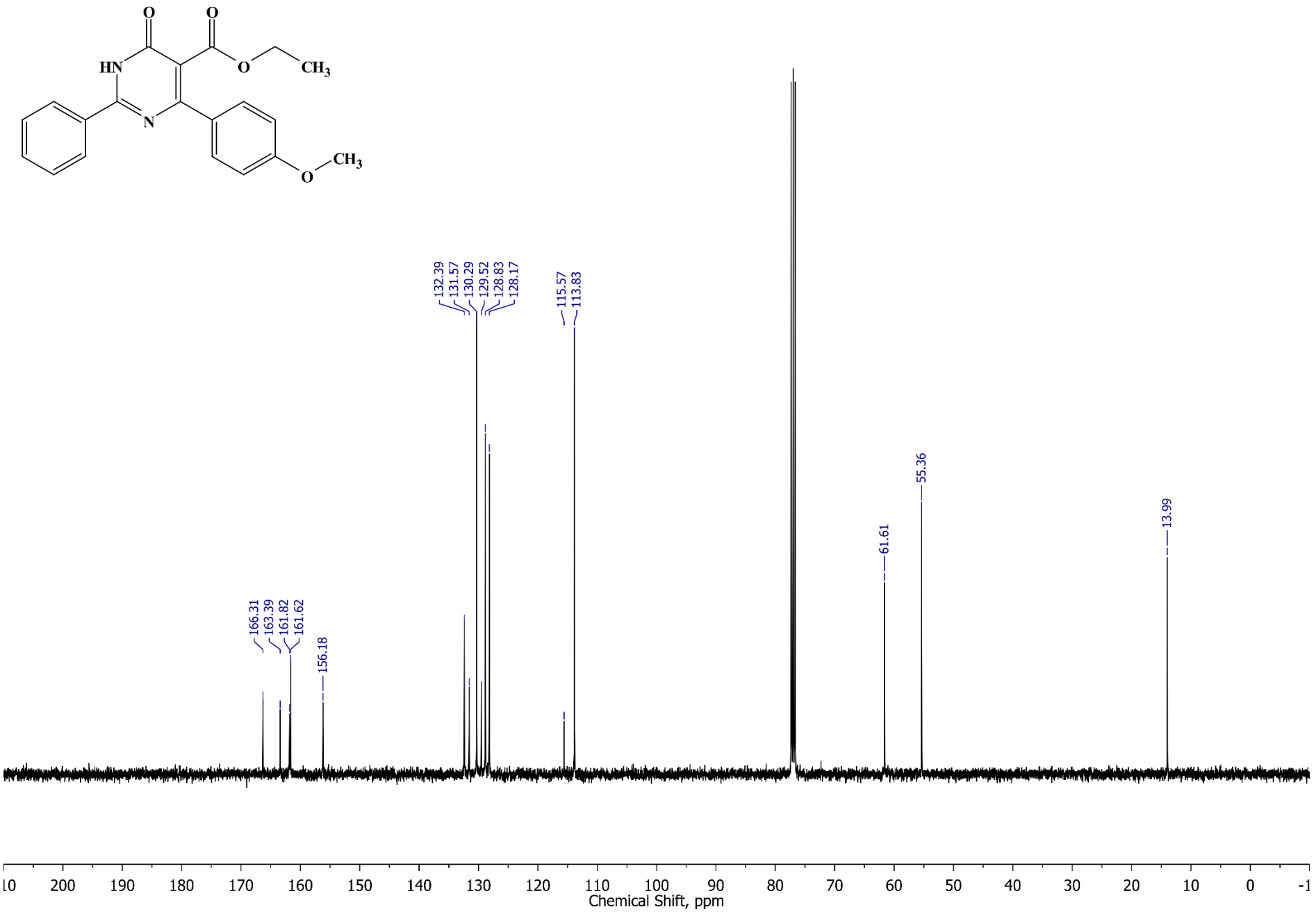
Ethyl 6-oxo-2-phenyl-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3a), DEPT, $CDCl_3$, 101 MHz



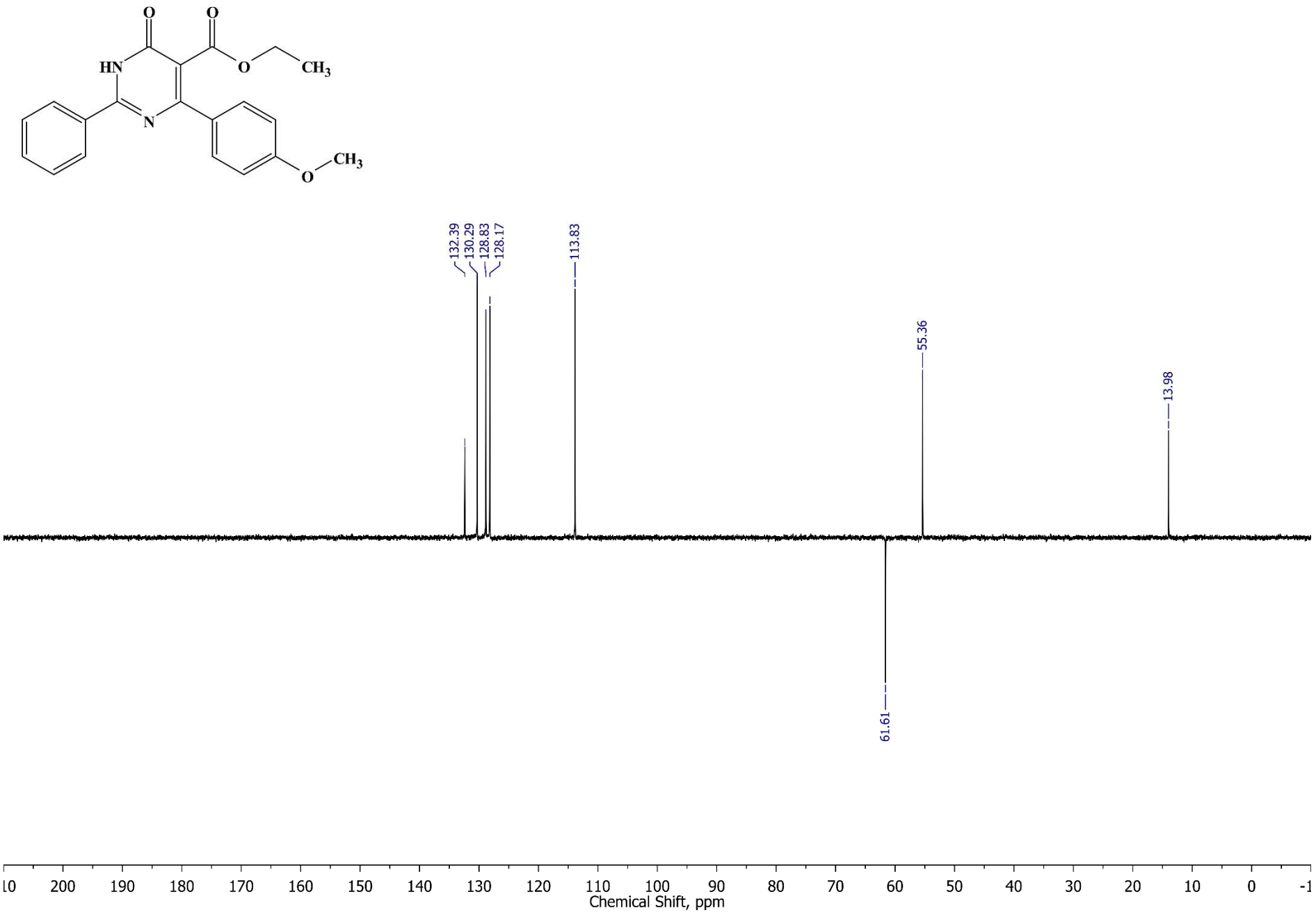
Ethyl 4-(4-methoxyphenyl)-6-oxo-2-phenyl-1,6-dihydropyrimidine-5-carboxylate (3b), ^{1}H NMR, $CDCl_3$, 400 MHz



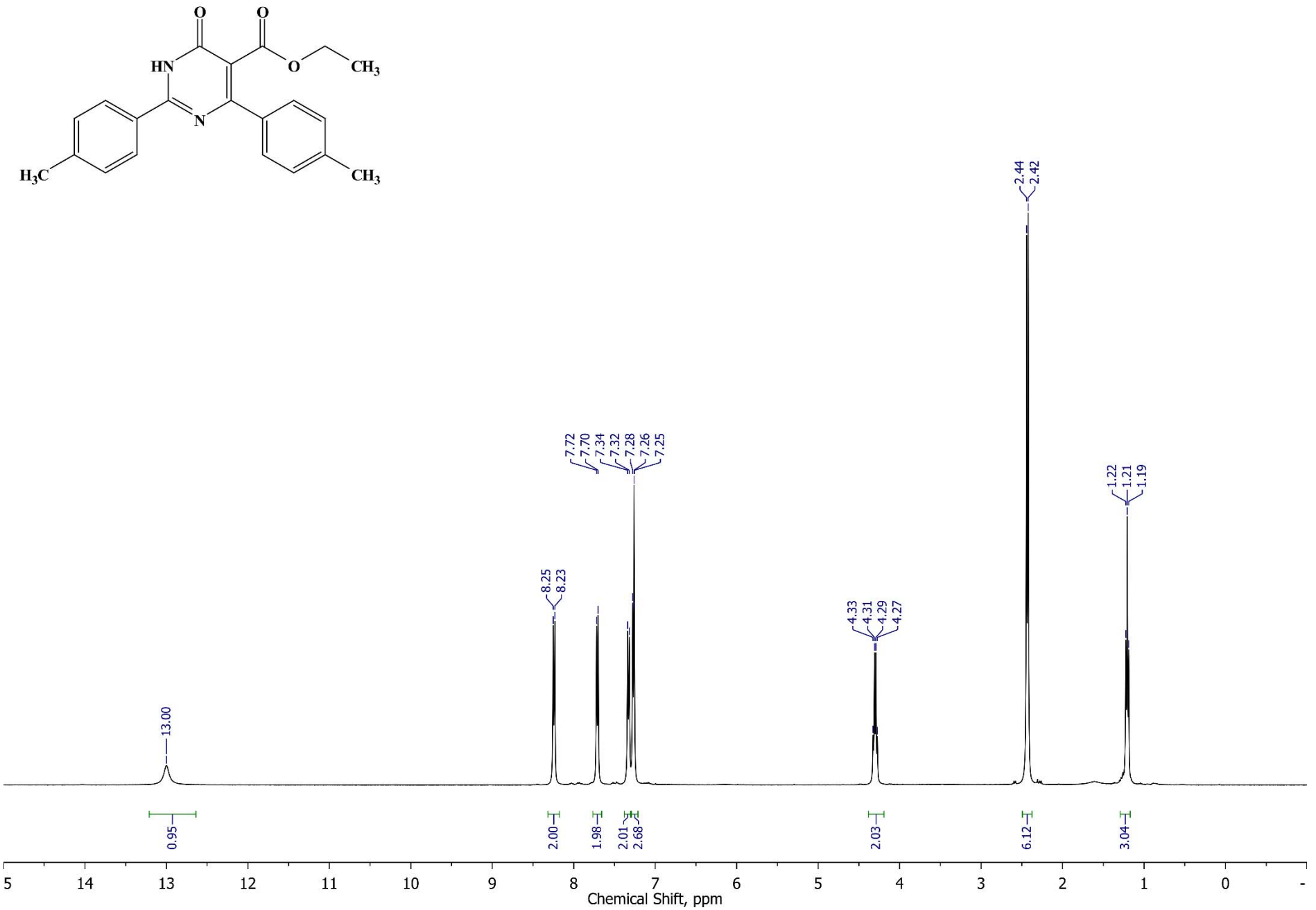
Ethyl 4-(4-methoxyphenyl)-6-oxo-2-phenyl-1,6-dihydropyrimidine-5-carboxylate (3b), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



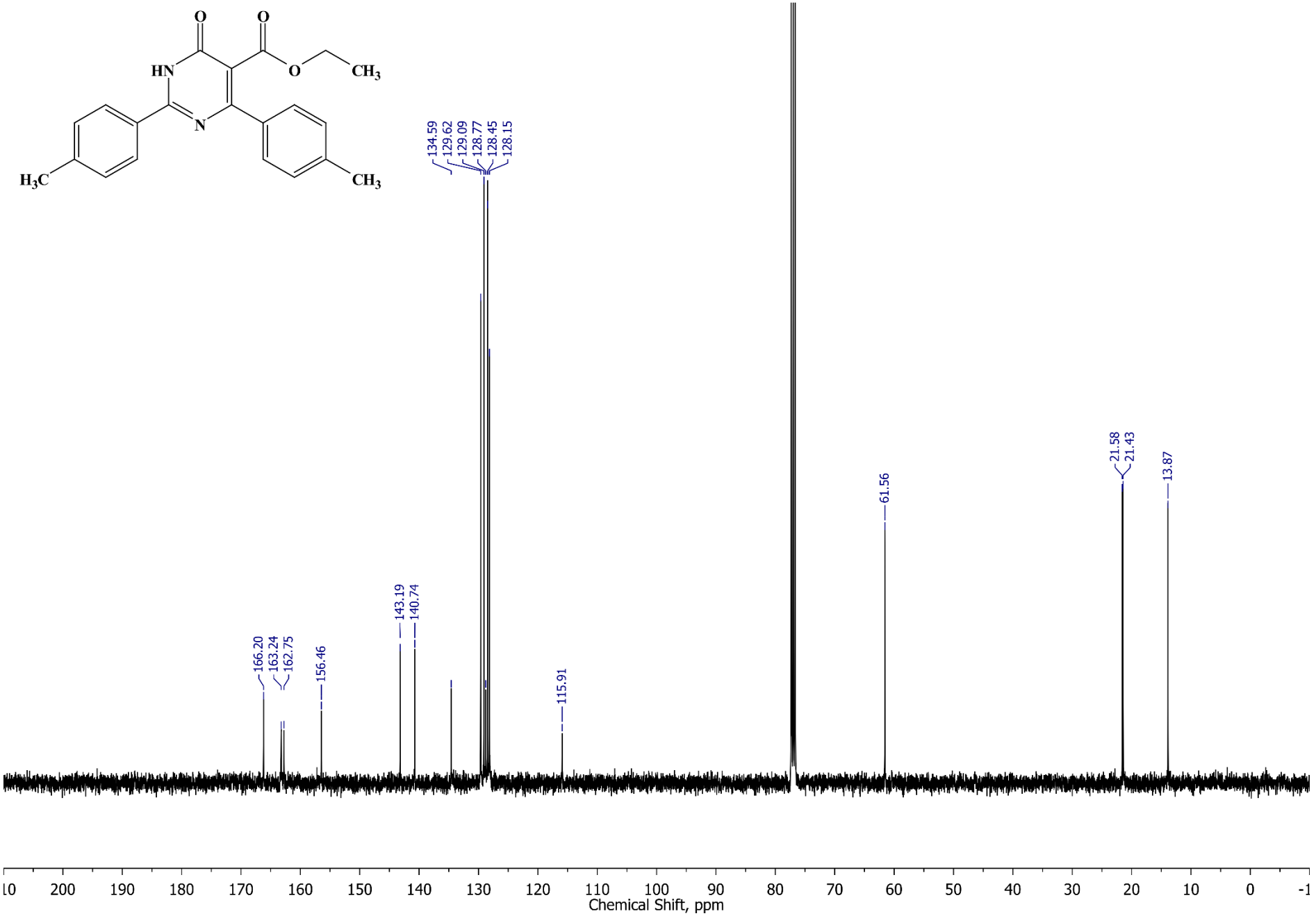
Ethyl 4-(4-methoxyphenyl)-6-oxo-2-phenyl-1,6-dihydropyrimidine-5-carboxylate (3b), DEPT, $CDCl_3$, 101 MHz



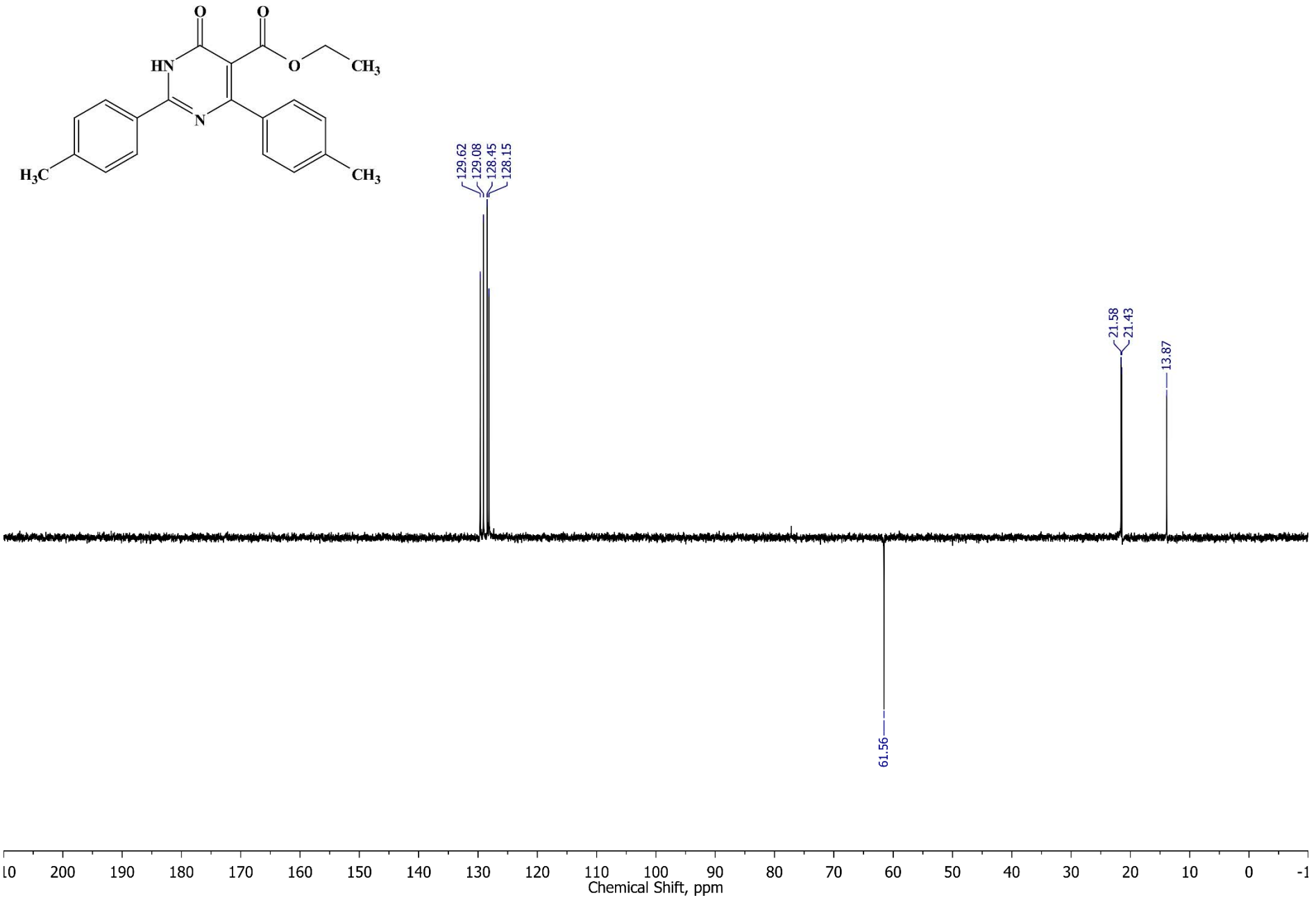
Ethyl 6-oxo-2,4-di-*p*-tolyl-1,6-dihydropyrimidine-5-carboxylate (3c), ^{1}H NMR, $CDCl_3$, 400 MHz



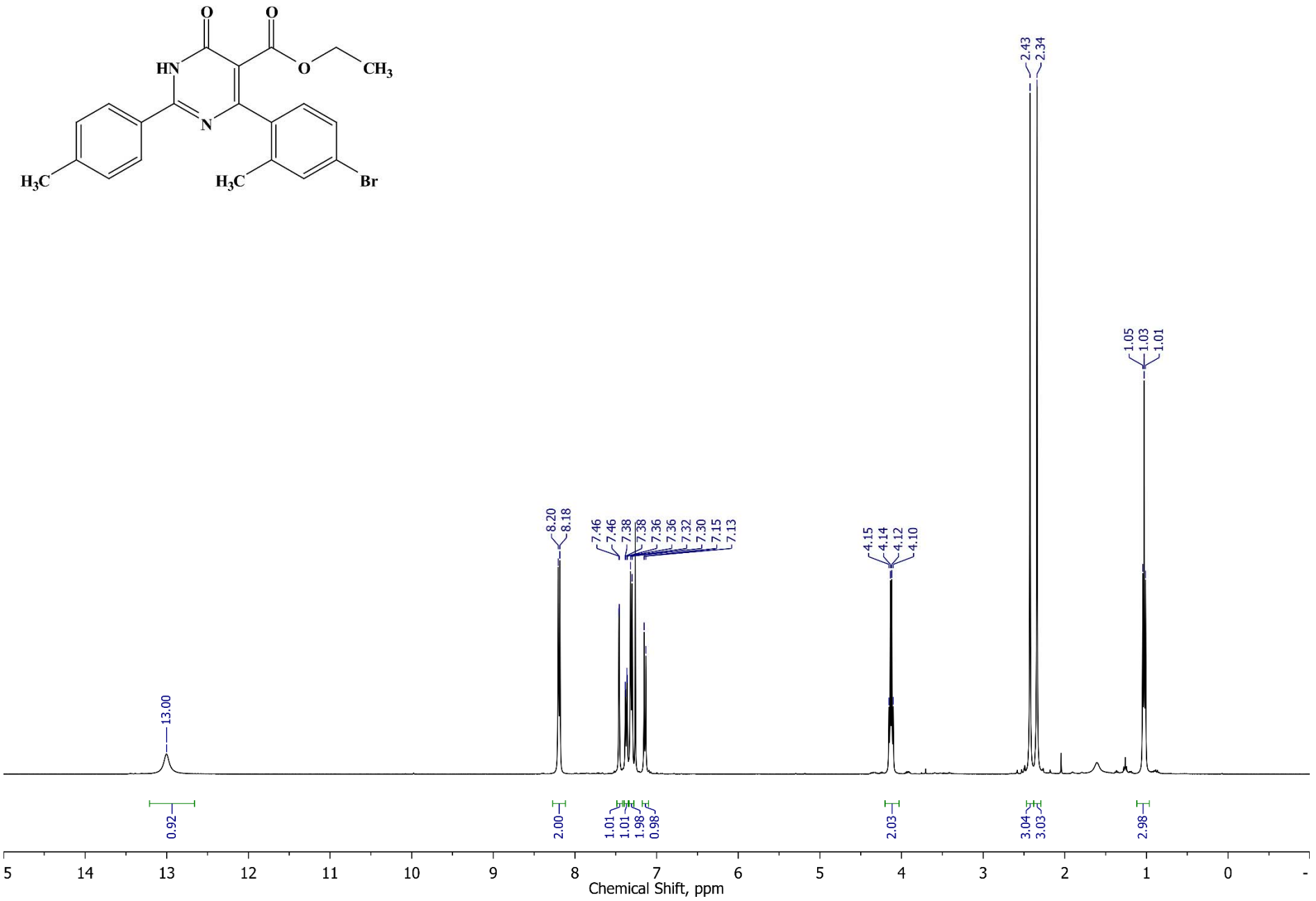
Ethyl 6-oxo-2,4-di-*p*-tolyl-1,6-dihydropyrimidine-5-carboxylate (3c), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



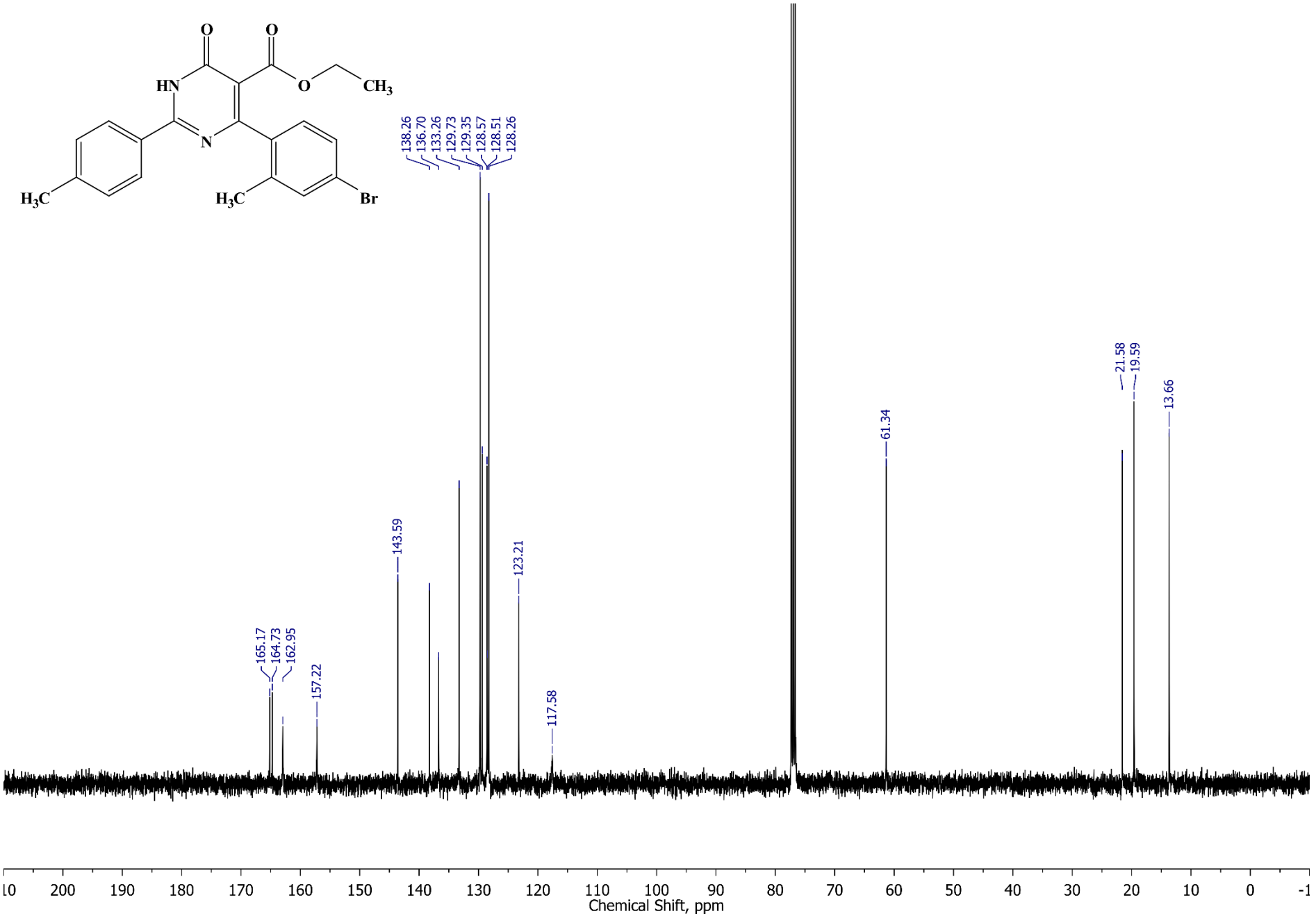
Ethyl 6-oxo-2,4-di-*p*-tolyl-1,6-dihydropyrimidine-5-carboxylate (3c), DEPT, $CDCl_3$, 101 MHz



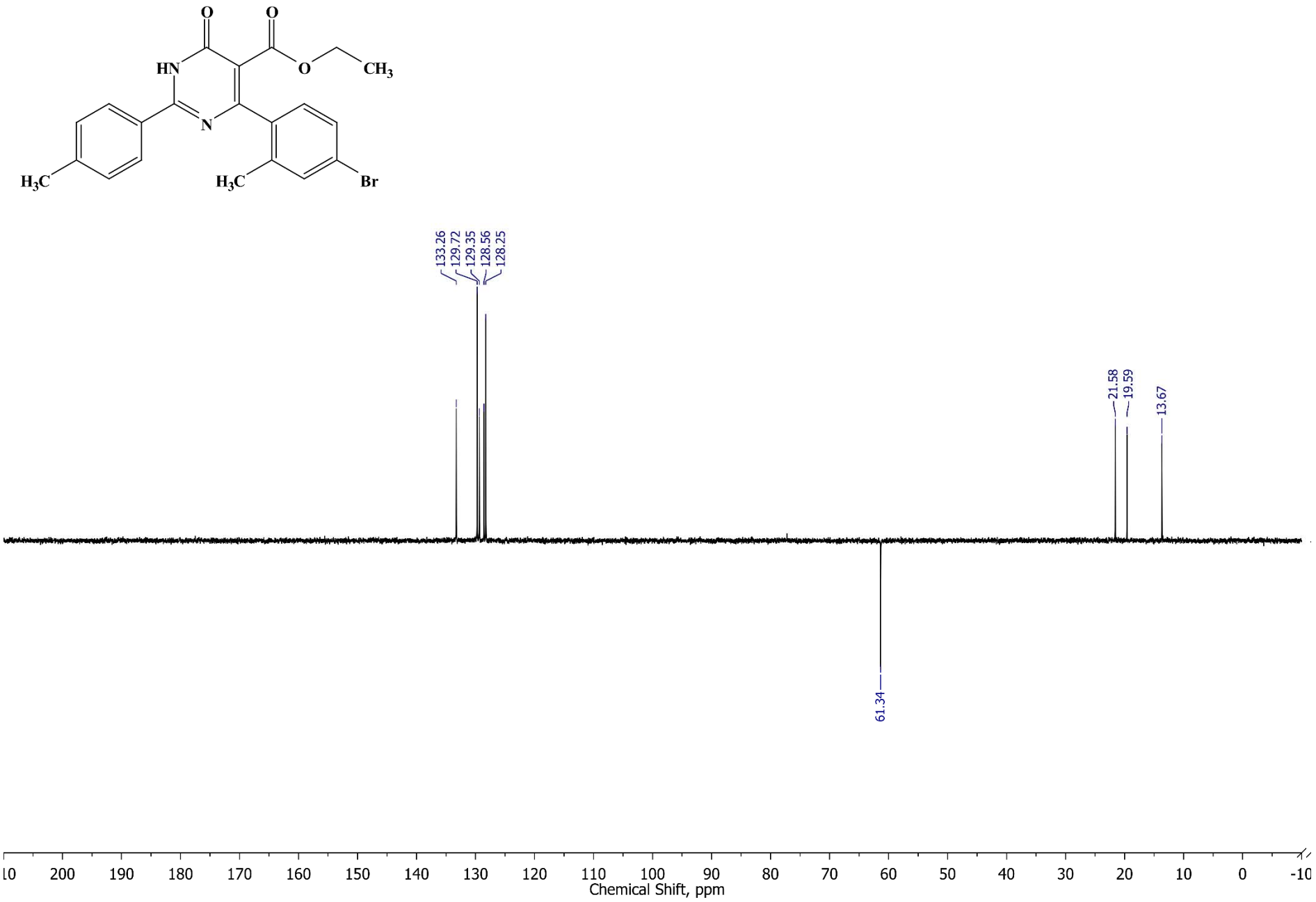
Ethyl 4-(4-bromo-2-methylphenyl)-6-oxo-2-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3d), ^{1}H NMR, $CDCl_3$, 400 MHz



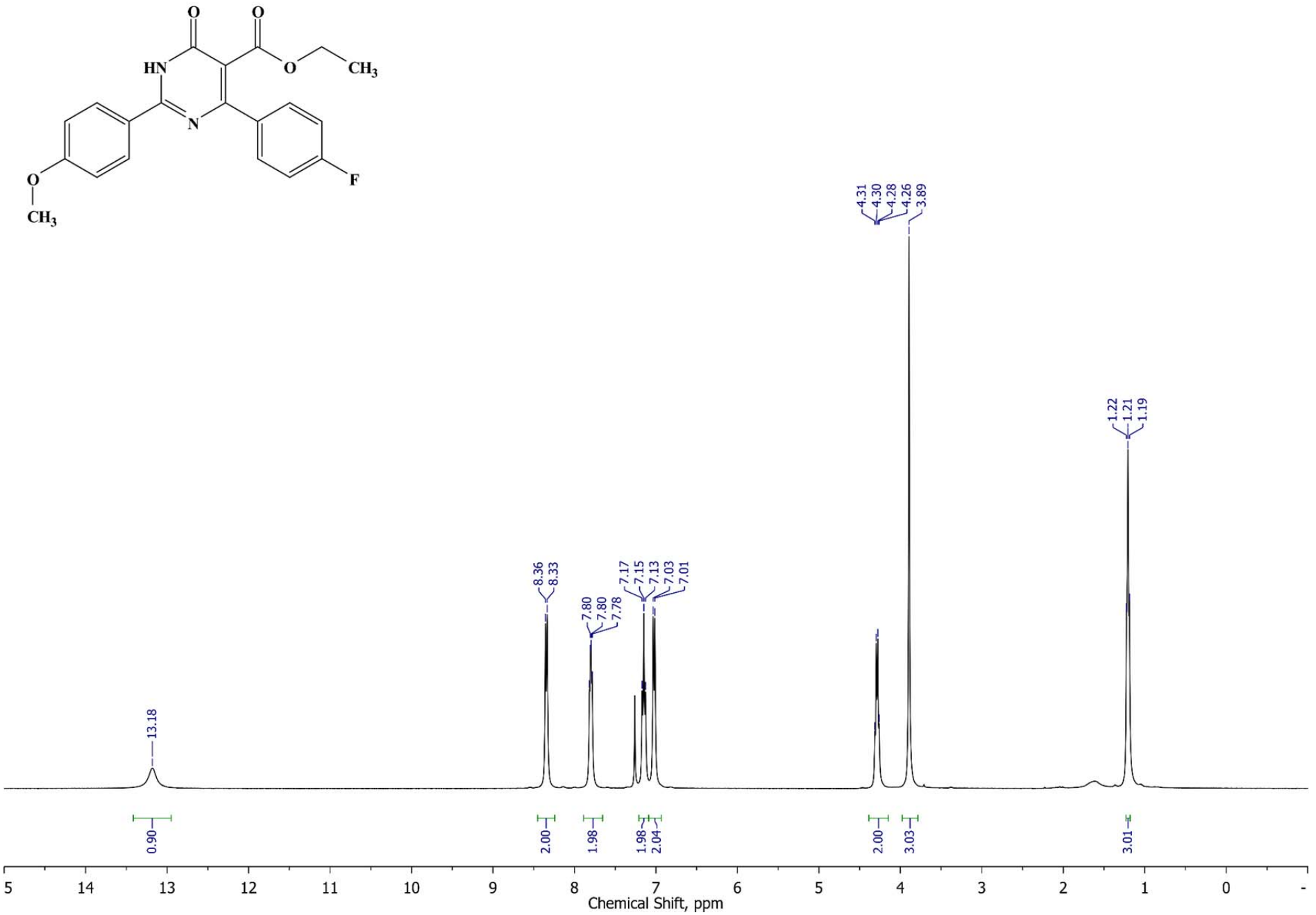
Ethyl 4-(4-bromo-2-methylphenyl)-6-oxo-2-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3d), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



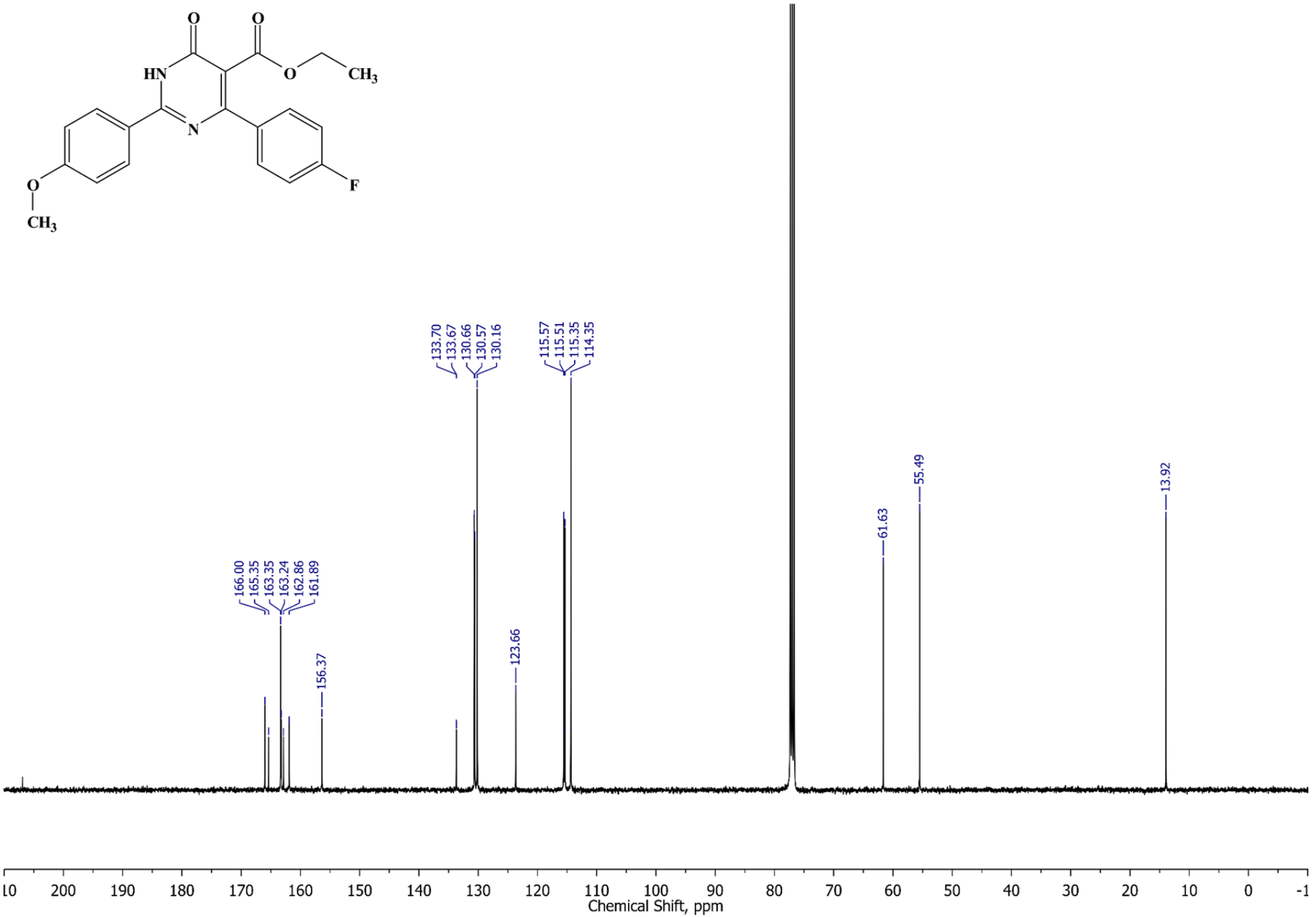
Ethyl 4-(4-bromo-2-methylphenyl)-6-oxo-2-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3d), DEPT, $CDCl_3$, 101 MHz



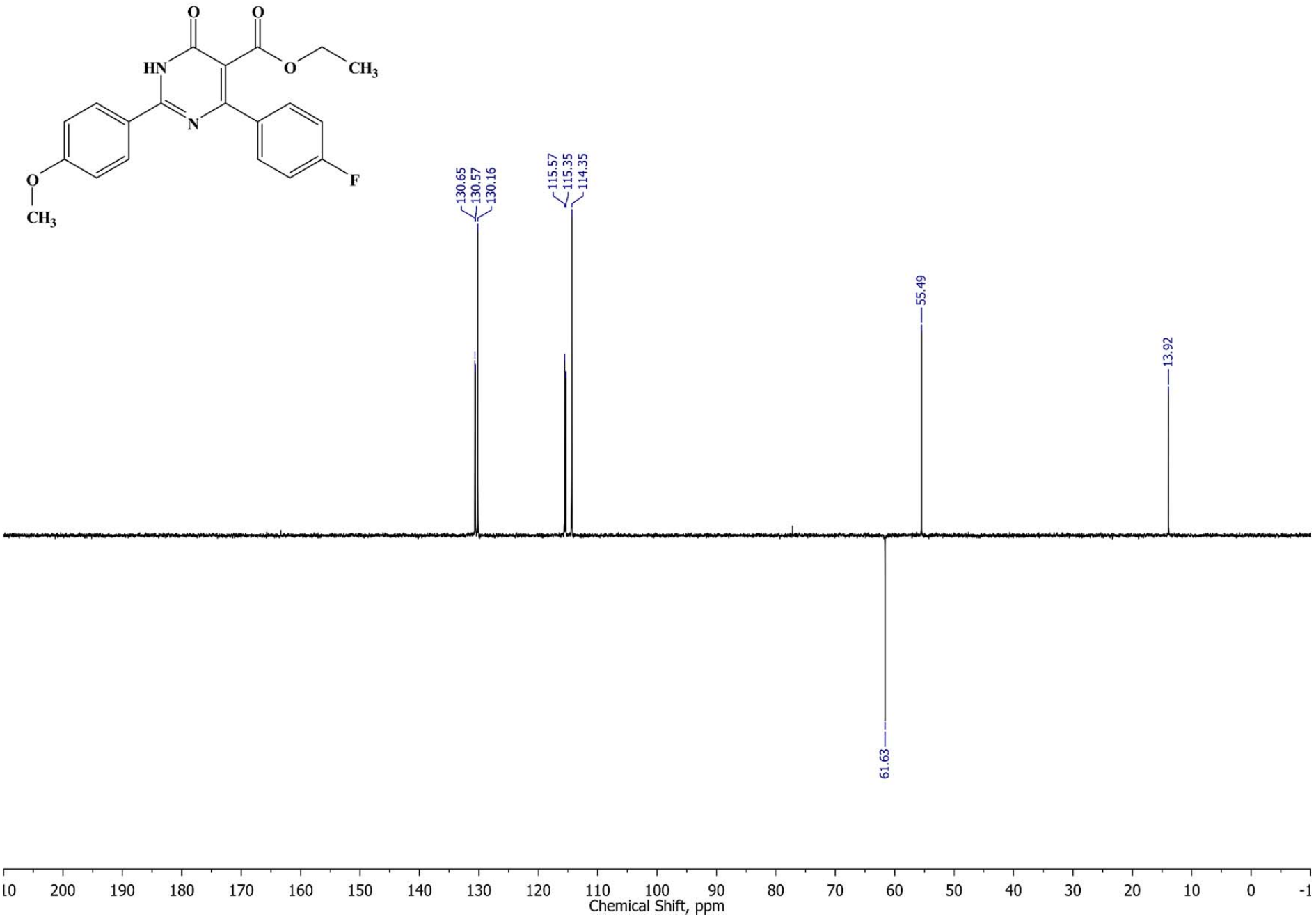
Ethyl 4-(4-fluorophenyl)-2-(4-methoxyphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3e), ^{1}H NMR, $CDCl_3$, 400 MHz



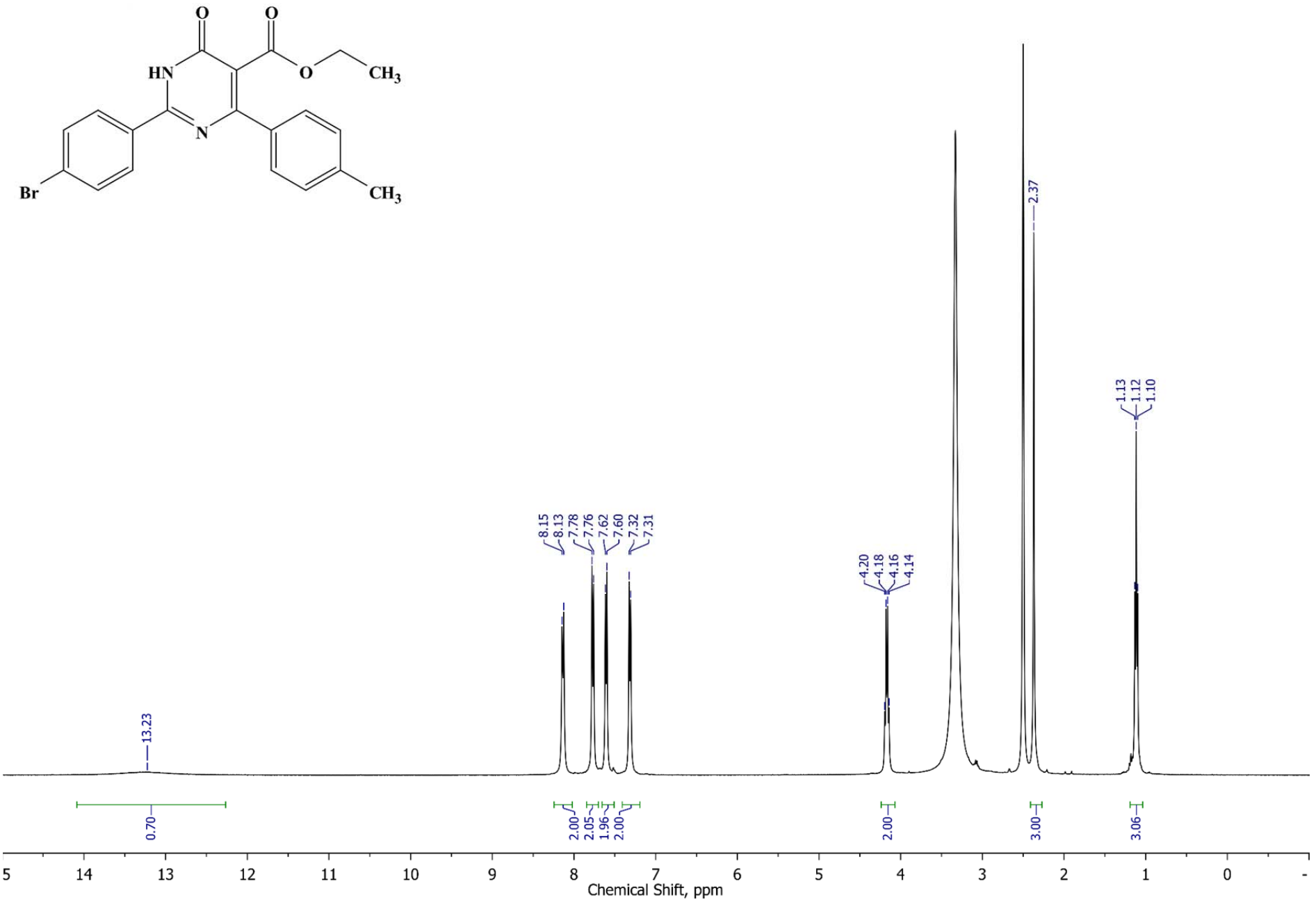
Ethyl 4-(4-fluorophenyl)-2-(4-methoxyphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3e), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



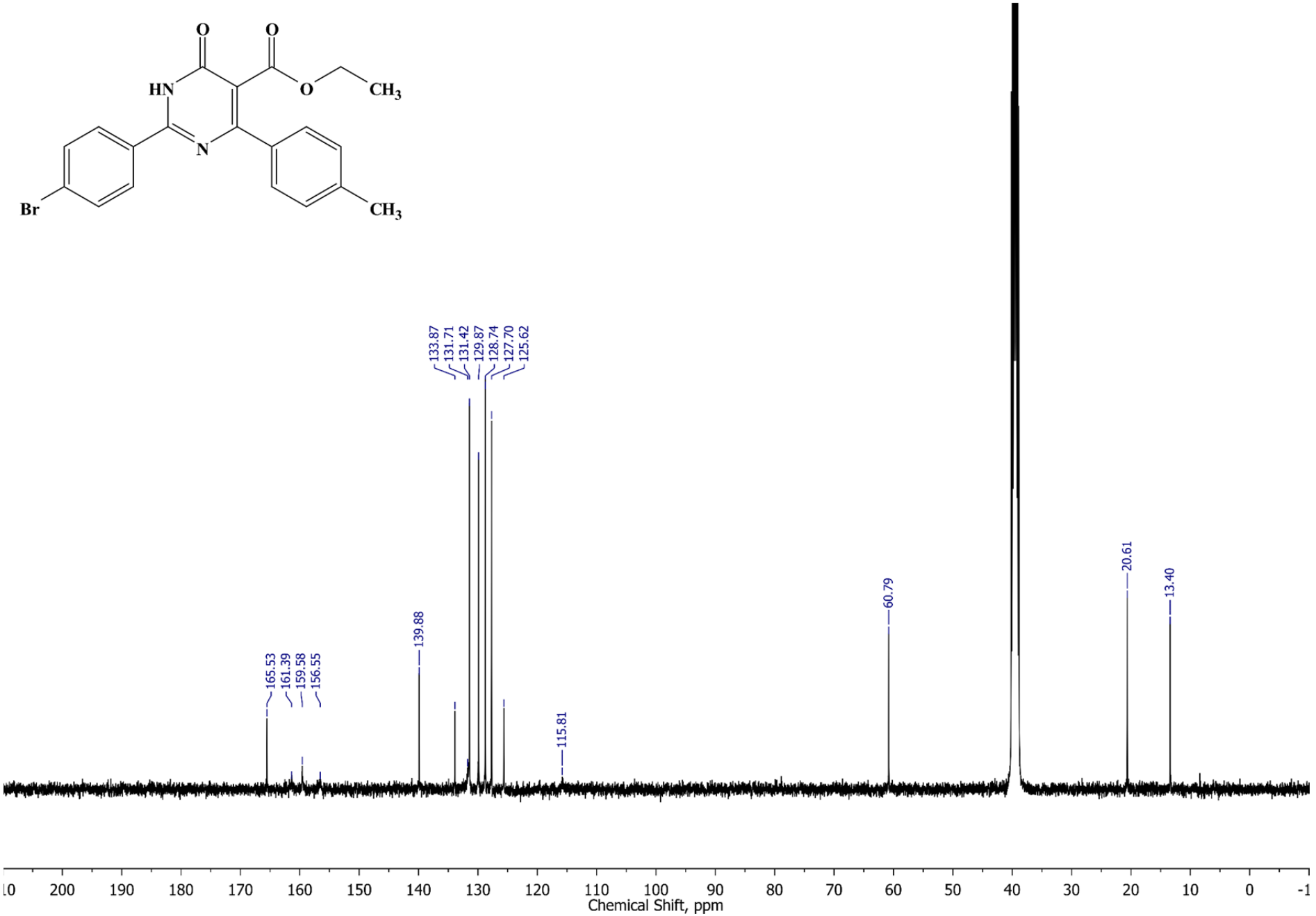
Ethyl 4-(4-fluorophenyl)-2-(4-methoxyphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3e), DEPT, $CDCl_3$, 101 MHz



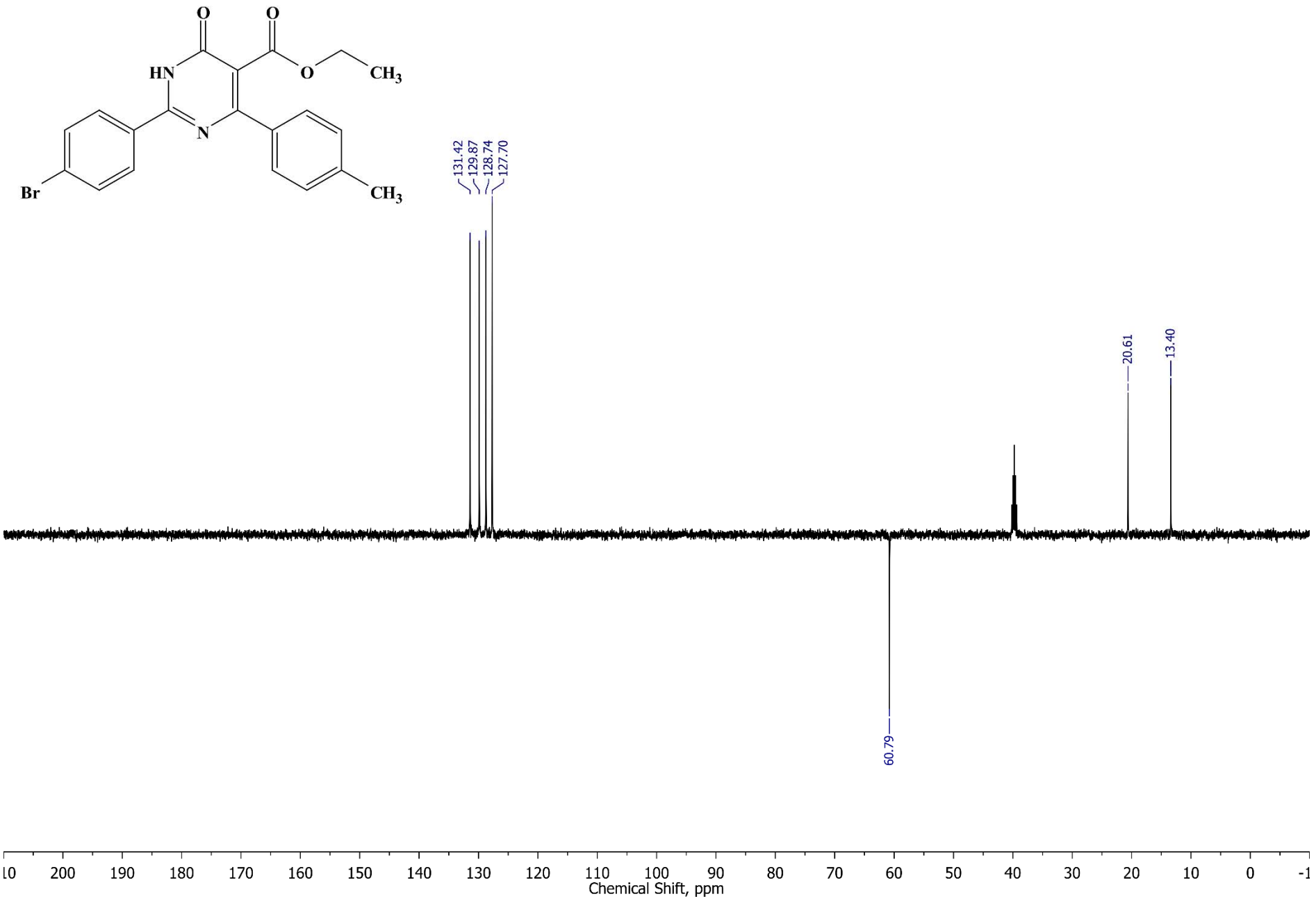
Ethyl 2-(4-bromophenyl)-6-oxo-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3f), ^{1}H NMR, DMSO-d$_6$, 400 MHz



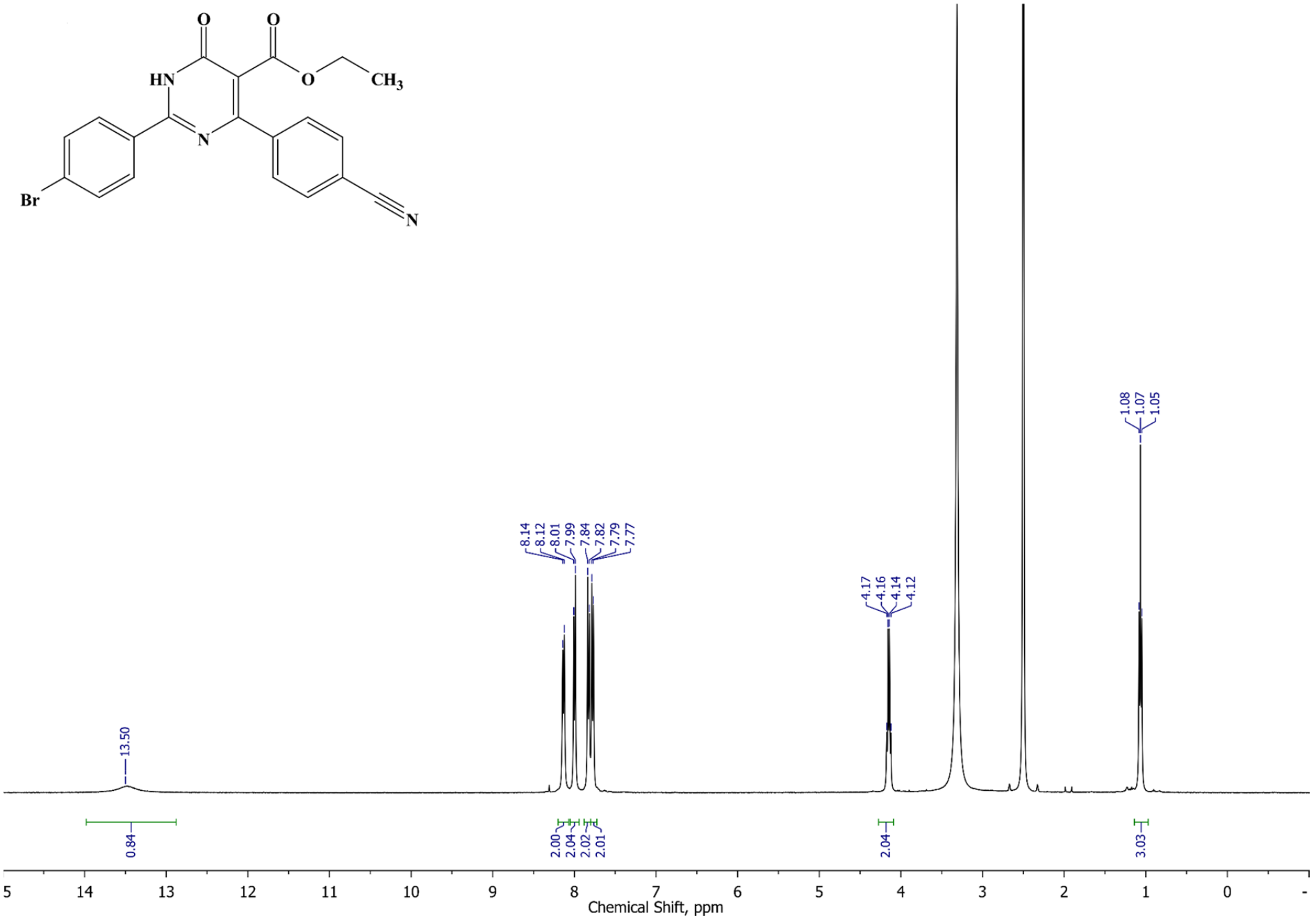
Ethyl 2-(4-bromophenyl)-6-oxo-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3f), $^{13}C\{^{1}H\}$ NMR, DMSO-d_6, 101 MHz



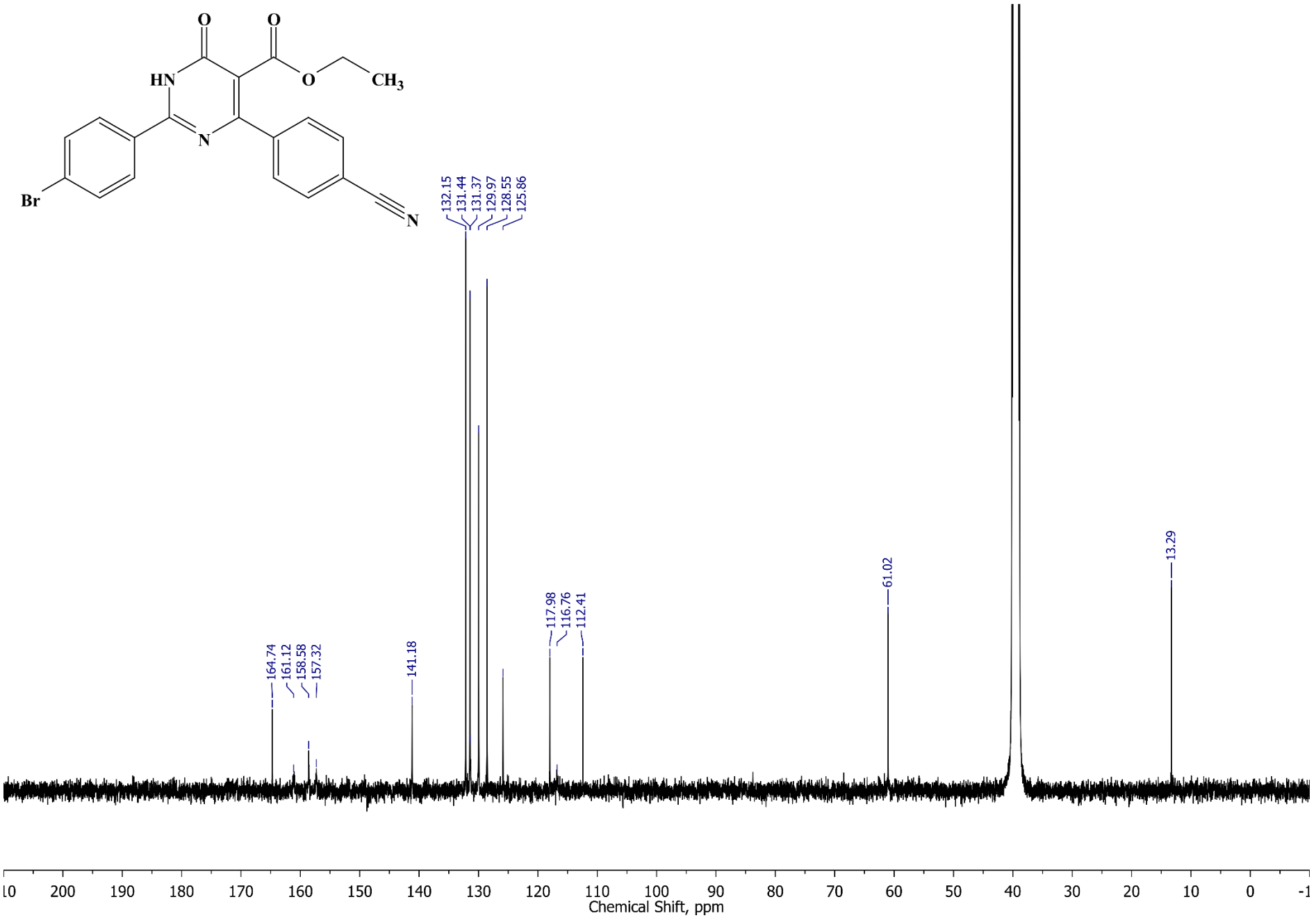
Ethyl 2-(4-bromophenyl)-6-oxo-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3f), DEPT, DMSO-d_6, 101 MHz



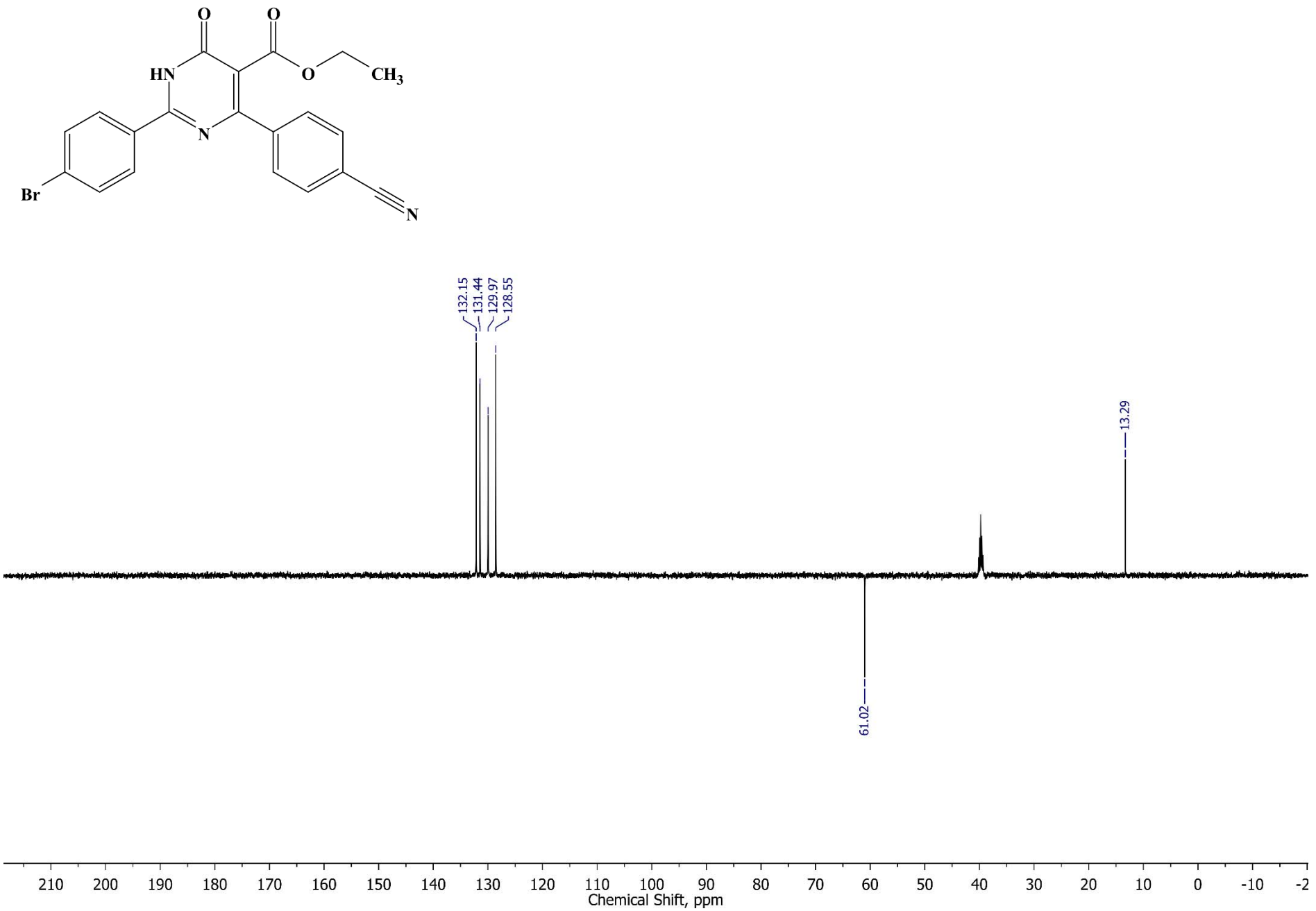
Ethyl 2-(4-bromophenyl)-4-(4-cyanophenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3g), ^{1}H NMR, DMSO-d_6, 400 MHz



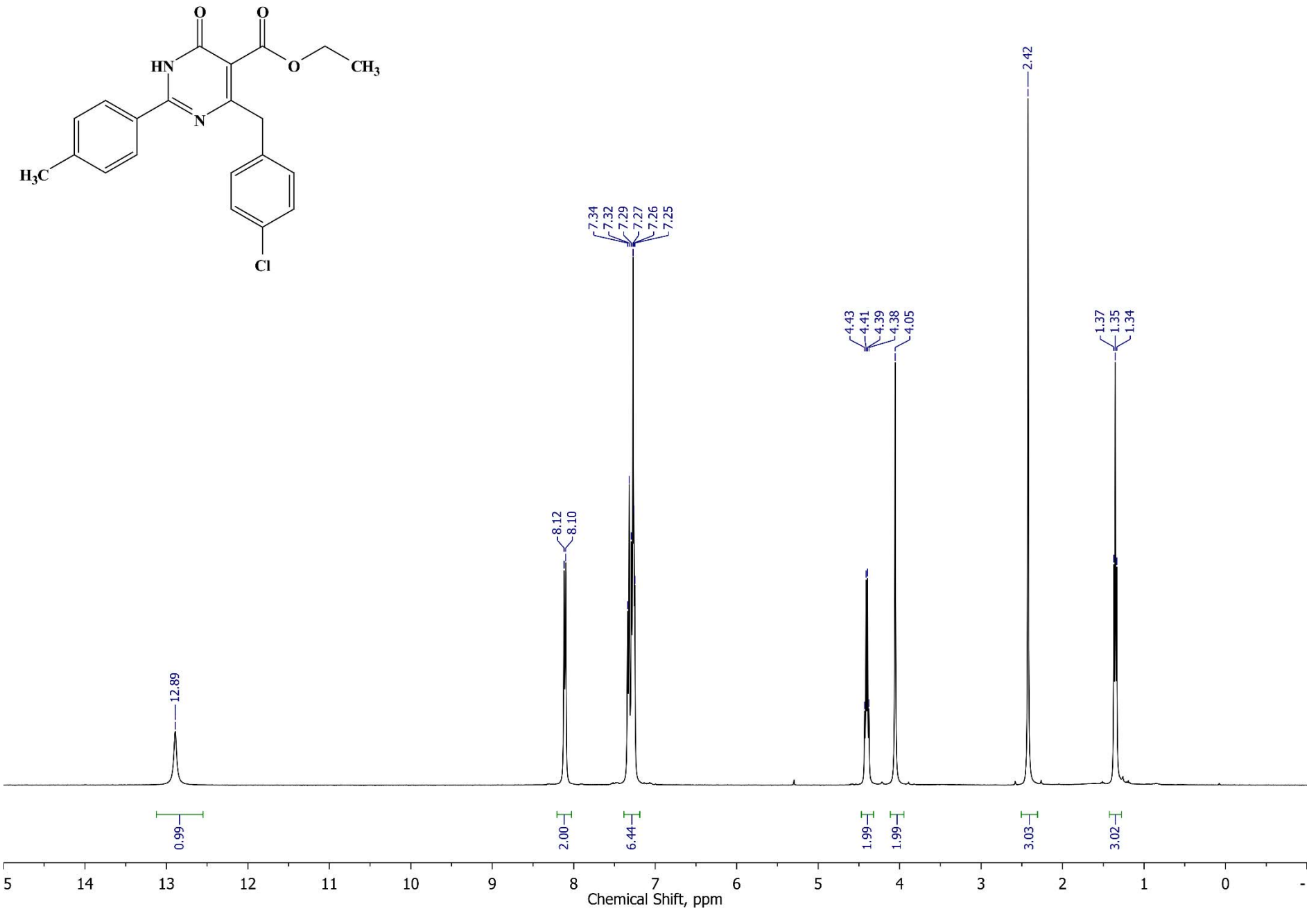
Ethyl 2-(4-bromophenyl)-4-(4-cyanophenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3g), $^{13}C\{^{1}H\}$ NMR, DMSO-d_6, 101 MHz



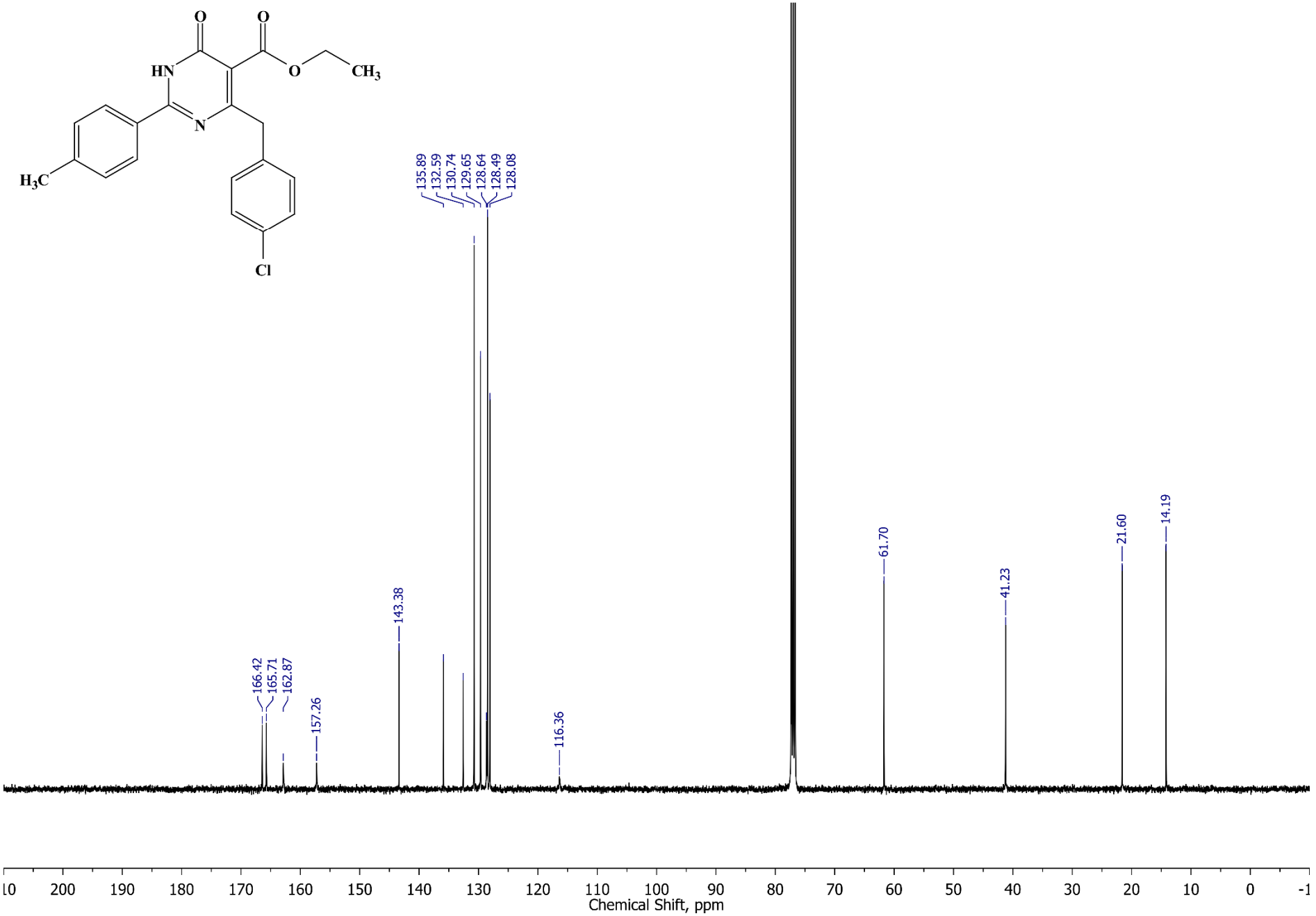
Ethyl 2-(4-bromophenyl)-4-(4-cyanophenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3g), DEPT, DMSO-d_6, 101 MHz



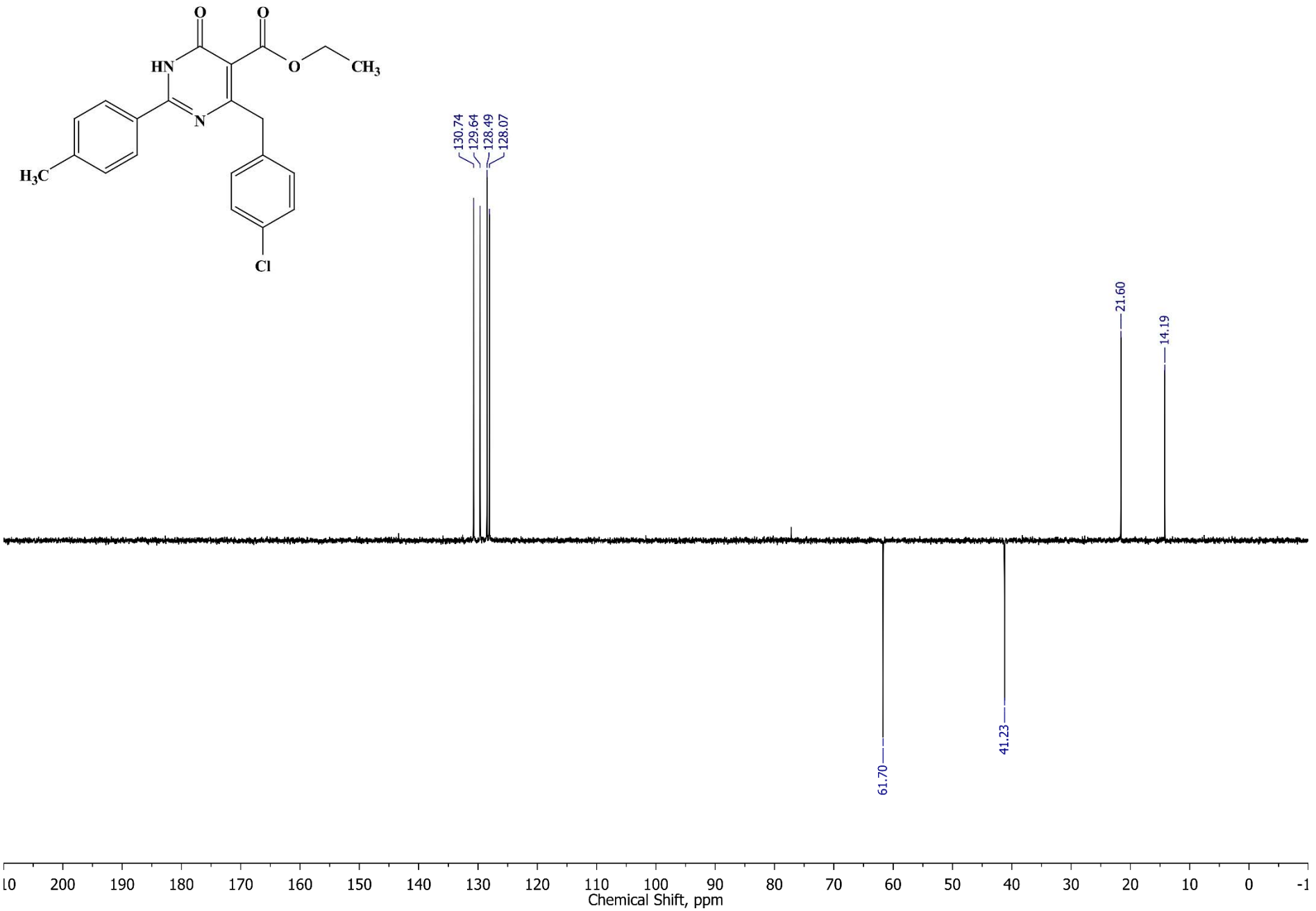
Ethyl 4-(4-chlorobenzyl)-6-oxo-2-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3h), ^{1}H NMR, $CDCl_3$, 400 MHz



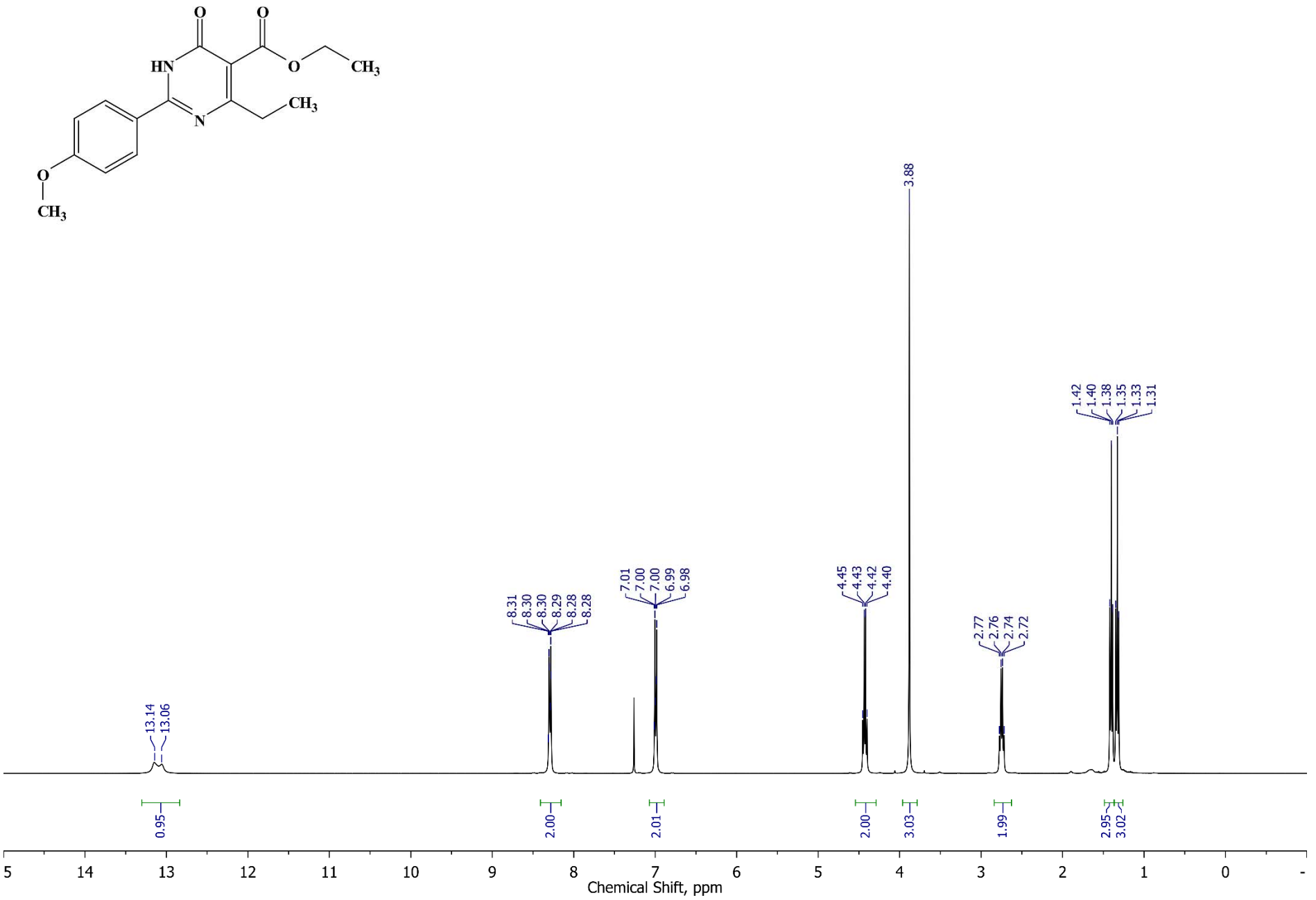
Ethyl 4-(4-chlorobenzyl)-6-oxo-2-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3h), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



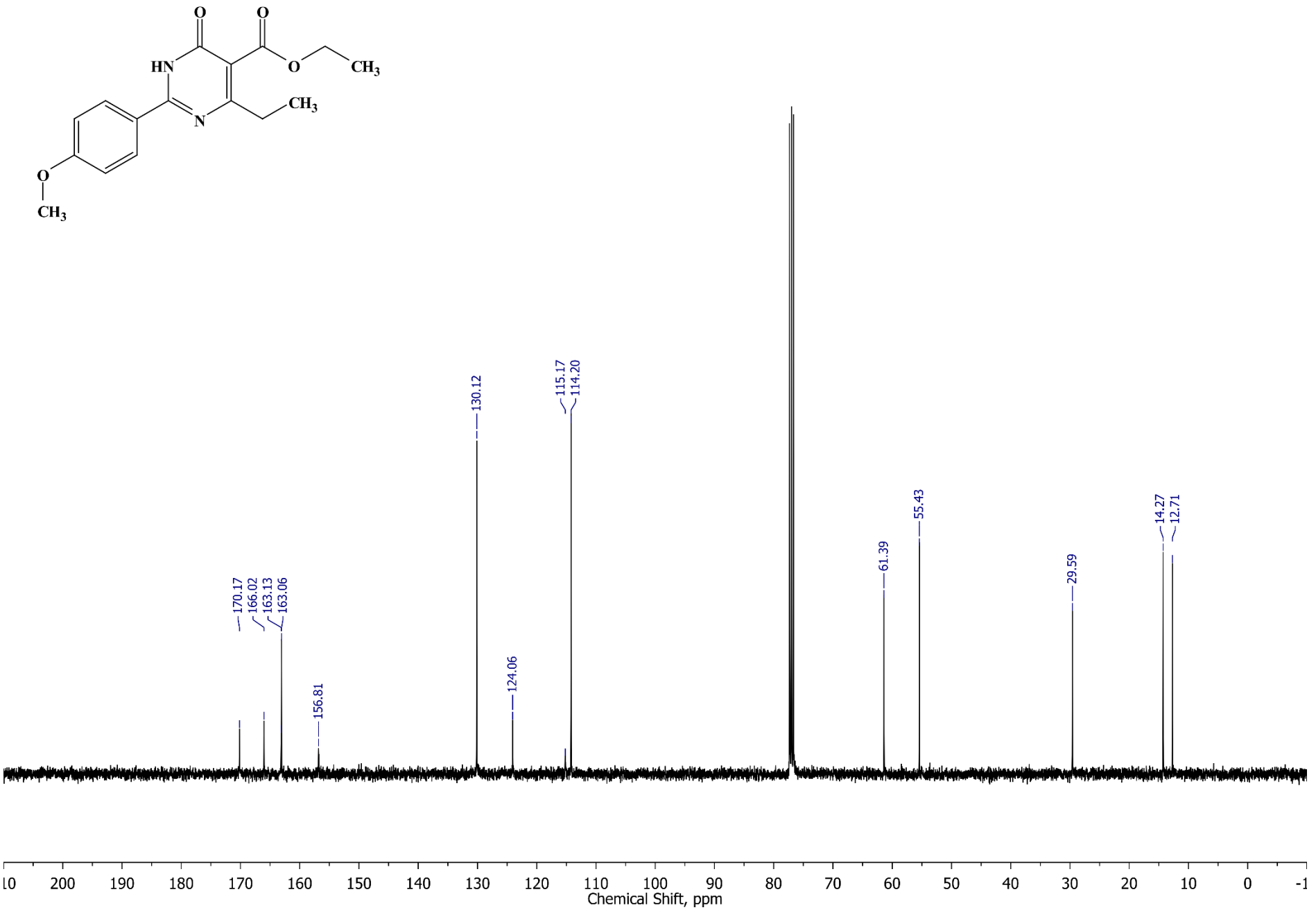
Ethyl 4-(4-chlorobenzyl)-6-oxo-2-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3h), DEPT, $CDCl_3$, 101 MHz



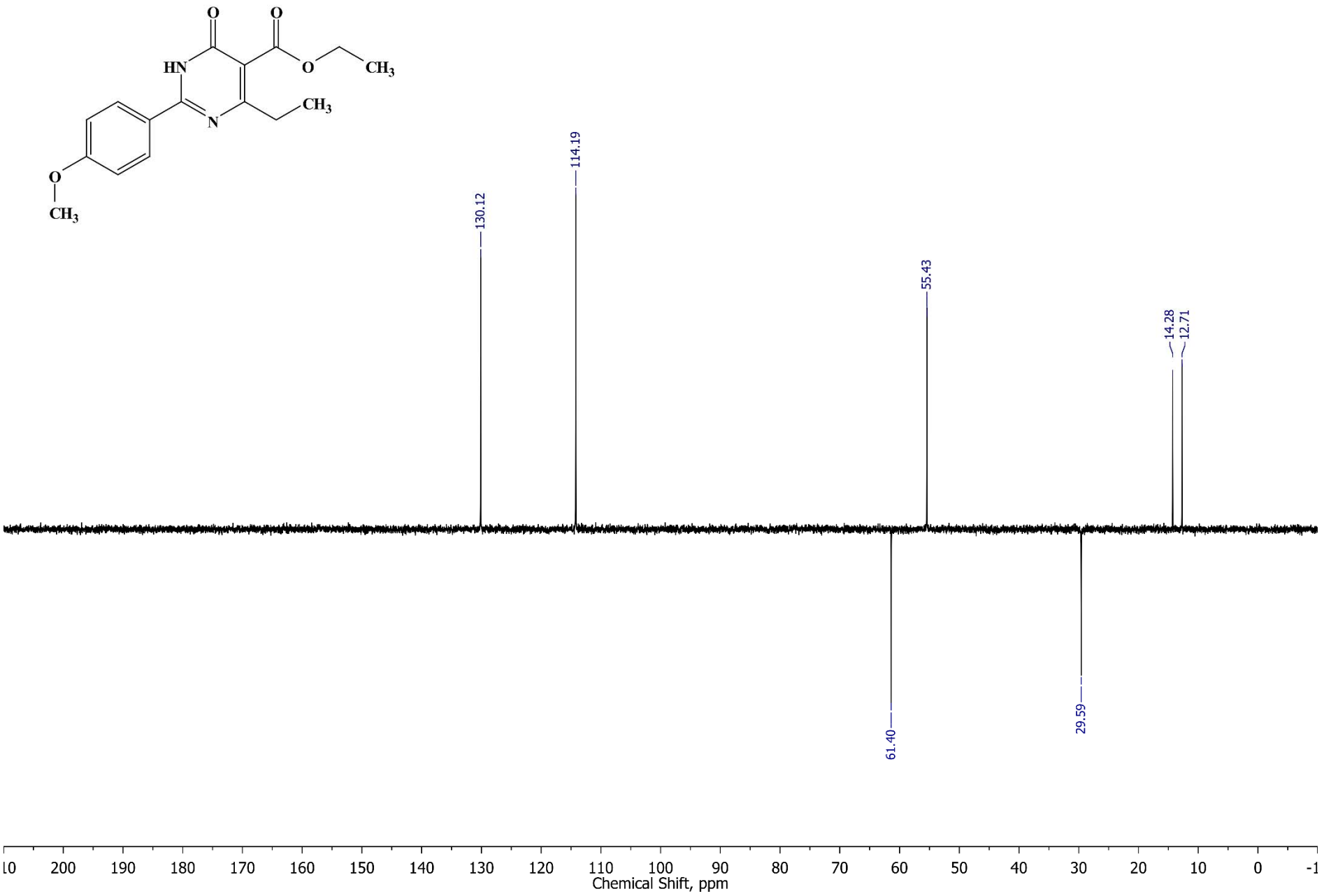
Ethyl 4-ethyl-2-(4-methoxyphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3i), ^{1}H NMR, $CDCl_3$, 400 MHz



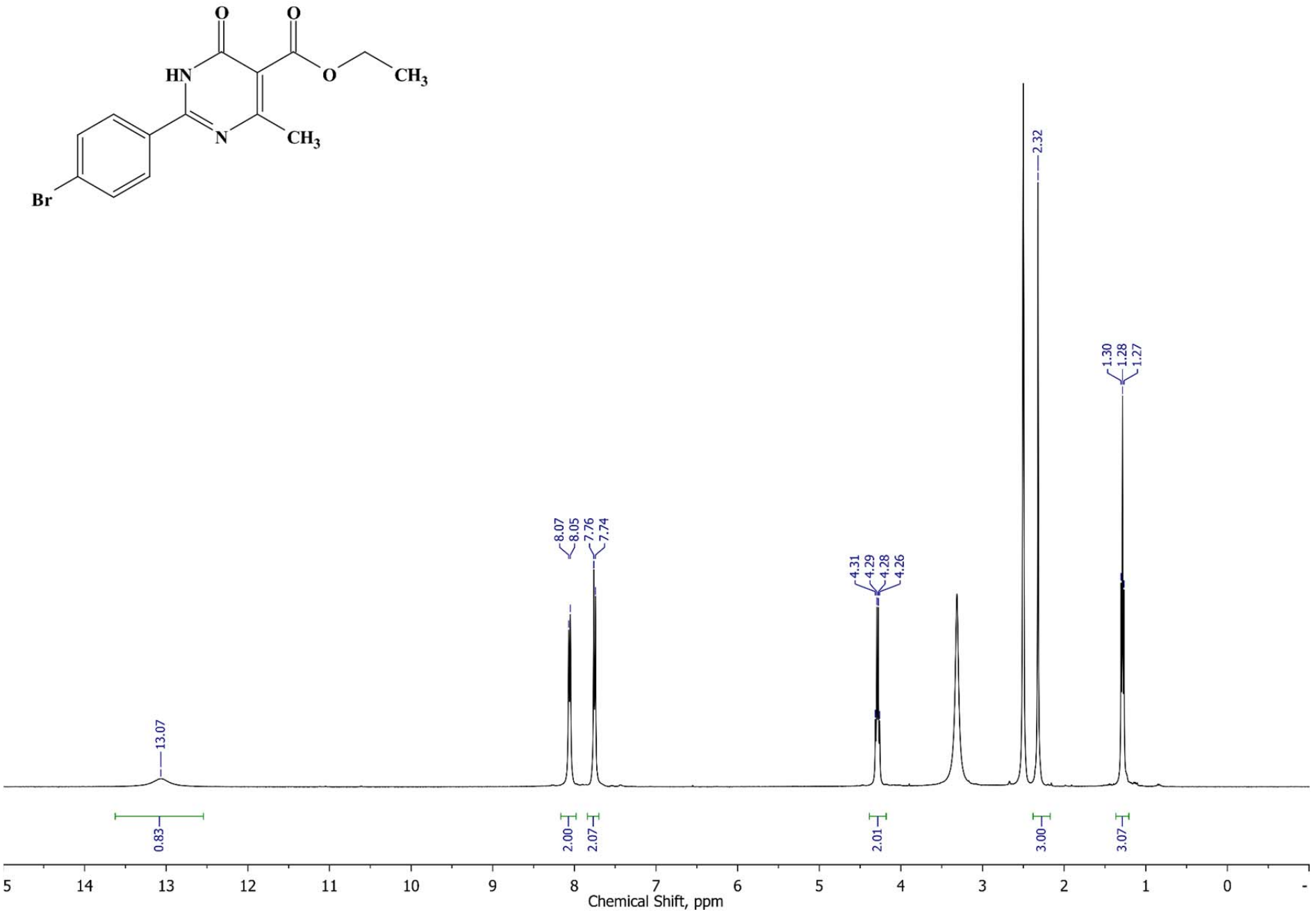
Ethyl 4-ethyl-2-(4-methoxyphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3i), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



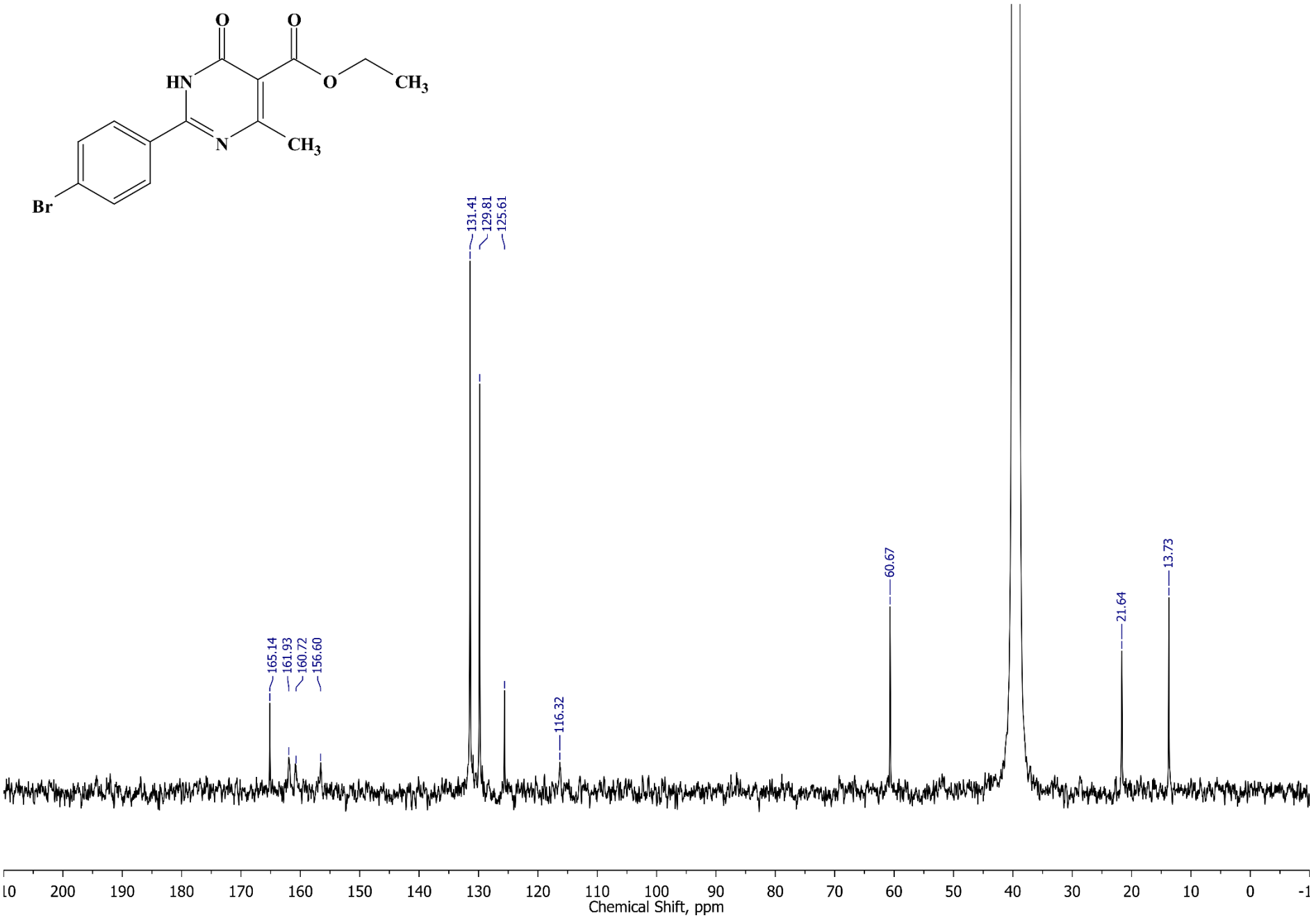
Ethyl 4-ethyl-2-(4-methoxyphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3i), DEPT, $CDCl_3$, 101 MHz



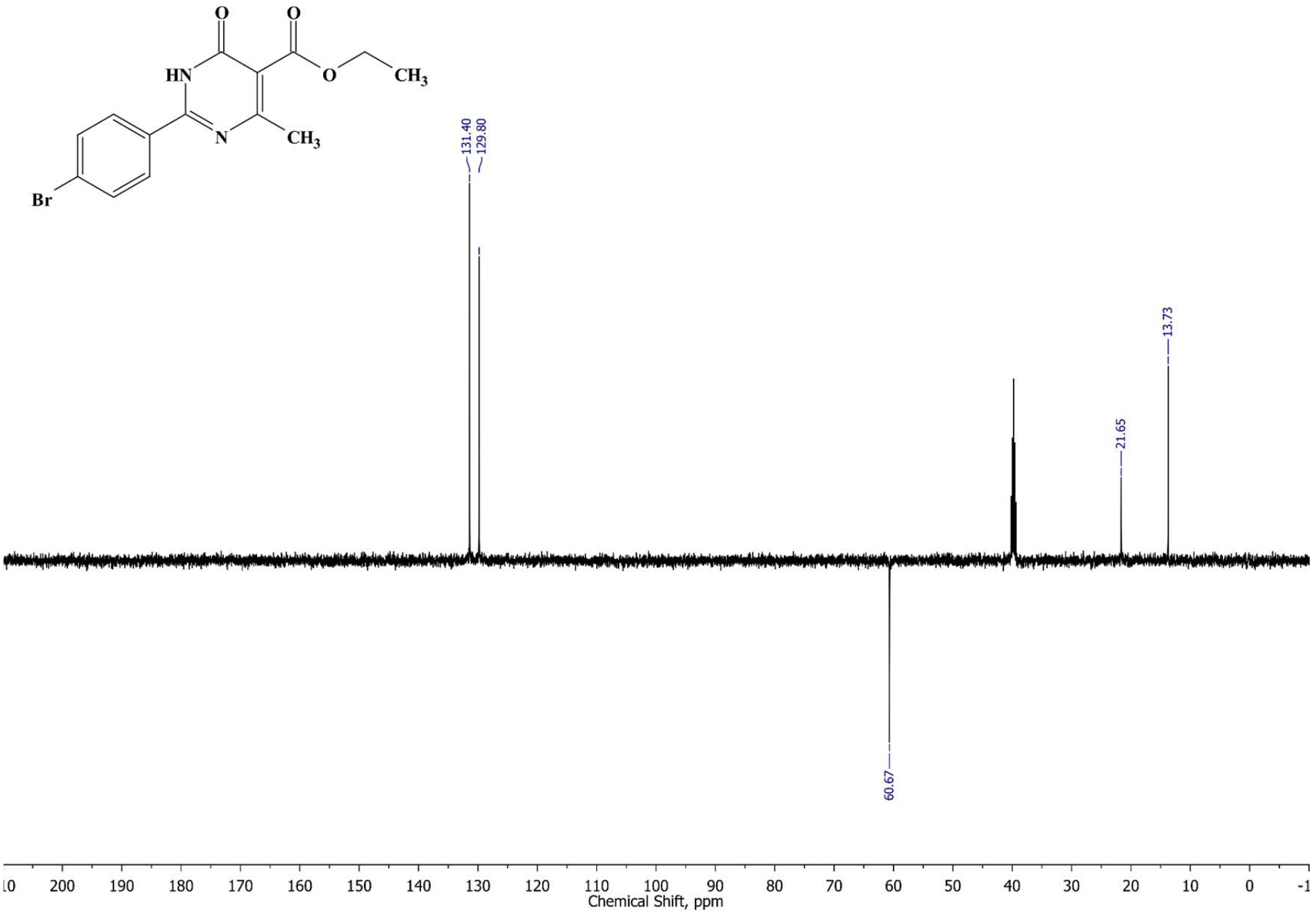
Ethyl 2-(4-bromophenyl)-4-methyl-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3j), ^{1}H NMR, DMSO-d$_6$, 400 MHz



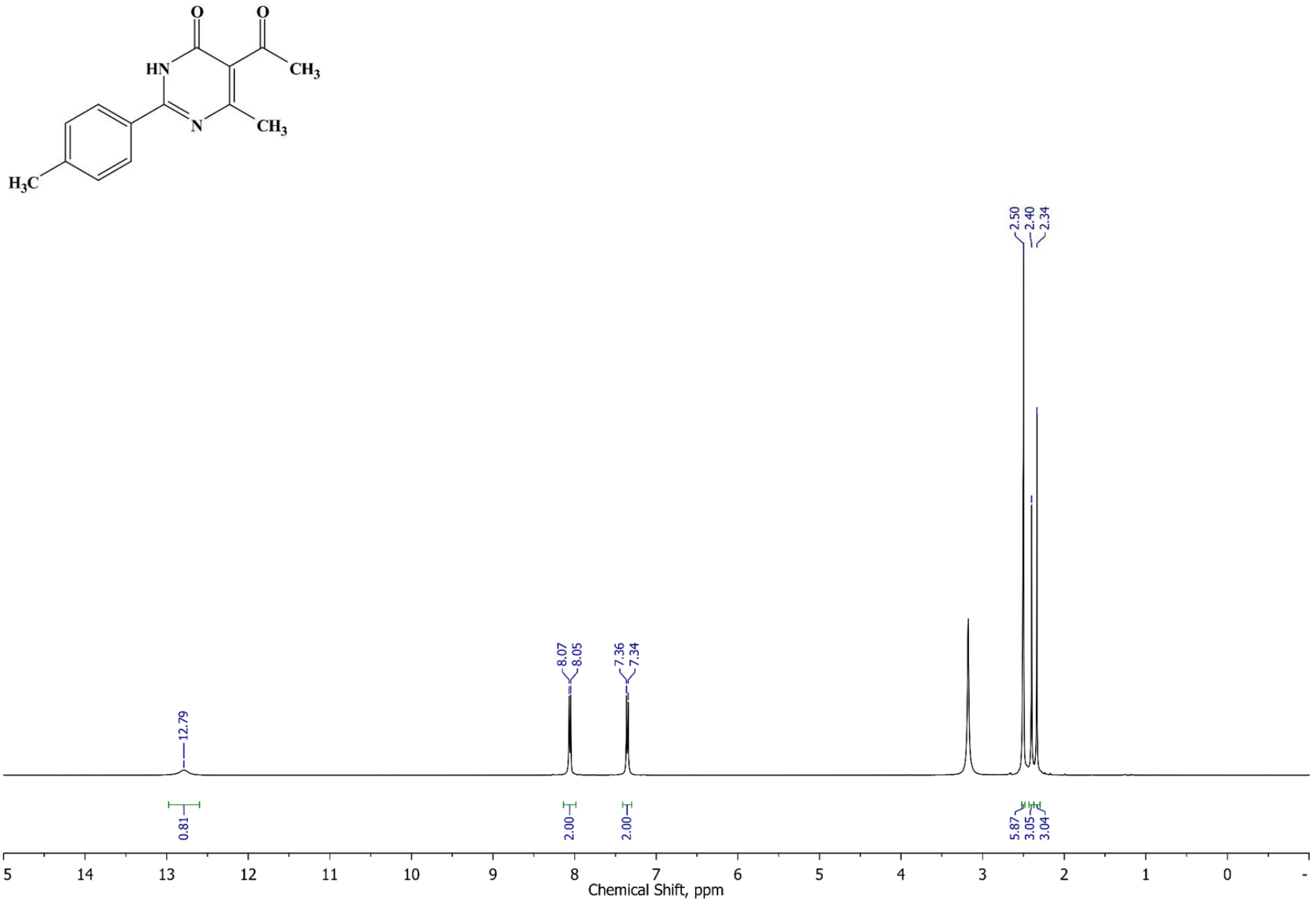
Ethyl 2-(4-bromophenyl)-4-methyl-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3j), $^{13}C\{^{1}H\}$ NMR, DMSO-d_6, 101 MHz



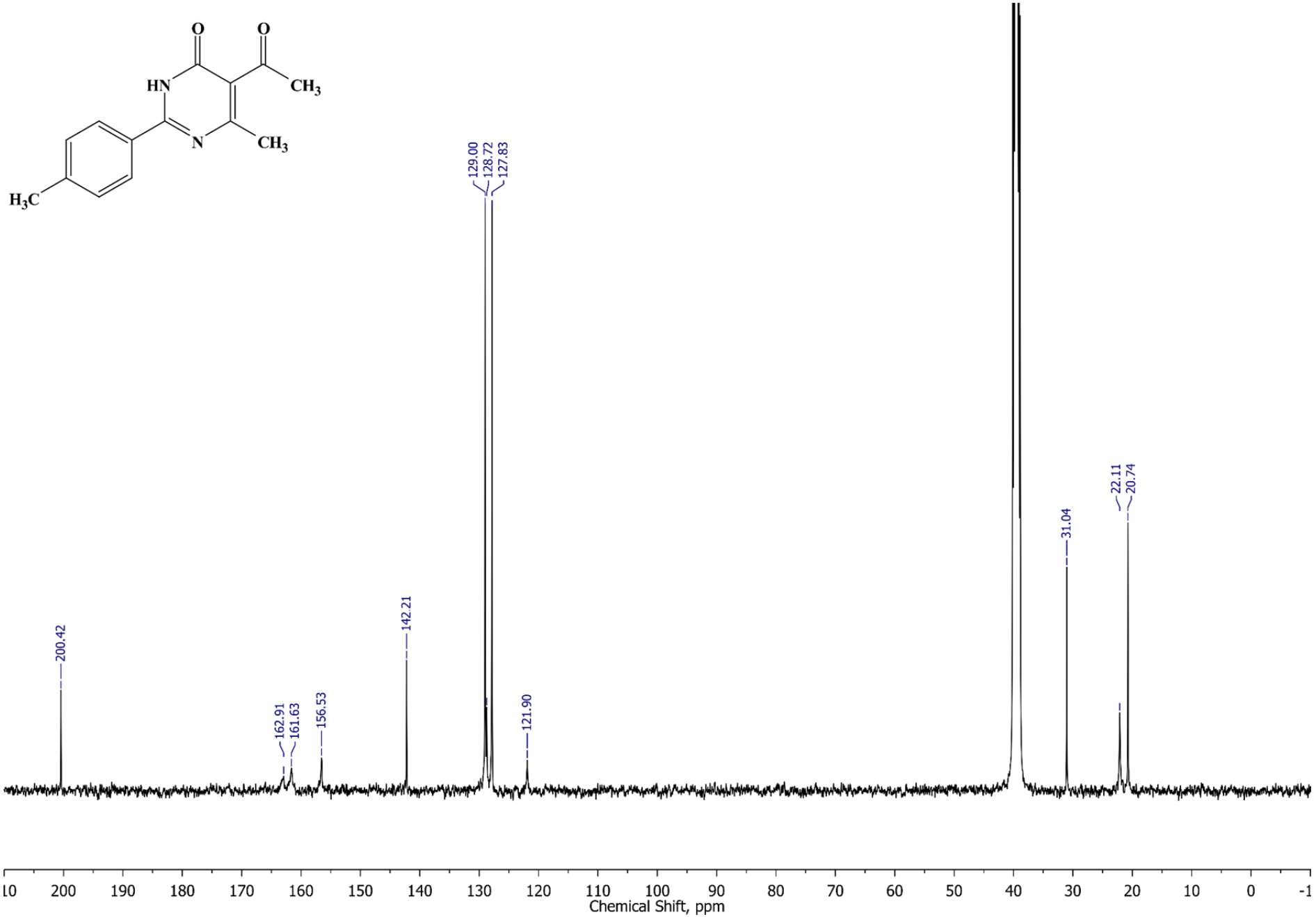
Ethyl 2-(4-bromophenyl)-4-methyl-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3j), DEPT, DMSO-d_6, 101 MHz



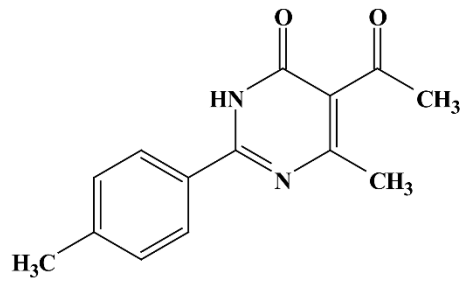
5-Acetyl-6-methyl-2-(*p*-tolyl)pyrimidin-4(3*H*)-one (3k), ^{1}H NMR, DMSO-d$_6$, 400 MHz

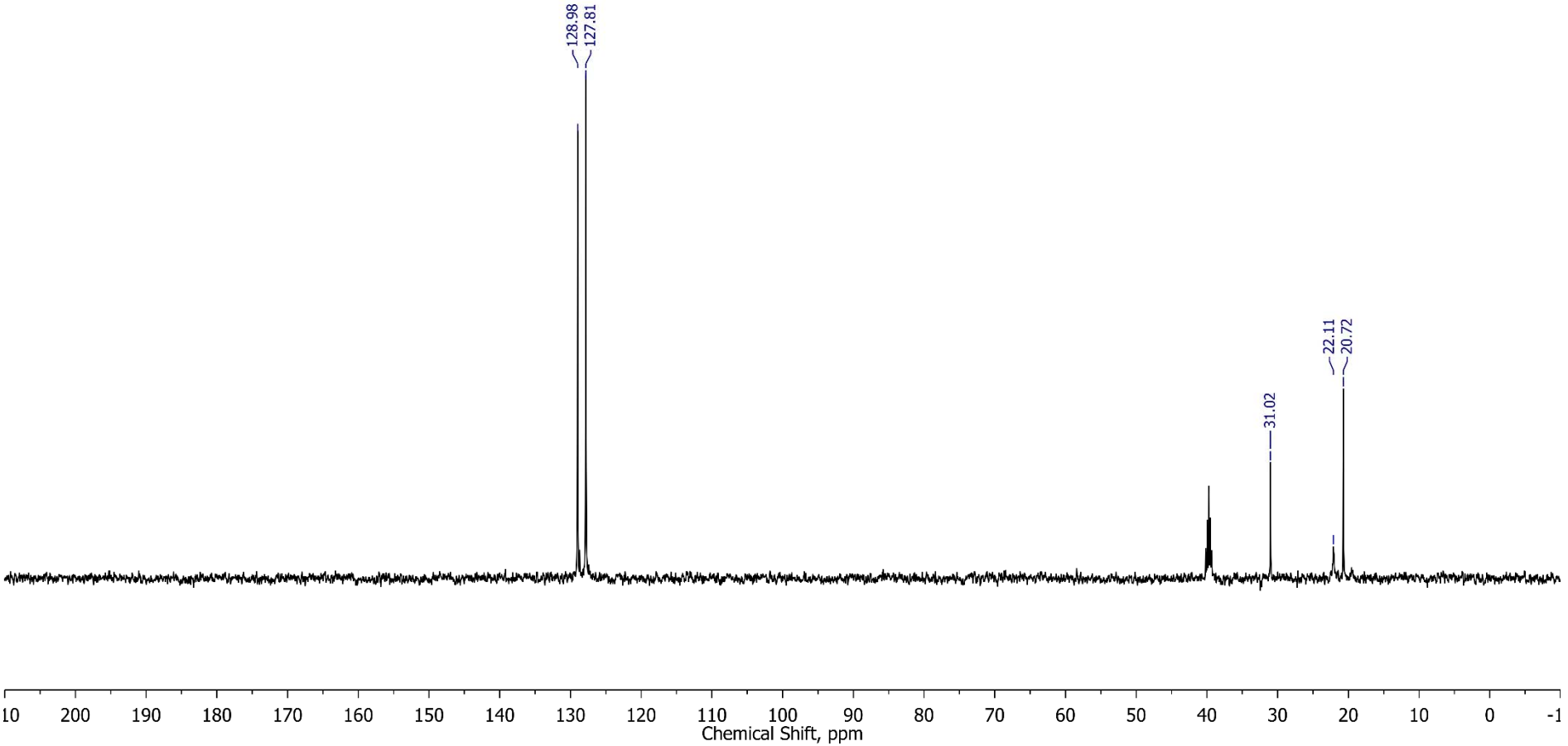


5-Acetyl-6-methyl-2-(*p*-tolyl)pyrimidin-4(3*H*)-one (3k), $^{13}C\{^{1}H\}$ NMR, DMSO-d_6, 101 MHz

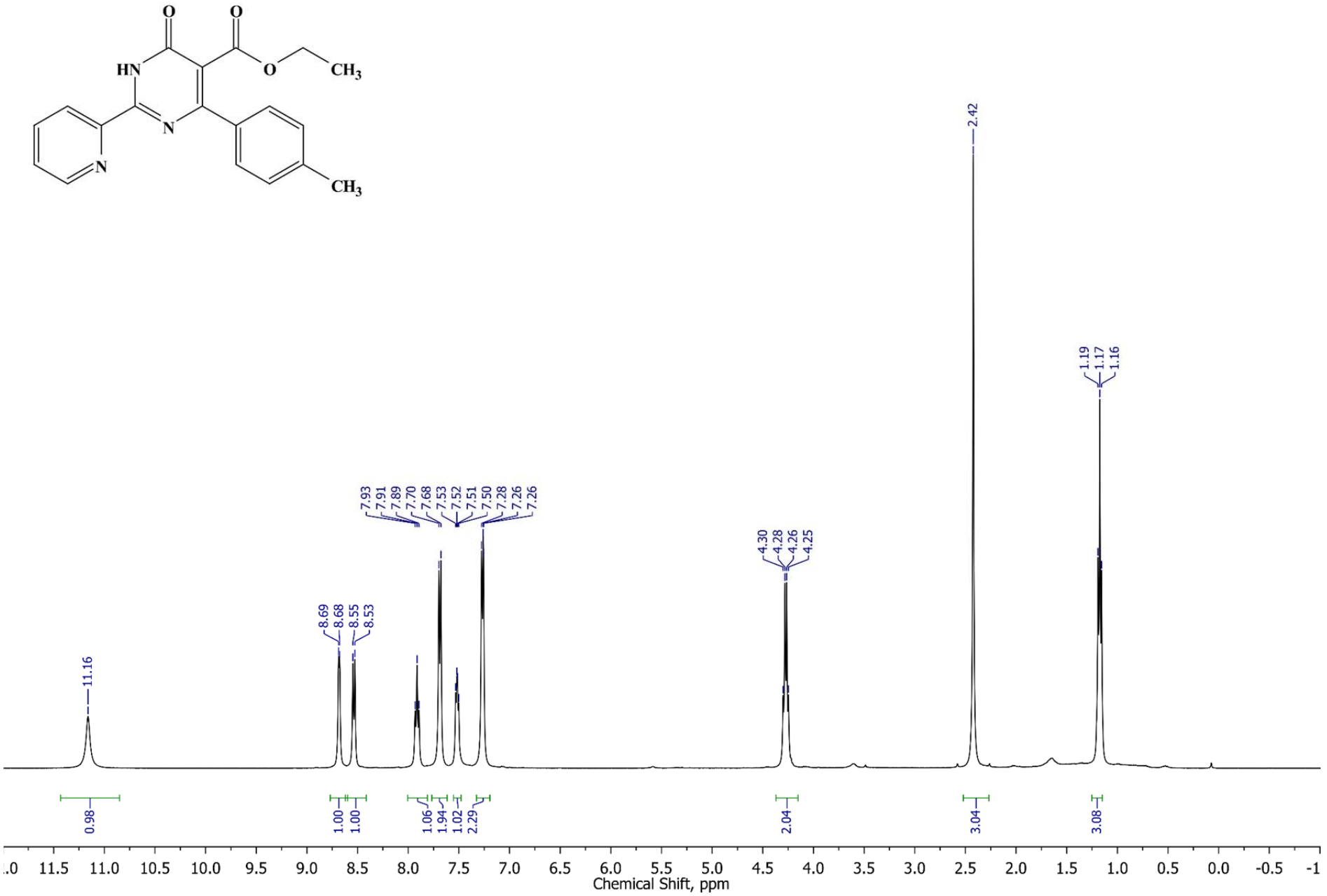


5-Acetyl-6-methyl-2-(*p*-tolyl)pyrimidin-4(3*H*)-one (3k), DEPT, DMSO-d_6, 101 MHz

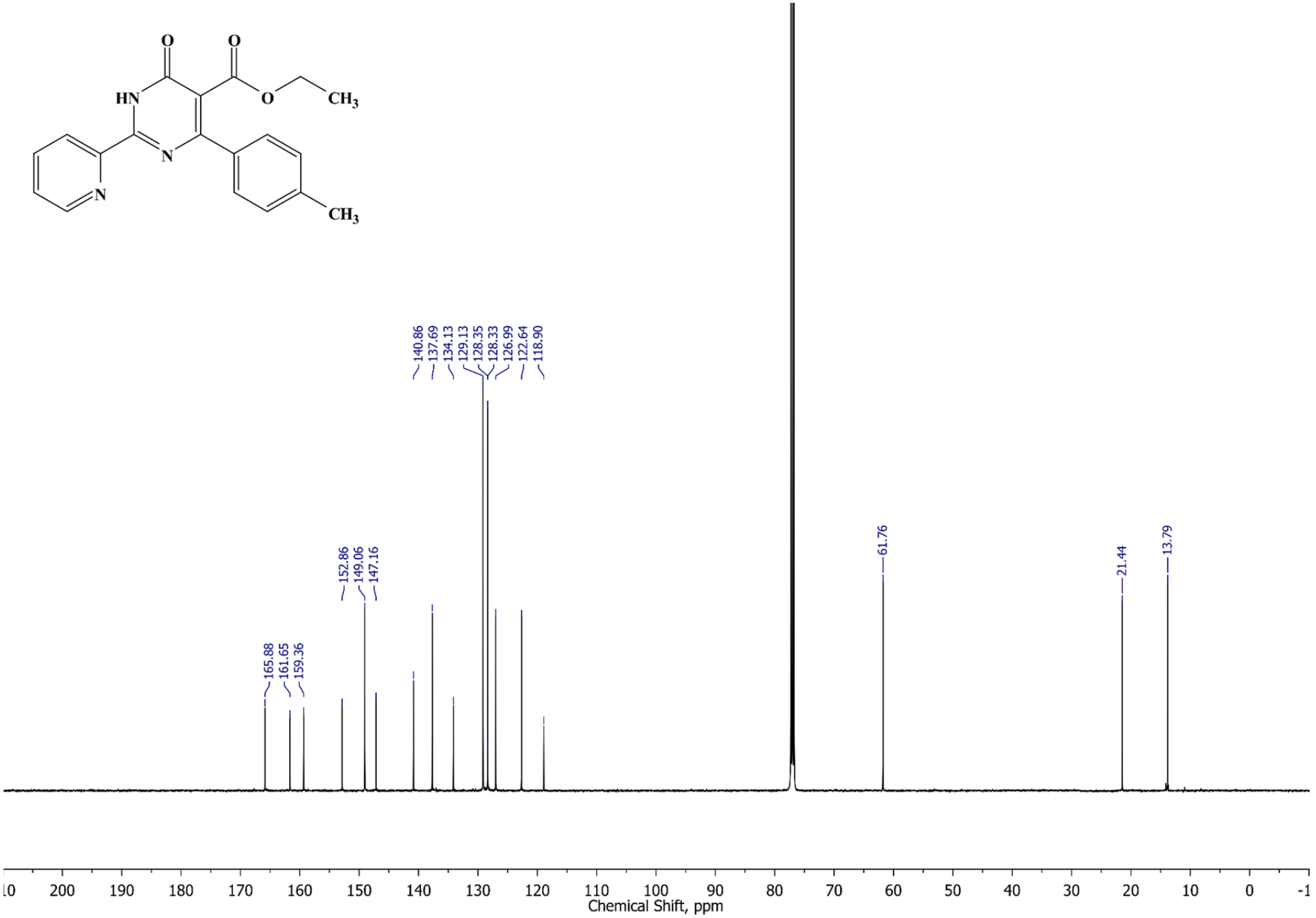




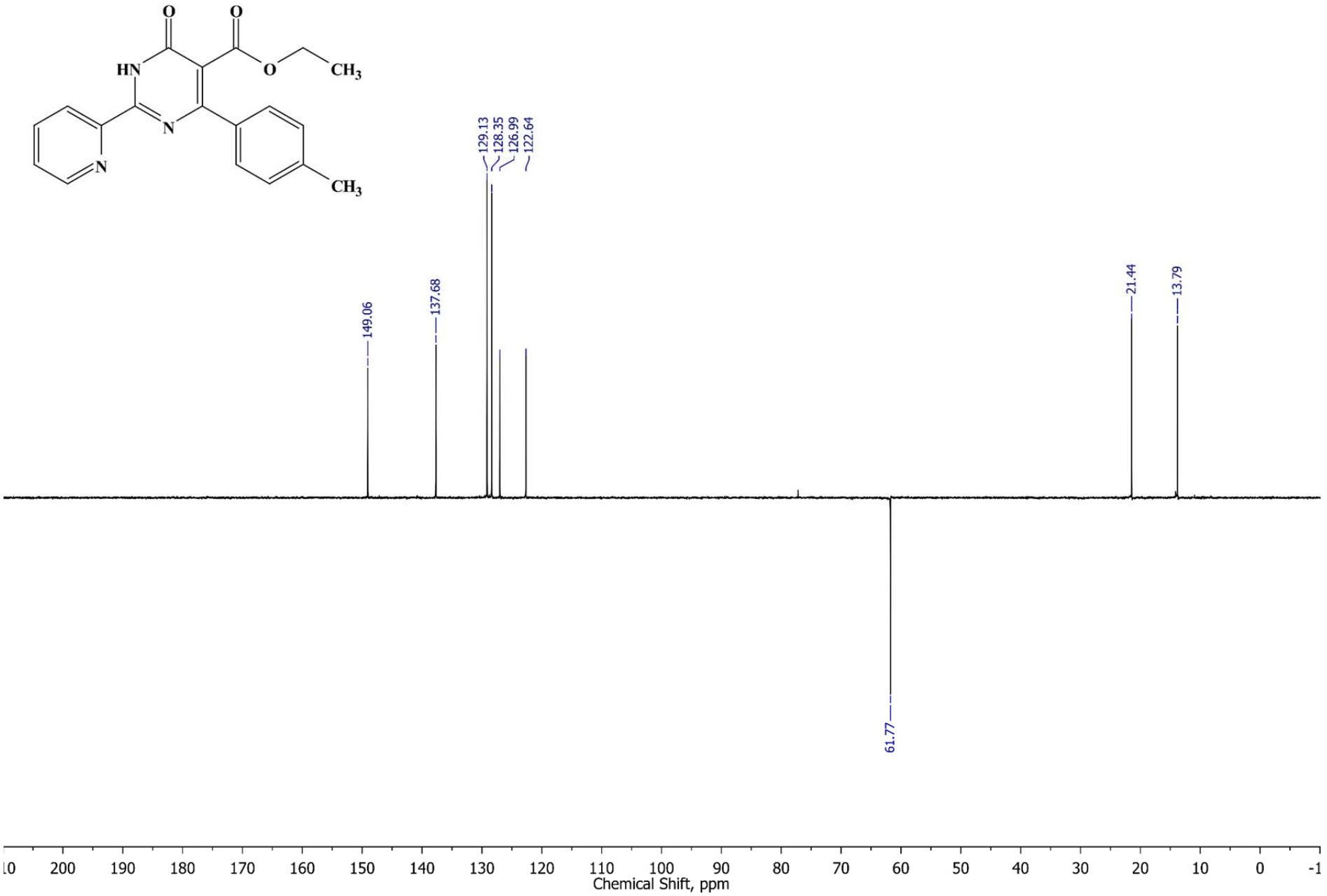
Ethyl 6-oxo-2-(pyridin-2-yl)-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3l), ^{1}H NMR, $CDCl_3$, 400 MHz



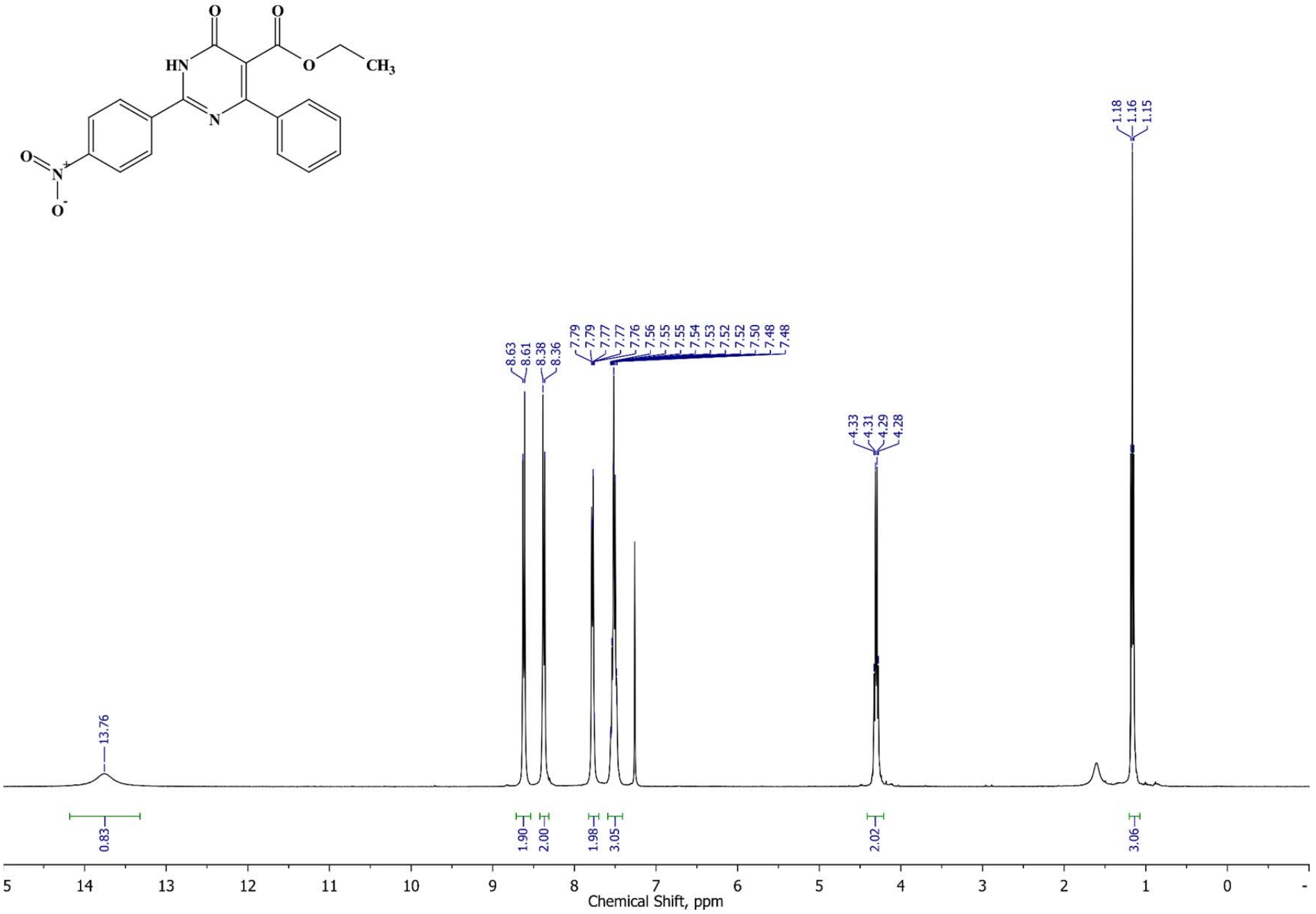
Ethyl 6-oxo-2-(pyridin-2-yl)-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3l), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



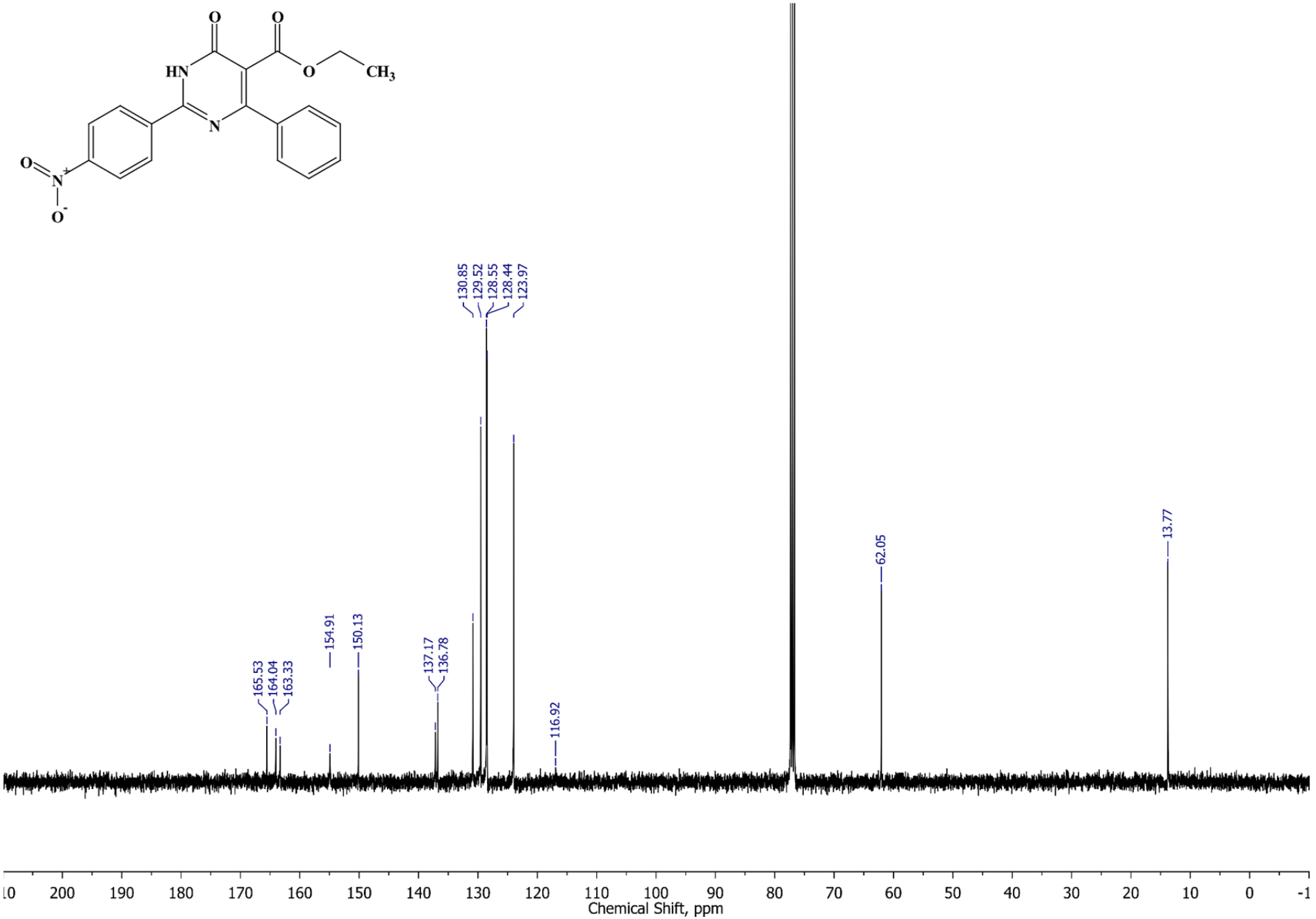
Ethyl 6-oxo-2-(pyridin-2-yl)-4-(*p*-tolyl)-1,6-dihydropyrimidine-5-carboxylate (3l), DEPT, $CDCl_3$, 101 MHz



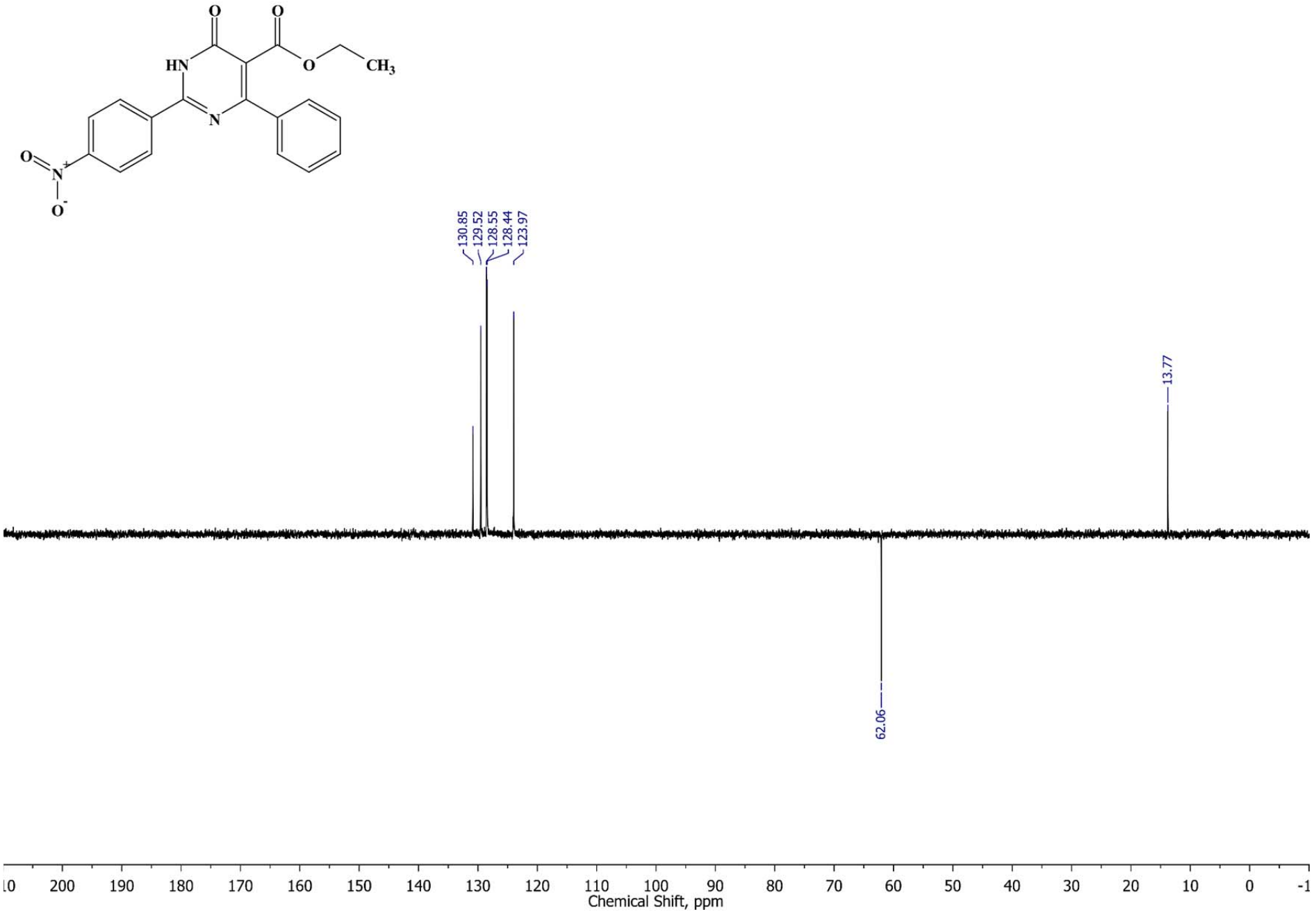
Ethyl 2-(4-nitrophenyl)-6-oxo-4-phenyl-1,6-dihydropyrimidine-5-carboxylate (3m), ^{1}H NMR, $CDCl_3$, 400 MHz



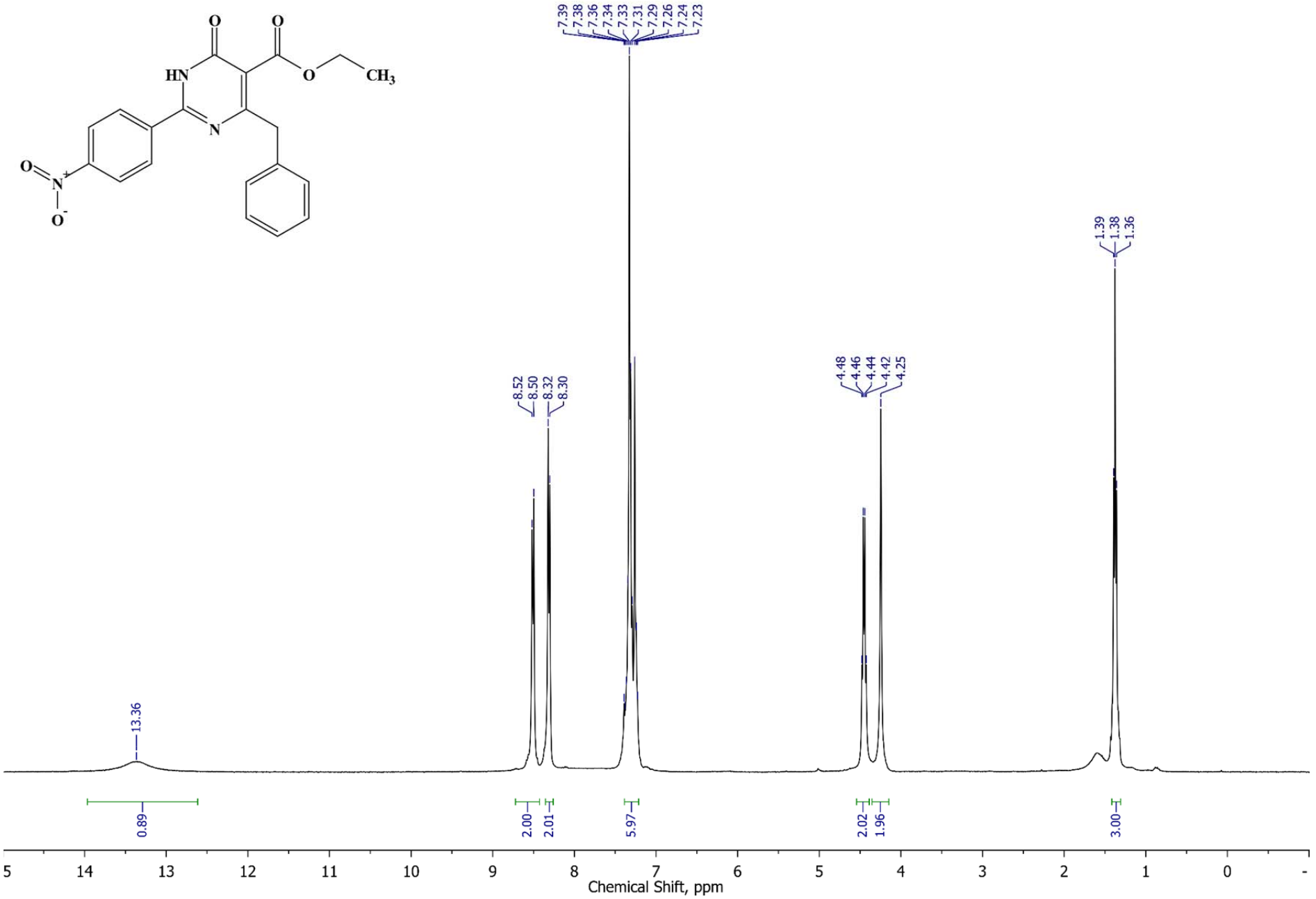
Ethyl 2-(4-nitrophenyl)-6-oxo-4-phenyl-1,6-dihydropyrimidine-5-carboxylate (3m), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



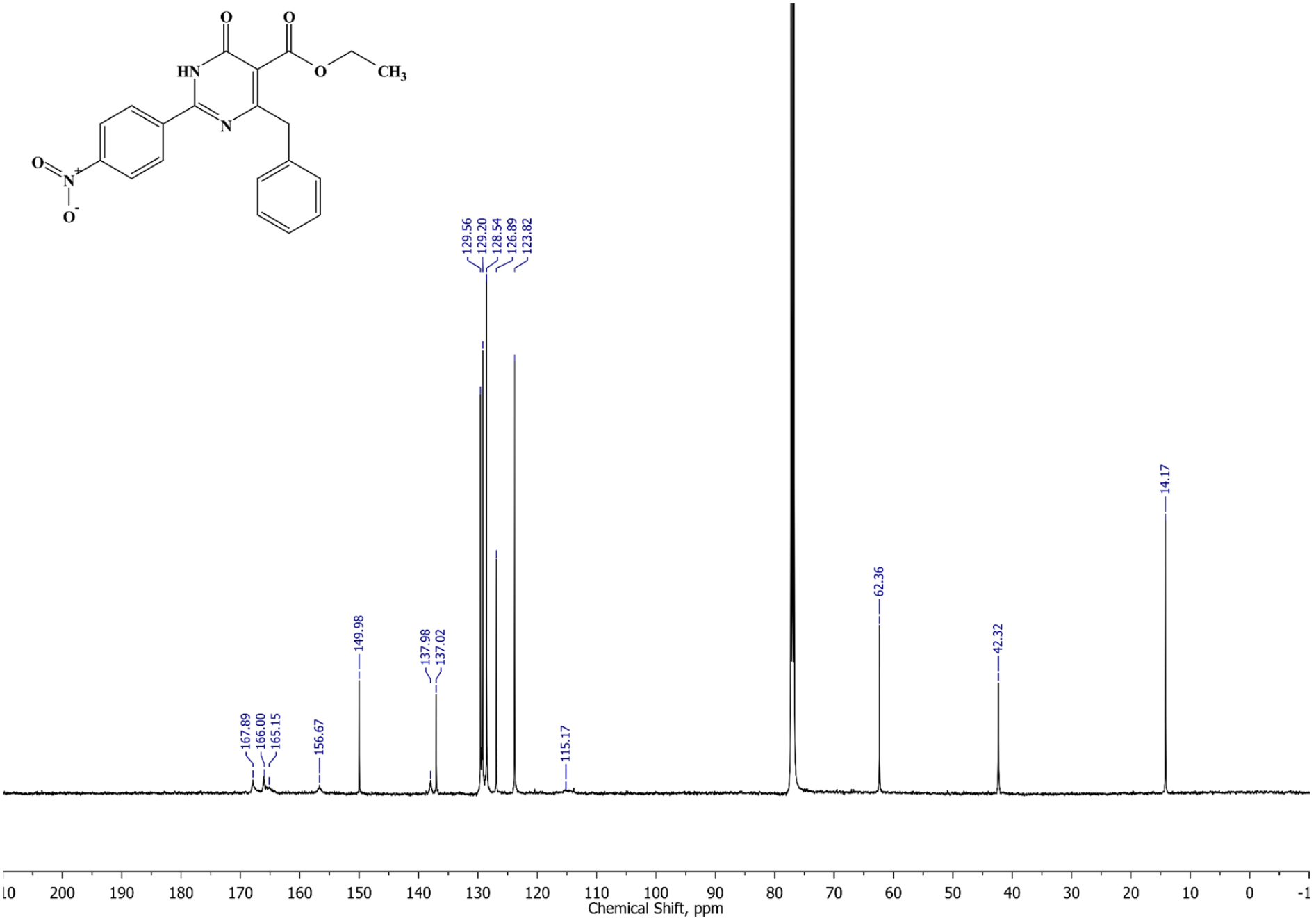
Ethyl 2-(4-nitrophenyl)-6-oxo-4-phenyl-1,6-dihydropyrimidine-5-carboxylate (3m), DEPT, $CDCl_3$, 101 MHz



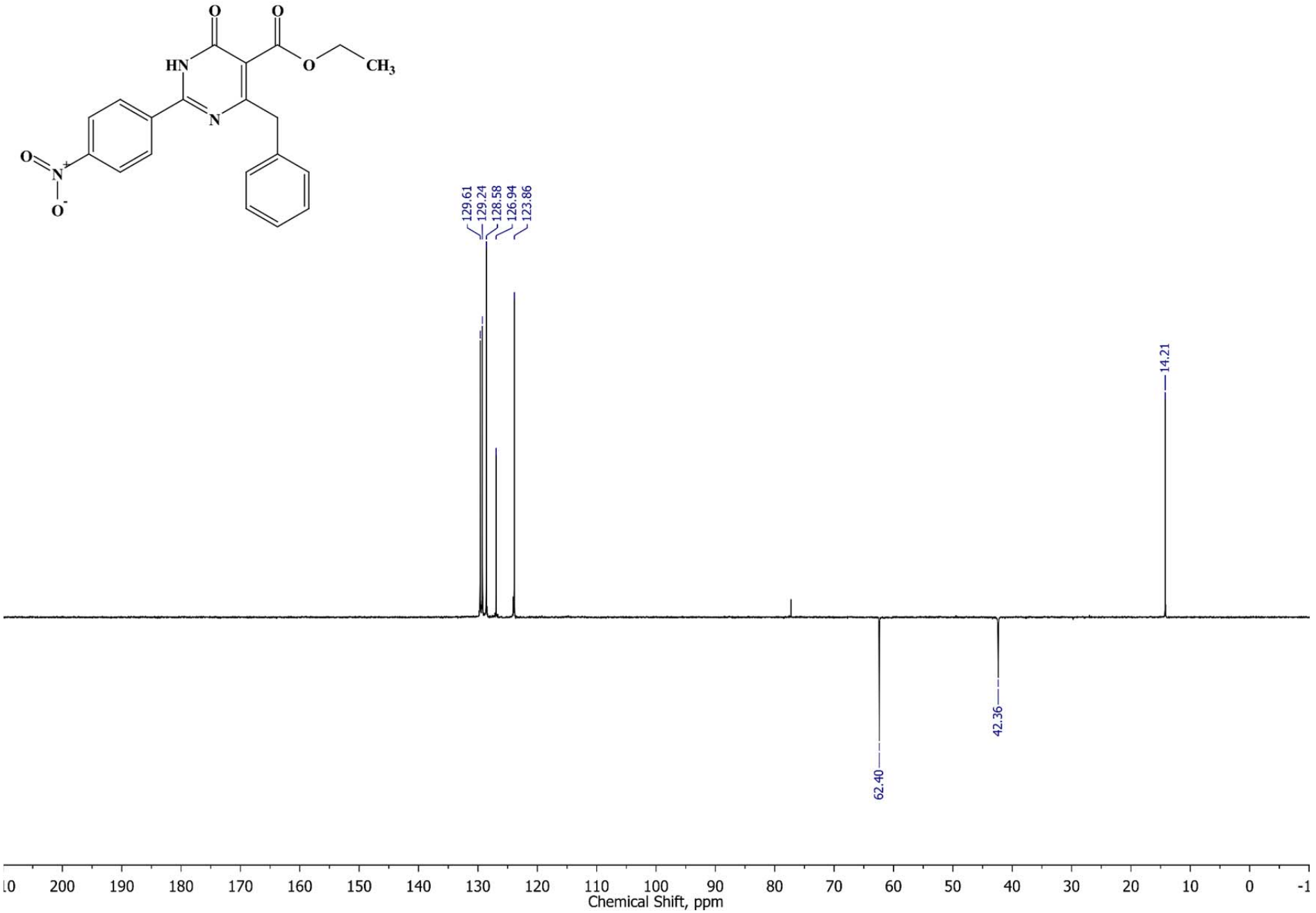
Ethyl 4-benzyl-2-(4-nitrophenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3n), ^{1}H NMR, $CDCl_3$, 400 MHz



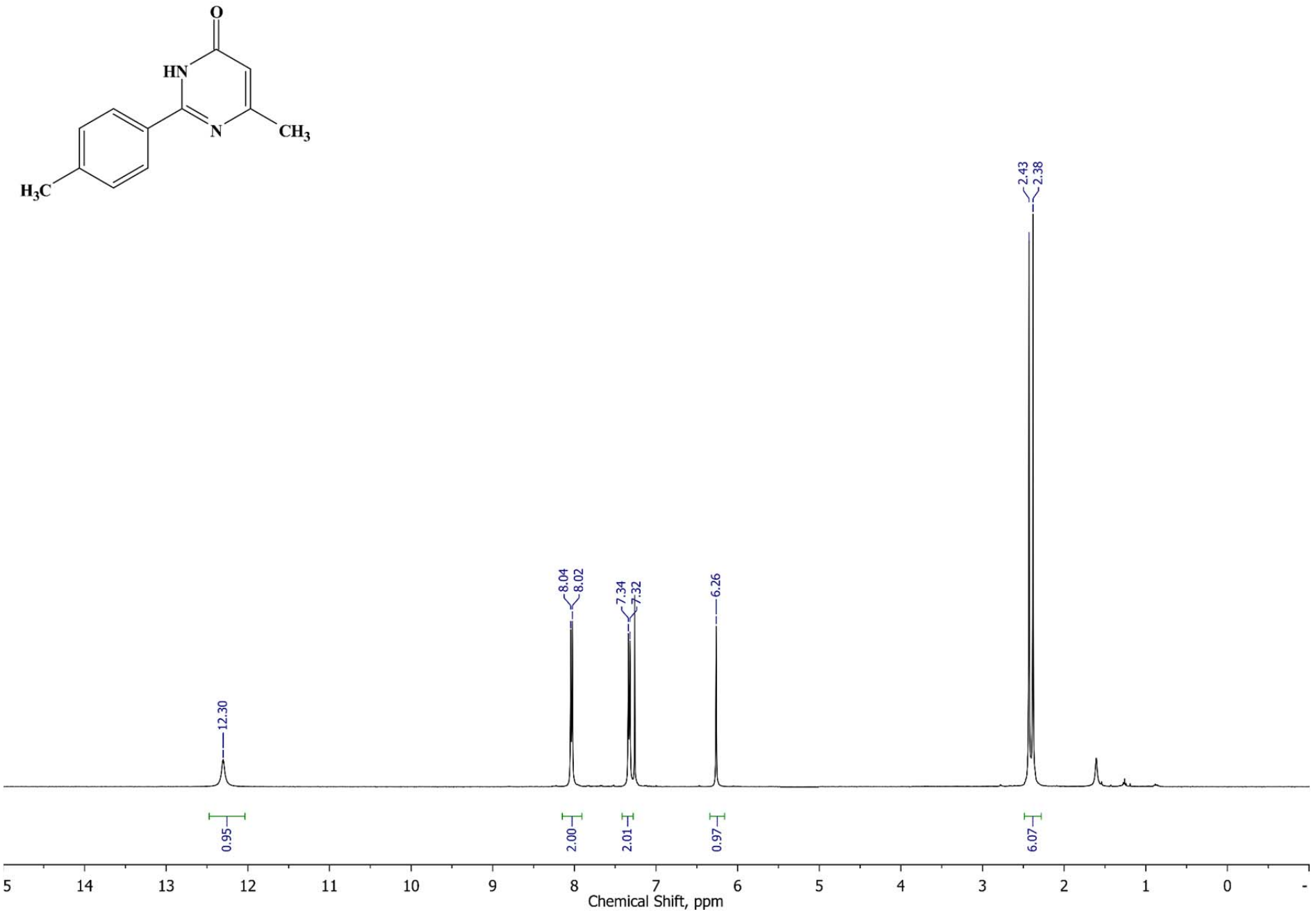
Ethyl 4-benzyl-2-(4-nitrophenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3n), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



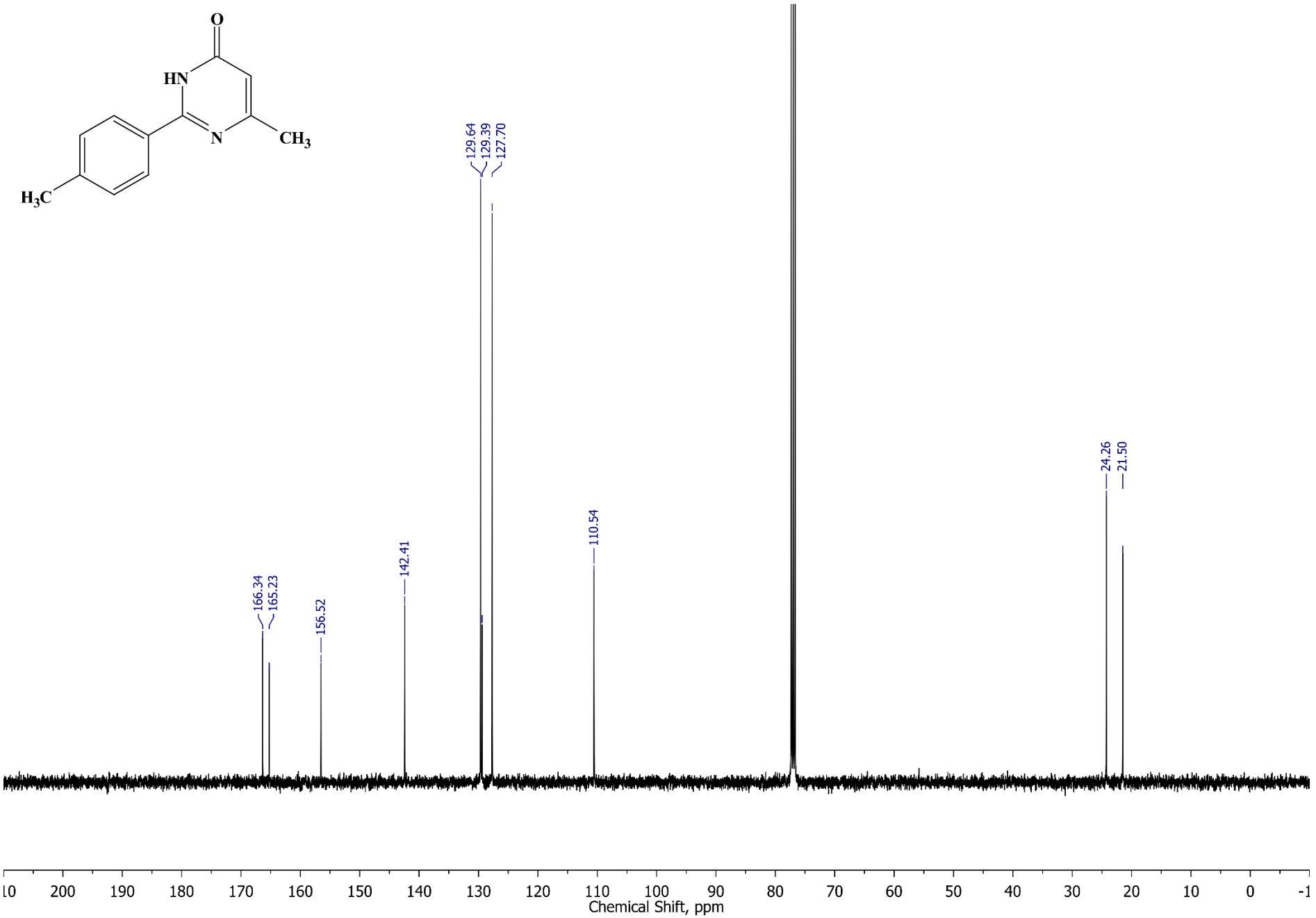
Ethyl 4-benzyl-2-(4-nitrophenyl)-6-oxo-1,6-dihydropyrimidine-5-carboxylate (3n), DEPT, $CDCl_3$, 101 MHz



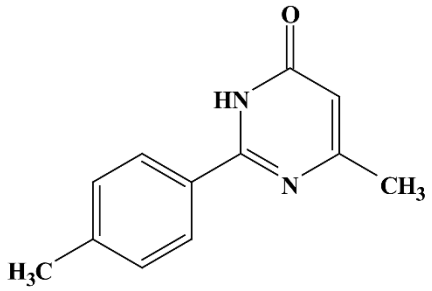
6-Methyl-2-(*p*-tolyl)pyrimidin-4(3*H*)-one (5a), ^{1}H NMR, $CDCl_3$, 400 MHz

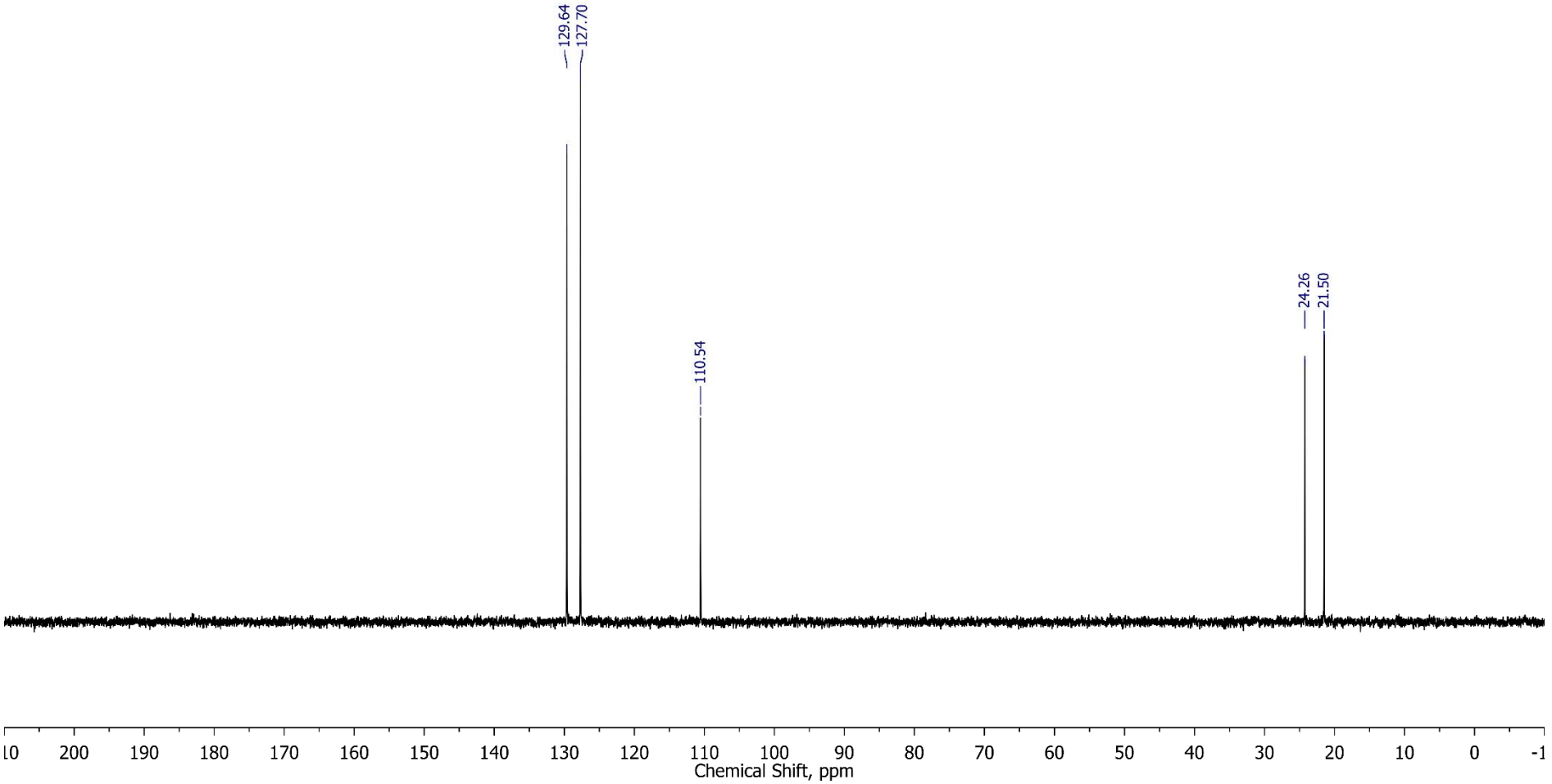


6-Methyl-2-(*p*-tolyl)pyrimidin-4(3*H*)-one (5a), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz

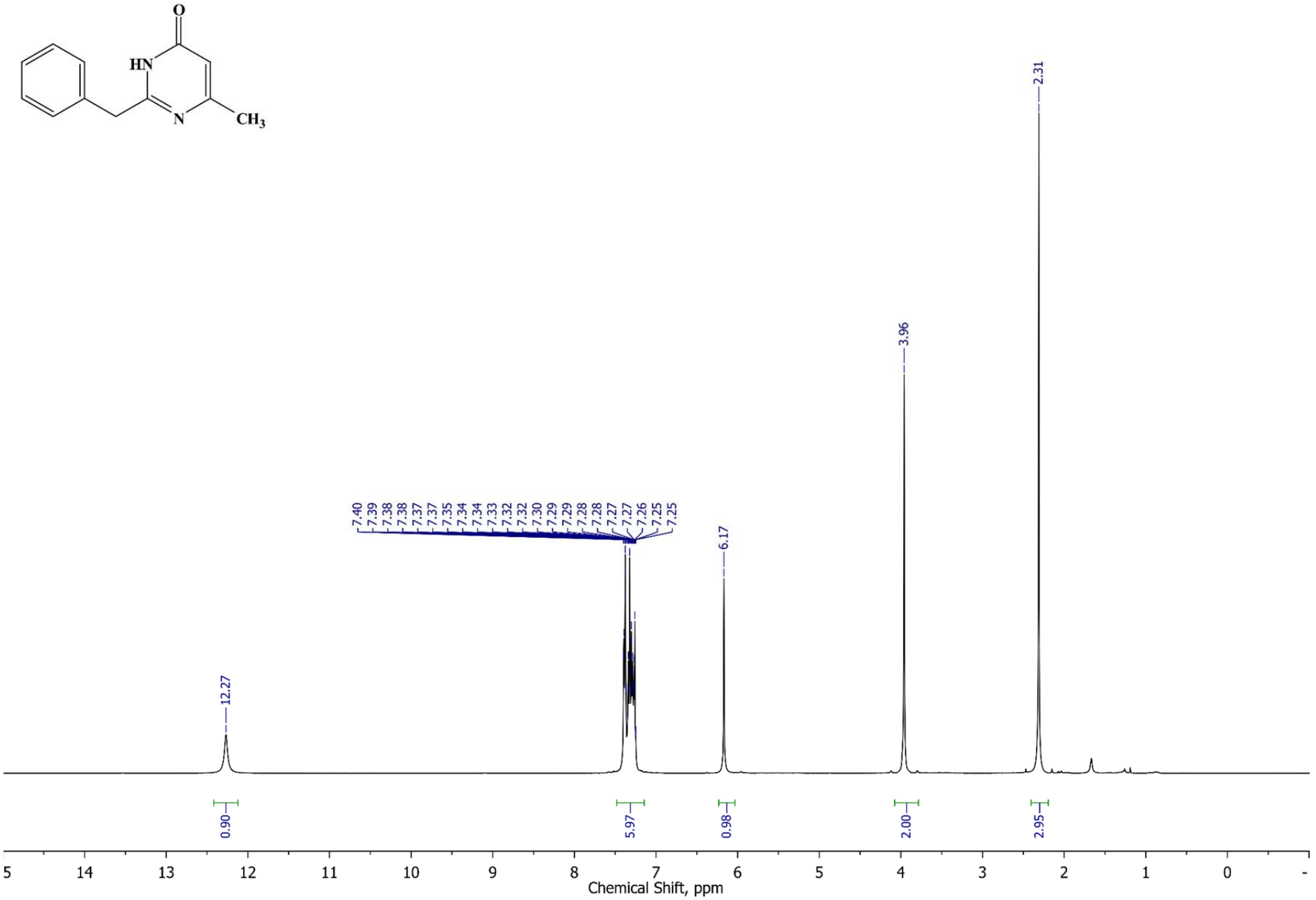


6-Methyl-2-(*p*-tolyl)pyrimidin-4(3*H*)-one (5a), DEPT, $CDCl_3$, 101 MHz

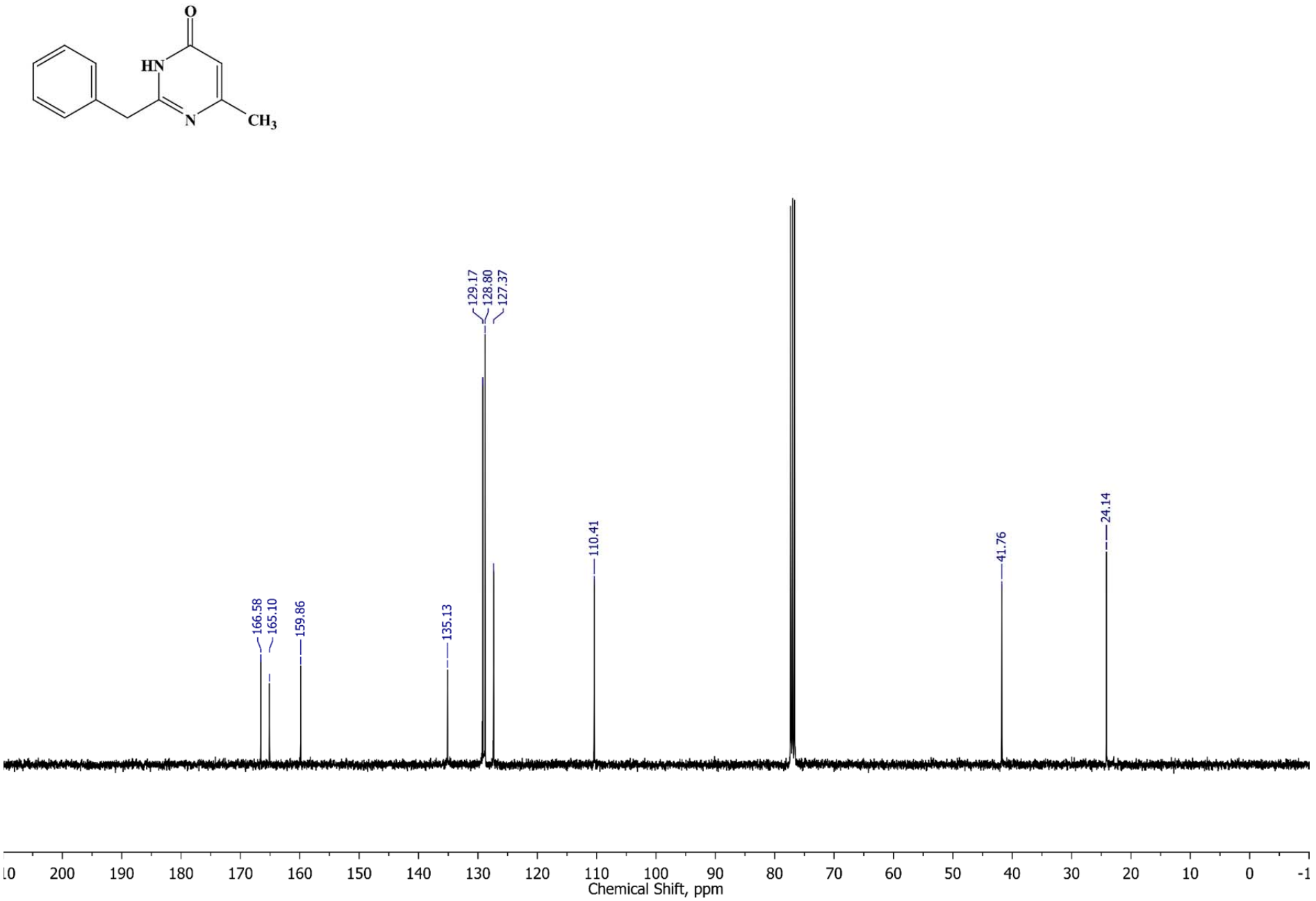




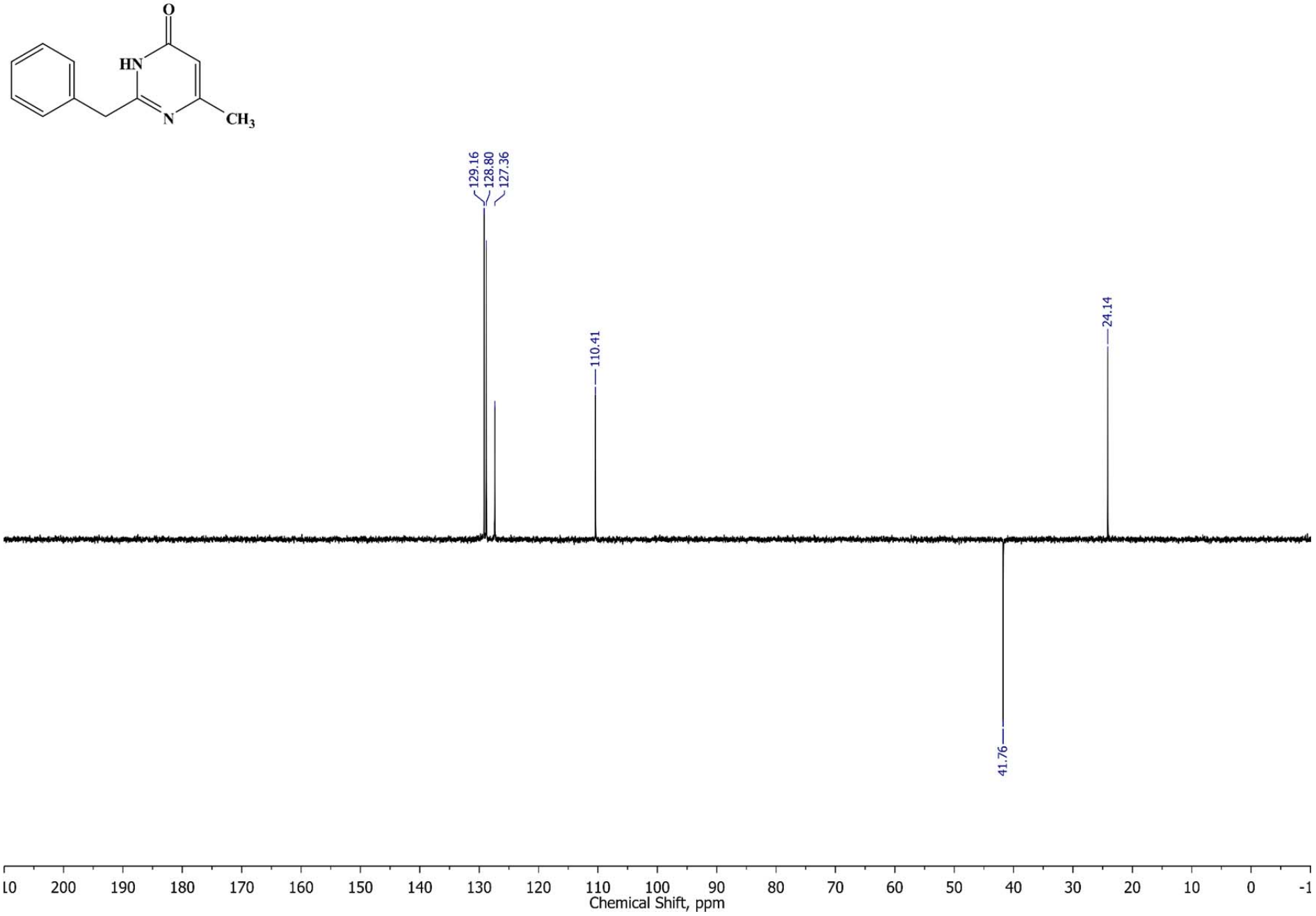
2-Benzyl-6-methylpyrimidin-4(3*H*)-one (5b), ^{1}H NMR, $CDCl_3$, 400 MHz



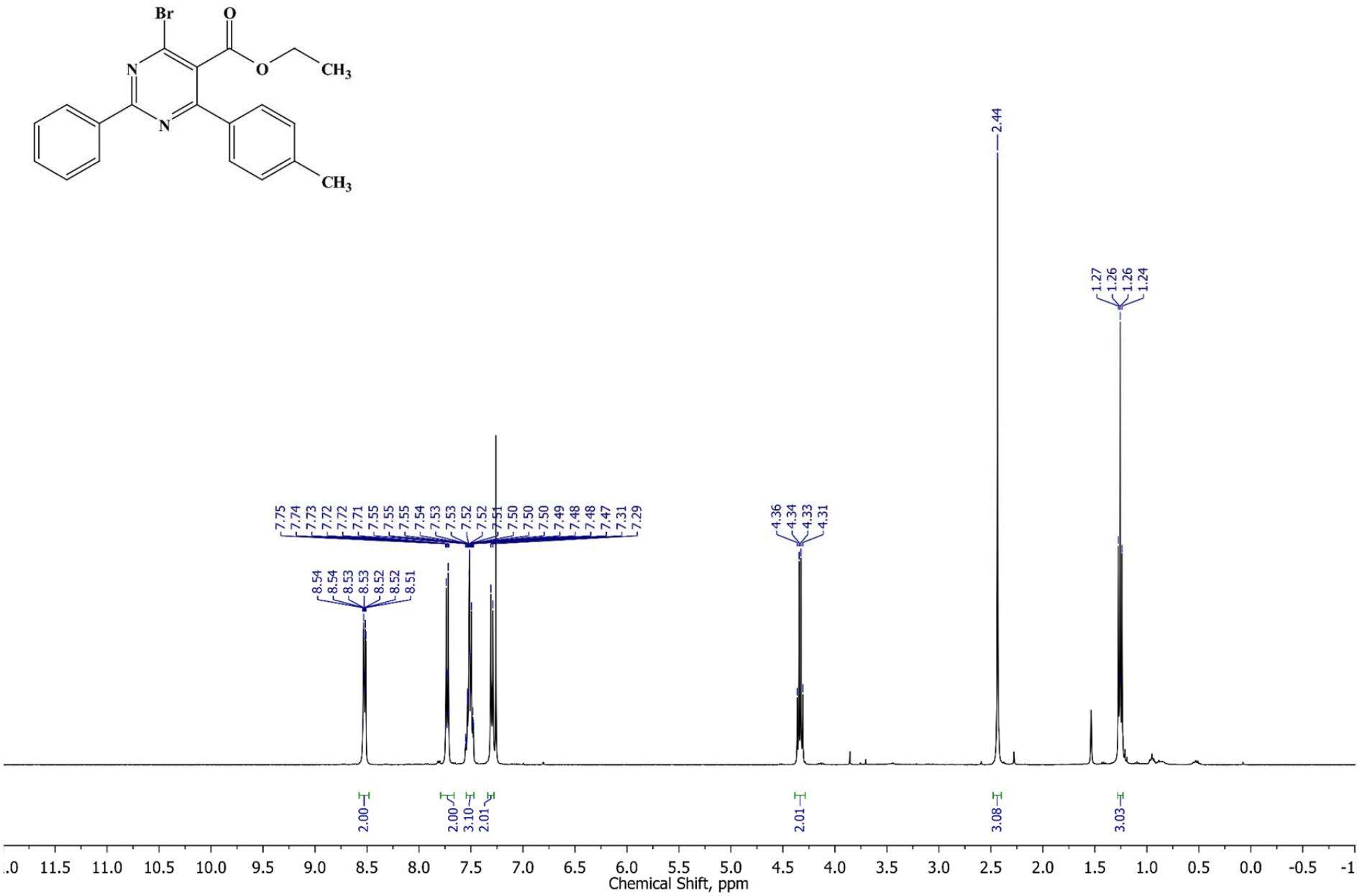
2-Benzyl-6-methylpyrimidin-4(3*H*)-one (5b), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



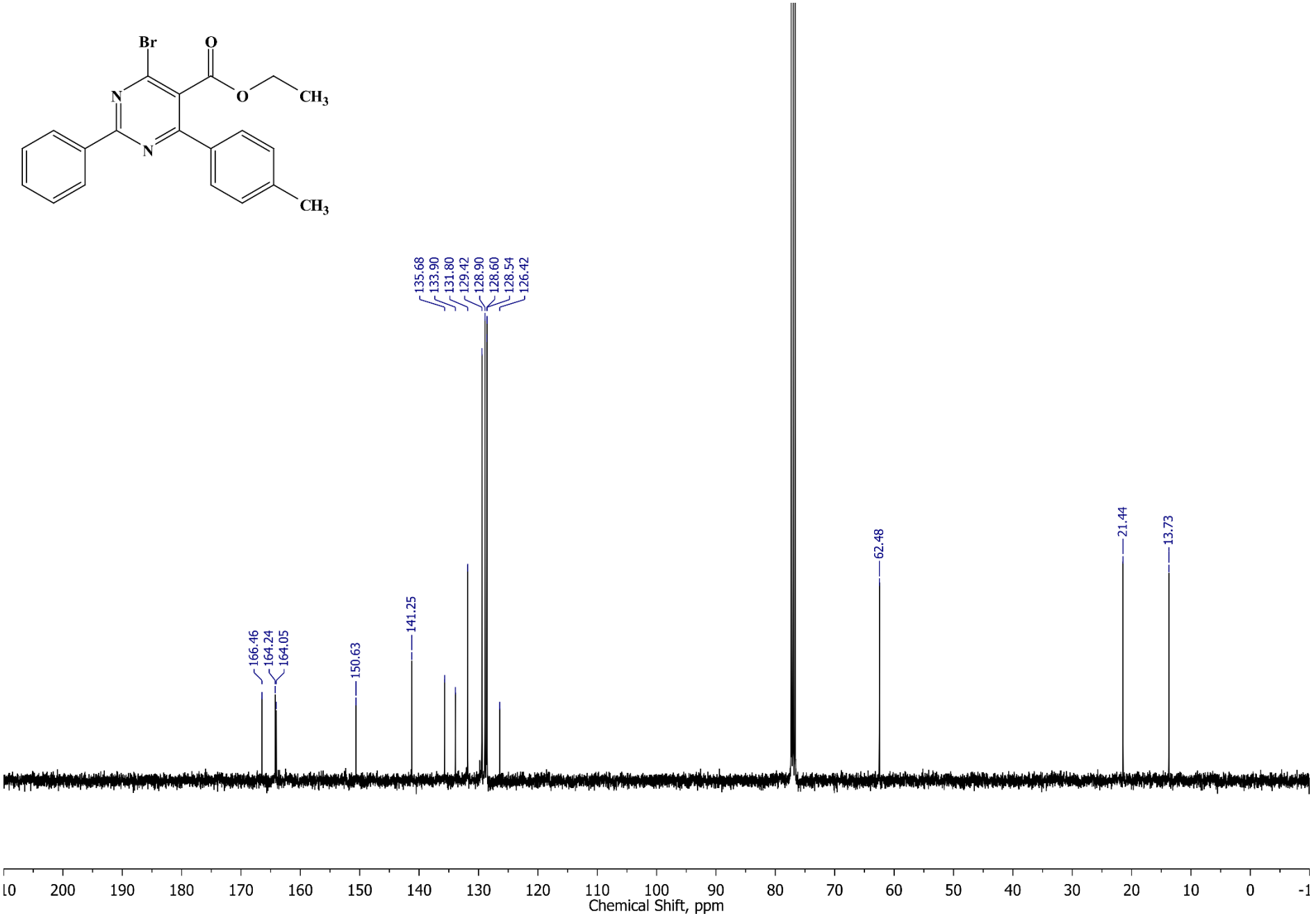
2-Benzyl-6-methylpyrimidin-4(3*H*)-one (5b), DEPT, $CDCl_3$, 101 MHz



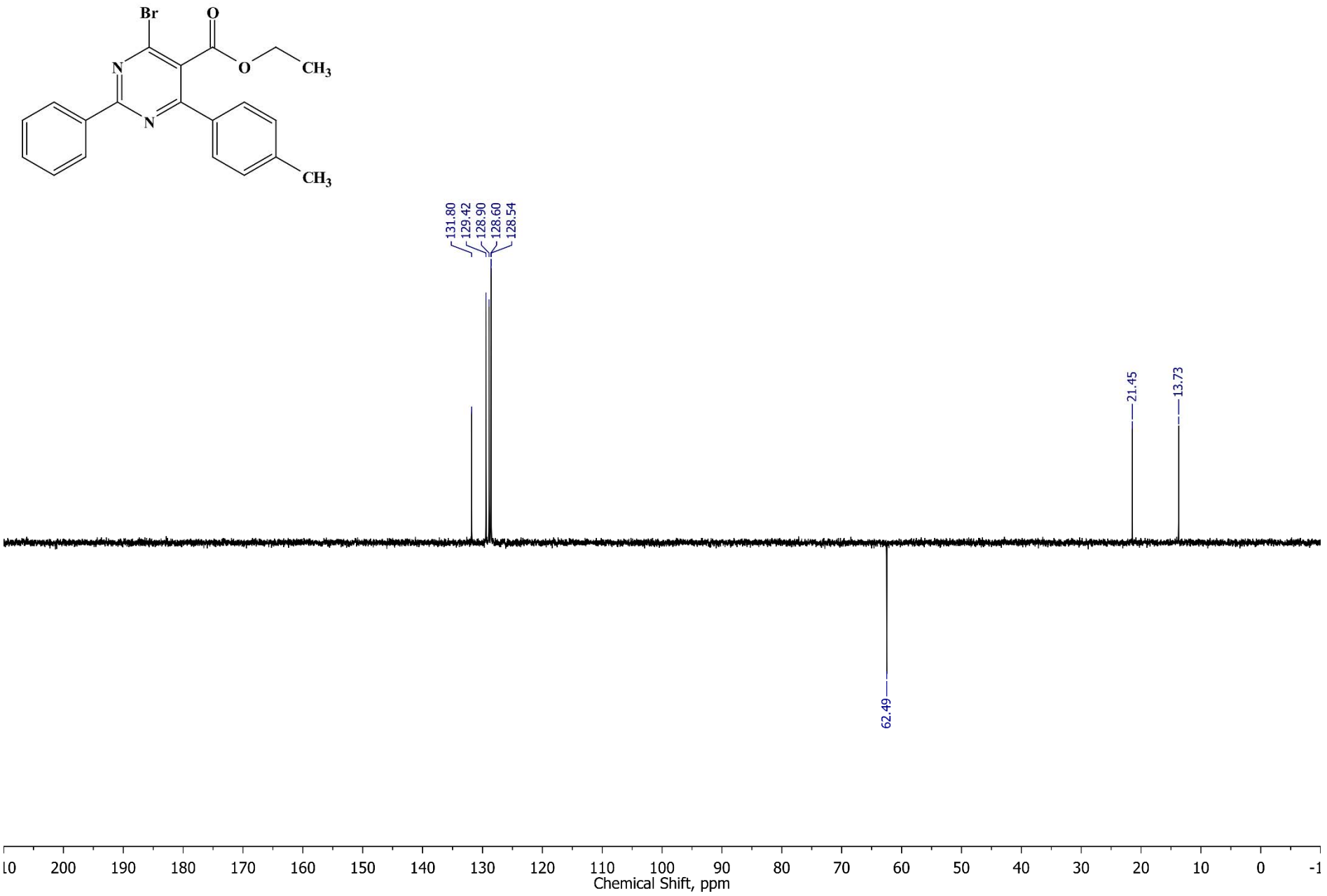
Ethyl 4-bromo-2-phenyl-6-(*p*-tolyl)pyrimidine-5-carboxylate (6), ^{1}H NMR, $CDCl_3$, 400 MHz



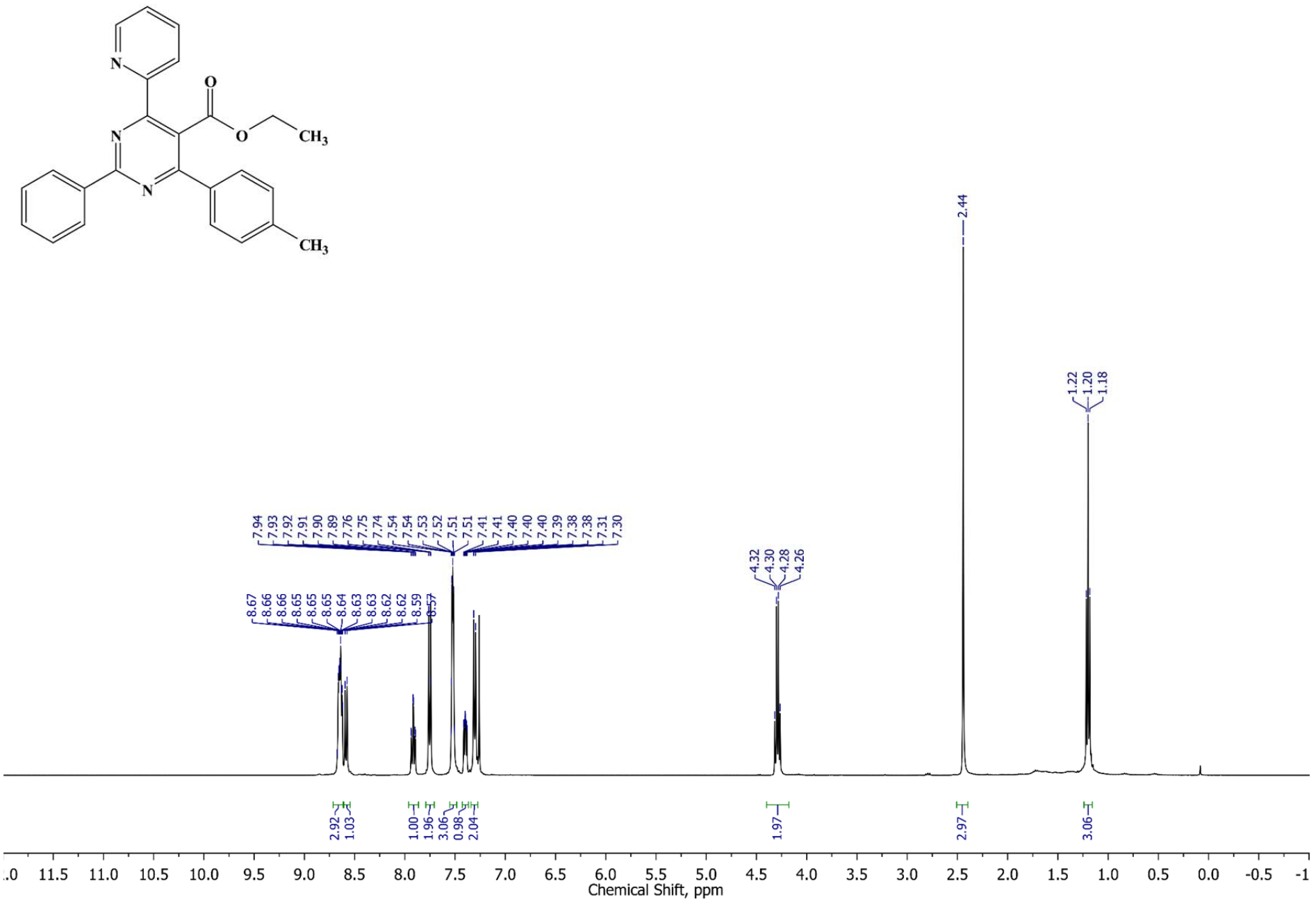
Ethyl 4-bromo-2-phenyl-6-(*p*-tolyl)pyrimidine-5-carboxylate (6), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



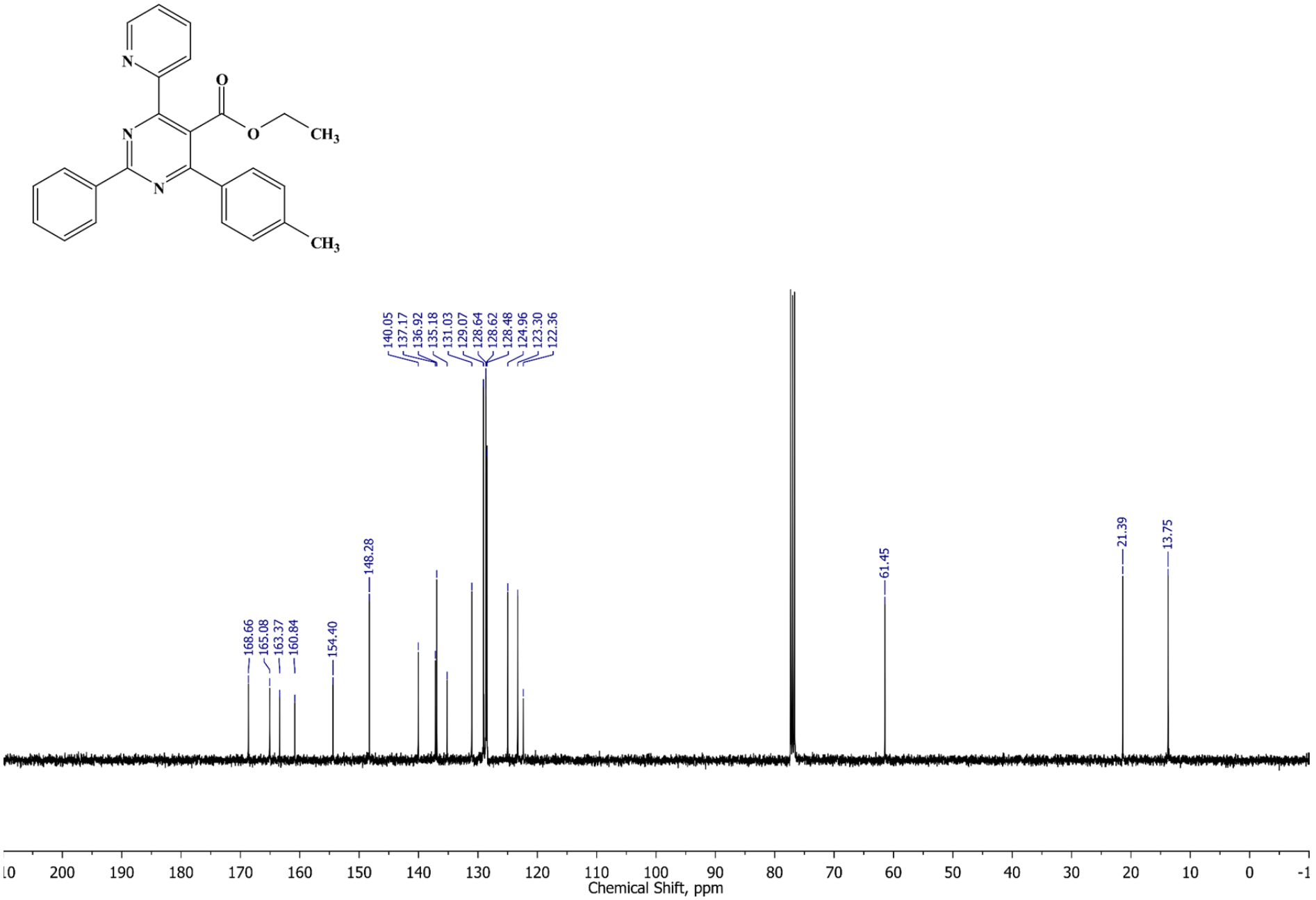
Ethyl 4-bromo-2-phenyl-6-(*p*-tolyl)pyrimidine-5-carboxylate (6), DEPT, $CDCl_3$, 101 MHz



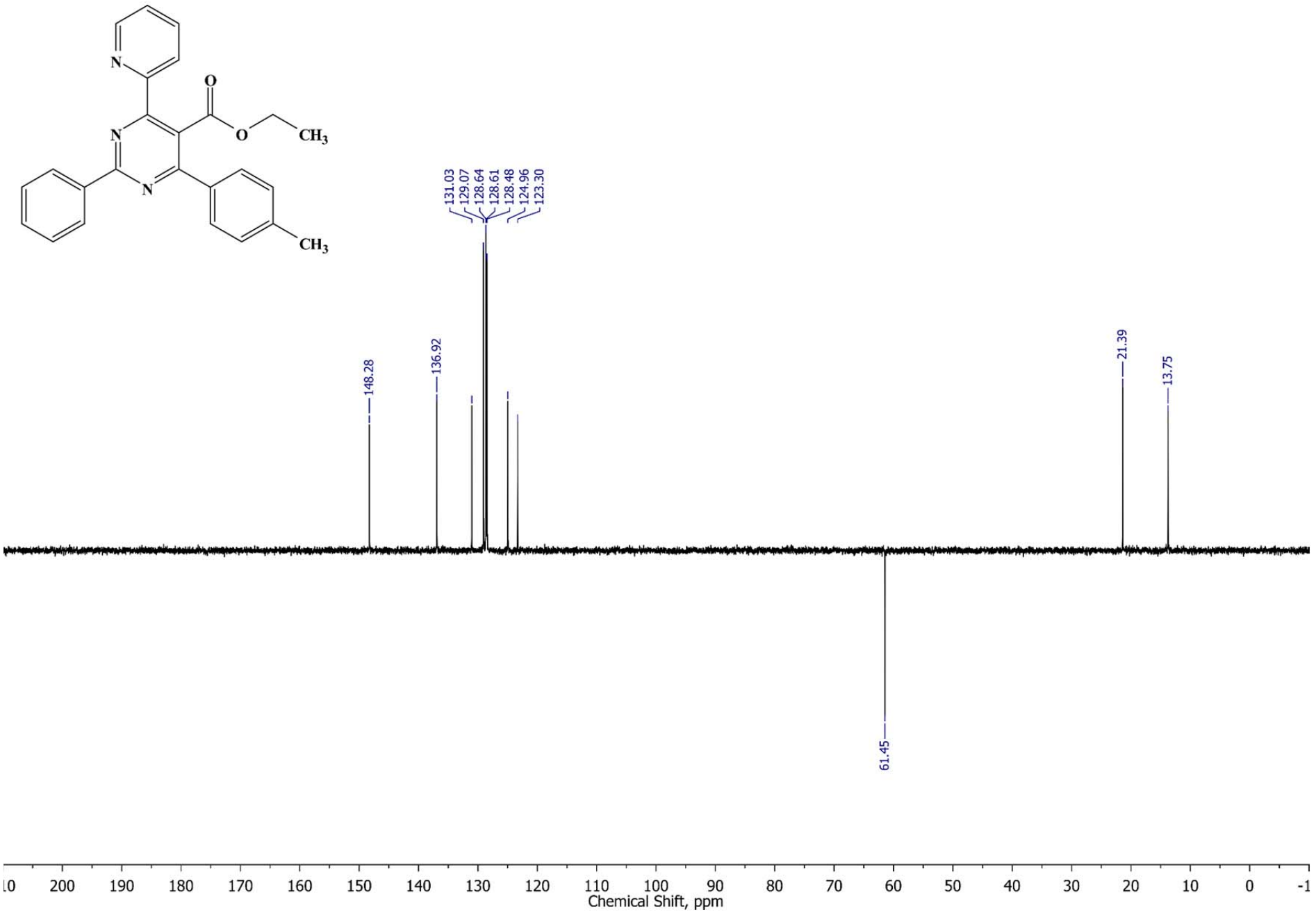
Ethyl 2-phenyl-4-(pyridin-2-yl)-6-(*p*-tolyl)pyrimidine-5-carboxylate (7), ^{1}H NMR, $CDCl_3$, 400 MHz



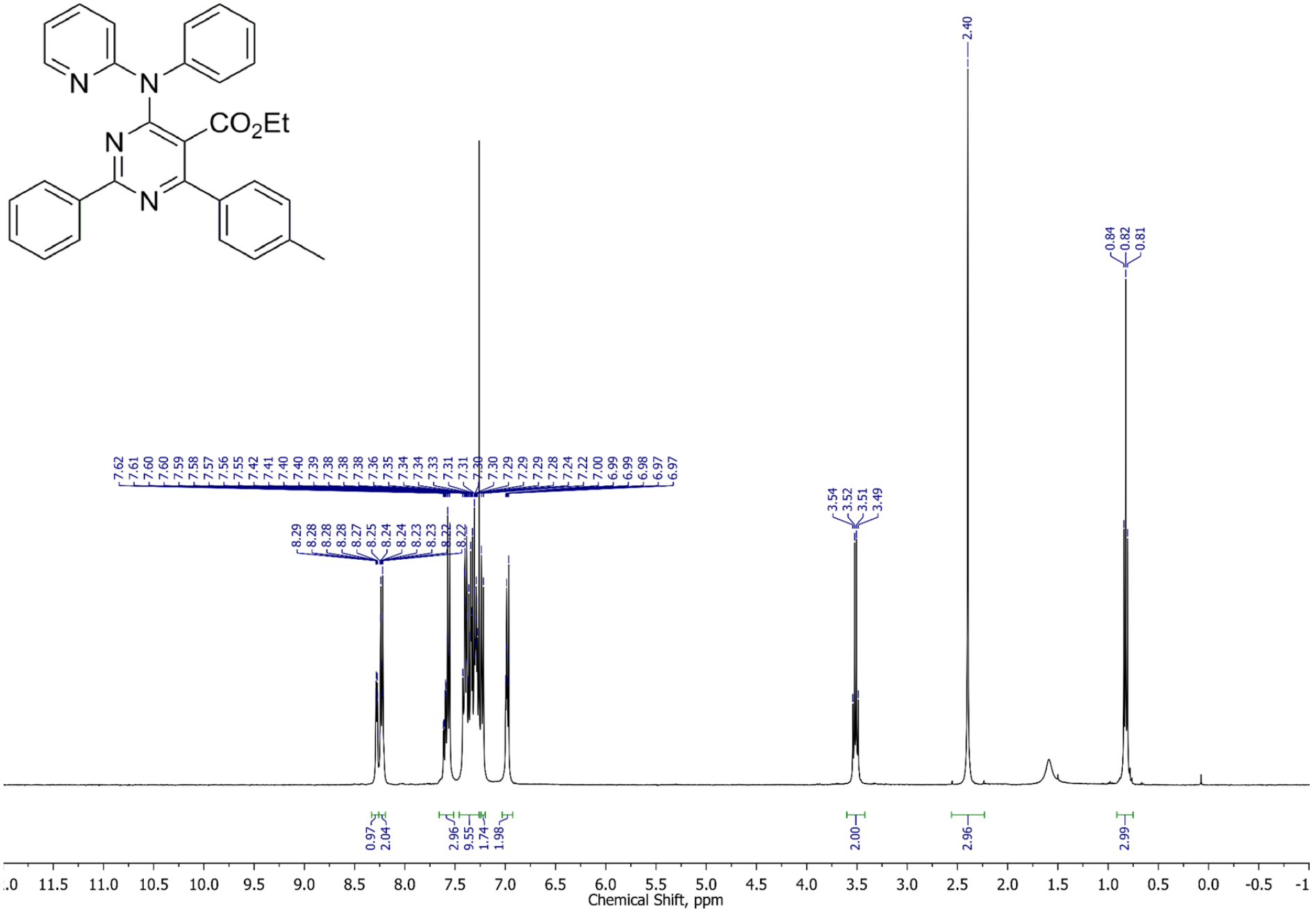
Ethyl 2-phenyl-4-(pyridin-2-yl)-6-(*p*-tolyl)pyrimidine-5-carboxylate (7), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



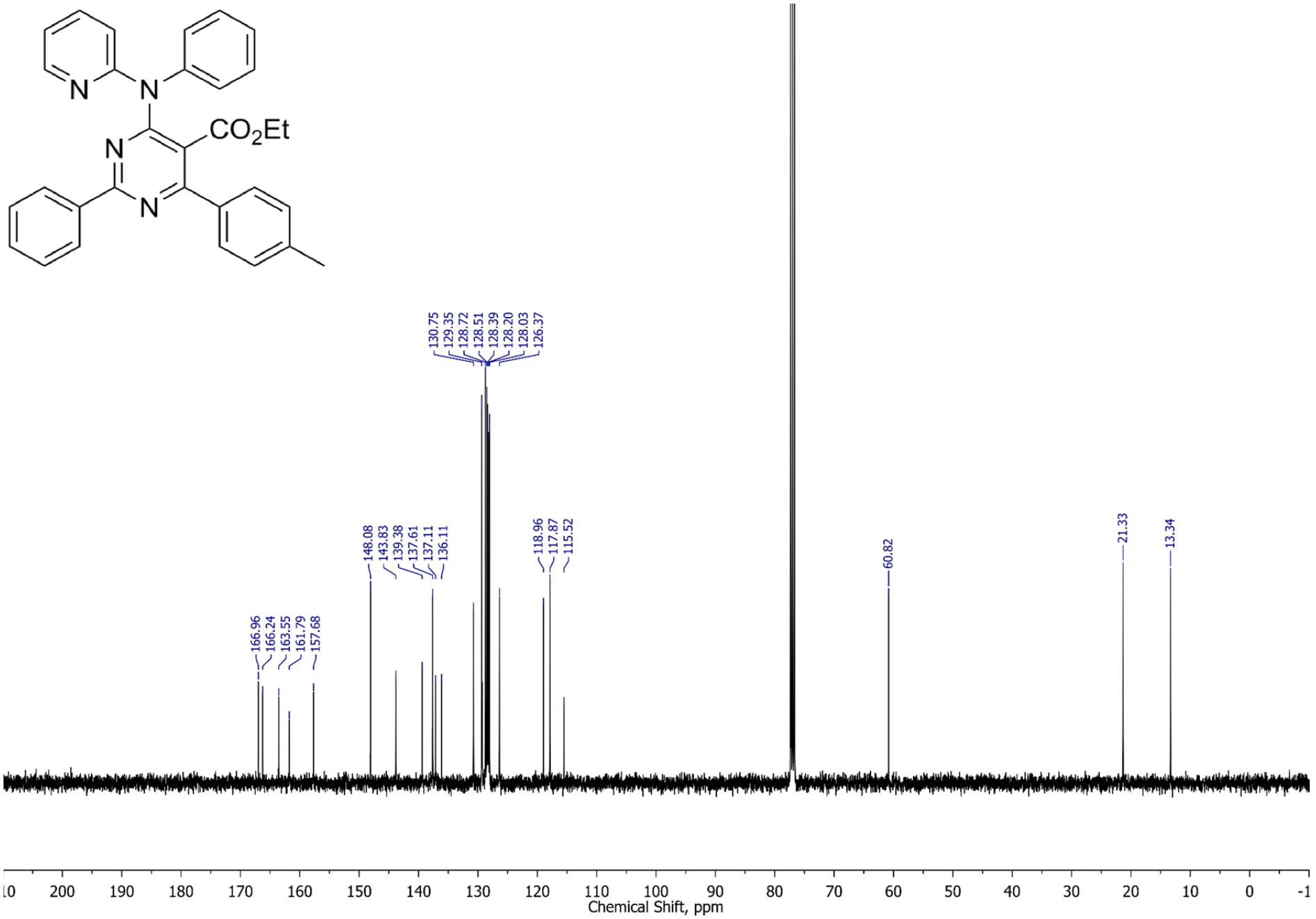
Ethyl 2-phenyl-4-(pyridin-2-yl)-6-(*p*-tolyl)pyrimidine-5-carboxylate (7), DEPT, $CDCl_3$, 101 MHz



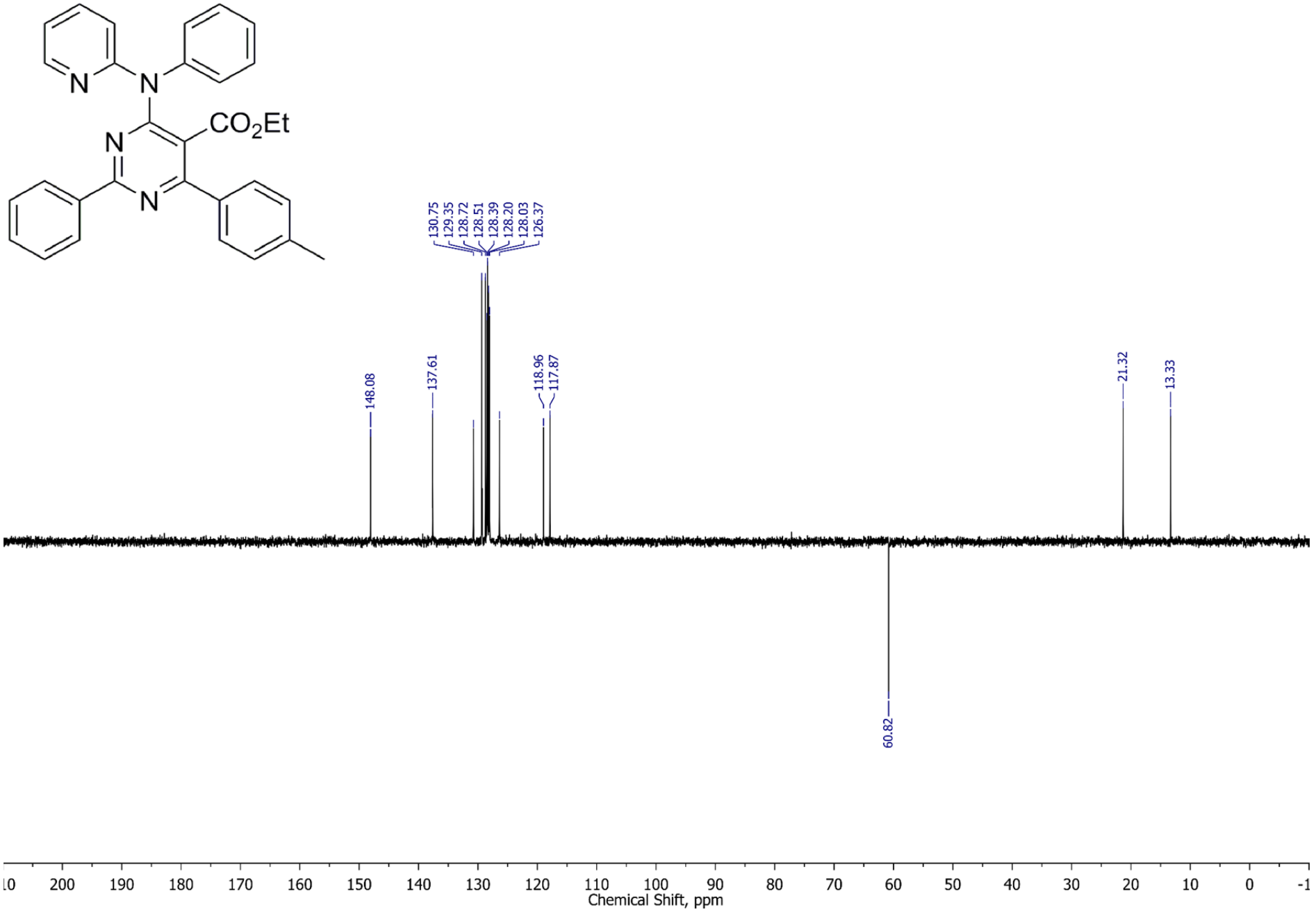
Ethyl 2-phenyl-4-(phenyl(pyridin-2-yl)amino)-6-(*p*-tolyl)pyrimidine-5-carboxylate (8), ^{1}H NMR, $CDCl_3$, 400 MHz



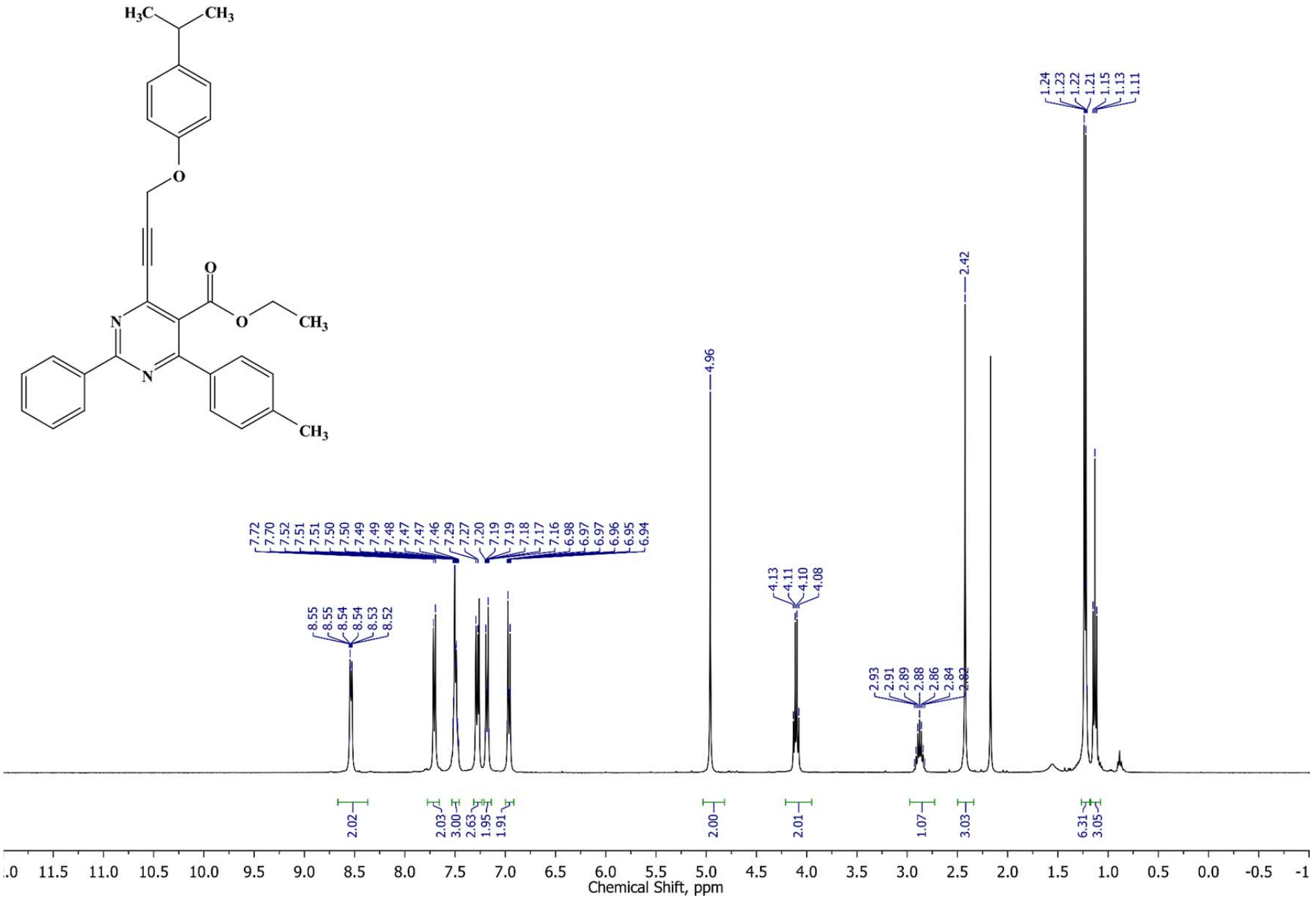
Ethyl 2-phenyl-4-(phenyl(pyridin-2-yl)amino)-6-(*p*-tolyl)pyrimidine-5-carboxylate (8), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



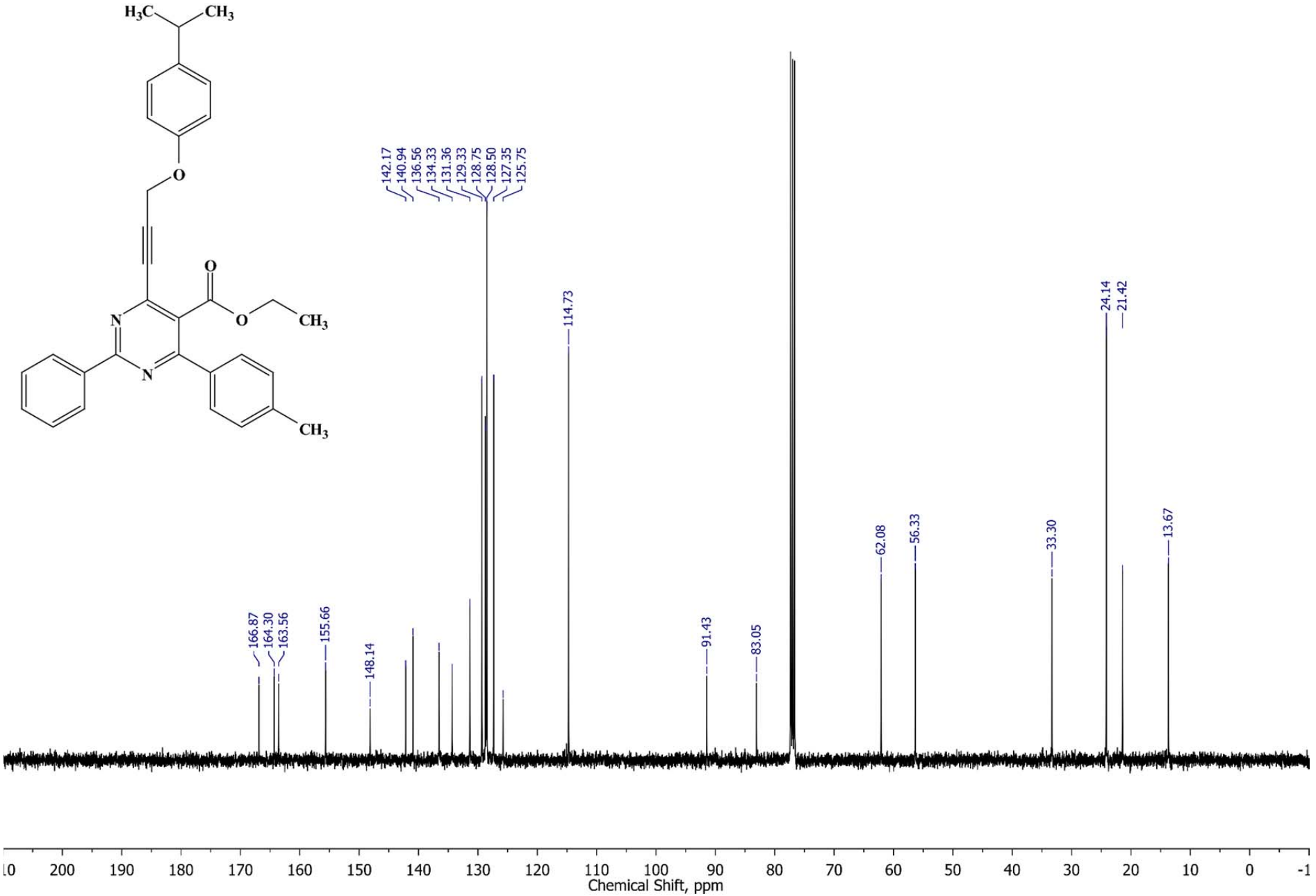
Ethyl 2-phenyl-4-(phenyl(pyridin-2-yl)amino)-6-(*p*-tolyl)pyrimidine-5-carboxylate (8), DEPT, $CDCl_3$, 101 MHz



Ethyl 4-(3-(4-isopropylphenoxy)prop-1-yn-1-yl)-2-phenyl-6-(*p*-tolyl)pyrimidine-5-carboxylate (9), ^{1}H NMR, $CDCl_3$, 400 MHz



Ethyl 4-(3-(4-isopropylphenoxy)prop-1-yn-1-yl)-2-phenyl-6-(*p*-tolyl)pyrimidine-5-carboxylate (9), $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, 101 MHz



Ethyl 4-(3-(4-isopropylphenoxy)prop-1-yn-1-yl)-2-phenyl-6-(*p*-tolyl)pyrimidine-5-carboxylate (9), DEPT, $CDCl_3$, 101 MHz