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Cascade synthesis of highly substituted tetrahydroquinolines using ethyl cyanoacetate via aza-Michael-Michael addition

Arunan Palanimuthu,[b] Chinpiao Chen*[a, b] and Gene-Hsian Lee[c]

[a] *Department of Nursing, Tzu Chi University of Science and Technology, Hualien 970, Taiwan, Fax: 886 3 856 1097; Tel: 886 3 857 2158 ext.2624; E-mail: chinpiao@ems.tcust.edu.tw*

[b] *Department of Chemistry, National Dong Hwa University, Soufeng, Hualien 974, Taiwan.*

[c] *Instrumentation Center, College of Science, National Taiwan University, Taipei 106, Taiwan.*

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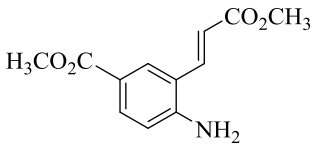
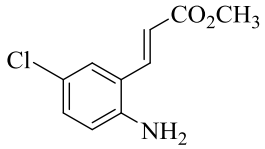
General procedure for synthesis of substituted *ortho*-amino cinnamates

Methyl (*E*)-4-amino-3-(3-methoxy-3-oxoprop-1-en-1-yl)benzoate (i).



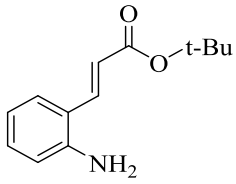
To the stirred solution of methyl 4-amino-3-iodobenzoate (3.61 mmol), palladium acetate (0.036 mmol), triphenylphosphine (0.072 mmol), potassium carbonate (7.22 mmol), and tetrabutylammonium bromide (0.072 mmol) in *N*,*N*′-dimethylformamide (10 mL) added methyl acrylate (7.22 mmol). The reaction mixture was stirred at 80 °C for 2 h in sealed tube. The mixture was cooled to room temperature, diluted with water (100 mL), and extracted with ethyl acetate (3 × 30 mL). The organic layer was washed with brine (10 mL), dried using $MgSO_4$, filtered, and concentrated in vacuo. The residue was purified by column chromatography (diethyl ether/petroleum ether, 1:4) to give (*E*)-methyl 4-amino-3-(3-methoxy-3-oxoprop-1-en-1-yl) benzoate (2.51 mmol) as light brown solid. Mp 174–176 °C; ^{1}H NMR (400 MHz, DMSO) δ 7.98 (1H, m), 7.88–7.84 (1H, d, J = 15.6 Hz)), 7.64 (1H, dd, J = 1.7, 8.6 Hz), 6.74–6.70 (1H, d, J = 15.6 Hz), 6.45 (2H, b), 6.40–6.36 (1H, d, J = 15.7 Hz), 3.76 (3H, s), 3.72 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 166.4, 15267, 140.3, 132.6, 129.8, 117.1, 116.9, 116.1, 51.9, 51.8; FT-IR (KBr) $\tilde{\nu}$ 3446, 3360, 3254, 1687, 1659, 1606, 1563, 1505, 1428, 1342, 1298, 1258, 1174, 1106, 980, 754, 484 cm^{-1}; LRMS-EI$^+$ (*m/z*) 258.45 ([M+Na]$^+$, 100), 236.27 ([M+H]$^+$, 42) 189.98 (11.71); HRMS-TOF-ES$^+$ (*m/*z) [M+Na]$^+$ calcd for $C_{12}H_{12}NNaO_4$, 258.0742 found 258.0742.

Methyl (*E*)-3-(2-amino-5-chlorophenyl) acrylate (ii).



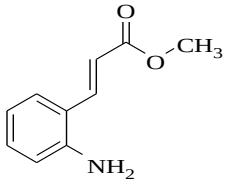
The reaction was carried out as described for the synthesis of (*E*)-methyl 4-amino-3-(3-methoxy-3-oxoprop-1-en-1-yl) benzoate (**i**) using 4-chloro-2-iodoaniline (3.95 mmol). The residue was purified by column chromatography (diethyl ether/petroleum ether, 1:4) to give (*E*)-methyl 4-amino-3-(3-methoxy-3-oxoprop-1-en-1-yl)benzoate (2.51 mmol) as yellow solid. Mp 182–184°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (1H, d, J = 15.8 Hz), 7.34 (1H, d, J = 2.2 Hz), 7.12 (1H, dd, J = 2.2, 8.6 Hz), 6.65–6.62 (1H, d, J = 8.6 Hz), 6.35 (1H, d, J = 15.8 Hz), 3.94 (3H, m), 3.81 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 144.0, 138.8, 131.0, 127.4, 123.8, 121.2, 119.1, 117.9, 51.7; LRMS-EI$^+$ (*m/z*) 211.0 ([M] $^+$); FT-IR (KBr) $\tilde{\nu}$ 3412, 3340, 2929, 1717, 1636, 1493, 1436, 1376, 1302, 1204, 1174, 1063, 823, 648, 5415 cm^{-1}.

***tert*-Butyl (*E*)-3-(2-aminophenyl)acrylate (iii).**



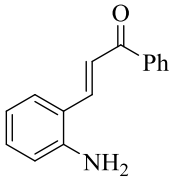
The reaction was carried out as described for the synthesis of (*E*)-methyl 4-amino-3-(3-methoxy-3-oxoprop-1-en-1-yl) benzoate **(i)** using 2-iodoaniline (9.17 mmol).The residue was purified by column chromatography (diethyl ether/petroleum ether, 1:4) to give (*E*)-*tert*-butyl 3-(2-aminophenyl) acrylate (6.85 mmol) as yellow solid. Mp 82–84 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (1H, d, J = 15.8 Hz), 7.37 (1H, d, J = 7.8 Hz), 7.16 (1H, t, J = 7.6 Hz), 6.76 (1H, t, J = 7.5 Hz), 6.69 (1H, d, J = 8.1 Hz), 6.29 (1H, d, J = 15.7 Hz), 3.94 (2H, b), 1.54 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 145.4, 139.0, 131.0, 128.2, 120.3, 120.2, 118.9, 116.6, 80.4, 28.2. EI^+ (*m/z*) 219.1 ($[M]^+$); FT-IR (KB,) $\tilde{\nu}$ 3375, 2978, 2931, 1697, 1623, 1573, 1490, 1459, 1367, 1256, 1206, 1169, 981, 865, 750, 598 cm^{-1}.

(*E*)-Methyl 3-(2-aminophenyl) acrylate (iv).



The reaction was carried out as described for the synthesis of (*E*)-methyl 4-amino-3-(3-methoxy-3-oxoprop-1-en-1-yl) benzoate **(i)** using 2-iodoaniline (9.17 mmol). Yellow solid; Mp 62–65 °C; H^1 NMR (400 MHz, $CDCl_3$) δ 7.83 (1H, d, J = 15.8 Hz), 7.39–7.36 (1H, m), 7.19–7.15 (1H, m), 6.78–6.69 (2H, m), 6.35 (1H, d, J = 15.8 Hz), 3.99 (2H, b), 3.80 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 145.0, 140.3, 131.4, 128.1, 119.8, 118.9, 117.6, 116.8, 51.7. EI^+ (*m/z*) 177.07 ($[M]^+$); FT-IR (KBr) $\tilde{\nu}$ 3377, 3240, 2951, 1703, 1623, 1573, 1490, 1460, 1434, 1265, 1198, 11697, 1035, 9817, 860, 758, 598 cm^{-1}.

(*E*)-3-(2-Aminophenyl)-1-phenylprop-2-en-1-one (v)[1]

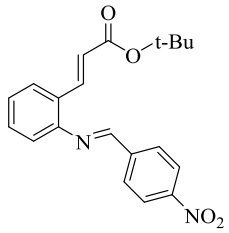


General Procedure for preparing benzylidene amino phenyl acrylate[2]

To the stirred solution of *(E)*-2-aminophenyl acrylate derivatives (1.0 equiv) and aldehyde (1.0 equiv) in anhydrous toluene (10 mL) added 4 Å molecular sieves (5.0 equiv). The reaction

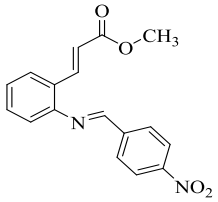
mixture was stirred at 110 °C for 18 h. After completion of the reaction molecular sieves were filtered and solvent was removed to obtain the substituted benzylidene amino phenyl acrylate.

(*E*)-*tert*-Butyl 3-(2-((*E*)-(4-nitrobenzylidene)amino)phenyl)acrylate (vi)



Yellow solid; Mp 143–145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (1H, s), 8.34 (2H, d, J = 8.7 Hz), 8.20–8.11 (3H, m), 7.67 (1H, d, J = 7.2 Hz), 7.45–7.40 (1H, t, J = 7.5 Hz), 7.30 (1H, t, J = 7.5 Hz), 7.04 (1H, d, J = 7.4 Hz), 6.40 (1H, d, J = 16.1 Hz), 1.52 (9H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 157.9, 149.9, 149.5, 141.3, 139.6, 131.0, 130.0, 129.1, 124.1, 121.3, 118.2, 80.5, 28.2.

(*E*)-Methyl 3-(2-((*E*)-(4-nitrobenzylidene) amino) phenyl) acrylate (vii)



Yellow solid; Mp 62–65 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (1H, s), 8.35 (2H, d, J = 8.6 Hz), 8.20 (1H, d, J = 16.2 Hz), 8.12 (2H, d, J = 8.5 Hz), 7.67 (1H, d, J = 7.6 Hz), 7.44 (1H, t, J = 7.3 Hz), 7.32 (1H, t, J = 7.4 Hz), 7.04 (1H, J = 7.8 Hz), 6.47 (1H, d, J = 16.1 Hz), 3.80 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 158.1, 150.2, 149.5, 141.2, 141.1, 131.3, 129.7, 128.7, 128.9, 127.6, 127.2, 124.1, 119.3, 118.4, 51.7.

General procedure for synthesis Knoevenagel intermediate

Ethyl (*Z*)-2-cyano-3-(2,4,6-trimethoxyphenyl)acrylate (5a1): To the stirred solution of ethyl cyanoacetate (1.02 mmol) and 2,4,6 trimethoxybenzaldehyde (1.02 mmol) in anhydrous DCM (10 mL) added (0.51 mmol) of DBU. The reaction mixture was stirred at room temperature and monitored by TLC for completion. Reaction mixture was concentrated using reduced pressure and purified using silica gel column chromatography to yield substituted Knoevenagel product. Yellow solid; Mp 101–102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (1H, s), 6.09 (2H, s), 4.33 (2H, q, J = 7.0 Hz), 3.88 (6H, s), 3.86 (3H, s), 1.36 (3H, t, J = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 164.0, 16.2, 147.4, 116.1, 104.6, 103.4, 90.4, 62.1, 55.6, 55.4, 14.3. LRMS-EI$^+$ (*m/z*) 292.32 ([M+H]$^+$, 100), ([M+H]$^+$ 246.37 (38.35); HRMS-TOF-ES$^+$ (*m/z*) [M+Na]$^+$ calcd for $C_{15}H_{17}NNaO_5$, 314.1004, found 314.1004.

Reference.

[1] G. T. Cin, S. Demirel and A. Cakici, Synthesis of novel ferrocenyl-containing pyrazolo[4,3-c]quinolines. *J. Organometallic Chem.* 2011**, 696** , 613.

[2] A. Patra, S. Mukherjee, T. K. Das, S. Jain, R. G. Gonnade, A. T. Biju, *N*-Heterocyclic-Carbene-Catalyzed Umpolung of Imines. *Angew. Chem. Int. Ed.* 2017**, 56**, 2730.

Crystallographic data of 3a

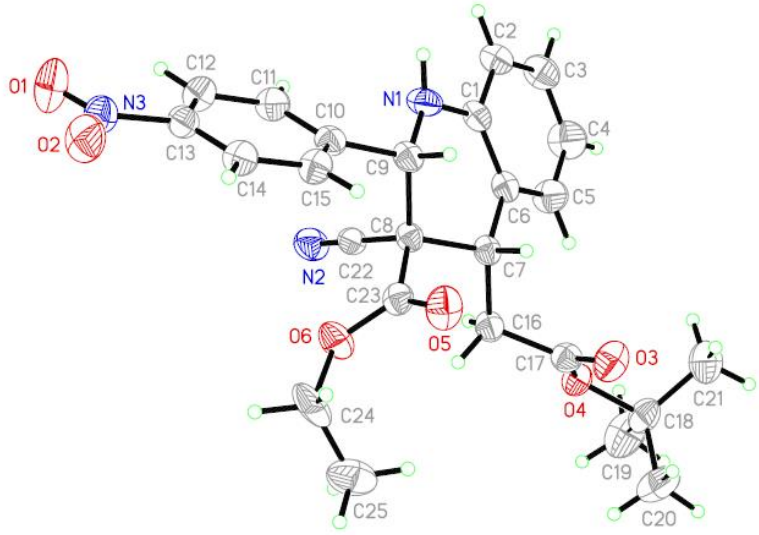


Fig. : The molecular structure of IC18499, thermal ellipsoids drawn at the 50% probability level.

Table 1. Crystal data and structure refinement for ic18499.

Identification code	ic18499
Empirical formula	C25 H27 N3 O6
Formula weight	465.49
Temperature	200(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 11.8148(3) Å = 90°.

	b = 9.6634(2) Å = 98.5727(10)°.
	c = 20.8234(5) Å = 90°.
Volume	2350.87(10) $Å^3$
Z	4
Density (calculated)	1.315 Mg/m^3
Absorption coefficient	0.784 mm^{-1}
F(000)	984
Crystal size	0.159 x 0.045 x 0.042 mm^3
Theta range for data collection	4.294 to 69.990°.
Index ranges	-14<=h<=14, -9<=k<=11, -24<=l<=25
Reflections collected	11420
Independent reflections	4394 [R(int) = 0.0208]
Completeness to theta = 67.679°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.6024
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4394 / 16 / 323
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0947
R indices (all data)	R1 = 0.0481, wR2 = 0.1040
Extinction coefficient	n/a
Largest diff. peak and hole	0.248 and -0.174 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)

for ic18499. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9079(1)	3230(2)	1826(1)	60(1)
O(2)	10128(1)	4781(2)	2361(1)	55(1)
O(3)	3844(1)	12926(1)	1363(1)	45(1)
O(4)	2813(1)	12513(1)	374(1)	33(1)
O(5)	6564(1)	10539(1)	1915(1)	45(1)
O(6)	6956(1)	9505(1)	1013(1)	43(1)
N(1)	4210(1)	7188(2)	1979(1)	38(1)
N(2)	4930(1)	7391(2)	344(1)	40(1)
N(3)	9204(1)	4350(2)	2098(1)	40(1)
C(1)	3173(1)	7820(2)	1748(1)	31(1)
C(2)	2154(1)	7126(2)	1809(1)	36(1)
C(3)	1112(1)	7671(2)	1548(1)	43(1)
C(4)	1061(1)	8911(2)	1218(1)	51(1)
C(5)	2060(1)	9613(2)	1162(1)	42(1)
C(6)	3127(1)	9095(2)	1426(1)	29(1)
C(7)	4220(1)	9888(2)	1386(1)	27(1)
C(8)	5240(1)	8866(2)	1410(1)	26(1)
C(9)	5289(1)	7919(2)	2023(1)	30(1)

C(10)	6293(1)	6916(2)	2070(1)	30(1)
C(11)	6178(1)	5597(2)	1805(1)	35(1)
C(12)	7126(1)	4738(2)	1824(1)	37(1)
C(13)	8184(1)	5230(2)	2105(1)	33(1)
C(14)	8324(1)	6519(2)	2385(1)	35(1)
C(15)	7369(1)	7355(2)	2370(1)	34(1)
C(16)	4158(1)	10842(2)	792(1)	31(1)
C(17)	3595(1)	12218(2)	888(1)	31(1)
C(18)	2181(1)	13841(2)	320(1)	40(1)
C(19)	1508(2)	13728(2)	-358(1)	65(1)
C(20)	3005(2)	15043(2)	363(1)	58(1)
C(21)	1400(2)	13883(2)	837(1)	59(1)
C(22)	5093(1)	8019(2)	812(1)	28(1)
C(23)	6337(1)	9731(2)	1477(1)	31(1)
C(24)	8045(5)	10212(7)	979(3)	56(1)
C(25)	7800(3)	11555(5)	618(2)	57(1)
C(24')	7978(8)	10401(11)	1150(4)	56(1)
C(25')	8292(5)	10842(7)	515(2)	57(1)

Table 3. Bond lengths [Å] and angles [°] for ic18499.

O(1)-N(3)	1.220(2)
O(2)-N(3)	1.2197(19)
O(3)-C(17)	1.2028(19)
O(4)-C(17)	1.3355(17)
O(4)-C(18)	1.4807(19)
O(5)-C(23)	1.1998(19)
O(6)-C(23)	1.3144(18)
O(6)-C(24)	1.468(6)
O(6)-C(24')	1.478(8)
N(1)-C(1)	1.3894(19)
N(1)-C(9)	1.4477(19)
N(2)-C(22)	1.140(2)
N(3)-C(13)	1.4767(19)
C(1)-C(6)	1.399(2)
C(1)-C(2)	1.401(2)
C(2)-C(3)	1.374(2)
C(3)-C(4)	1.378(3)
C(4)-C(5)	1.382(2)
C(5)-C(6)	1.392(2)
C(6)-C(7)	1.5136(19)
C(7)-C(16)	1.5360(19)
C(7)-C(8)	1.5532(18)

C(8)-C(22)	1.4779(19)
C(8)-C(23)	1.5313(19)
C(8)-C(9)	1.5648(19)
C(9)-C(10)	1.5235(19)
C(10)-C(11)	1.388(2)
C(10)-C(15)	1.396(2)
C(11)-C(12)	1.390(2)
C(12)-C(13)	1.383(2)
C(13)-C(14)	1.375(2)
C(14)-C(15)	1.384(2)
C(16)-C(17)	1.513(2)
C(18)-C(20)	1.510(3)
C(18)-C(19)	1.517(2)
C(18)-C(21)	1.520(3)
C(24)-C(25)	1.506(7)
C(24')-C(25')	1.488(7)

C(17)-O(4)-C(18)	121.84(12)
C(23)-O(6)-C(24)	123.1(3)
C(23)-O(6)-C(24')	106.8(3)
C(1)-N(1)-C(9)	121.96(13)
O(2)-N(3)-O(1)	123.29(14)
O(2)-N(3)-C(13)	118.44(15)
O(1)-N(3)-C(13)	118.27(14)

N(1)-C(1)-C(6)	121.52(13)
N(1)-C(1)-C(2)	118.90(14)
C(6)-C(1)-C(2)	119.50(13)
C(3)-C(2)-C(1)	120.79(16)
C(2)-C(3)-C(4)	120.05(15)
C(3)-C(4)-C(5)	119.64(15)
C(4)-C(5)-C(6)	121.67(16)
C(5)-C(6)-C(1)	118.32(14)
C(5)-C(6)-C(7)	121.73(14)
C(1)-C(6)-C(7)	119.93(12)
C(6)-C(7)-C(16)	114.18(11)
C(6)-C(7)-C(8)	109.92(12)
C(16)-C(7)-C(8)	110.50(11)
C(22)-C(8)-C(23)	111.79(11)
C(22)-C(8)-C(7)	109.44(11)
C(23)-C(8)-C(7)	107.34(12)
C(22)-C(8)-C(9)	110.39(12)
C(23)-C(8)-C(9)	108.44(11)
C(7)-C(8)-C(9)	109.35(10)
N(1)-C(9)-C(10)	111.30(13)
N(1)-C(9)-C(8)	107.99(11)
C(10)-C(9)-C(8)	111.02(11)
C(11)-C(10)-C(15)	119.04(14)
C(11)-C(10)-C(9)	121.94(13)

C(15)-C(10)-C(9)	118.98(14)
C(10)-C(11)-C(12)	120.43(14)
C(13)-C(12)-C(11)	118.69(15)
C(14)-C(13)-C(12)	122.39(14)
C(14)-C(13)-N(3)	118.60(13)
C(12)-C(13)-N(3)	119.01(15)
C(13)-C(14)-C(15)	118.18(14)
C(14)-C(15)-C(10)	121.22(15)
C(17)-C(16)-C(7)	113.06(11)
O(3)-C(17)-O(4)	126.27(15)
O(3)-C(17)-C(16)	123.35(13)
O(4)-C(17)-C(16)	110.38(12)
O(4)-C(18)-C(20)	110.38(13)
O(4)-C(18)-C(19)	101.39(14)
C(20)-C(18)-C(19)	110.77(17)
O(4)-C(18)-C(21)	108.76(14)
C(20)-C(18)-C(21)	113.05(17)
C(19)-C(18)-C(21)	111.85(16)
N(2)-C(22)-C(8)	176.82(15)
O(5)-C(23)-O(6)	125.46(14)
O(5)-C(23)-C(8)	121.07(13)
O(6)-C(23)-C(8)	113.46(12)
O(6)-C(24)-C(25)	108.7(5)
O(6)-C(24')-C(25')	107.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ic18499. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2} U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	50(1)	52(1)	78(1)	-16(1)	3(1)	17(1)
O(2)	29(1)	57(1)	77(1)	3(1)	3(1)	7(1)
O(3)	56(1)	40(1)	35(1)	-5(1)	-5(1)	6(1)
O(4)	32(1)	31(1)	33(1)	2(1)	-1(1)	5(1)
O(5)	37(1)	46(1)	51(1)	-16(1)	1(1)	-5(1)
O(6)	27(1)	54(1)	49(1)	-2(1)	13(1)	-3(1)
N(1)	29(1)	45(1)	40(1)	18(1)	9(1)	4(1)
N(2)	47(1)	41(1)	33(1)	-4(1)	10(1)	-7(1)
N(3)	36(1)	42(1)	44(1)	5(1)	8(1)	9(1)
C(1)	28(1)	40(1)	26(1)	0(1)	7(1)	2(1)
C(2)	34(1)	42(1)	34(1)	3(1)	8(1)	-3(1)
C(3)	27(1)	54(1)	47(1)	0(1)	6(1)	-6(1)
C(4)	25(1)	61(1)	64(1)	10(1)	0(1)	4(1)
C(5)	30(1)	43(1)	51(1)	9(1)	3(1)	4(1)
C(6)	26(1)	36(1)	26(1)	-1(1)	4(1)	4(1)
C(7)	26(1)	32(1)	24(1)	0(1)	4(1)	4(1)
C(8)	24(1)	31(1)	24(1)	0(1)	4(1)	2(1)
C(9)	28(1)	38(1)	25(1)	4(1)	4(1)	4(1)
C(10)	29(1)	36(1)	25(1)	7(1)	4(1)	4(1)

C(11)	30(1)	38(1)	37(1)	3(1)	1(1)	0(1)
C(12)	37(1)	33(1)	40(1)	0(1)	3(1)	2(1)
C(13)	30(1)	37(1)	33(1)	6(1)	6(1)	7(1)
C(14)	29(1)	40(1)	34(1)	4(1)	0(1)	2(1)
C(15)	34(1)	35(1)	31(1)	0(1)	-1(1)	3(1)
C(16)	31(1)	34(1)	27(1)	2(1)	5(1)	5(1)
C(17)	31(1)	34(1)	29(1)	4(1)	4(1)	1(1)
C(18)	36(1)	33(1)	48(1)	4(1)	-1(1)	9(1)
C(19)	64(1)	60(1)	60(1)	7(1)	-21(1)	22(1)
C(20)	60(1)	35(1)	77(1)	12(1)	2(1)	1(1)
C(21)	48(1)	56(1)	75(1)	2(1)	18(1)	17(1)
C(22)	27(1)	30(1)	29(1)	4(1)	7(1)	1(1)
C(23)	25(1)	32(1)	34(1)	2(1)	1(1)	4(1)
C(24)	28(1)	81(3)	66(4)	-11(2)	26(2)	-10(2)
C(25)	57(2)	63(3)	51(2)	0(2)	8(1)	-25(2)
C(24')	28(1)	81(3)	66(4)	-11(2)	26(2)	-10(2)
C(25')	57(2)	63(3)	51(2)	0(2)	8(1)	-25(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ic18499.

	x	y	z	U(eq)
H(1)	4161(16)	6590(20)	2286(10)	46(5)
H(2A)	2183	6267	2033	44
H(3)	427	7194	1596	51
H(4)	342	9281	1030	61
H(5)	2017	10471	937	50
H(7)	4372	10485	1782	33
H(9)	5384	8516	2420	36
H(11)	5446	5279	1609	42
H(12)	7049	3830	1647	45
H(14)	9057	6827	2584	42
H(15)	7448	8244	2566	40
H(16A)	4943	11010	698	37
H(16B)	3724	10369	411	37
H(19A)	2035	13551	-671	97
H(19B)	1096	14596	-471	97
H(19C)	958	12966	-372	97
H(20A)	3418	15110	806	87
H(20B)	2580	15901	251	87
H(20C)	3553	14897	59	87

H(21A)	902	13067	794	88
H(21B)	929	14722	782	88
H(21C)	1864	13889	1268	88
H(24A)	8541	9621	750	67
H(24B)	8448	10396	1422	67
H(25A)	8514	12074	624	86
H(25B)	7261	12104	828	86
H(25C)	7465	11362	168	86
H(24C)	8618	9885	1403	67
H(24D)	7807	11219	1405	67
H(25D)	9020	11346	588	86
H(25E)	7692	11447	292	86
H(25F)	8370	10025	246	86

Crystallographic data of 4a

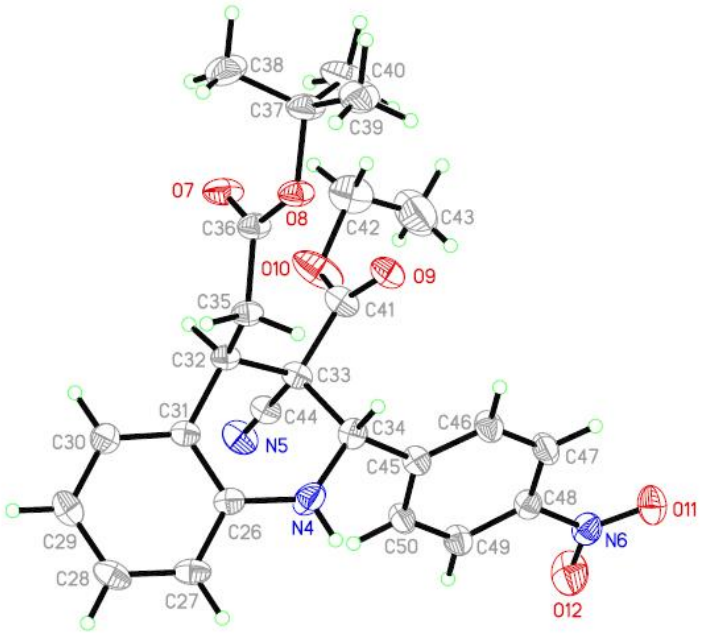


Fig. 2: The molecular structure of IC18555, thermal ellipsoids drawn at the 30% probability level.

Table 1. Crystal data and structure refinement for ic18555.

Identification code	ic18555	
Empirical formula	C25 H27 N3 O6	
Formula weight	465.49	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4969(2) Å	= 89.5889(12)°.
	b = 12.7230(3) Å	= 87.0347(11)°.
	c = 20.1047(5) Å	= 88.2917(12)°.
Volume	2424.86(10) $Å^3$	

Z	4
Density (calculated)	1.275 Mg/m^3
Absorption coefficient	0.760 mm^{-1}
F(000)	984
Crystal size	0.131 x 0.100 x 0.086 mm^3
Theta range for data collection	3.475 to 69.998°.
Index ranges	-11<=h<=11, -15<=k<=13, -24<=l<=24
Reflections collected	15799
Independent reflections	9164 [R(int) = 0.0158]
Completeness to theta = 67.679°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.6439
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9164 / 6 / 644
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0468, wR2 = 0.1169
R indices (all data)	R1 = 0.0559, wR2 = 0.1267
Extinction coefficient	n/a
Largest diff. peak and hole	0.474 and -0.507 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)

for ic18555. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8547(2)	2594(2)	1016(1)	69(1)
O(2)	6354(1)	2236(1)	1410(1)	51(1)
O(3)	8697(1)	820(1)	2180(1)	51(1)
O(4)	10961(2)	934(1)	1819(1)	76(1)
O(5)	10604(2)	-2381(1)	4764(1)	57(1)
O(6)	12589(2)	-1652(1)	4894(1)	63(1)
N(1)	9689(2)	2938(1)	3706(1)	59(1)
N(2)	12747(2)	2591(1)	2639(1)	60(1)
N(3)	11411(2)	-1650(1)	4676(1)	44(1)
C(1)	9633(2)	3945(1)	3449(1)	45(1)
C(2)	9782(2)	4802(2)	3870(1)	55(1)
C(3)	9847(2)	5803(2)	3618(1)	62(1)
C(4)	9756(2)	5987(2)	2944(1)	60(1)
C(5)	9578(2)	5145(2)	2527(1)	51(1)
C(6)	9511(2)	4122(1)	2768(1)	41(1)
C(7)	9345(2)	3219(1)	2296(1)	40(1)
C(8)	10059(2)	2206(1)	2593(1)	38(1)
C(9)	9415(2)	2022(1)	3316(1)	40(1)

C(10)	7797(2)	3096(2)	2126(1)	43(1)
C(11)	7637(2)	2606(2)	1455(1)	46(1)
C(12)	5910(2)	1764(2)	787(1)	59(1)
C(13)	4411(3)	1467(3)	971(1)	88(1)
C(14)	5924(3)	2588(2)	243(1)	80(1)
C(15)	6839(4)	812(3)	614(2)	106(1)
C(16)	9817(2)	1233(2)	2179(1)	43(1)
C(17)	10906(5)	63(3)	1357(2)	63(1)
C(18)	11439(8)	-839(4)	1785(3)	103(2)
C(17')	10787(10)	-238(6)	1648(5)	63(1)
C(18')	12116(12)	-728(8)	1446(8)	103(2)
C(19)	11584(2)	2403(1)	2616(1)	42(1)
C(20)	9990(2)	1039(1)	3650(1)	37(1)
C(21)	9185(2)	144(1)	3682(1)	41(1)
C(22)	9645(2)	-746(1)	4014(1)	43(1)
C(23)	10929(2)	-728(1)	4301(1)	37(1)
C(24)	11771(2)	131(2)	4262(1)	46(1)
C(25)	11287(2)	1023(2)	3938(1)	47(1)
O(7)	6283(1)	7883(1)	1067(1)	60(1)
O(8)	8522(1)	7368(1)	1262(1)	49(1)
O(9)	6209(1)	5922(1)	2095(1)	55(1)
O(10)	3959(2)	6430(2)	1875(1)	50(1)
O(10')	3953(6)	5935(5)	2220(3)	50(1)
O(11)	3805(2)	2609(1)	4626(1)	69(1)

O(12)	2181(2)	3657(1)	5022(1)	82(1)
N(4)	6072(2)	7819(1)	3797(1)	60(1)
N(5)	2458(2)	7785(1)	3132(1)	56(1)
N(6)	3251(2)	3485(1)	4682(1)	51(1)
C(26)	5820(2)	8862(1)	3641(1)	39(1)
C(27)	5778(2)	9623(2)	4139(1)	46(1)
C(28)	5527(2)	10666(2)	3989(1)	50(1)
C(29)	5294(2)	10973(2)	3343(1)	52(1)
C(30)	5338(2)	10218(1)	2847(1)	45(1)
C(31)	5617(2)	9169(1)	2984(1)	36(1)
C(32)	5699(2)	8350(1)	2443(1)	37(1)
C(33)	5074(2)	7311(1)	2744(1)	39(1)
C(34)	5926(2)	6948(1)	3354(1)	43(1)
C(35)	7205(2)	8204(2)	2133(1)	40(1)
C(36)	7250(2)	7793(2)	1430(1)	44(1)
C(37)	8868(2)	6995(2)	576(1)	59(1)
C(38)	8834(3)	7927(2)	104(1)	84(1)
C(39)	10364(2)	6557(2)	623(1)	70(1)
C(40)	7894(3)	6130(3)	403(1)	87(1)
C(41)	5157(2)	6433(2)	2226(1)	50(1)
C(42)	3910(3)	5639(2)	1341(1)	61(1)
C(43)	3431(5)	4662(3)	1636(3)	91(1)
C(42')	4084(11)	5002(8)	1805(5)	61(1)
C(43')	2801(15)	4821(15)	1449(10)	91(1)

C(44)	3588(2)	7562(1)	2958(1)	42(1)
C(45)	5244(2)	6030(1)	3718(1)	41(1)
C(46)	5741(2)	5010(2)	3596(1)	50(1)
C(47)	5092(2)	4169(1)	3908(1)	52(1)
C(48)	3940(2)	4367(1)	4339(1)	42(1)
C(49)	3441(2)	5368(1)	4483(1)	46(1)
C(50)	4114(2)	6202(1)	4173(1)	45(1)

Table 3. Bond lengths [Å] and angles [°] for ic18555.

O(1)-C(11)	1.203(2)
O(2)-C(11)	1.327(2)
O(2)-C(12)	1.481(2)
O(3)-C(16)	1.200(2)
O(4)-C(16)	1.321(2)
O(4)-C(17)	1.455(4)
O(4)-C(17')	1.548(7)
O(5)-N(3)	1.228(2)
O(6)-N(3)	1.223(2)
N(1)-C(1)	1.378(3)
N(1)-C(9)	1.447(2)
N(2)-C(19)	1.140(2)
N(3)-C(23)	1.464(2)
C(1)-C(6)	1.397(3)
C(1)-C(2)	1.399(3)
C(2)-C(3)	1.369(3)
C(3)-C(4)	1.381(3)
C(4)-C(5)	1.385(3)
C(5)-C(6)	1.387(3)
C(6)-C(7)	1.512(2)
C(7)-C(10)	1.539(2)
C(7)-C(8)	1.567(2)

C(8)-C(19)	1.480(2)
C(8)-C(16)	1.526(2)
C(8)-C(9)	1.566(2)
C(9)-C(20)	1.516(2)
C(10)-C(11)	1.507(2)
C(12)-C(15)	1.509(4)
C(12)-C(14)	1.509(3)
C(12)-C(13)	1.510(3)
C(17)-C(18)	1.520(7)
C(17')-C(18')	1.431(15)
C(20)-C(25)	1.388(2)
C(20)-C(21)	1.391(2)
C(21)-C(22)	1.381(3)
C(22)-C(23)	1.377(2)
C(23)-C(24)	1.374(2)
C(24)-C(25)	1.382(3)
O(7)-C(36)	1.204(2)
O(8)-C(36)	1.337(2)
O(8)-C(37)	1.479(2)
O(9)-C(41)	1.194(2)
O(10)-C(41)	1.369(3)
O(10)-C(42)	1.480(3)
O(10')-C(41)	1.324(6)
O(10')-C(42')	1.456(8)

O(11)-N(6)	1.222(2)
O(12)-N(6)	1.210(2)
N(4)-C(26)	1.378(2)
N(4)-C(34)	1.442(2)
N(5)-C(44)	1.140(2)
N(6)-C(48)	1.466(2)
C(26)-C(31)	1.396(2)
C(26)-C(27)	1.396(2)
C(27)-C(28)	1.375(3)
C(28)-C(29)	1.379(3)
C(29)-C(30)	1.388(3)
C(30)-C(31)	1.382(2)
C(31)-C(32)	1.508(2)
C(32)-C(35)	1.537(2)
C(32)-C(33)	1.569(2)
C(33)-C(44)	1.480(2)
C(33)-C(41)	1.532(2)
C(33)-C(34)	1.563(2)
C(34)-C(45)	1.518(2)
C(35)-C(36)	1.509(2)
C(37)-C(40)	1.513(4)
C(37)-C(38)	1.515(3)
C(37)-C(39)	1.518(3)
C(42)-C(43)	1.449(5)

C(42')-C(43')	1.470(9)
C(45)-C(50)	1.386(2)
C(45)-C(46)	1.387(2)
C(46)-C(47)	1.383(3)
C(47)-C(48)	1.378(3)
C(48)-C(49)	1.373(2)
C(49)-C(50)	1.383(3)

C(11)-O(2)-C(12)	121.45(14)
C(16)-O(4)-C(17)	119.9(2)
C(16)-O(4)-C(17')	106.6(4)
C(1)-N(1)-C(9)	122.66(16)
O(6)-N(3)-O(5)	122.97(16)
O(6)-N(3)-C(23)	118.62(15)
O(5)-N(3)-C(23)	118.40(14)
N(1)-C(1)-C(6)	120.98(16)
N(1)-C(1)-C(2)	119.67(17)
C(6)-C(1)-C(2)	119.24(18)
C(3)-C(2)-C(1)	120.8(2)
C(2)-C(3)-C(4)	120.52(19)
C(3)-C(4)-C(5)	118.97(19)
C(4)-C(5)-C(6)	121.73(19)
C(5)-C(6)-C(1)	118.70(17)
C(5)-C(6)-C(7)	120.34(16)

C(1)-C(6)-C(7)	120.95(16)
C(6)-C(7)-C(10)	111.83(14)
C(6)-C(7)-C(8)	108.67(13)
C(10)-C(7)-C(8)	114.50(14)
C(19)-C(8)-C(16)	110.80(14)
C(19)-C(8)-C(9)	109.67(14)
C(16)-C(8)-C(9)	108.50(14)
C(19)-C(8)-C(7)	107.12(13)
C(16)-C(8)-C(7)	111.95(13)
C(9)-C(8)-C(7)	108.77(13)
N(1)-C(9)-C(20)	109.98(14)
N(1)-C(9)-C(8)	107.78(14)
C(20)-C(9)-C(8)	113.83(13)
C(11)-C(10)-C(7)	113.34(14)
O(1)-C(11)-O(2)	125.33(17)
O(1)-C(11)-C(10)	123.60(17)
O(2)-C(11)-C(10)	111.02(14)
O(2)-C(12)-C(15)	109.64(17)
O(2)-C(12)-C(14)	109.31(19)
C(15)-C(12)-C(14)	113.1(2)
O(2)-C(12)-C(13)	102.36(17)
C(15)-C(12)-C(13)	111.9(3)
C(14)-C(12)-C(13)	110.0(2)
O(3)-C(16)-O(4)	125.44(17)

O(3)-C(16)-C(8)	122.52(15)
O(4)-C(16)-C(8)	112.02(15)
O(4)-C(17)-C(18)	100.5(4)
C(18')-C(17')-O(4)	111.0(8)
N(2)-C(19)-C(8)	177.6(2)
C(25)-C(20)-C(21)	119.32(16)
C(25)-C(20)-C(9)	121.39(15)
C(21)-C(20)-C(9)	119.26(15)
C(22)-C(21)-C(20)	120.65(15)
C(23)-C(22)-C(21)	118.34(15)
C(24)-C(23)-C(22)	122.54(16)
C(24)-C(23)-N(3)	118.33(15)
C(22)-C(23)-N(3)	119.12(15)
C(23)-C(24)-C(25)	118.52(16)
C(24)-C(25)-C(20)	120.57(16)
C(36)-O(8)-C(37)	120.80(14)
C(41)-O(10)-C(42)	116.93(18)
C(41)-O(10')-C(42')	111.6(6)
C(26)-N(4)-C(34)	125.29(16)
O(12)-N(6)-O(11)	122.71(17)
O(12)-N(6)-C(48)	118.91(16)
O(11)-N(6)-C(48)	118.35(17)
N(4)-C(26)-C(31)	120.45(16)
N(4)-C(26)-C(27)	120.13(16)

C(31)-C(26)-C(27)	119.42(16)
C(28)-C(27)-C(26)	120.64(17)
C(27)-C(28)-C(29)	120.34(17)
C(28)-C(29)-C(30)	119.13(18)
C(31)-C(30)-C(29)	121.55(17)
C(30)-C(31)-C(26)	118.89(15)
C(30)-C(31)-C(32)	121.74(15)
C(26)-C(31)-C(32)	119.37(15)
C(31)-C(32)-C(35)	111.81(13)
C(31)-C(32)-C(33)	107.97(13)
C(35)-C(32)-C(33)	113.58(14)
C(44)-C(33)-C(41)	110.56(14)
C(44)-C(33)-C(34)	110.41(14)
C(41)-C(33)-C(34)	108.76(14)
C(44)-C(33)-C(32)	106.66(14)
C(41)-C(33)-C(32)	110.85(14)
C(34)-C(33)-C(32)	109.59(13)
N(4)-C(34)-C(45)	110.94(15)
N(4)-C(34)-C(33)	109.94(14)
C(45)-C(34)-C(33)	111.56(14)
C(36)-C(35)-C(32)	113.26(13)
O(7)-C(36)-O(8)	125.38(16)
O(7)-C(36)-C(35)	123.94(15)
O(8)-C(36)-C(35)	110.61(14)

O(8)-C(37)-C(40)	110.23(18)
O(8)-C(37)-C(38)	108.89(18)
C(40)-C(37)-C(38)	113.8(2)
O(8)-C(37)-C(39)	102.38(16)
C(40)-C(37)-C(39)	110.3(2)
C(38)-C(37)-C(39)	110.6(2)
O(9)-C(41)-O(10')	116.7(3)
O(9)-C(41)-O(10)	125.32(17)
O(9)-C(41)-C(33)	122.96(16)
O(10')-C(41)-C(33)	111.1(3)
O(10)-C(41)-C(33)	111.01(15)
C(43)-C(42)-O(10)	108.5(3)
O(10')-C(42')-C(43')	112.4(10)
N(5)-C(44)-C(33)	177.76(19)
C(50)-C(45)-C(46)	119.44(16)
C(50)-C(45)-C(34)	120.44(15)
C(46)-C(45)-C(34)	120.12(16)
C(47)-C(46)-C(45)	120.39(17)
C(48)-C(47)-C(46)	118.55(16)
C(49)-C(48)-C(47)	122.48(16)
C(49)-C(48)-N(6)	118.19(16)
C(47)-C(48)-N(6)	119.28(16)
C(48)-C(49)-C(50)	118.26(16)
C(49)-C(50)-C(45)	120.82(16)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ic18555. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	47(1)	122(1)	37(1)	-13(1)	4(1)	-12(1)
O(2)	42(1)	75(1)	36(1)	-6(1)	-6(1)	-9(1)
O(3)	45(1)	56(1)	53(1)	-11(1)	-3(1)	-11(1)
O(4)	43(1)	94(1)	90(1)	-54(1)	4(1)	1(1)
O(5)	74(1)	46(1)	51(1)	3(1)	-7(1)	-8(1)
O(6)	60(1)	61(1)	69(1)	-6(1)	-23(1)	9(1)
N(1)	101(1)	43(1)	32(1)	-5(1)	-1(1)	-1(1)
N(2)	41(1)	64(1)	74(1)	10(1)	-8(1)	-10(1)
N(3)	50(1)	44(1)	37(1)	-10(1)	-2(1)	3(1)
C(1)	46(1)	43(1)	45(1)	-6(1)	-5(1)	0(1)
C(2)	60(1)	51(1)	56(1)	-14(1)	-14(1)	3(1)
C(3)	56(1)	45(1)	87(2)	-17(1)	-20(1)	2(1)
C(4)	50(1)	40(1)	92(2)	1(1)	-14(1)	-1(1)
C(5)	41(1)	50(1)	61(1)	8(1)	-6(1)	-1(1)
C(6)	33(1)	45(1)	45(1)	-2(1)	-3(1)	-3(1)
C(7)	35(1)	49(1)	34(1)	1(1)	1(1)	-4(1)
C(8)	33(1)	45(1)	35(1)	-4(1)	0(1)	-5(1)
C(9)	42(1)	43(1)	35(1)	-4(1)	4(1)	-2(1)
C(10)	36(1)	59(1)	36(1)	-4(1)	-1(1)	-1(1)

C(11)	38(1)	66(1)	35(1)	-1(1)	-3(1)	-1(1)
C(12)	56(1)	82(2)	42(1)	-10(1)	-16(1)	-6(1)
C(13)	74(2)	132(3)	64(2)	1(2)	-23(1)	-44(2)
C(14)	72(2)	122(2)	49(1)	12(1)	-23(1)	-18(2)
C(15)	112(2)	103(2)	108(2)	-52(2)	-49(2)	20(2)
C(16)	38(1)	52(1)	39(1)	-8(1)	-2(1)	-1(1)
C(17)	67(2)	72(3)	50(2)	-24(2)	0(2)	9(2)
C(18)	117(5)	60(2)	134(6)	-19(3)	-30(3)	5(3)
C(17')	67(2)	72(3)	50(2)	-24(2)	0(2)	9(2)
C(18')	117(5)	60(2)	134(6)	-19(3)	-30(3)	5(3)
C(19)	39(1)	46(1)	43(1)	2(1)	-2(1)	-5(1)
C(20)	36(1)	42(1)	34(1)	-4(1)	4(1)	-6(1)
C(21)	29(1)	49(1)	45(1)	1(1)	-1(1)	-7(1)
C(22)	37(1)	44(1)	48(1)	-2(1)	1(1)	-10(1)
C(23)	36(1)	41(1)	33(1)	-6(1)	3(1)	1(1)
C(24)	37(1)	56(1)	46(1)	-2(1)	-9(1)	-10(1)
C(25)	47(1)	48(1)	47(1)	1(1)	-10(1)	-18(1)
O(7)	46(1)	95(1)	38(1)	-14(1)	-7(1)	13(1)
O(8)	39(1)	73(1)	36(1)	-6(1)	3(1)	7(1)
O(9)	50(1)	56(1)	58(1)	-14(1)	4(1)	6(1)
O(10)	42(1)	55(1)	55(1)	-15(1)	-10(1)	-5(1)
O(10')	42(1)	55(1)	55(1)	-15(1)	-10(1)	-5(1)
O(11)	90(1)	37(1)	81(1)	6(1)	-2(1)	-7(1)
O(12)	72(1)	67(1)	104(1)	19(1)	28(1)	-13(1)

N(4)	92(1)	47(1)	45(1)	8(1)	-25(1)	-25(1)
N(5)	39(1)	59(1)	68(1)	-12(1)	6(1)	-4(1)
N(6)	57(1)	43(1)	54(1)	4(1)	-9(1)	-13(1)
C(26)	36(1)	45(1)	36(1)	-1(1)	1(1)	-14(1)
C(27)	40(1)	63(1)	36(1)	-8(1)	6(1)	-17(1)
C(28)	35(1)	60(1)	56(1)	-22(1)	6(1)	-7(1)
C(29)	42(1)	44(1)	71(1)	-12(1)	-6(1)	2(1)
C(30)	42(1)	48(1)	46(1)	-1(1)	-5(1)	1(1)
C(31)	29(1)	43(1)	35(1)	-4(1)	2(1)	-5(1)
C(32)	33(1)	45(1)	33(1)	-3(1)	-1(1)	-3(1)
C(33)	31(1)	44(1)	42(1)	-7(1)	1(1)	-4(1)
C(34)	38(1)	43(1)	48(1)	2(1)	-3(1)	-7(1)
C(35)	34(1)	54(1)	33(1)	-3(1)	0(1)	-4(1)
C(36)	37(1)	59(1)	36(1)	-4(1)	2(1)	1(1)
C(37)	52(1)	85(2)	38(1)	-12(1)	5(1)	15(1)
C(38)	87(2)	118(2)	44(1)	11(1)	18(1)	37(2)
C(39)	56(1)	94(2)	58(1)	-5(1)	13(1)	21(1)
C(40)	72(2)	114(2)	75(2)	-48(2)	1(1)	8(2)
C(41)	40(1)	51(1)	58(1)	-17(1)	3(1)	-6(1)
C(42)	52(1)	70(2)	61(2)	-10(1)	-9(1)	-9(1)
C(43)	81(3)	75(2)	119(4)	-27(2)	-2(2)	-16(2)
C(42')	52(1)	70(2)	61(2)	-10(1)	-9(1)	-9(1)
C(43')	81(3)	75(2)	119(4)	-27(2)	-2(2)	-16(2)
C(44)	37(1)	44(1)	45(1)	-7(1)	0(1)	-6(1)

C(45)	37(1)	39(1)	48(1)	-2(1)	-1(1)	-3(1)
C(46)	45(1)	45(1)	57(1)	-1(1)	11(1)	6(1)
C(47)	61(1)	34(1)	59(1)	-4(1)	5(1)	4(1)
C(48)	42(1)	38(1)	47(1)	1(1)	-5(1)	-8(1)
C(49)	41(1)	43(1)	51(1)	0(1)	6(1)	0(1)
C(50)	48(1)	34(1)	52(1)	-4(1)	6(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ic18555.

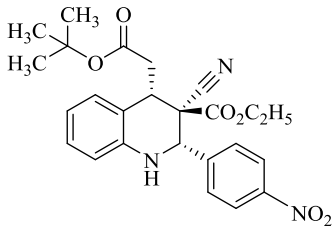
	x	y	z	U(eq)
H(1)	9590(20)	2855(19)	4127(13)	64(7)
H(2)	9840	4688	4335	66
H(3)	9956	6376	3910	74
H(4A)	9815	6681	2769	73
H(5A)	9499	5271	2064	61
H(7)	9887	3390	1872	48
H(9)	8371	1963	3294	48
H(10A)	7323	2655	2473	52
H(10B)	7316	3797	2135	52
H(13A)	4407	953	1336	133
H(13B)	3994	1161	584	133
H(13C)	3858	2097	1113	133
H(14A)	5362	3207	395	120
H(14B)	5523	2302	-155	120
H(14C)	6898	2790	135	120
H(15A)	7787	1038	473	159
H(15B)	6440	427	252	159
H(15C)	6895	353	1006	159

H(17A)	11531	169	954	76
H(17B)	9932	-47	1223	76
H(18A)	11458	-1493	1529	155
H(18B)	12394	-696	1916	155
H(18C)	10811	-909	2183	155
H(17C)	10377	-610	2042	76
H(17D)	10129	-291	1284	76
H(18D)	11978	-1467	1340	155
H(18E)	12516	-366	1051	155
H(18F)	12763	-685	1808	155
H(21)	8310	143	3474	49
H(22)	9090	-1355	4043	51
H(24)	12666	114	4452	55
H(25)	11847	1630	3913	56
H(4)	6220(30)	7653(19)	4200(13)	67(7)
H(27)	5923	9418	4586	55
H(28)	5514	11177	4331	60
H(29)	5106	11692	3240	63
H(30)	5172	10428	2403	54
H(32)	5079	8600	2084	44
H(34)	6891	6711	3184	51
H(35A)	7676	8887	2134	48
H(35B)	7742	7708	2413	48
H(38A)	7879	8242	114	127

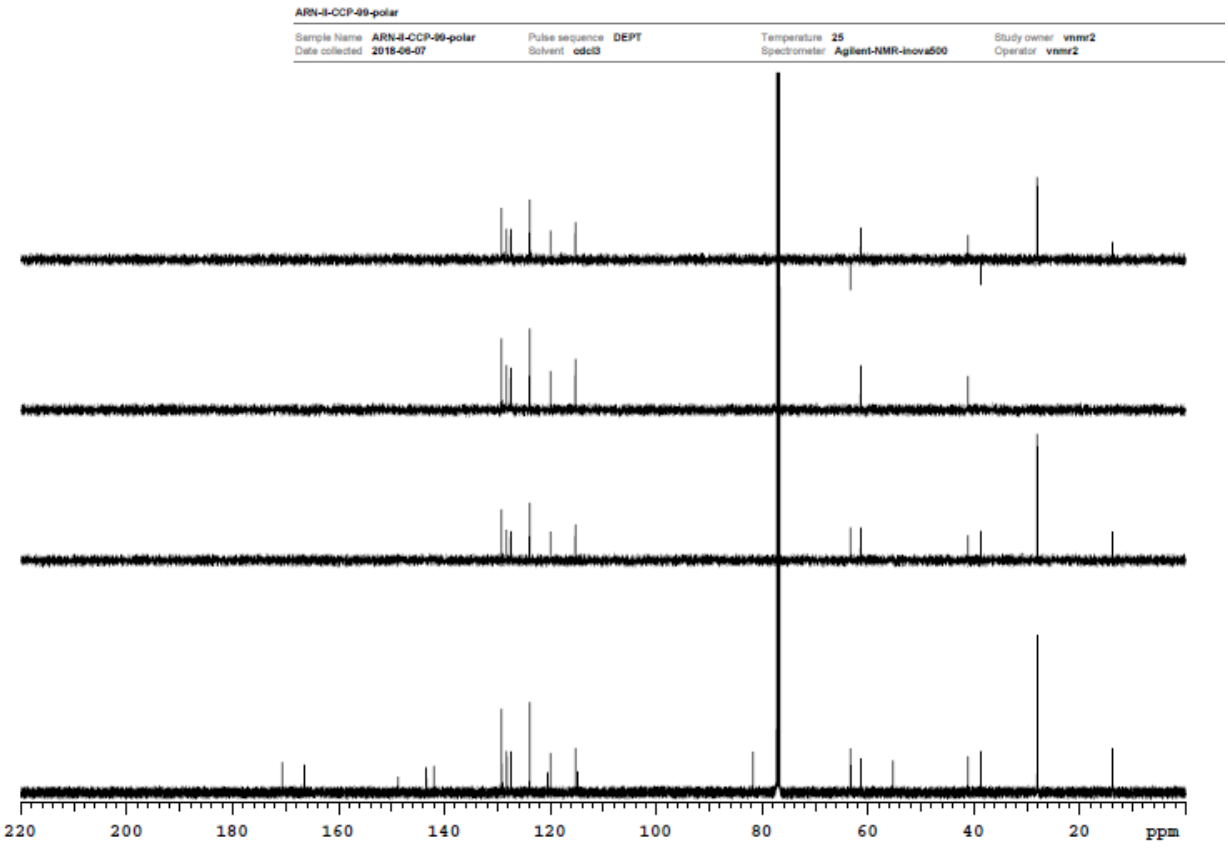
H(38B)	9106	7692	-349	127
H(38C)	9496	8450	241	127
H(39A)	10958	7101	793	105
H(39B)	10736	6337	181	105
H(39C)	10364	5951	927	105
H(40A)	7861	5605	762	131
H(40B)	8245	5795	-13	131
H(40C)	6944	6429	348	131
H(42A)	3255	5887	1001	73
H(42B)	4859	5530	1120	73
H(43A)	3392	4129	1288	137
H(43B)	4087	4420	1969	137
H(43C)	2488	4776	1851	137
H(42C)	4290	4382	2088	73
H(42D)	4889	5078	1477	73
H(43D)	2939	4187	1177	137
H(43E)	2004	4730	1772	137
H(43F)	2603	5426	1161	137
H(46)	6533	4889	3294	60
H(47)	5433	3469	3828	62
H(49)	2654	5484	4787	55
H(50)	3797	6901	4273	54

^{1}H, ^{13}C and IR Spectra

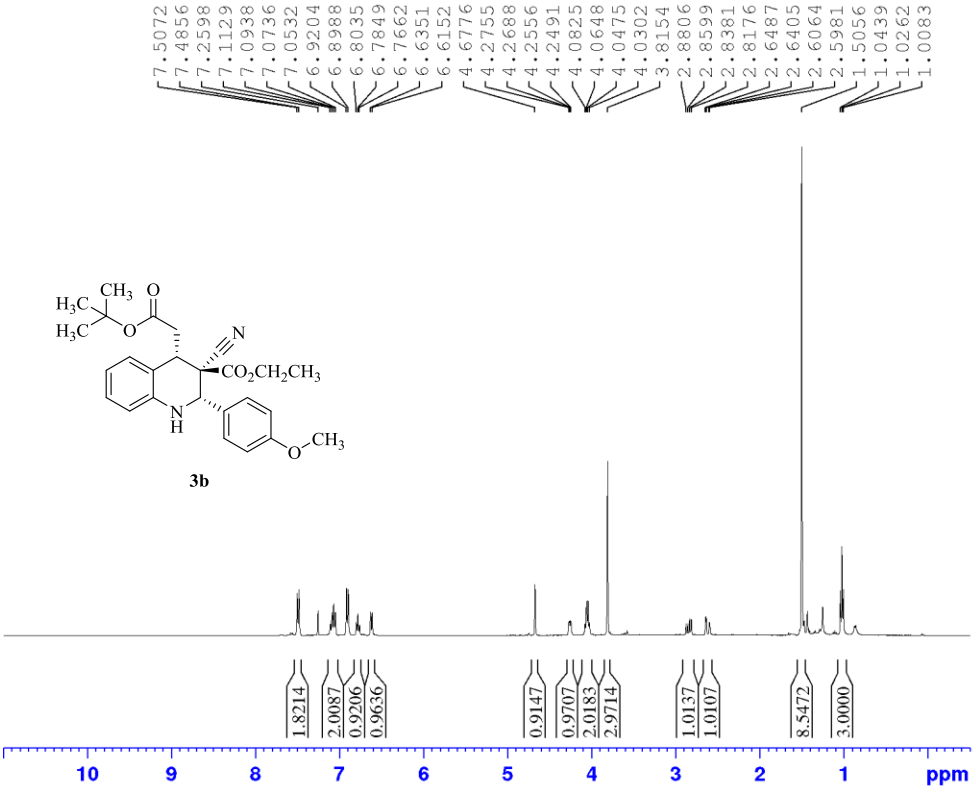
Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3a**, major isomer)



3a



Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate **(3b)**



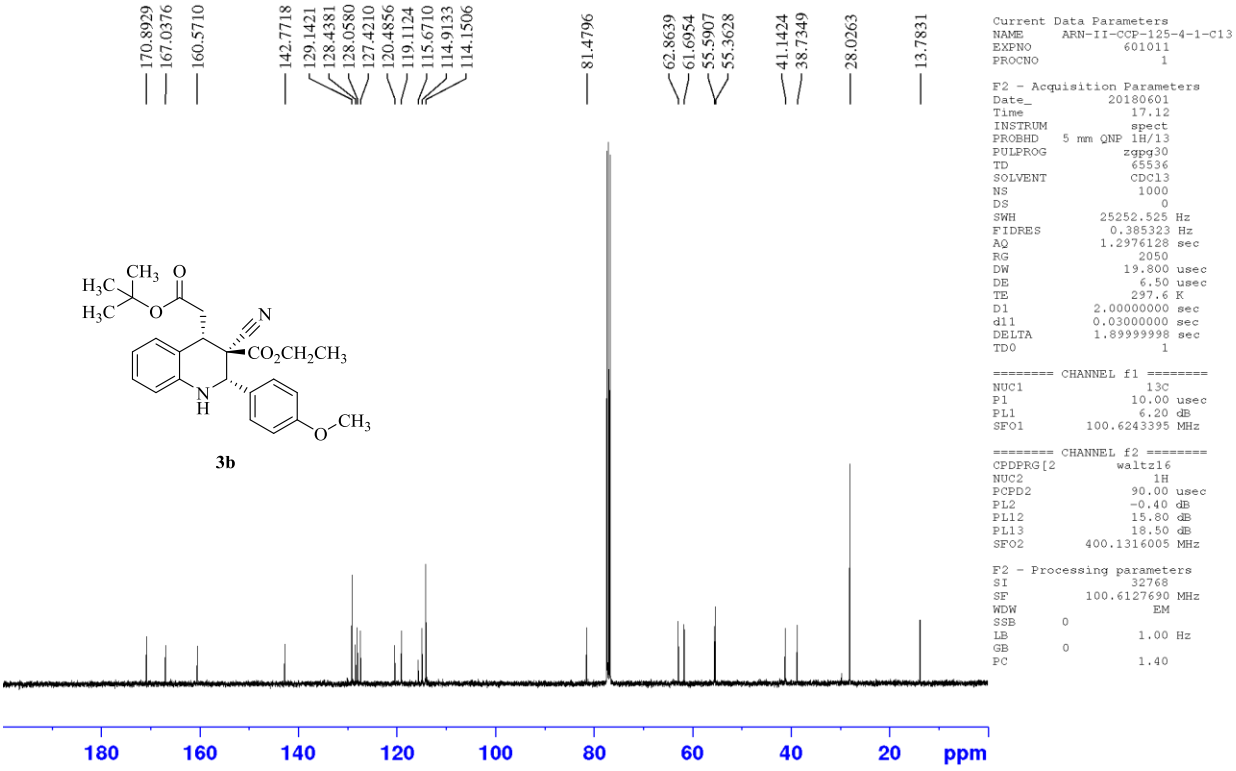

```
Current Data Parameters
NAME      ARN-II-CCP-125-4-1
EXPNO              601011
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180601
Time              16.15
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    9
DS                    0
SWH            6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                  181
DW                83.200 usec
DE                 6.50 usec
TE                297.5 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1                15.00 usec
PL1                0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300090 MHz
WDW                 EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3b**)

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Current Data Parameters
NAME      ARN-II-CCP-125-4-1-C13
EXPNO              601011
PROCNO                1

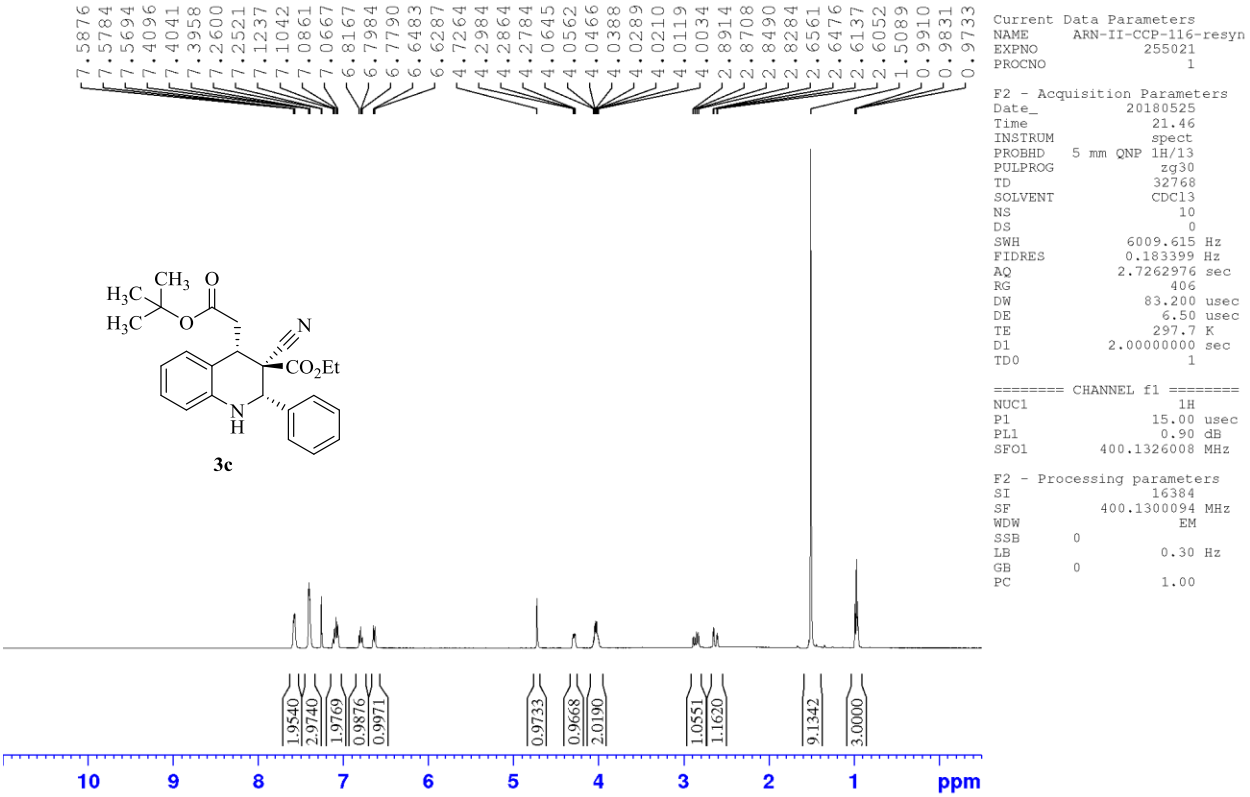
F2 - Acquisition Parameters
Date_           20180601
Time              17.12
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1000
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE                297.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PL1               6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2              -0.40 dB
PL12             15.80 dB
PL13             18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3c**)



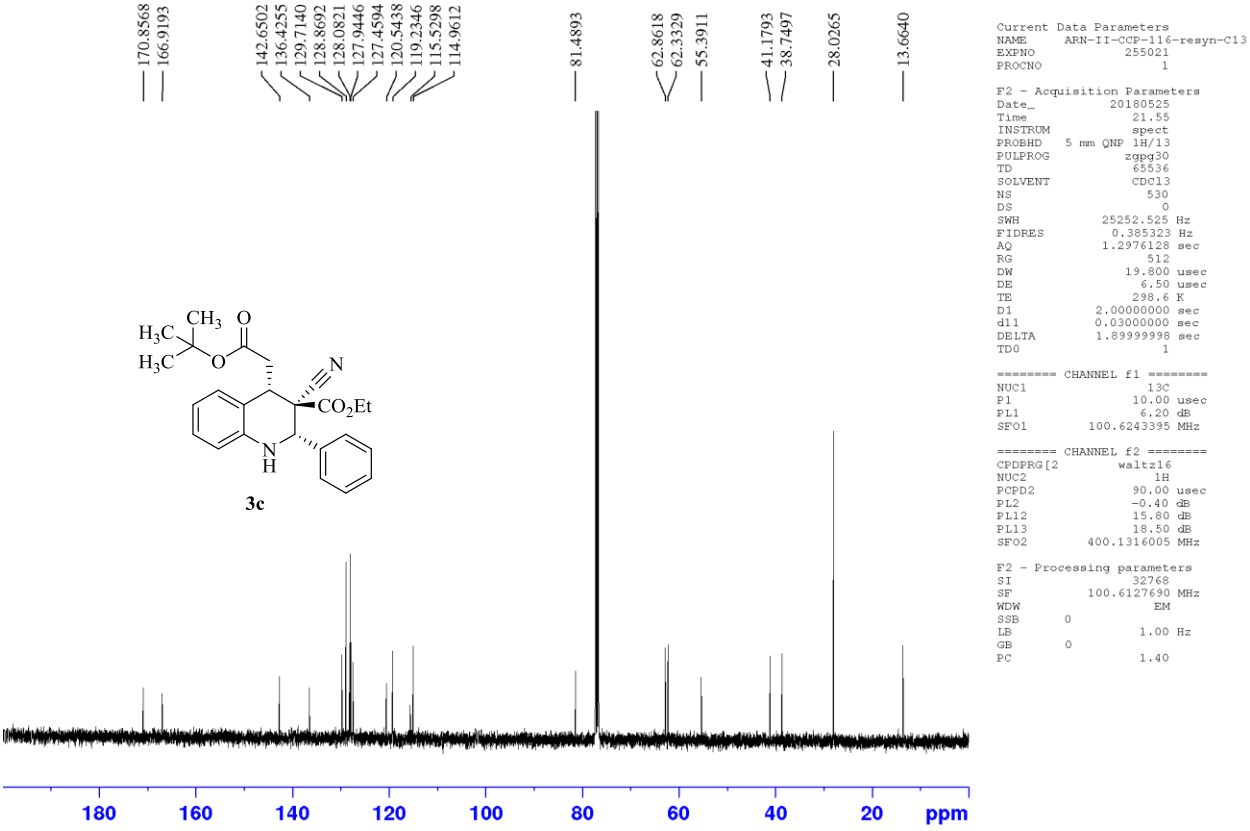

```
Current Data Parameters
NAME      ARN-II-CCP-116-resyn
EXPNO               255021
PROCNO                   1

F2 - Acquisition Parameters
Date_            20180525
Time                21.46
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                   406
DW                83.200 usec
DE                 6.50 usec
TE                297.7 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300094 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-phenyl-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3c**)

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Current Data Parameters
NAME      ARN-II-CCP-116-resyn-C13
EXPNO               255021
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180525
Time                21.55
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   530
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976128 sec
RG                   512
DW                19.800 usec
DE                 6.50 usec
TE                298.6 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```
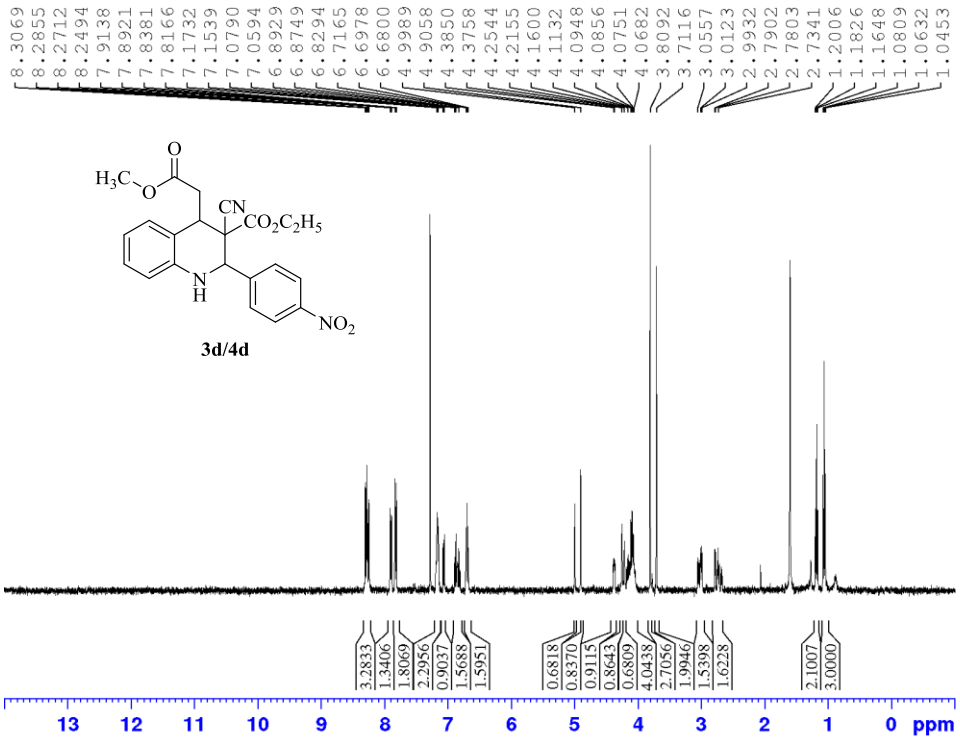
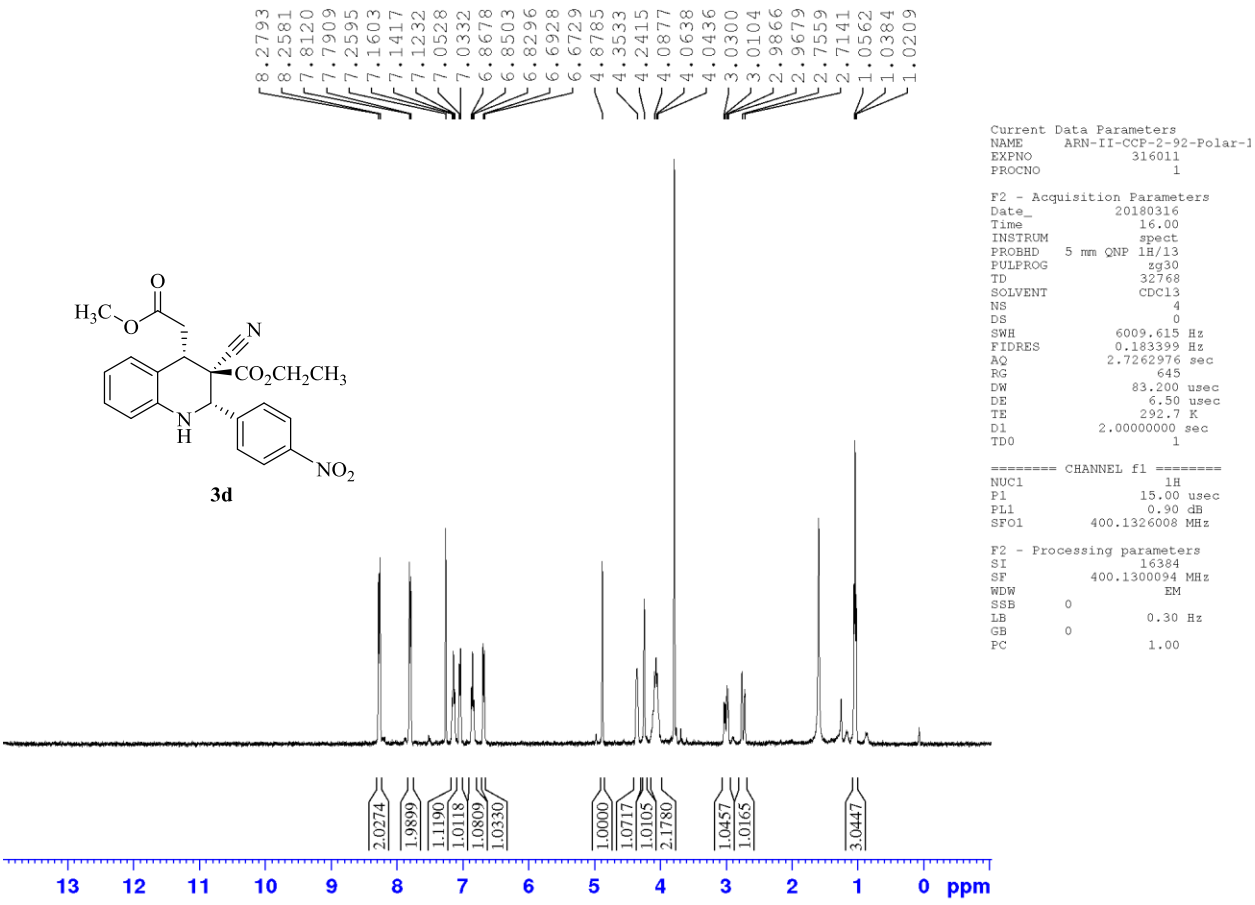

Ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3d/4d,** mixture**)**



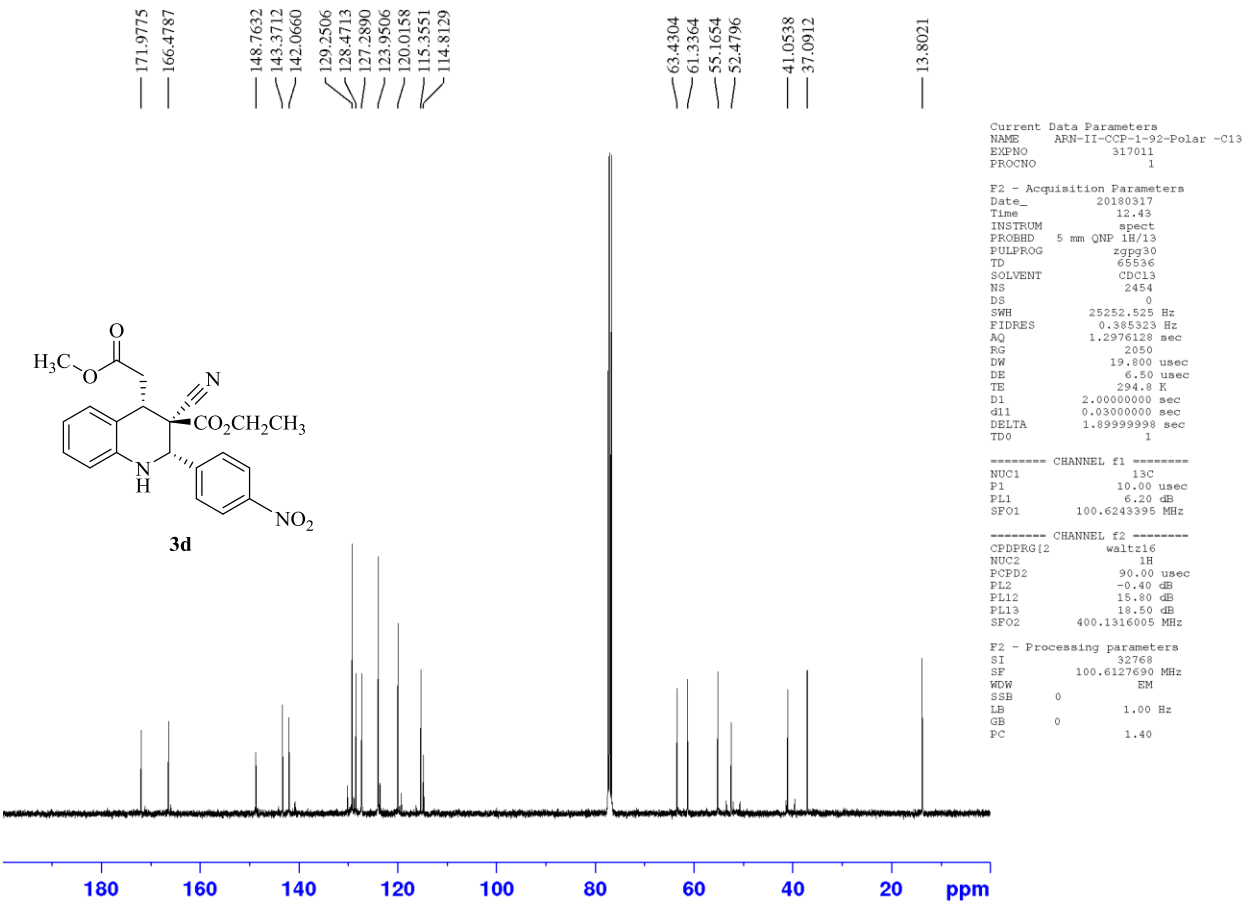
3d/4d

```
Current Data Parameters
NAME      ARN-CCP-092-1
EXPNO              315011
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180315
Time                15.44
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                   724
DW                83.200 usec
DE                 6.50 usec
TE                292.5 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3d**, major isomer)

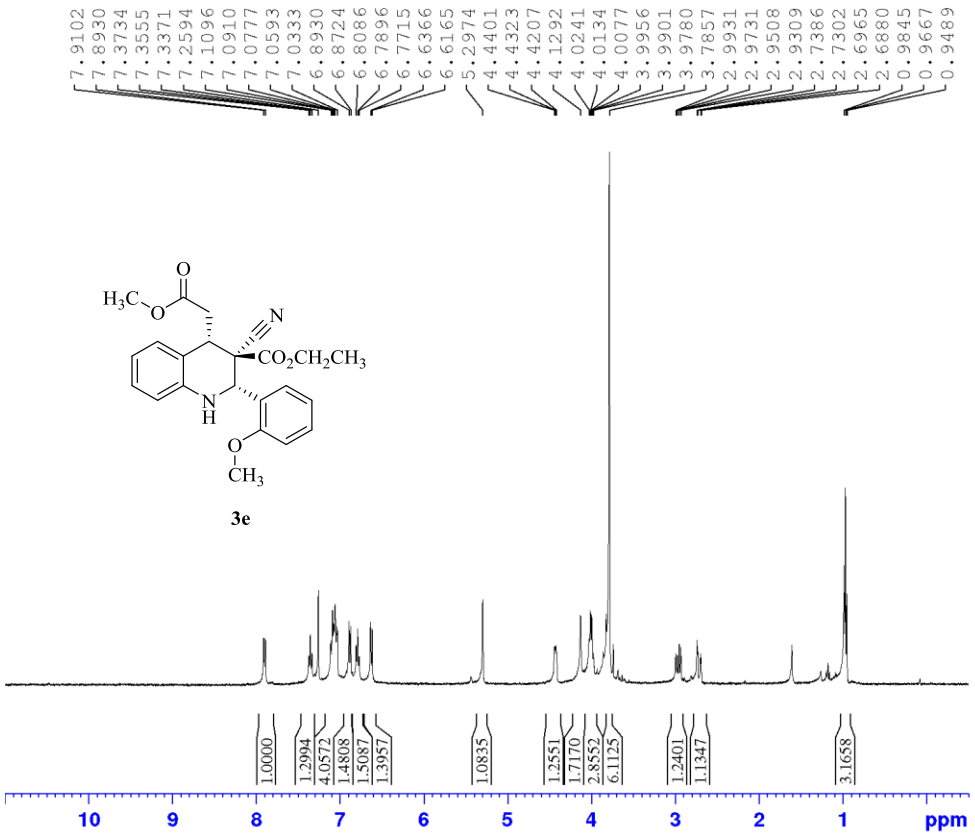


Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3d**, major isomer)




```
Current Data Parameters
NAME      ARN-II-CCP-1-92-Polar -C13
EXPNO              317011
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180317
Time               12.43
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                 2454
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE                294.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PL1               6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2              -0.40 dB
PL12             15.80 dB
PL13             18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

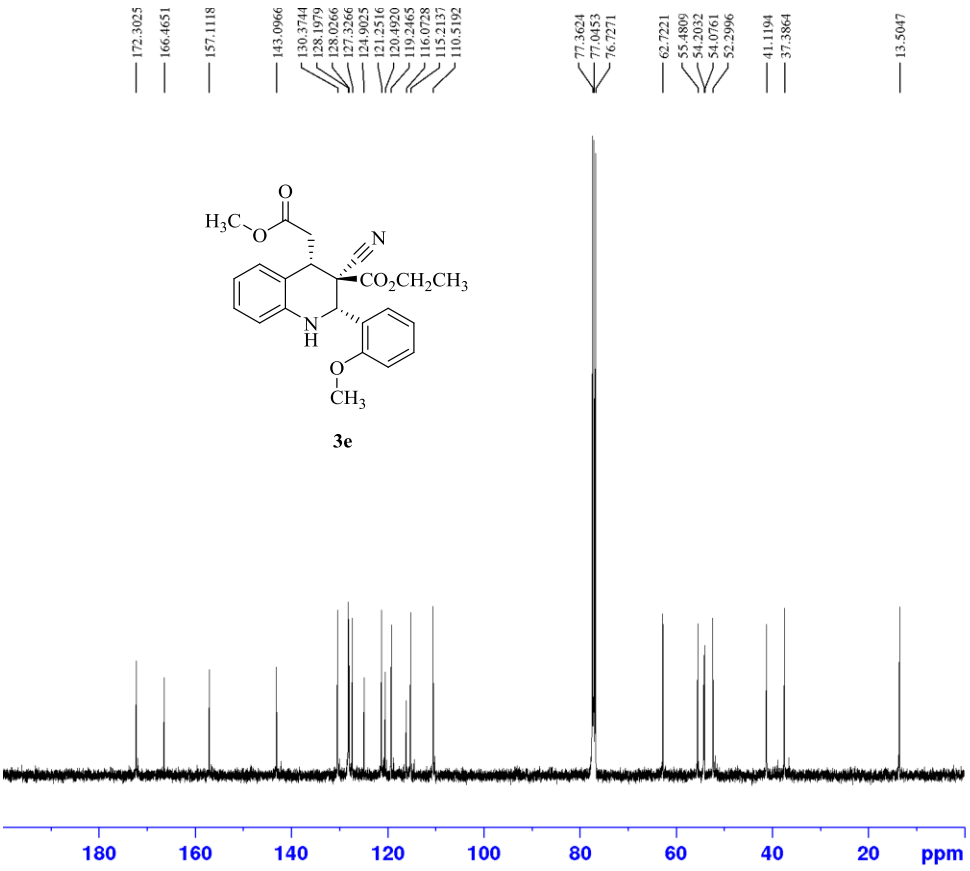
Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3e**)



3e

```
Current Data Parameters
NAME      ARN-II-CCP-057-Prep-2-1
EXPNO              1125011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171125
Time               19.55
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    1
DS                    0
SWH            6009.615 Hz
FIDRES         0.183399 Hz
AQ            2.7262976 sec
RG                  362
DW               83.200 usec
DE                6.50 usec
TE                299.4 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300061 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

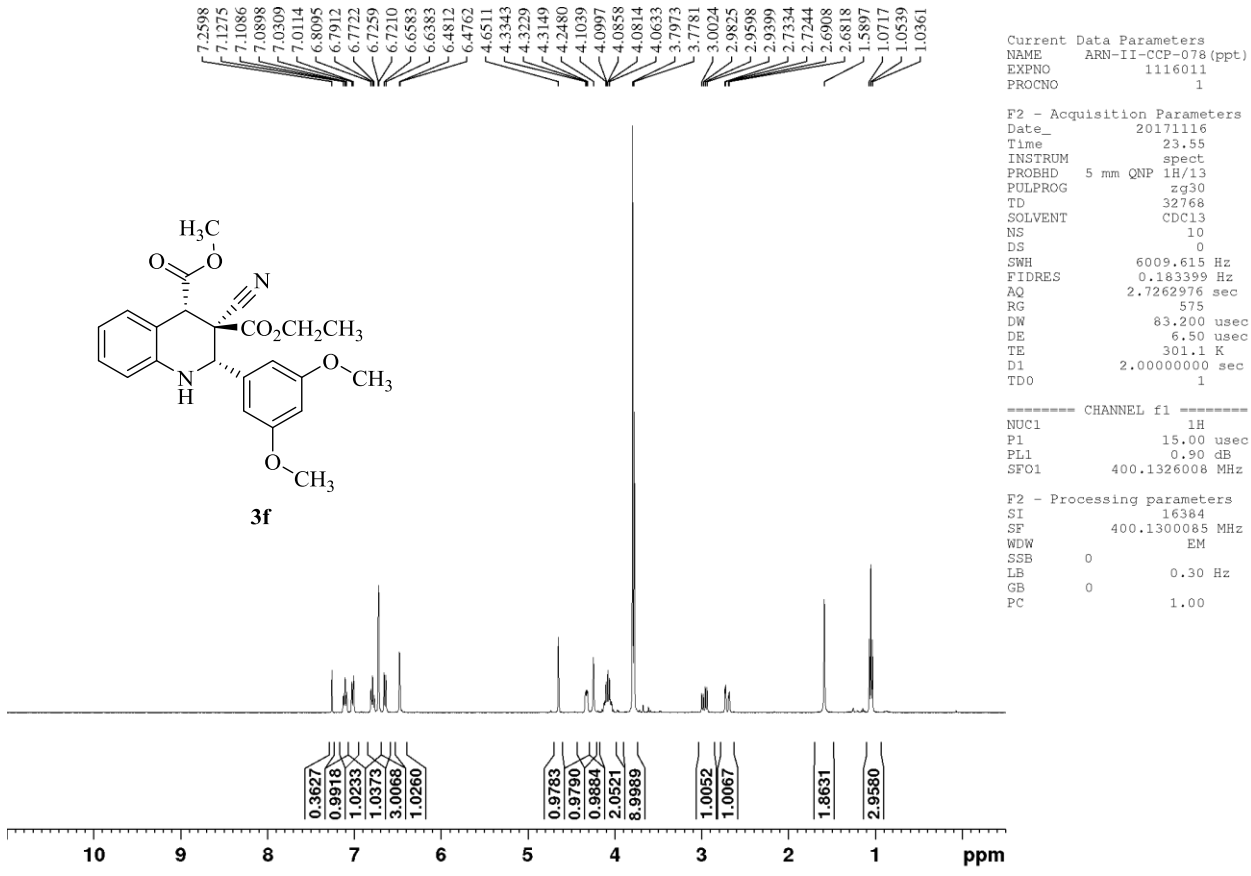
Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**3e**)



3e

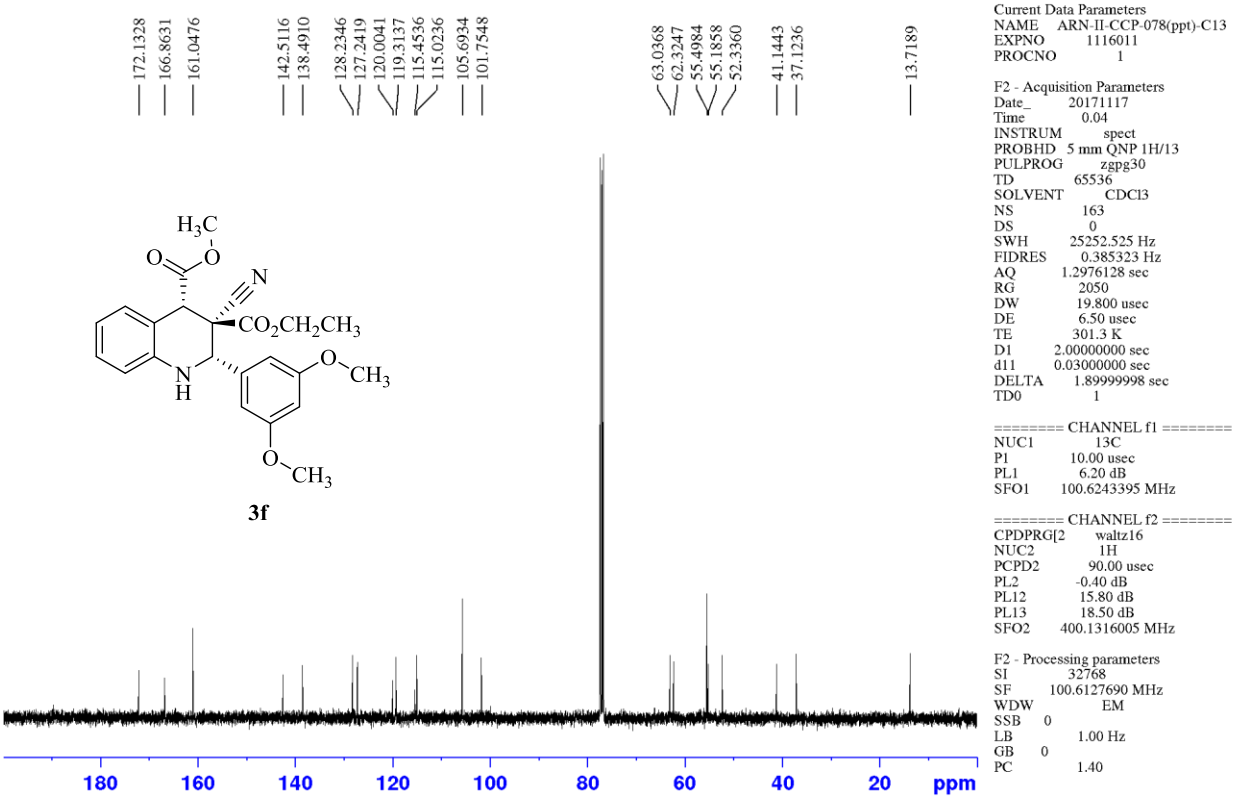
```
Current Data Parameters
NAME      ARN-II-CCP-057-Prep-2-1-C13
EXPNO              1125011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171125
Time              20.53
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1000
DS                    0
SWH           25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE               299.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Racemate of 3-ethyl 4-methyl-3-cyano-2-(3,5-dimethoxyphenyl)-1,2,3,4-tetrahydroquinoline-3,4-dicarboxylate (**3f**)




```
Current Data Parameters
NAME      ARN-II-CCP-078(ppt)
EXPNO              1116011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171116
Time               23.55
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                   575
DW                83.200 usec
DE                 6.50 usec
TE                301.1 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300085 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of 3-ethyl 4-methyl 3-cyano-2-(3,5-dimethoxyphenyl)-1,2,3,4-tetrahydroquinoline-3,4-dicarboxylate (**3f**)



Current Data Parameters
NAME ARN-II-CCP-078(ppt)-C13
EXPNO 1116011
PROCNO 1

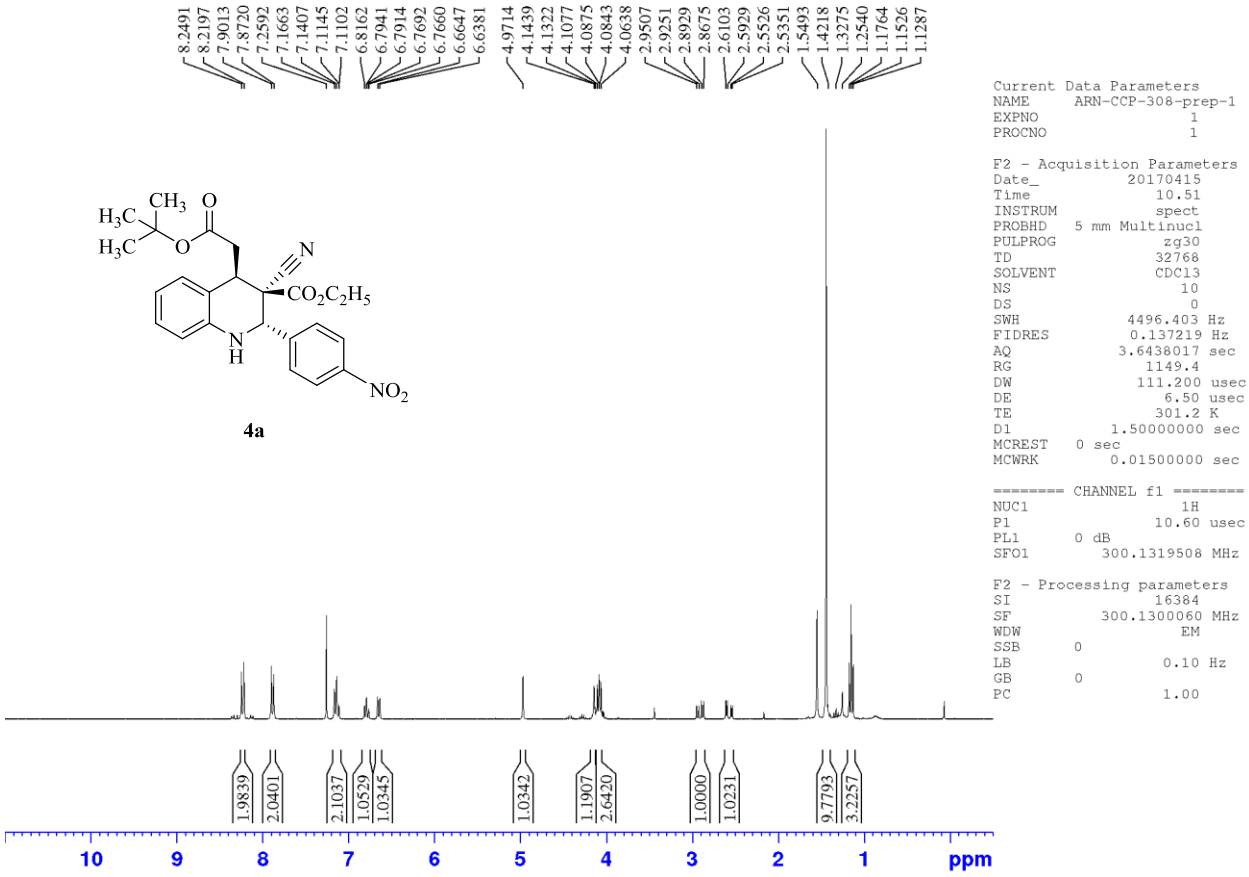
F2 - Acquisition Parameters
Date_ 20171117
Time 0.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 163
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 301.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.20 dB
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.40 dB
PL12 15.80 dB
PL13 18.50 dB
SFO2 400.1316005 MHz

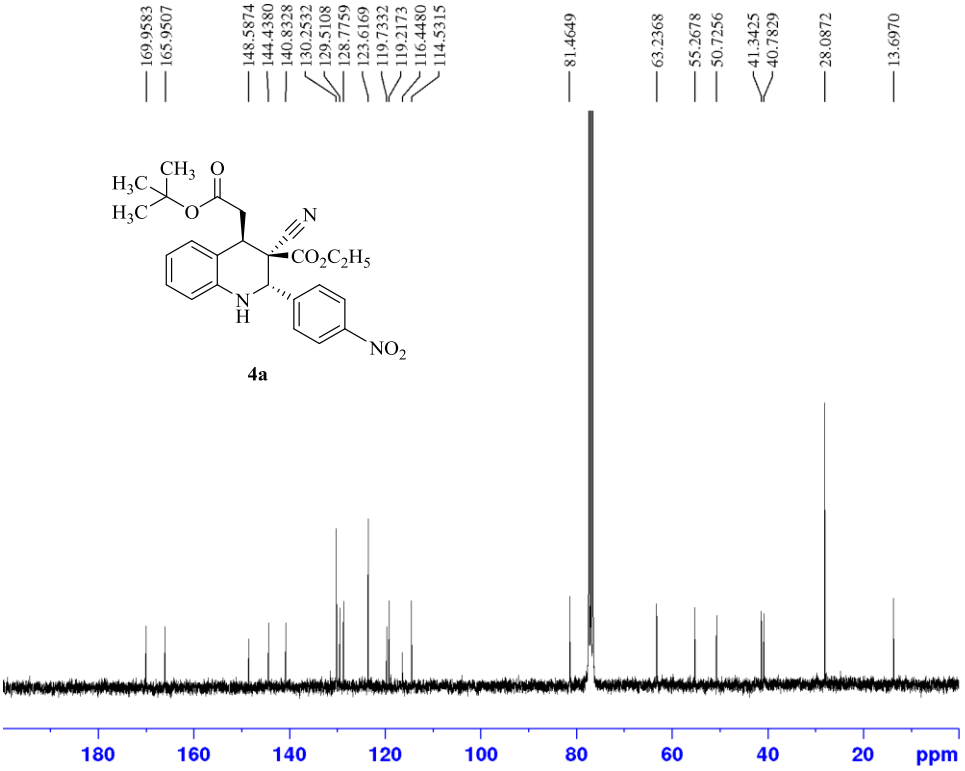
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**4a**, minor isomer)



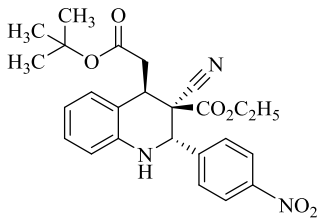

```
Current Data Parameters
NAME      ARN-CCP-308-prep-1
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_           20170415
Time              10.51
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   10
DS                    0
SWH            4496.403 Hz
FIDRES         0.137219 Hz
AQ             3.6438017 sec
RG                1149.4
DW               111.200 usec
DE                 6.50 usec
TE                301.2 K
D1             1.50000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.60 usec
PL1       0 dB
SFO1         300.1319508 MHz

F2 - Processing parameters
SI                16384
SF           300.1300060 MHz
WDW                  EM
SSB       0
LB                0.10 Hz
GB        0
PC                1.00
```

Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**4a**, minor)

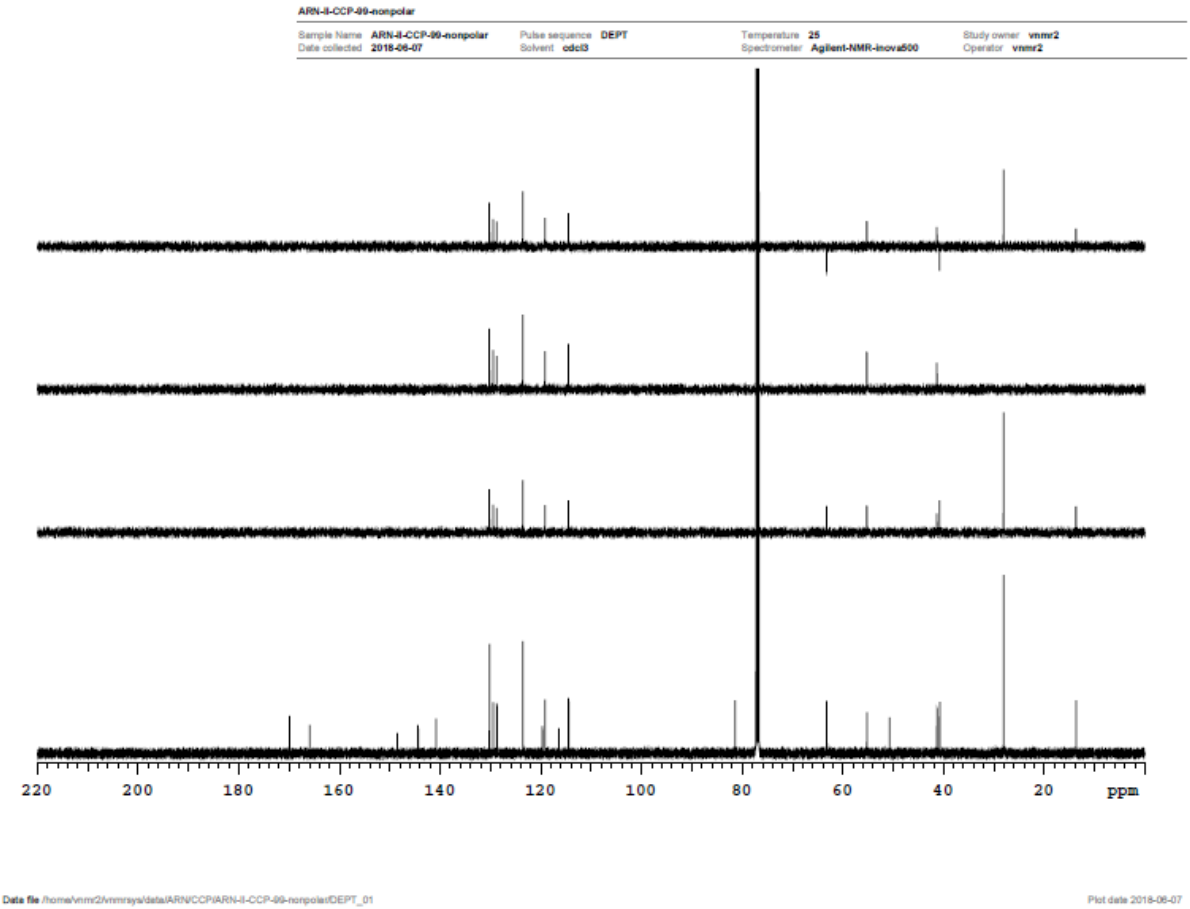



```
Current Data Parameters
NAME      ARN-CCP-308-1-1-C13
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20170419
Time                23.27
INSTRUM             spect
PROBHD    5 mm Multinucl
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   9999
DS                      0
SWH            18832.393 Hz
FIDRES          0.287360 Hz
AQ              1.7399808 sec
RG                   8192
DW                26.550 usec
DE                 6.50 usec
TE                298.2 K
D1            1.50000000 sec
d11           0.03000000 sec
DELTA         1.39999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 11.10 usec
PL1       0 dB
SFO1          75.4763978 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2       0 dB
PL12               18.80 dB
PL13               21.80 dB
SFO2         300.1313506 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677477 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

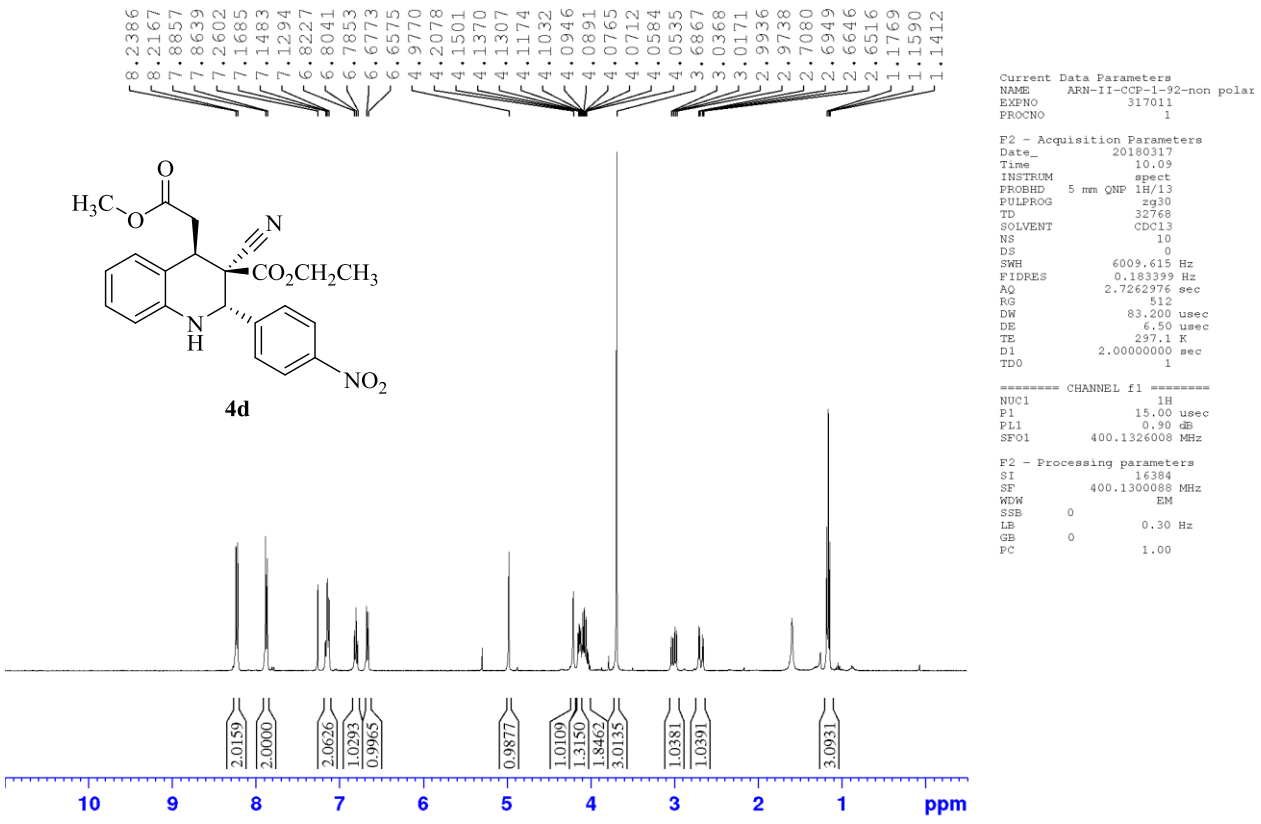
Racemate of ethyl 4-(2-(*tert*-butoxy)-2-oxoethyl)-3-cyano-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**4a**, minor)



4a

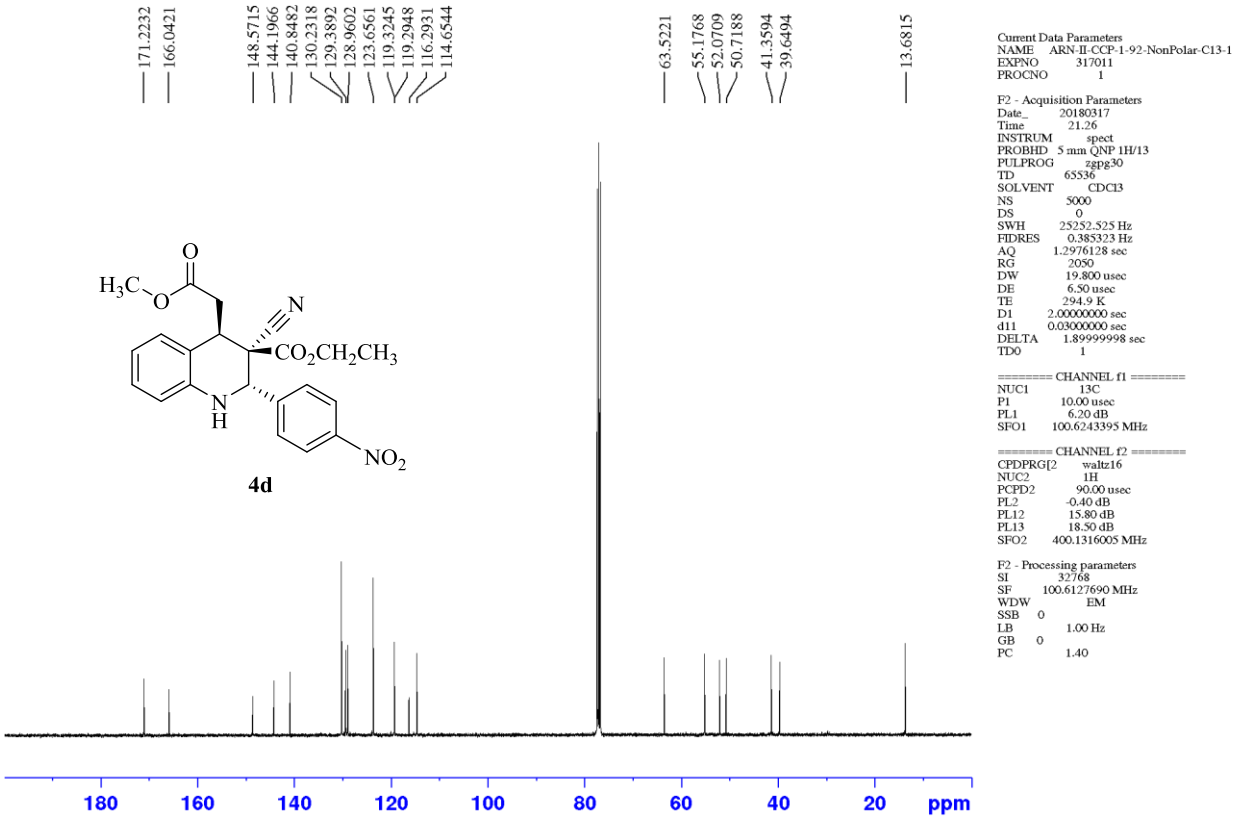


Ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**4d**, minor isomer)




```
Current Data Parameters
NAME      ARN-II-CCP-1-92-non polar
EXPNO             317011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180317
Time               10.09
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDC13
NS                   10
DS                    0
SWH            6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                  512
DW                83.200 usec
DE                 6.50 usec
TE                297.1 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300088 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(4-nitrophenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**4d**, minor isomer)



Current Data Parameters
NAME ARN-II-CCP-1-92-NonPolar-C13-1
EXPNO 317011
PROCNO 1

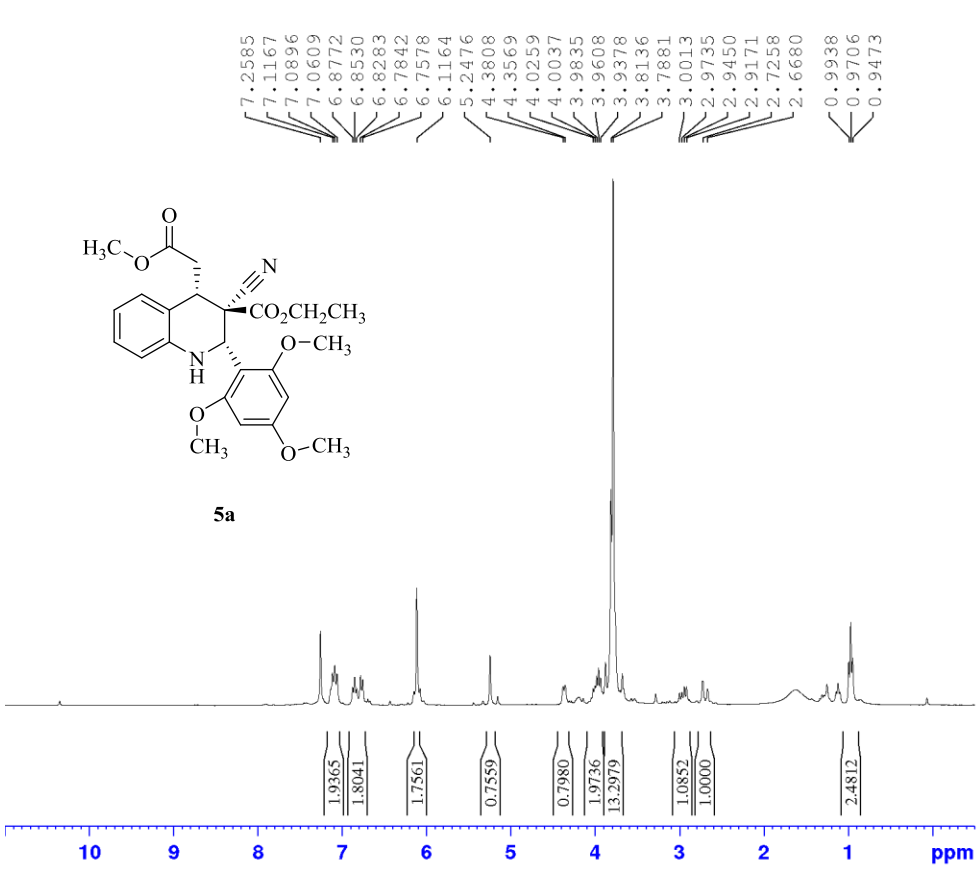
F2 - Acquisition Parameters
Date_ 20180317
Time 21.26
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5000
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.20 dB
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.40 dB
PL12 15.80 dB
PL13 18.50 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

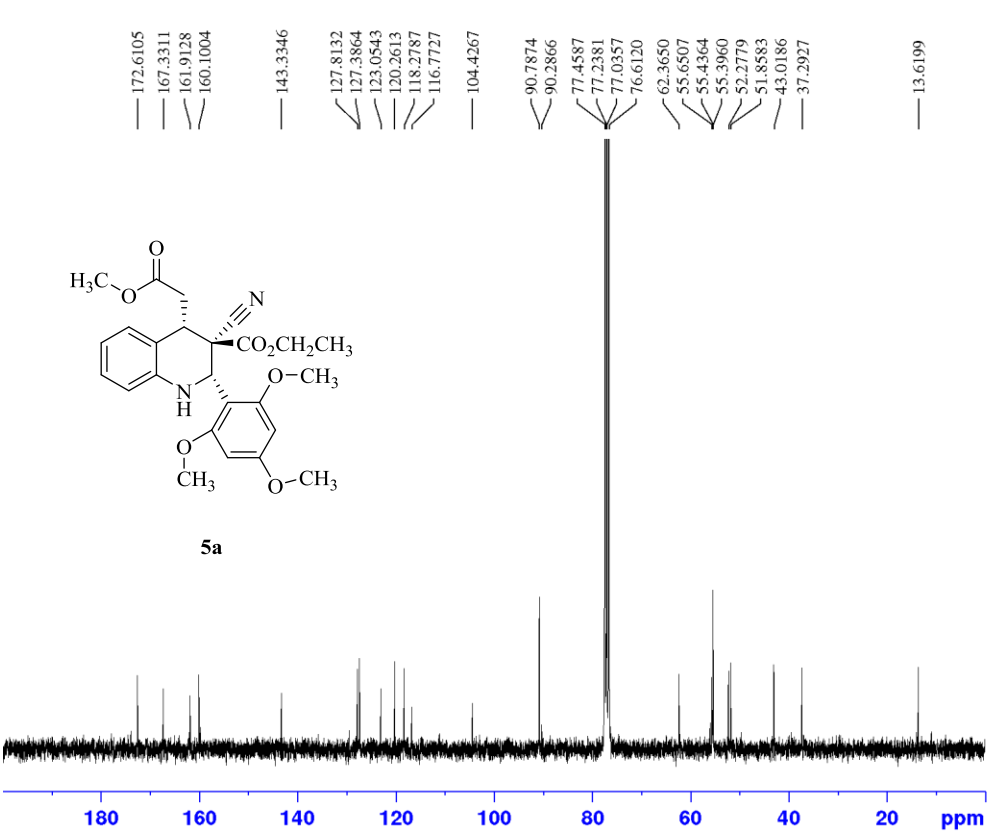
Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(2,4,6-trimethoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**5a**)



5a

```
Current Data Parameters
NAME      ARN-II-CCP-132-prep
EXPNO              623014
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180623
Time              14.03
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG           zgdc30
TD                4096
SOLVENT             D2O
NS                  10
DS                   0
SWH            5995.204 Hz
FIDRES         1.463673 Hz
AQ            0.3416064 sec
RG                812.7
DW               83.400 usec
DE                6.50 usec
TE               299.2 K
D1            1.00000000 sec
d11           0.03000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.20 usec
PL1       0 dB
SFO1         300.1313506 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                11B
PCPD2            65.00 usec
PL2              16.00 dB
PL12             19.00 dB
SFO2          96.2933370 MHz

F2 - Processing parameters
SI                32768
SF           300.1300060 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
```

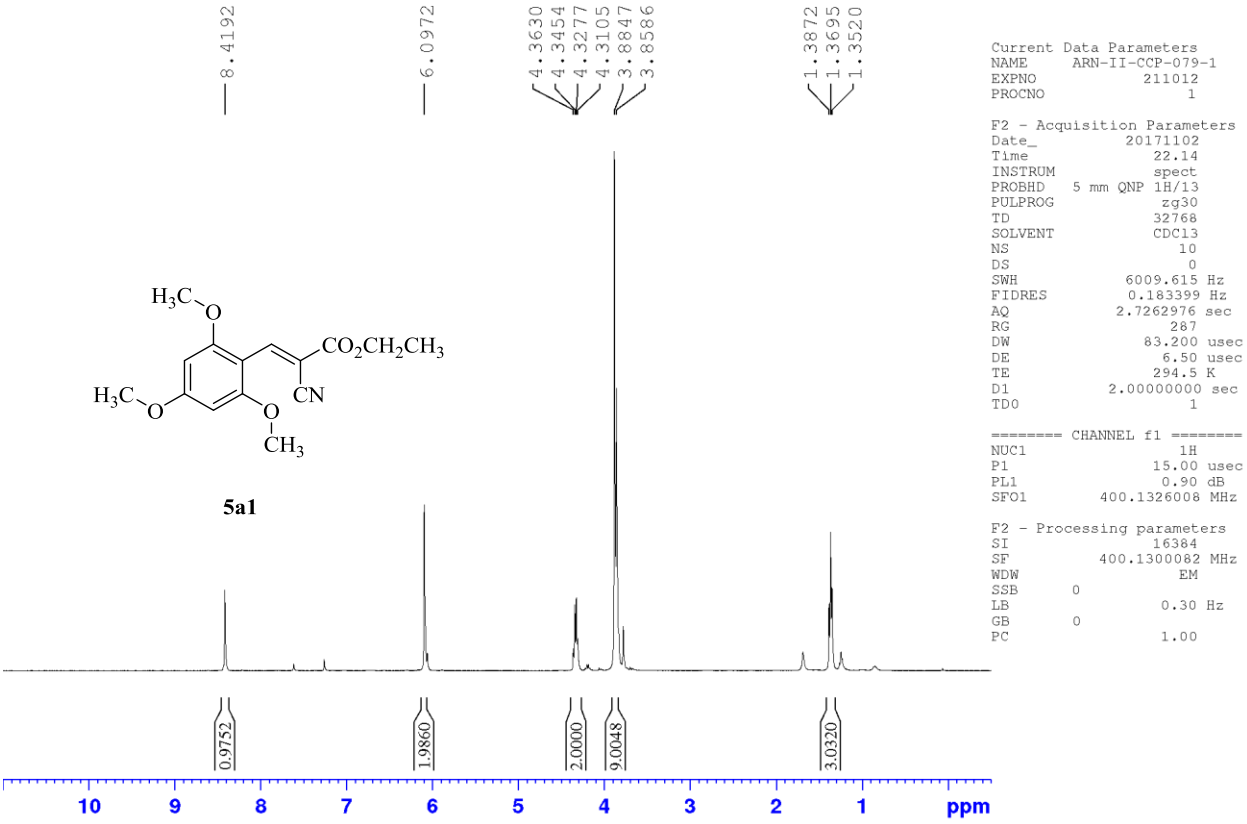
Racemate of methyl 2-((3-cyano-3-((ethylperoxy)-l2-methyl)-2-(2,4,6-trimethoxyphenyl)-1,2,3,4-tetrahydroquinolin-4-yl)acetate (**5a**)



5a

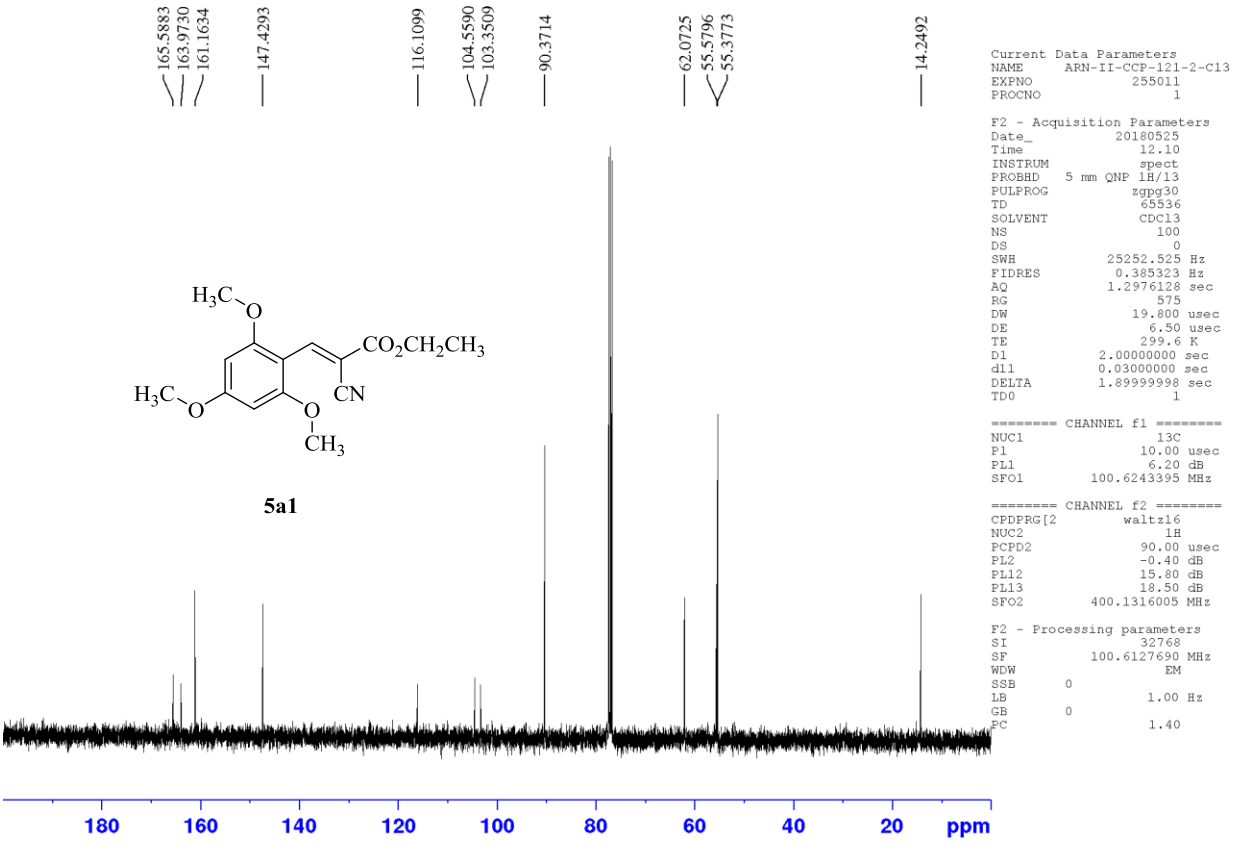
```
Current Data Parameters
NAME      ARN-II-CCP-132-2-C13
EXPNO              623014
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180623
Time               17.06
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 7443
DS                    0
SWH           18832.393 Hz
FIDRES         0.287360 Hz
AQ             1.7399808 sec
RG              5792.6
DW                26.550 usec
DE                 6.50 usec
TE               299.2 K
D1            1.50000000 sec
d11           0.03000000 sec
DELTA         1.39999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                11.10 usec
PL1       0 dB
SFO1          75.4763978 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                1H
PCPD2             90.00 usec
PL2       0 dB
PL12              18.80 dB
PL13              21.80 dB
SFO2         300.1313506 MHz

F2 - Processing parameters
SI                32768
SF          75.4677477 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

Ethyl (*Z*)-2-cyano-3-(2,4,6-trimethoxyphenyl)acrylate (**5a1**)



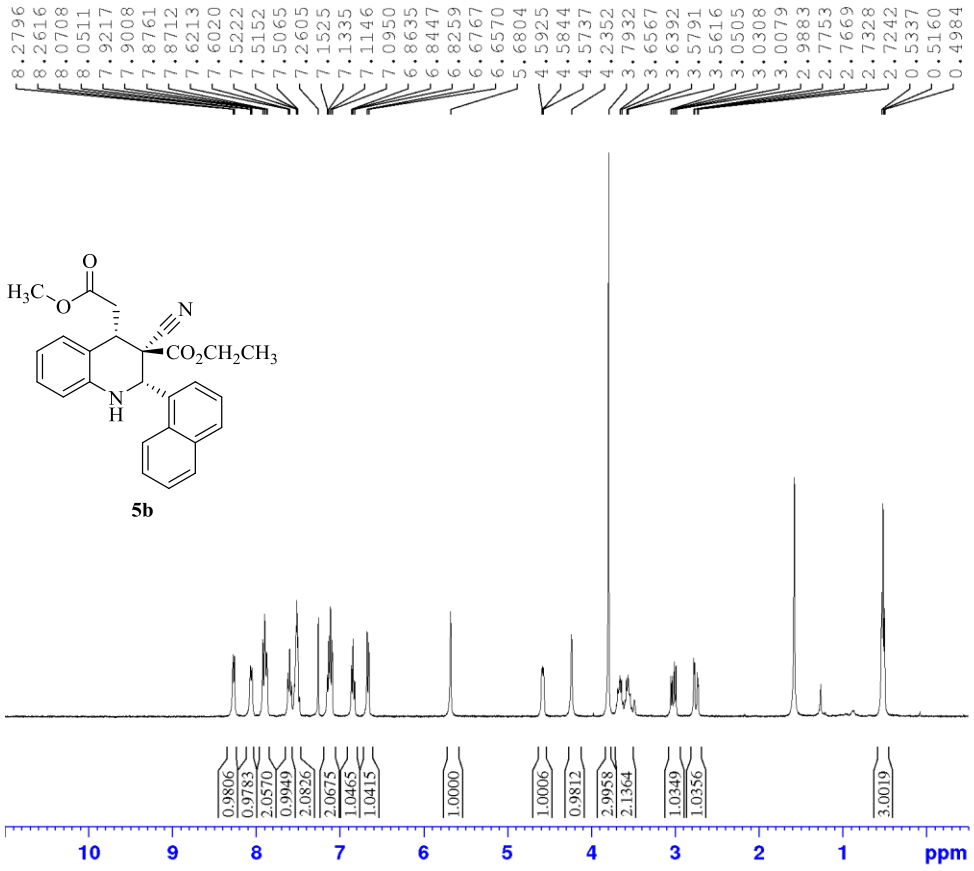

```
Current Data Parameters
NAME      ARN-II-CCP-079-1
EXPNO              211012
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171102
Time               22.14
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ            2.7262976 sec
RG                   287
DW                83.200 usec
DE                 6.50 usec
TE                294.5 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300082 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Ethyl (*Z*)-2-cyano-3-(2,4,6-trimethoxyphenyl)acrylate (**5a1**)



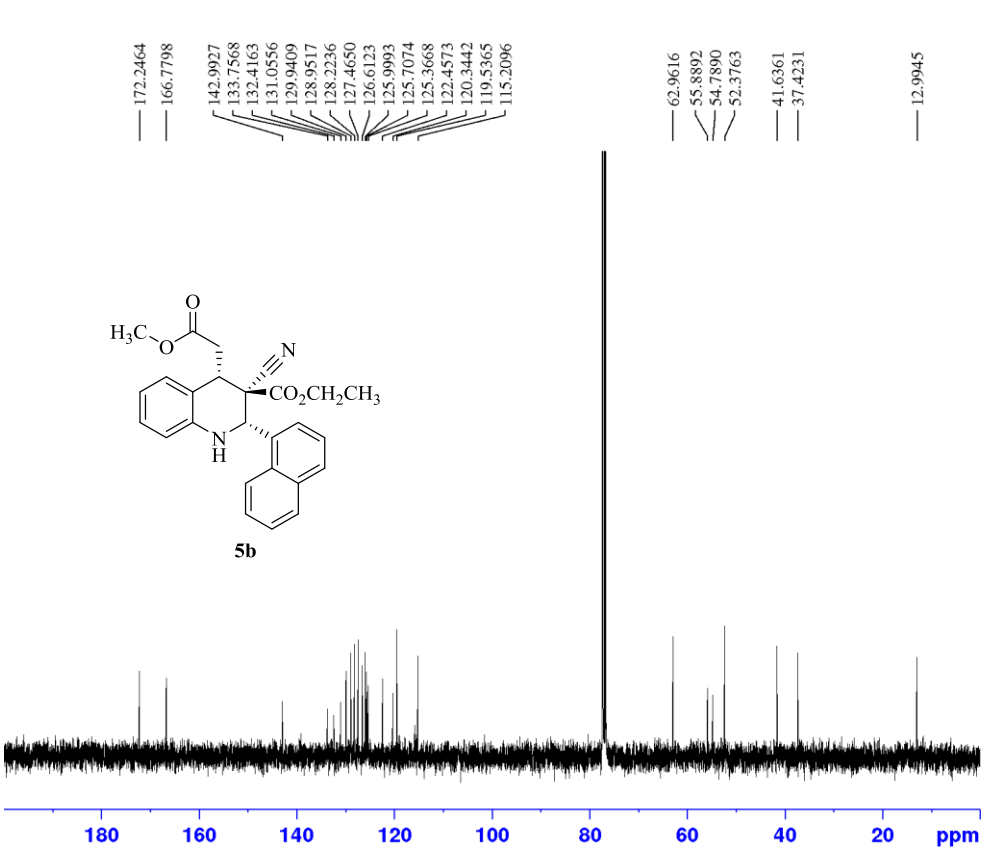

```
Current Data Parameters
NAME      ARN-II-CCP-121-2-C13
EXPNO               255011
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180525
Time                12.10
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    100
DS                      0
SWH             25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976128 sec
RG                    575
DW                19.800 usec
DE                 6.50 usec
TE                299.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Racemate ofethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-1-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**5b**)



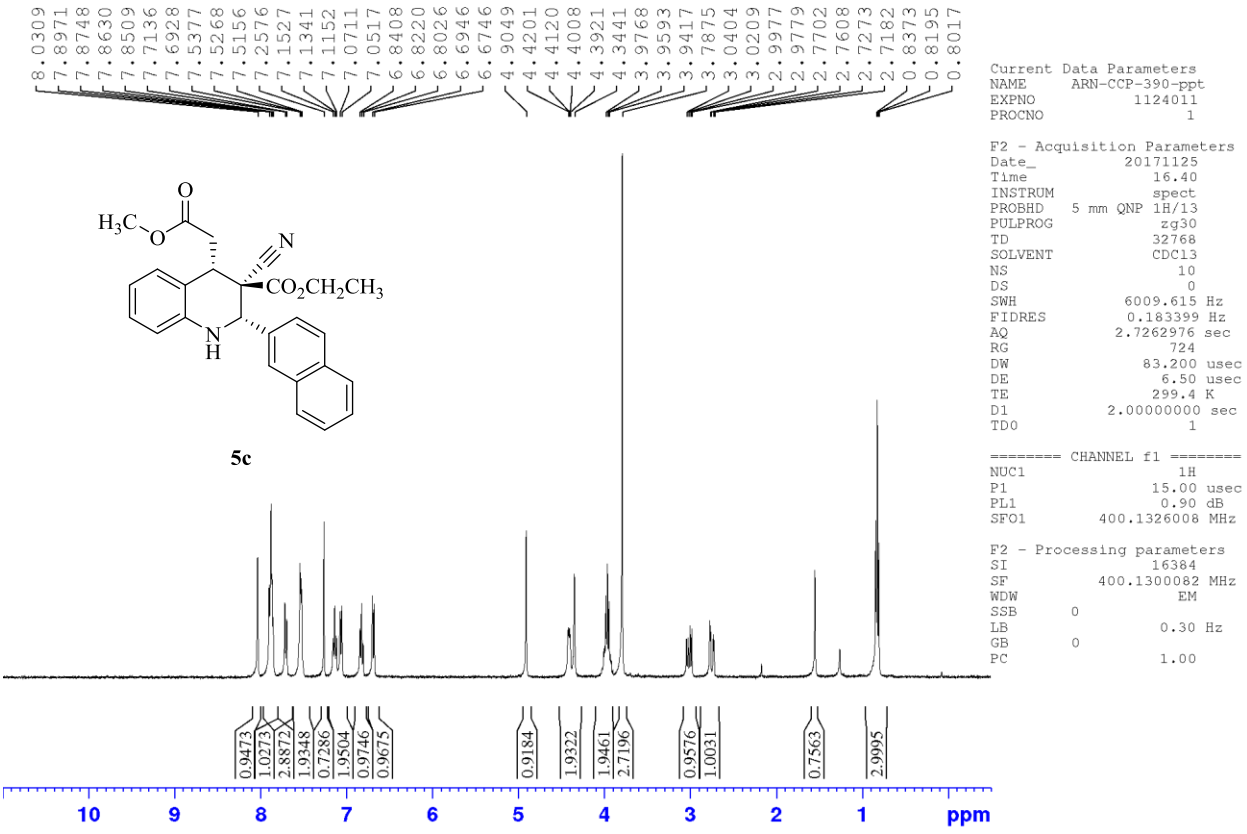

```
Current Data Parameters
NAME      ARN-CCP-372 (ppt)
EXPNO            1026011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171026
Time               14.05
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    11
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                   645
DW                83.200 usec
DE                 6.50 usec
TE                300.8 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300089 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-1-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**5b**)



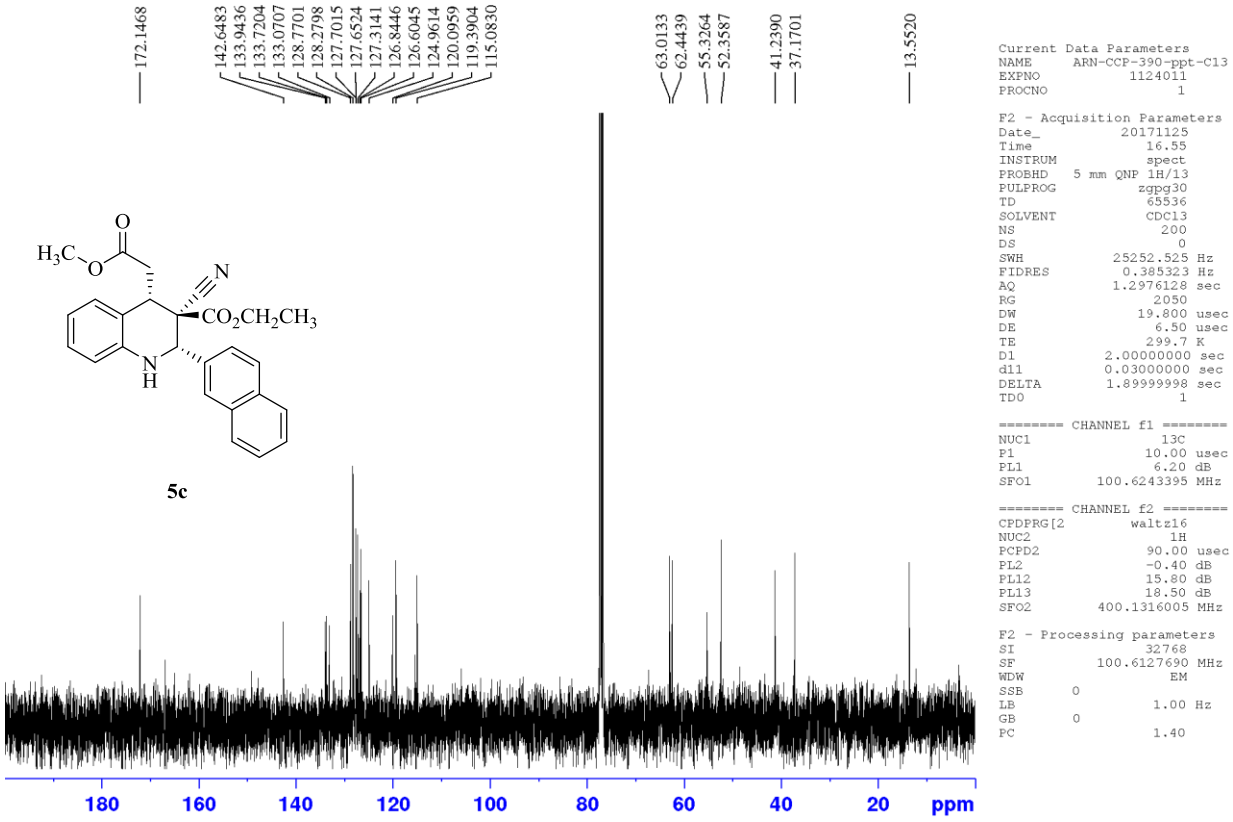

```
Current Data Parameters
NAME      ARN-CCP-392 C13-1
EXPNO           1026021
PROCNO                1

F2 - Acquisition Parameters
Date_          20171026
Time              21.44
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 285
DS                   0
SWH          25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.2976128 sec
RG                2050
DW               19.800 usec
DE                6.50 usec
TE               299.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**5c**)



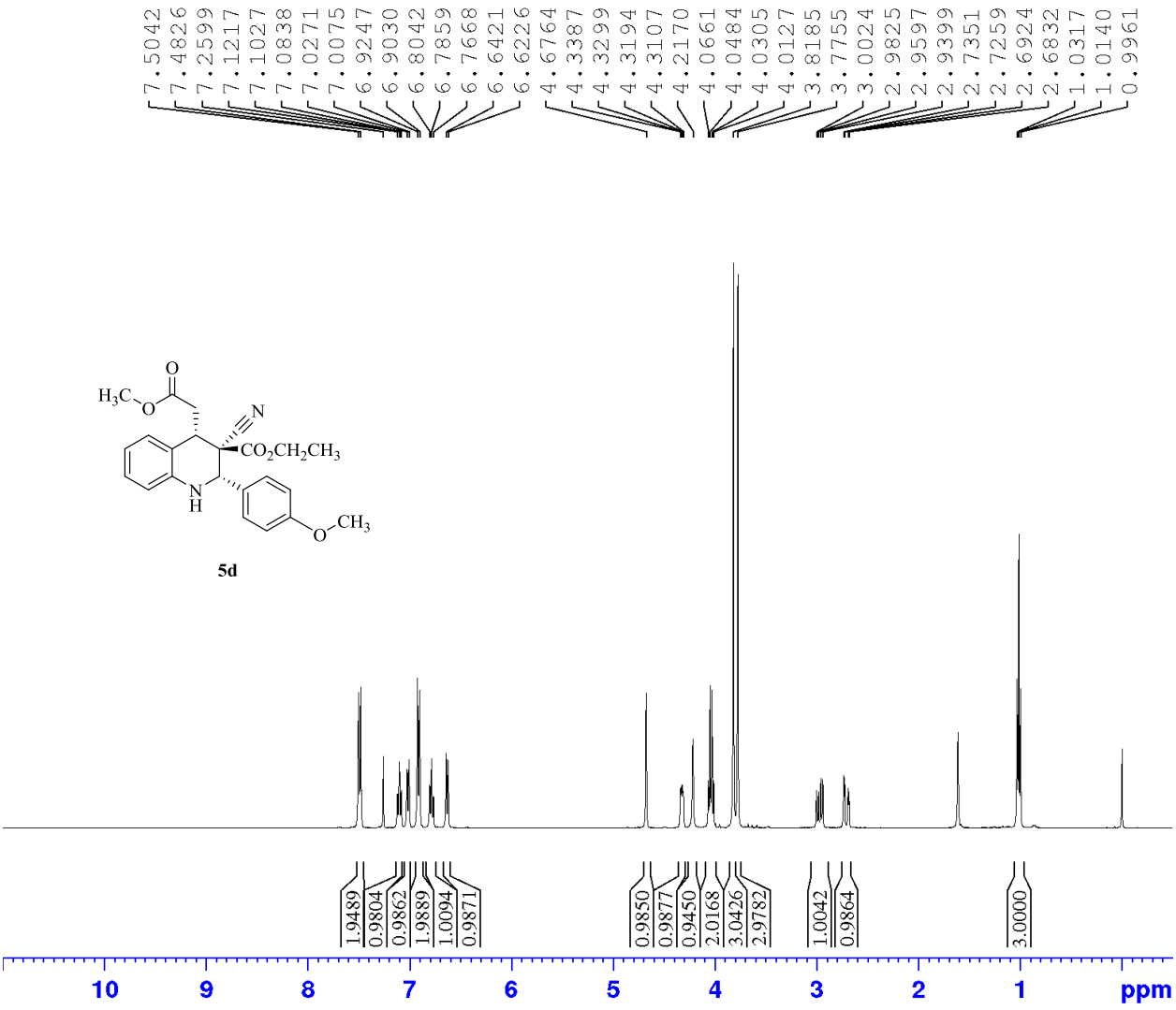

```
Current Data Parameters
NAME      ARN-CCP-390-ppt
EXPNO            1124011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171125
Time               16.40
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDC13
NS                   10
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG                  724
DW                83.200 usec
DE                 6.50 usec
TE                299.4 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300082 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**5c**)

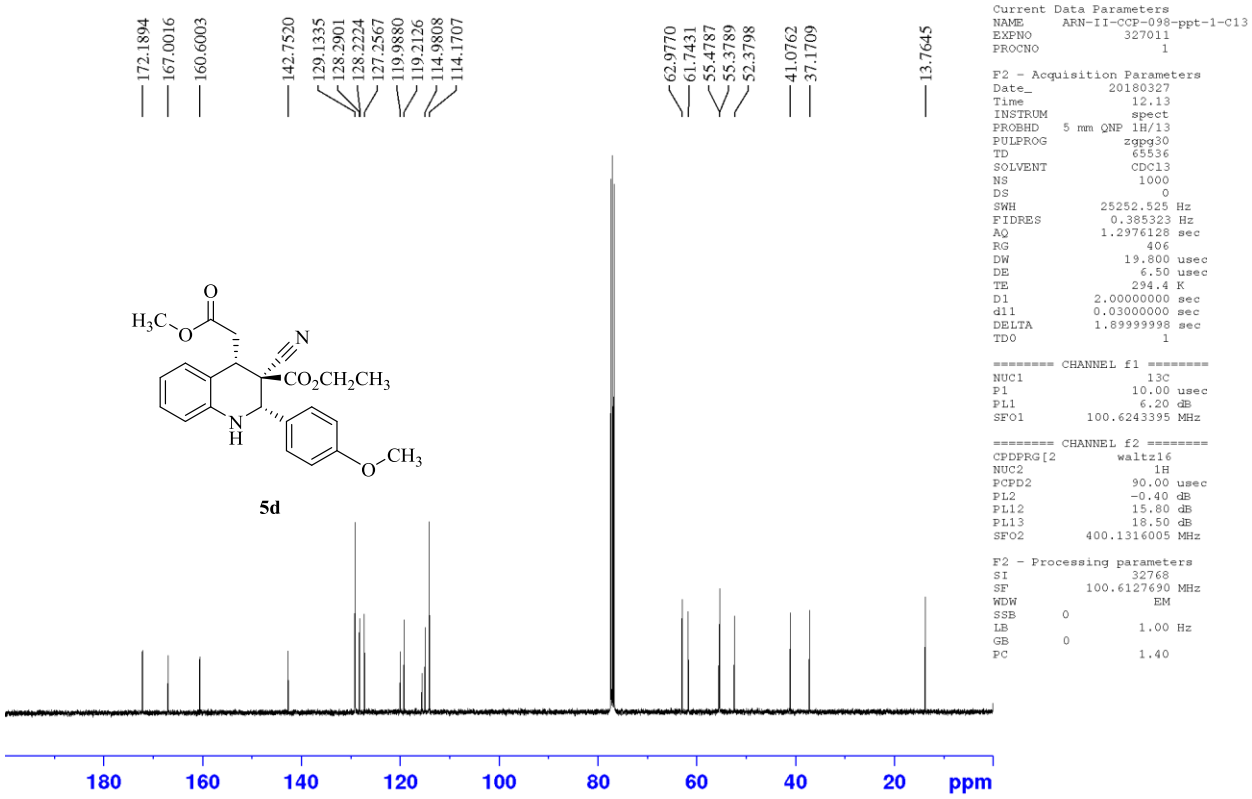



```
Current Data Parameters
NAME      ARN-CCP-390-ppt-C13
EXPNO              1124011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171125
Time              16.55
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    0
SWH           25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE                299.7 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**5d**)

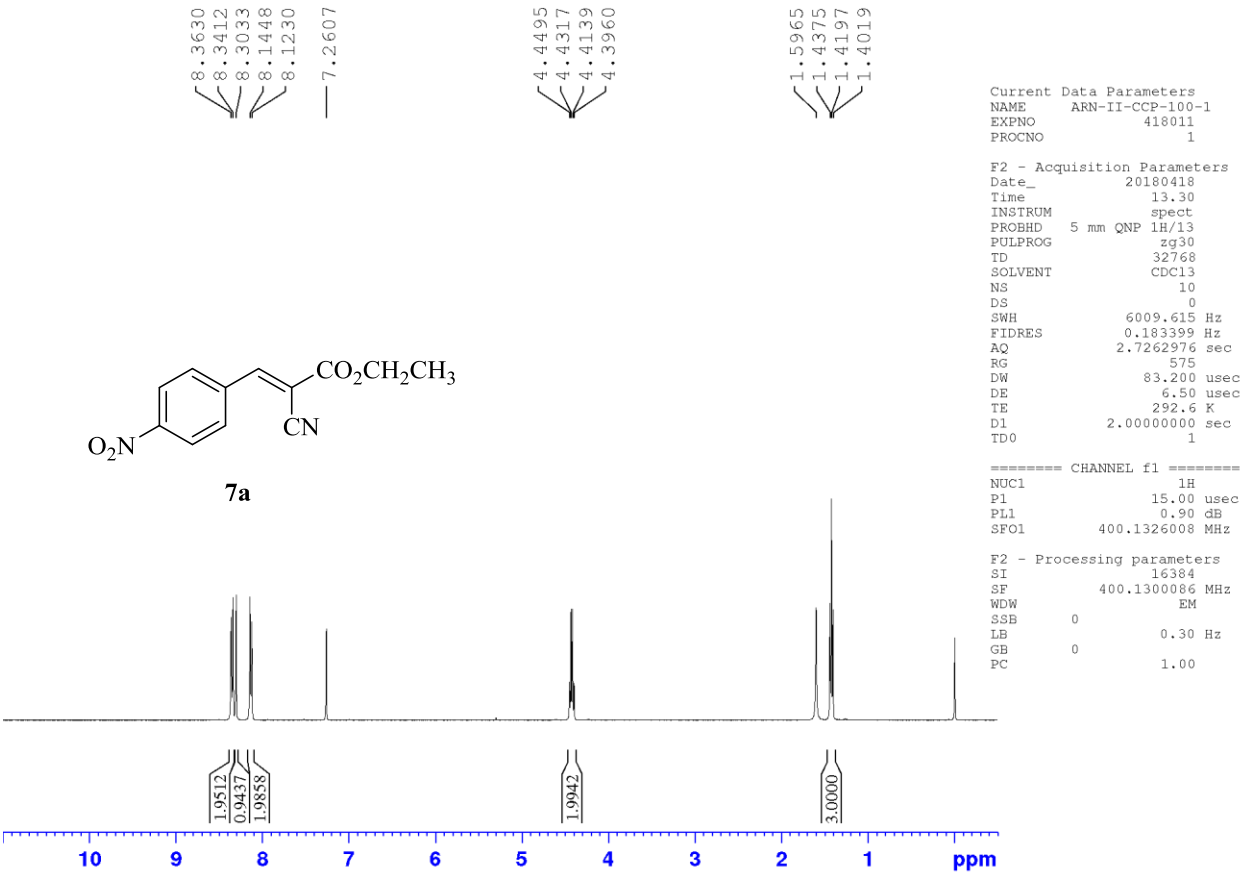


Racemate of ethyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(4-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**5d**)

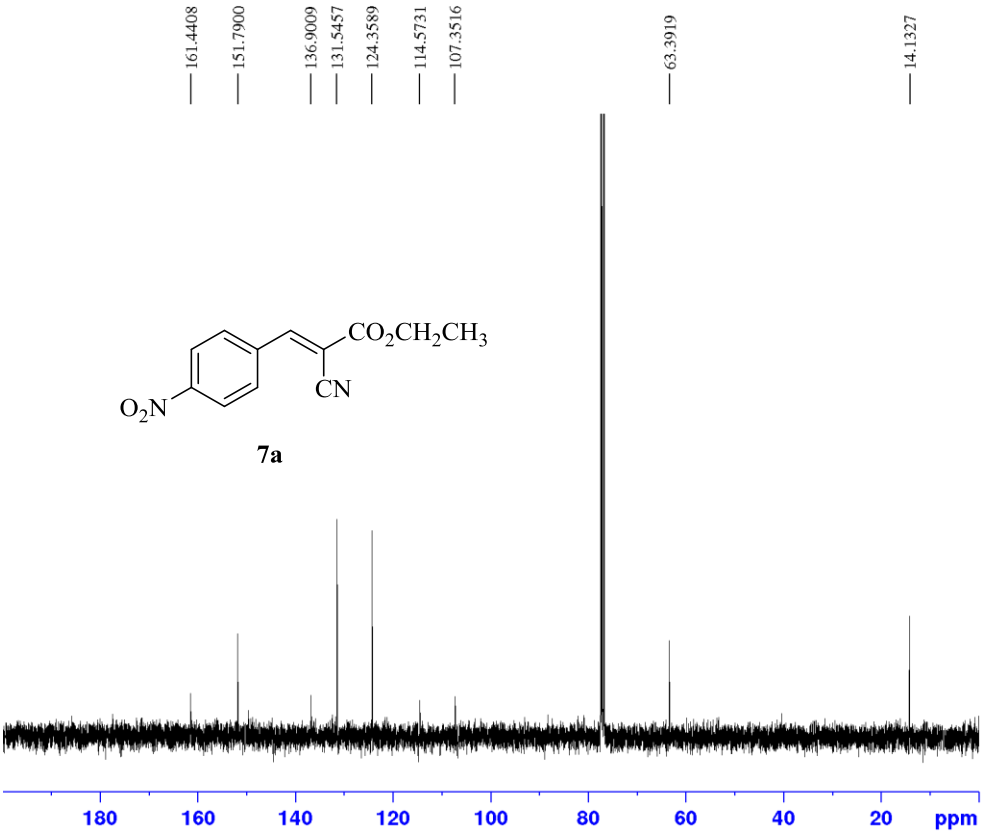



```
Current Data Parameters
NAME      ARN-II-CCP-098-ppt-1-C13
EXPNO              327011
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180327
Time                12.13
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDC13
NS                  1000
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976128 sec
RG                   406
DW                19.800 usec
DE                 6.50 usec
TE                294.4 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

Ethyl (*Z*)-2-cyano-3-(4-nitrophenyl)acrylate (**7a**)

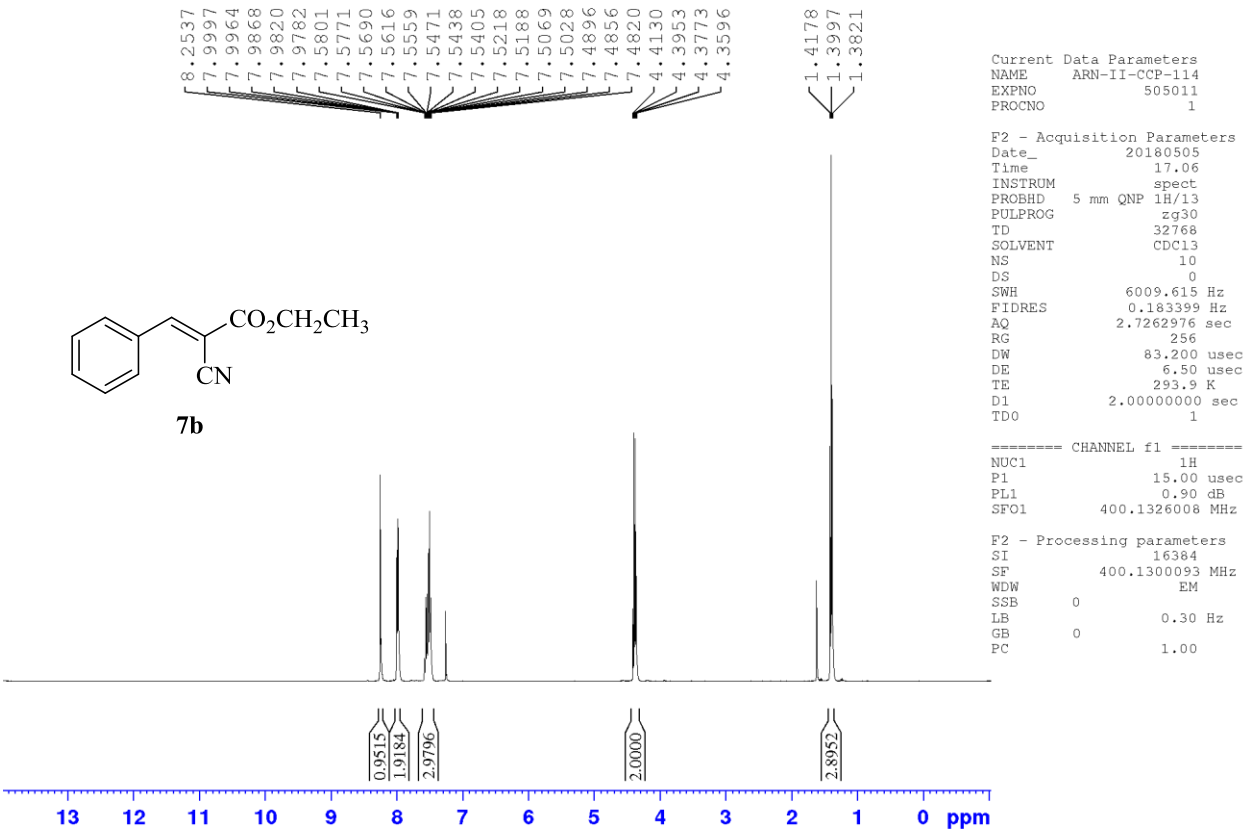


Ethyl (*Z*)-2-cyano-3-(4-nitrophenyl)acrylate (**7a**)



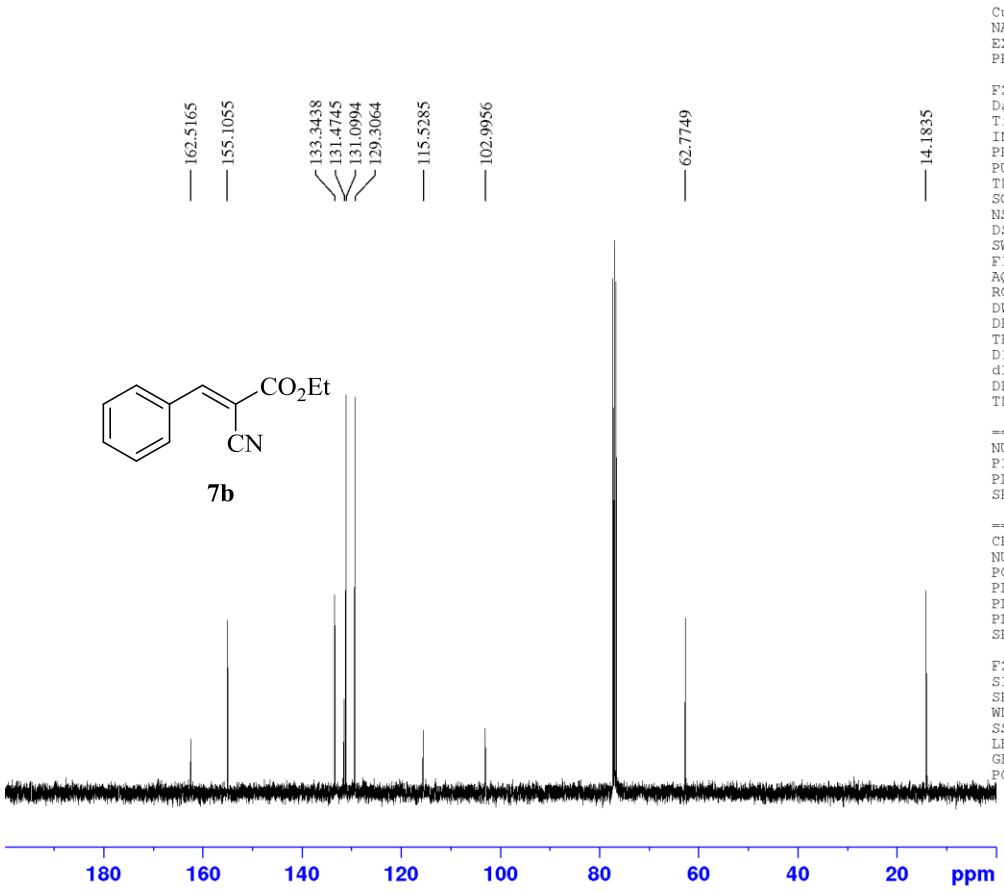

```
Current Data Parameters
NAME      ARN-II-CCP-100-1-C13
EXPNO               418011
PROCNO                   1

F2 - Acquisition Parameters
Date_            20180418
Time                13.39
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   100
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976128 sec
RG                   406
DW                19.800 usec
DE                 6.50 usec
TE                293.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

Ethyl (*E*)-2-cyano-3-phenylacrylate (**7b**)



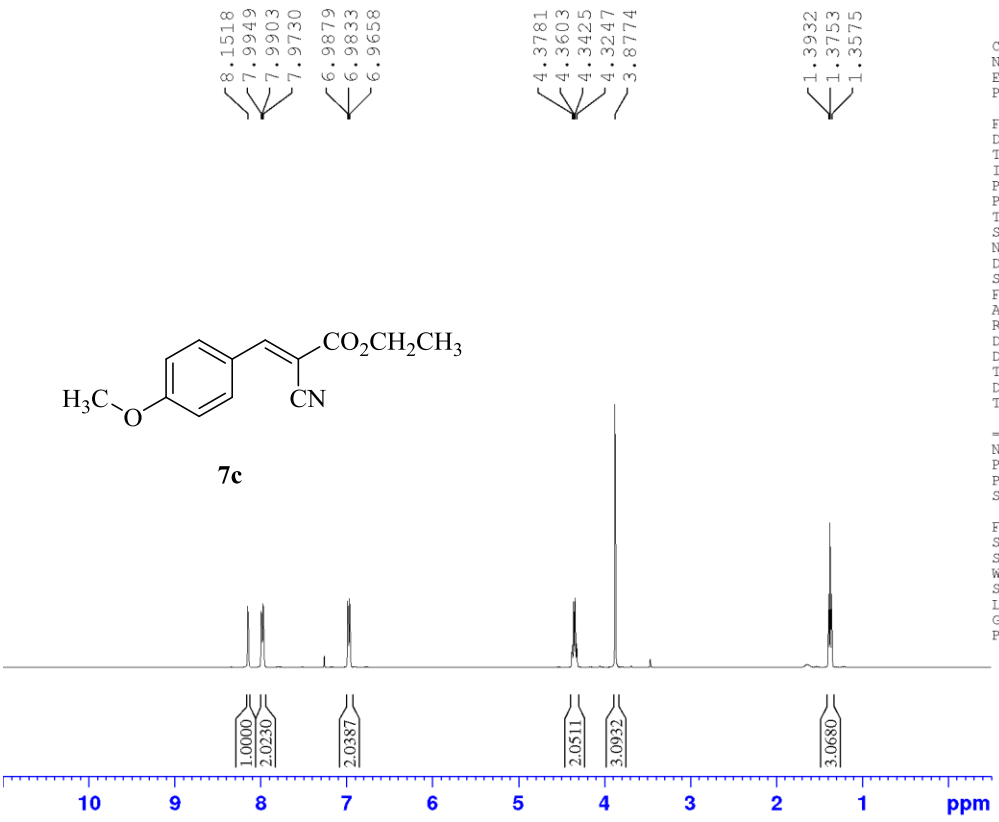

```
Current Data Parameters
NAME      ARN-II-CCP-114
EXPNO             505011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180505
Time               17.06
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                   256
DW                83.200 usec
DE                 6.50 usec
TE                293.9 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300093 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Ethyl (*E*)-2-cyano-3-phenylacrylate (**7b**)



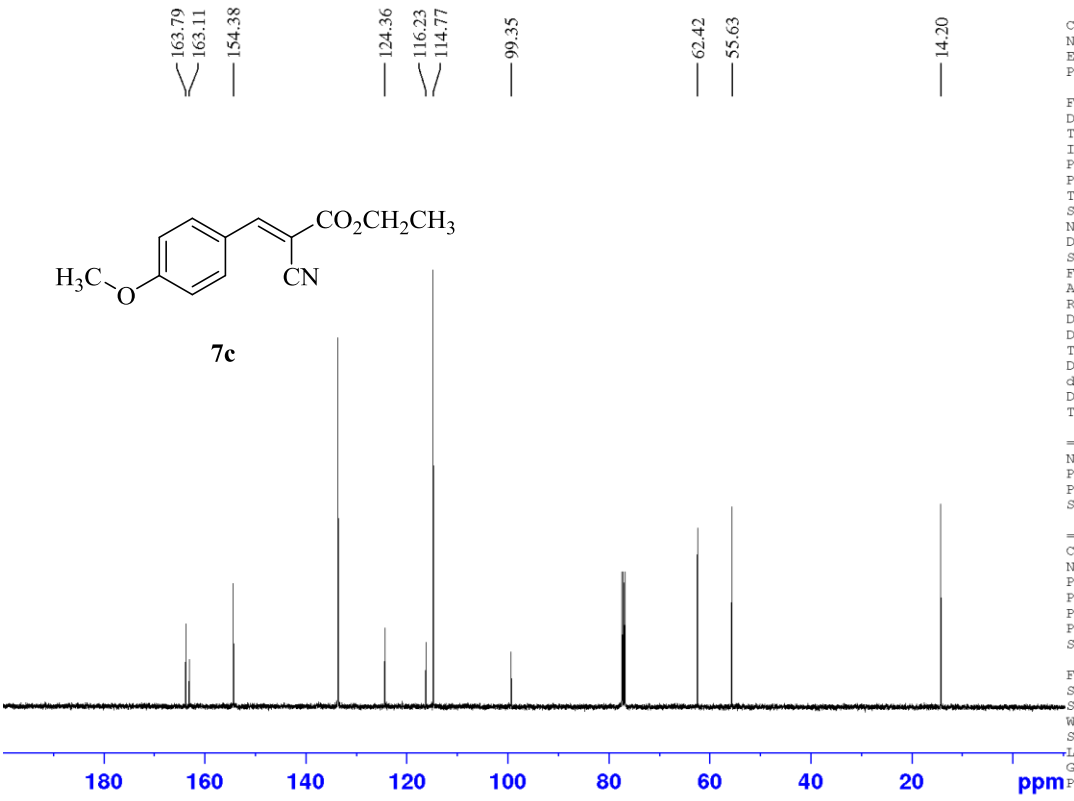

```
Current Data Parameters
NAME      ARN-II-CCP-114-c13
EXPNO              505011
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180505
Time               17.15
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDC13
NS                  100
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                  724
DW               19.800 usec
DE                6.50 usec
TE               294.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Ethyl (*Z*)-2-cyano-3-(4-methoxyphenyl) acrylate (**7c**)



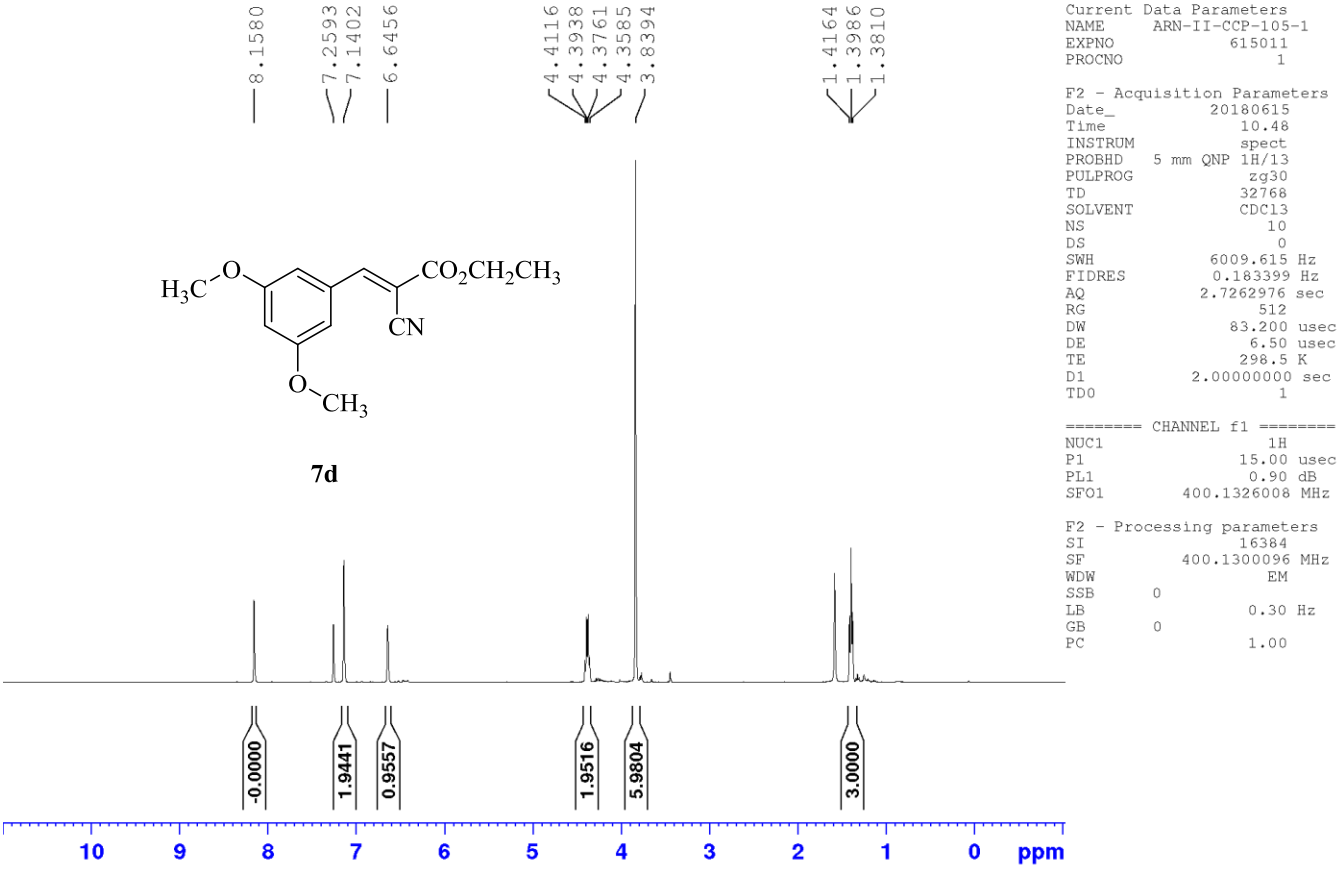

```
Current Data Parameters
NAME      ARN-II-CCP-112
EXPNO             205011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180521
Time               20.33
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   10
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG                  101
DW               83.200 usec
DE                6.50 usec
TE                297.3 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300087 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Ethyl (*Z*)-2-cyano-3-(4-methoxyphenyl) acrylate (**7c**)



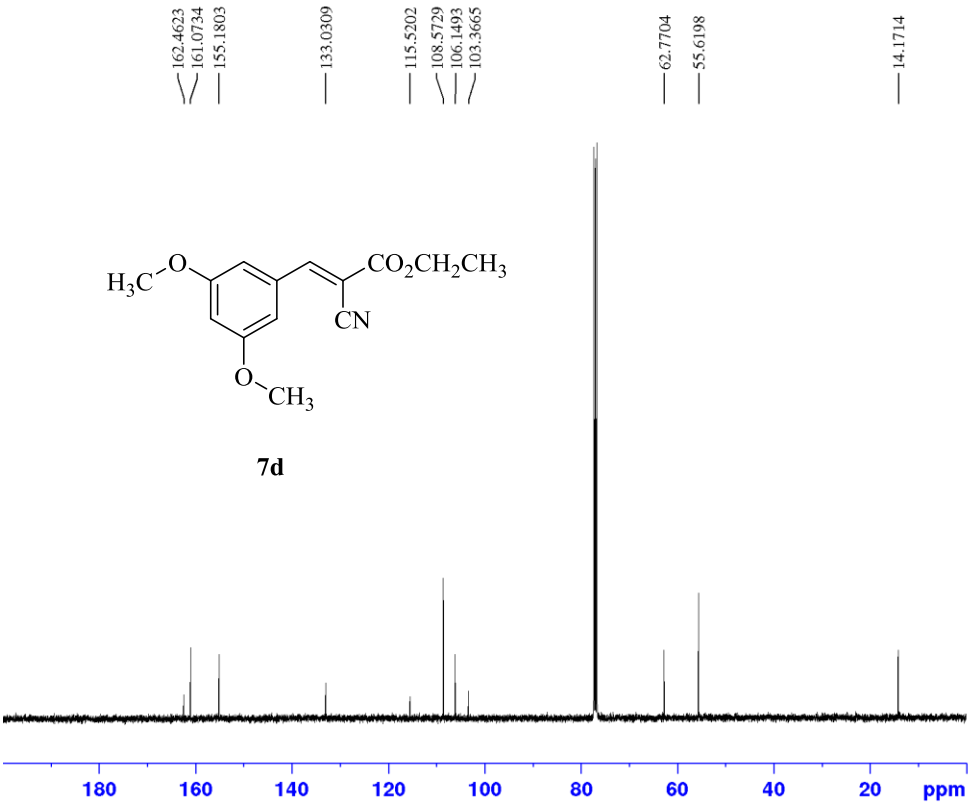

```
Current Data Parameters
NAME      ARN-II-CCP-112-C13
EXPNO              205011
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180521
Time               20.48
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                  724
DW               19.800 usec
DE                6.50 usec
TE                297.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PL1               6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2              -0.40 dB
PL12             15.80 dB
PL13             18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Ethyl (Z)-2-cyano-3-(3,5-dimethoxyphenyl)acrylate (**7d**)



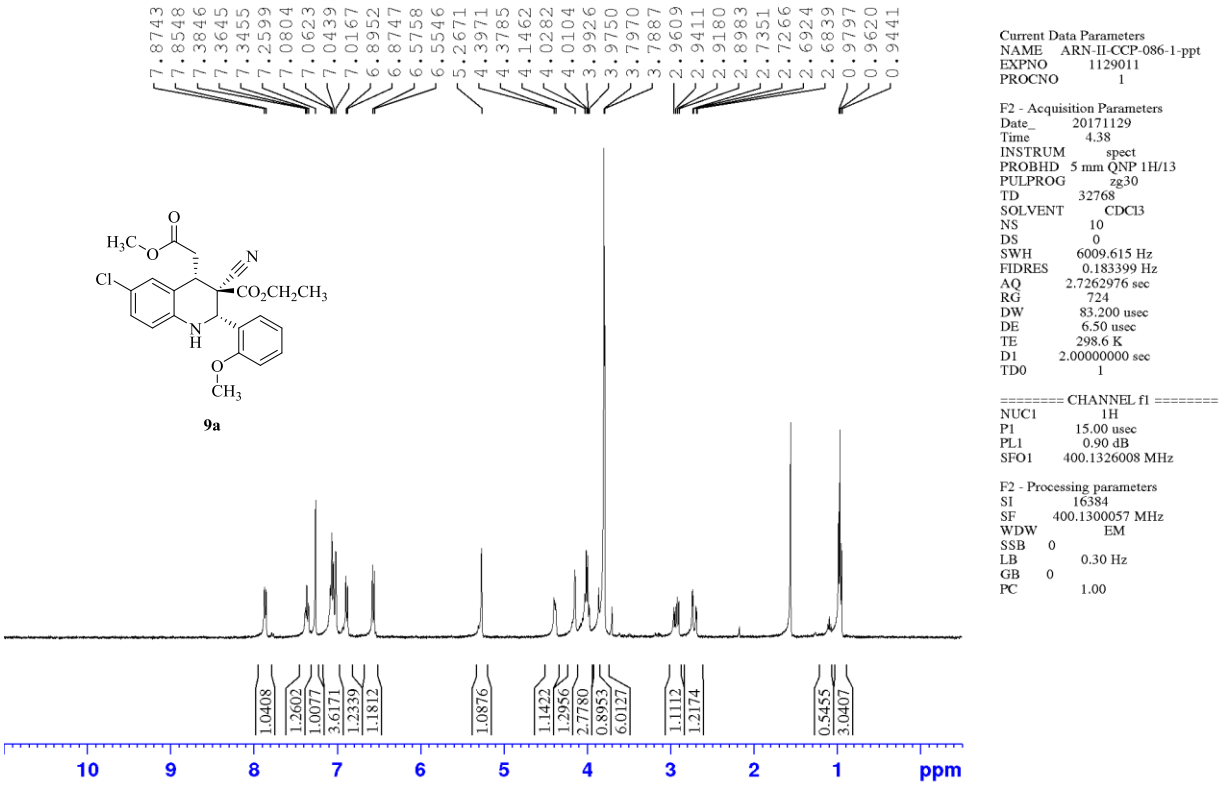

```
Current Data Parameters
NAME      ARN-II-CCP-105-1
EXPNO              615011
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180615
Time               10.48
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                   512
DW                83.200 usec
DE                 6.50 usec
TE                298.5 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300096 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Ethyl (*Z*)-2-cyano-3-(3,5-dimethoxyphenyl)acrylate (**7d**)




```
Current Data Parameters
NAME      ARN-II-CCP-105-1-c13
EXPNO              615011
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180615
Time                10.58
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   685
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976128 sec
RG                  1150
DW                19.800 usec
DE                 6.50 usec
TE                298.8 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9a**)



9a

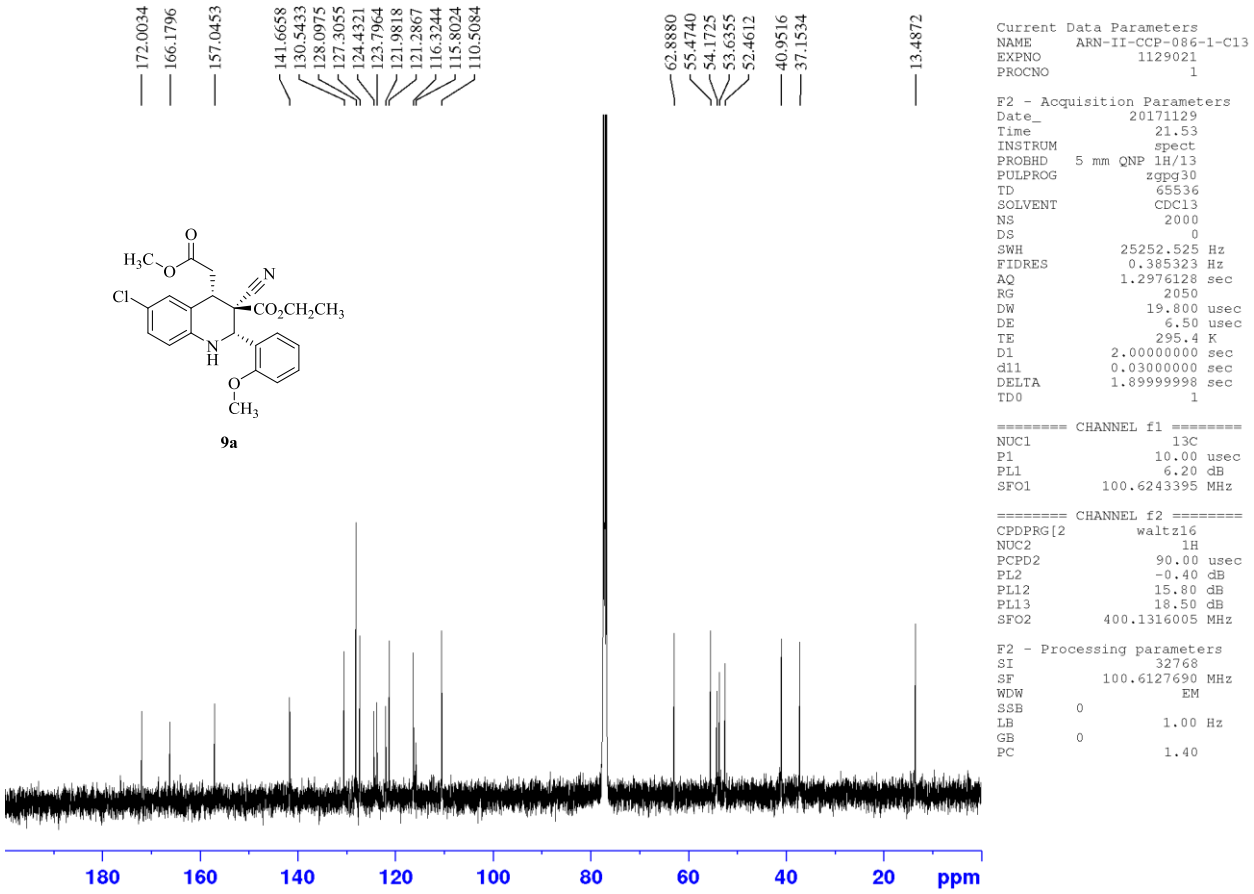
Current Data Parameters
NAME ARN-II-CCP-086-1-ppt
EXPNO 1129011
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171129
Time 4.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 724
DW 83.200 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 0.90 dB
SFO1 400.1326008 MHz

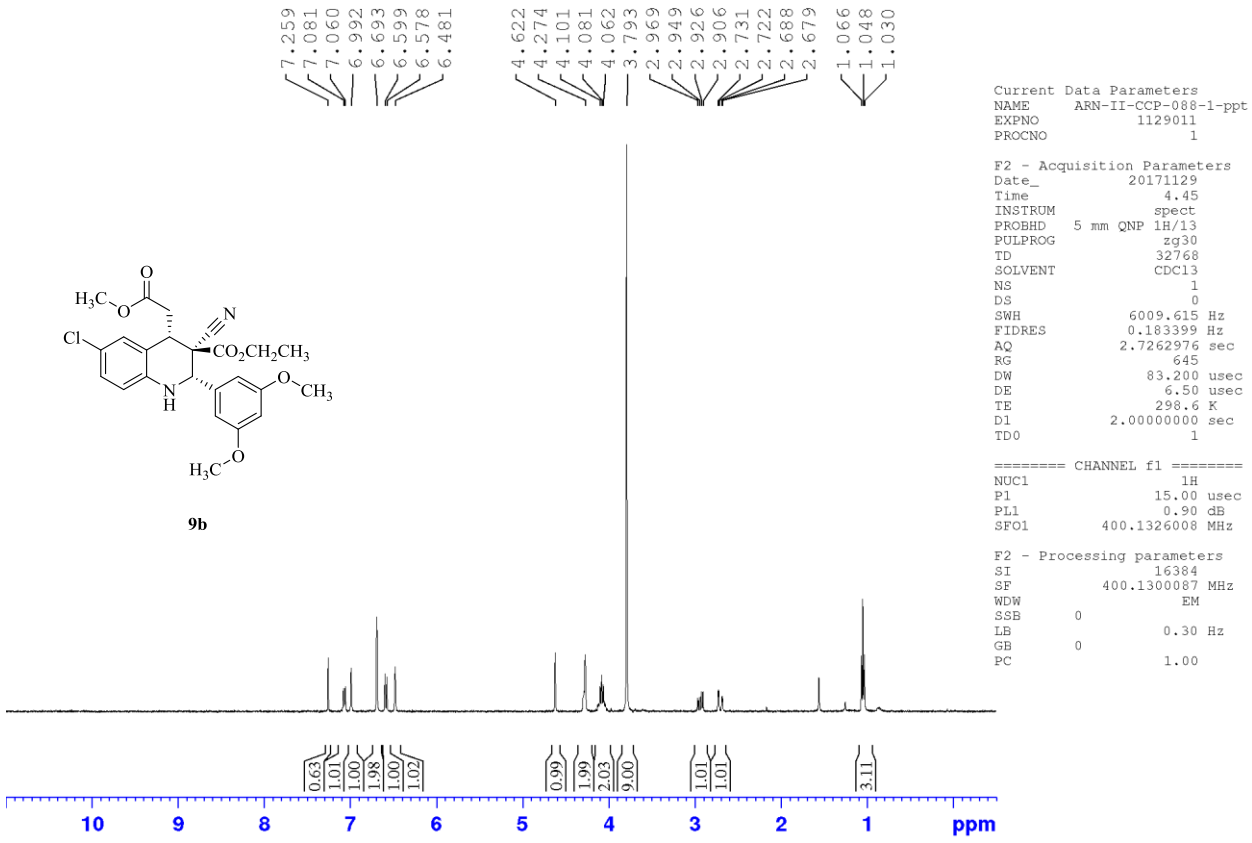
F2 - Processing parameters
SI 16384
SF 400.1300057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9a**)

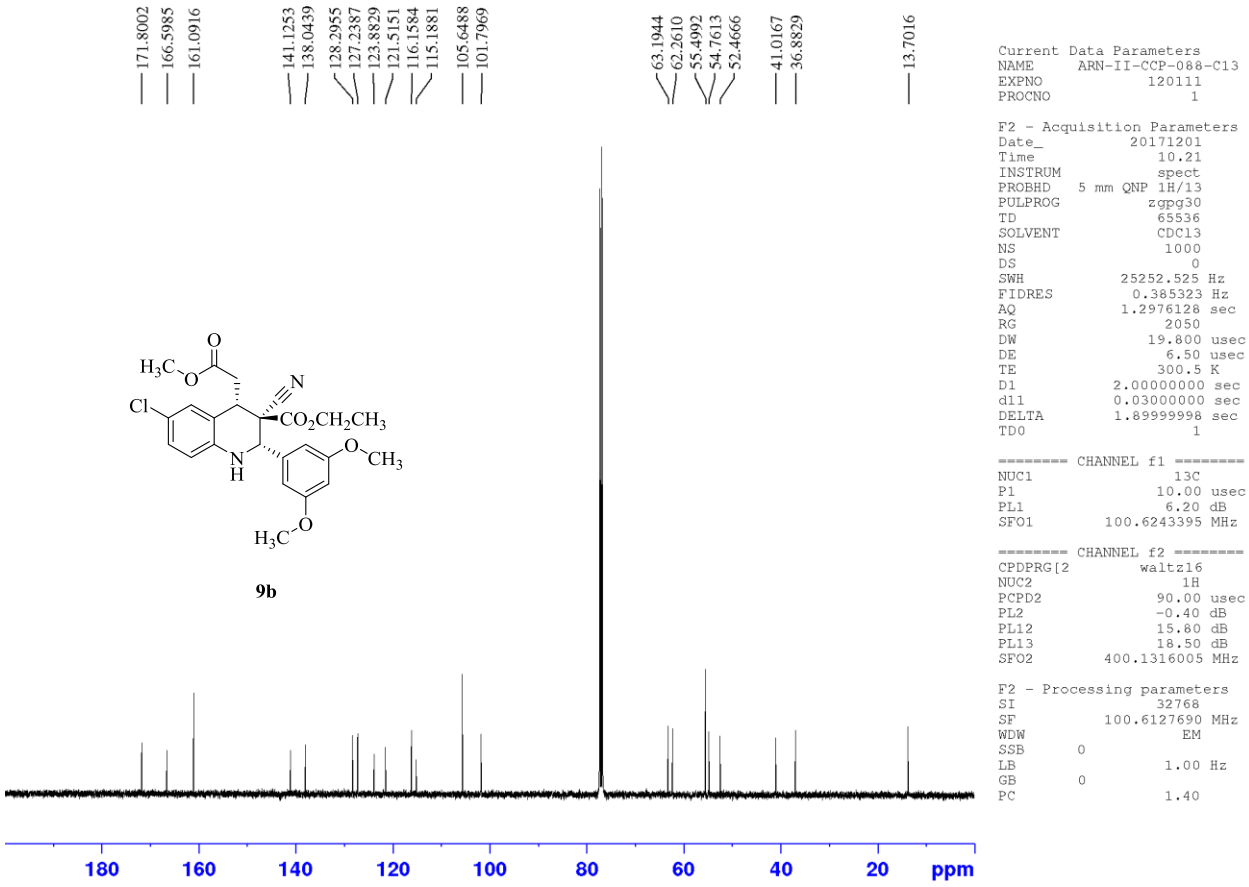



```
Current Data Parameters
NAME      ARN-II-CCP-086-1-C13
EXPNO              1129021
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171129
Time                21.53
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2000
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976128 sec
RG                  2050
DW                19.800 usec
DE                 6.50 usec
TE                295.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9b**)

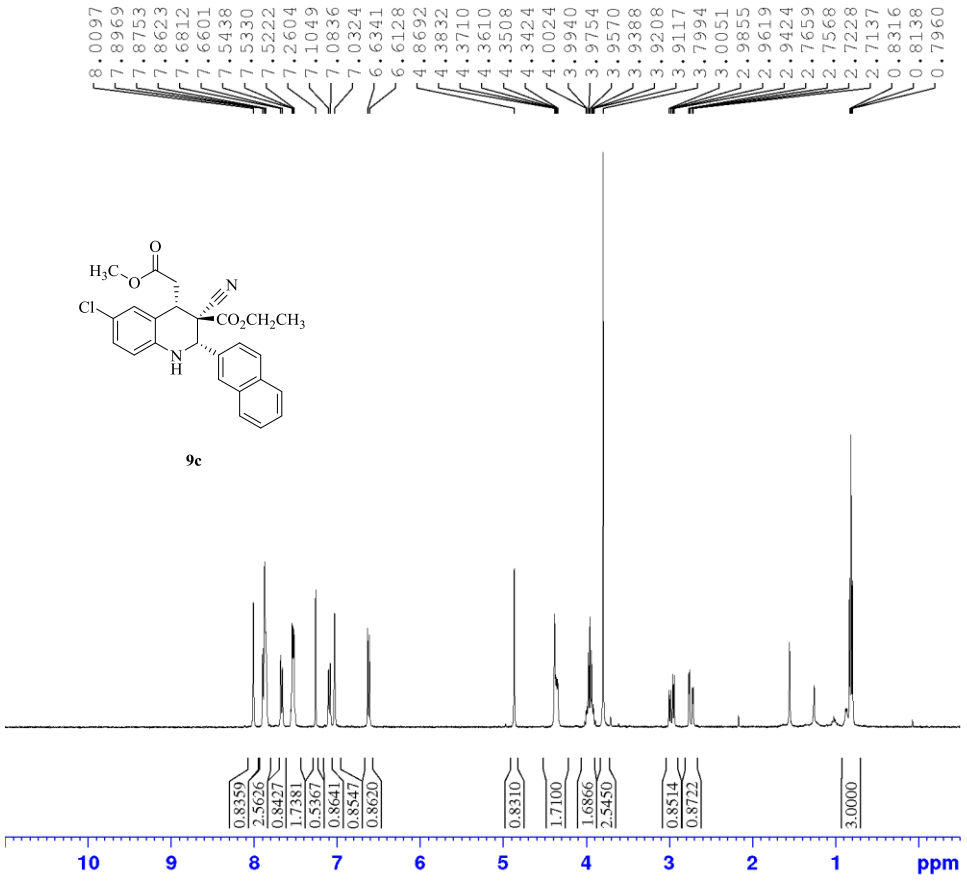


Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9b**)




```
Current Data Parameters
NAME      ARN-II-CCP-088-C13
EXPNO              120111
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171201
Time               10.21
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1000
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE                300.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

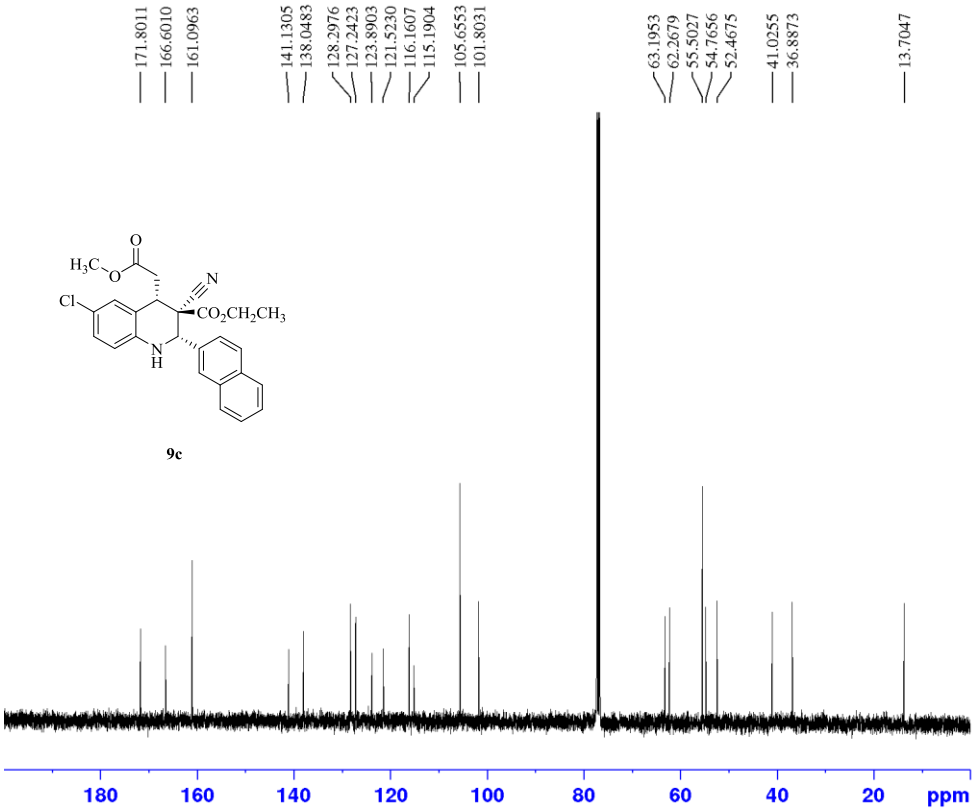
Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9c**)



9c

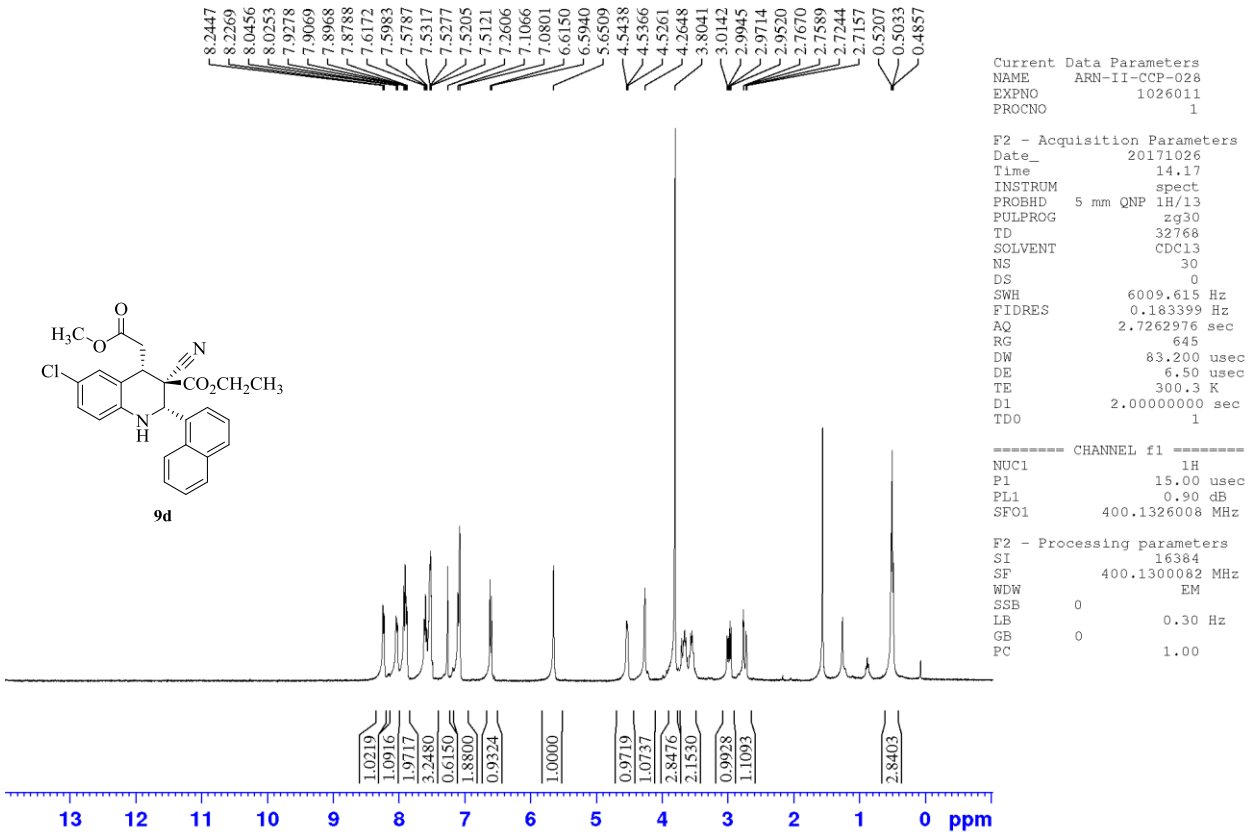
```
Current Data Parameters
NAME      ARN-II-CCP-85-ppt
EXPNO           1129011
PROCNO                1

F2 - Acquisition Parameters
Date_          20171129
Time               4.30
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  10
DS                   0
SWH           6009.615 Hz
FIDRES         0.183399 Hz
AQ            2.7262976 sec
RG                 645
DW              83.200 usec
DE               6.50 usec
TE              298.6 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1              15.00 usec
PL1              0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300081 MHz
WDW                  EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9c**)



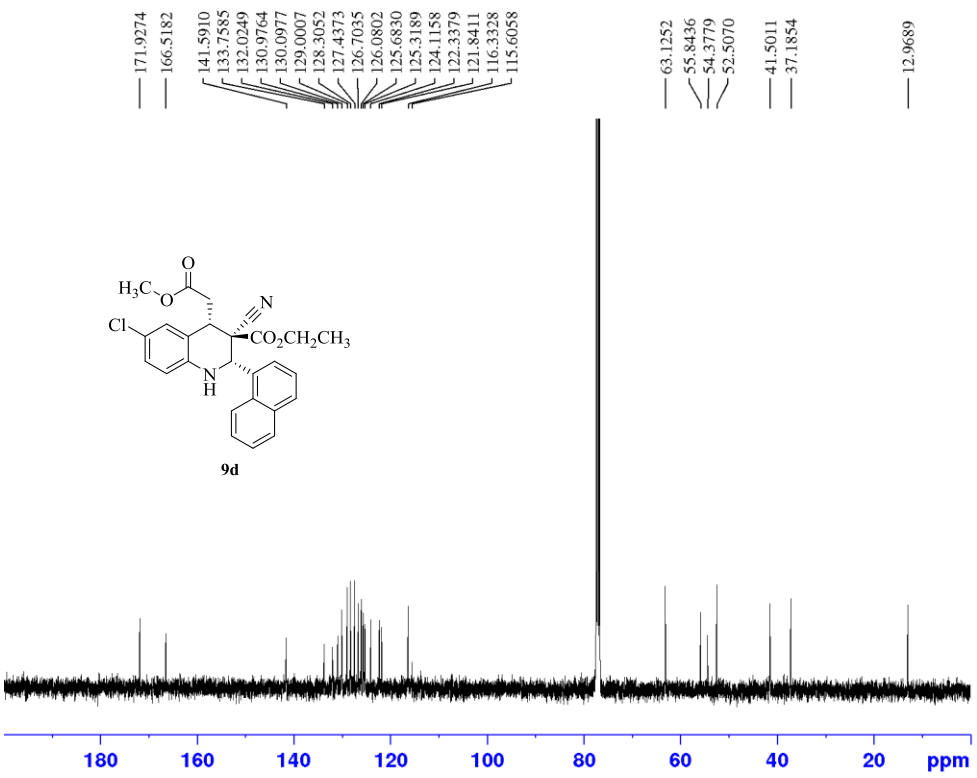

```
Current Data Parameters
NAME      ARN-II-CCP-85-ppt-C13-1
EXPNO               1129021
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171130
Time                  15.31
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      509
DS                        0
SWH               25252.525 Hz
FIDRES            0.385323 Hz
AQ                1.2976128 sec
RG                     2050
DW                   19.800 usec
DE                    6.50 usec
TE                   300.9 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.00 usec
PL1                    6.20 dB
SFO1          100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                    1H
PCPD2                 90.00 usec
PL2                   -0.40 dB
PL12                  15.80 dB
PL13                  18.50 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF            100.6127690 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-1-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9d**)



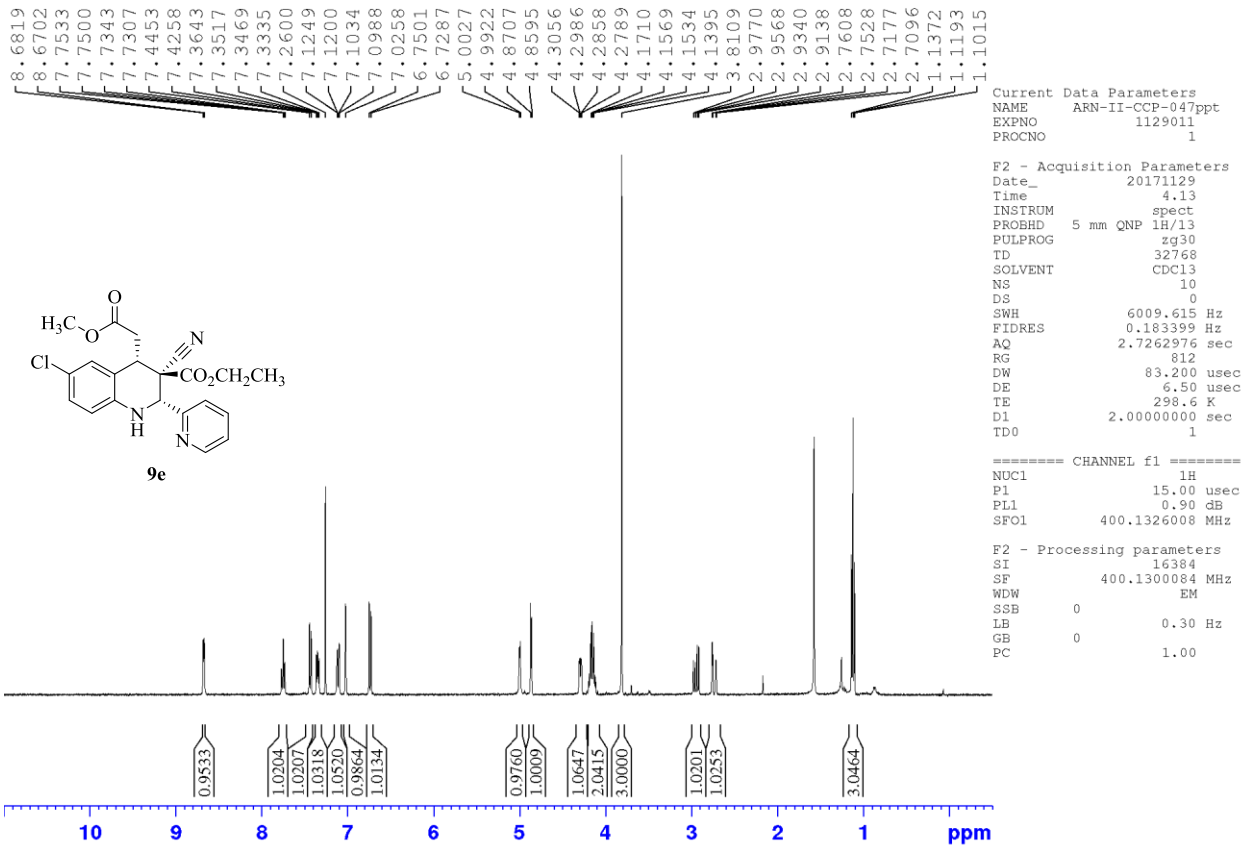

```
Current Data Parameters
NAME      ARN-II-CCP-028
EXPNO            1026011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171026
Time               14.17
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   30
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG                  645
DW               83.200 usec
DE                6.50 usec
TE                300.3 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300082 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-1-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9d**)



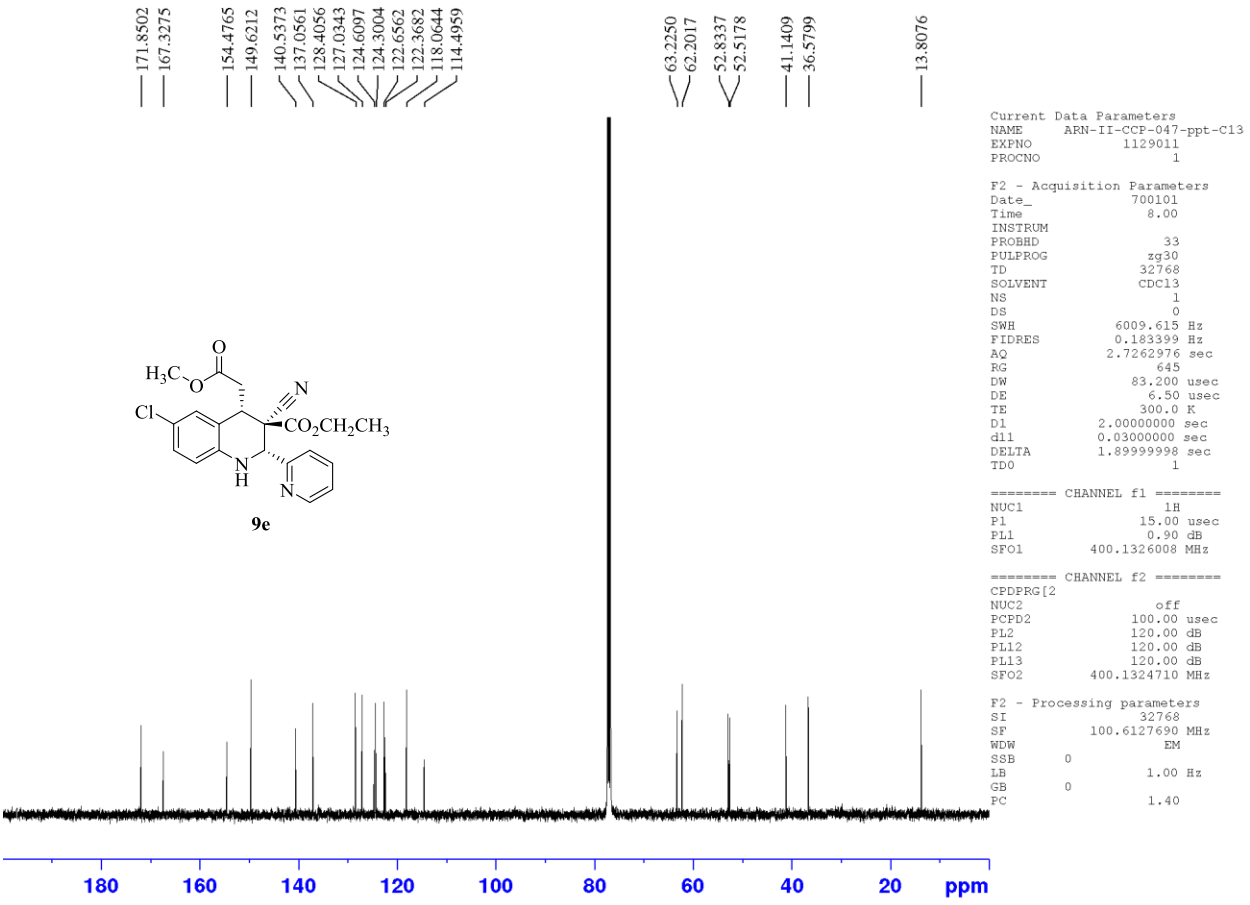

```
Current Data Parameters
NAME      ARN-II-CCP-028 C13-1
EXPNO            1026021
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171026
Time              21.23
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  976
DS                    0
SWH           25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE               299.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Racemeate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(pyridin-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9e**)



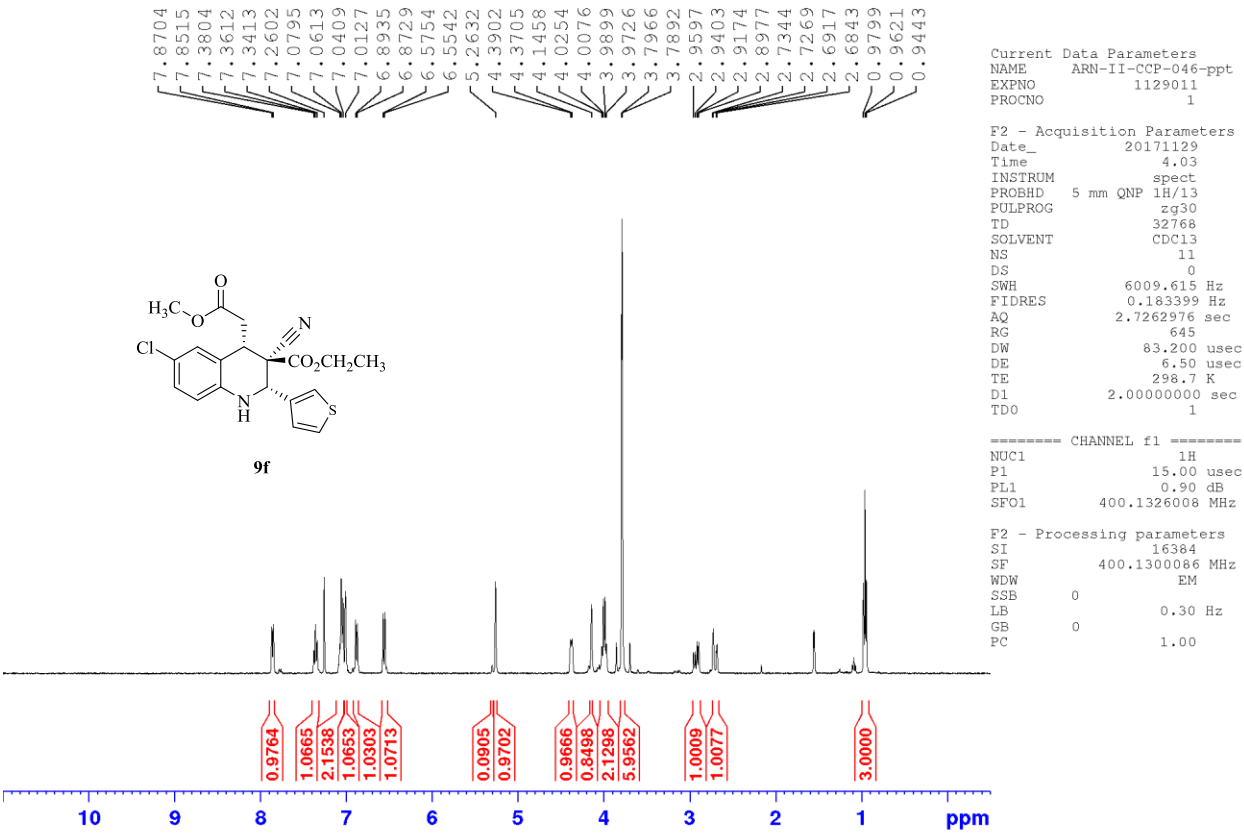
9e

Racemeate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(pyridin-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9e**)



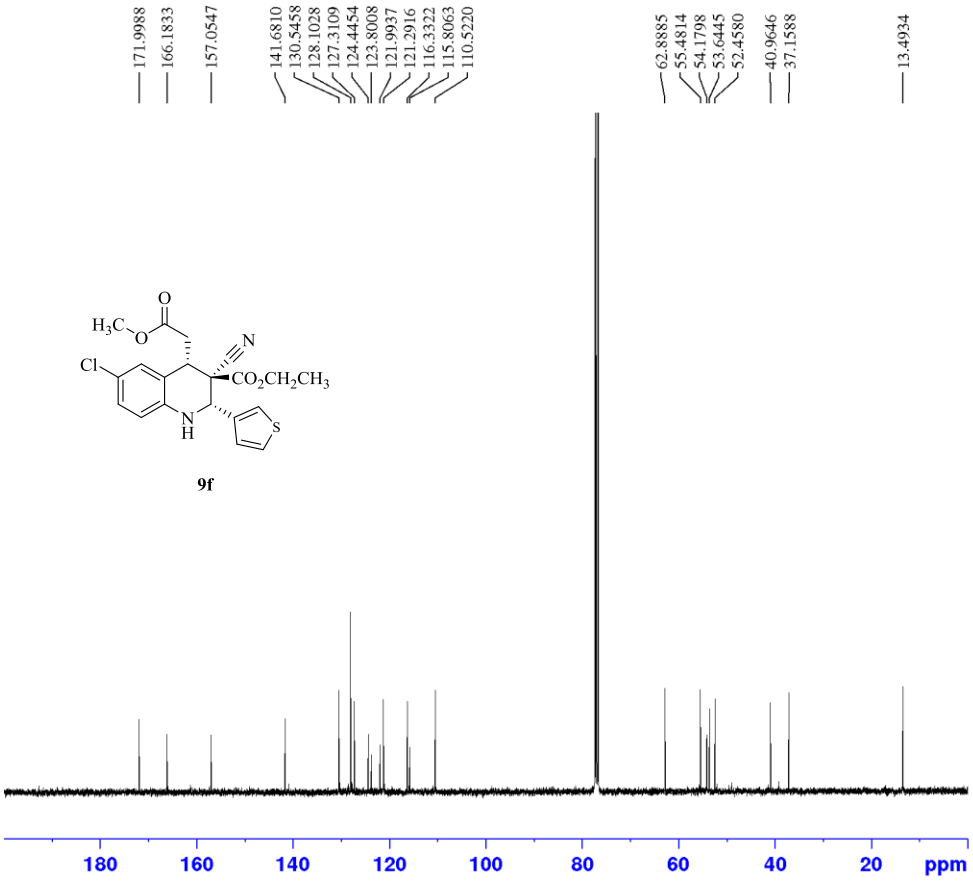

```
Current Data Parameters
NAME      ARN-II-CCP-047-ppt-C13
EXPNO               1129011
PROCNO                    1

F2 - Acquisition Parameters
Date_               700101
Time                  8.00
INSTRUM
PROBHD                  33
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                        1
DS                        0
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                      645
DW                   83.200 usec
DE                    6.50 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    15.00 usec
PL1                    0.90 dB
SFO1          400.1326008 MHz

======== CHANNEL f2 ========
CPDPRG[2
NUC2                   off
PCPD2               100.00 usec
PL2                 120.00 dB
PL12                120.00 dB
PL13                120.00 dB
SFO2          400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF             100.6127690 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(thiophen-3-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9f**)



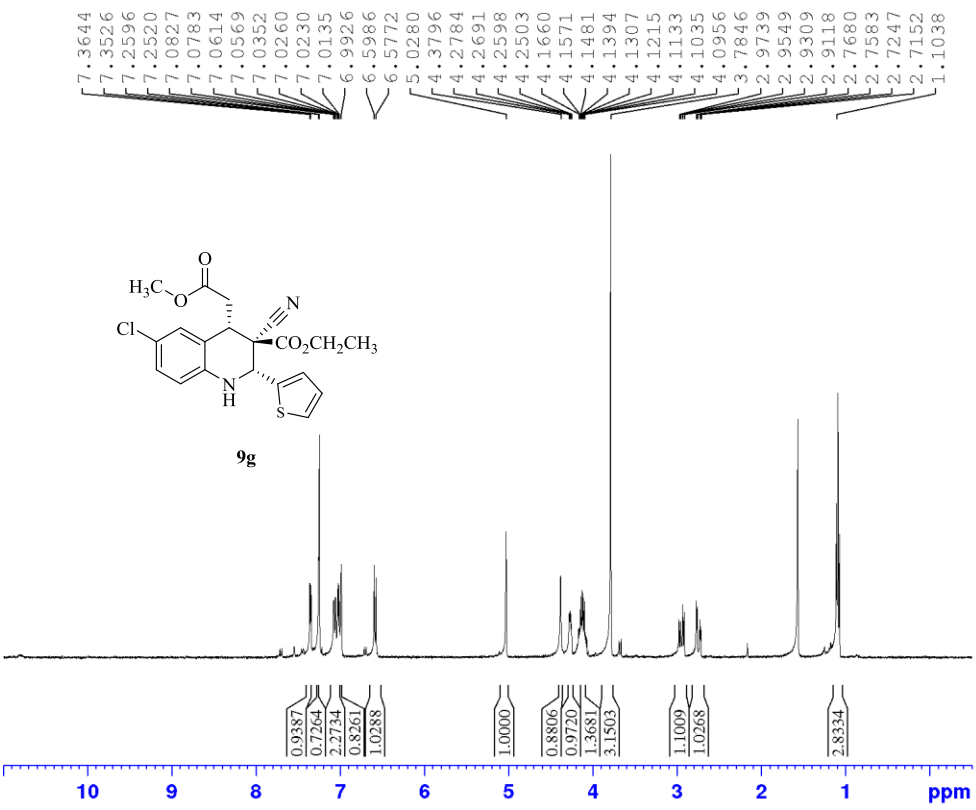

```
Current Data Parameters
NAME      ARN-II-CCP-046-ppt
EXPNO              1129011
PROCNO                   1

F2 - Acquisition Parameters
Date_            20171129
Time                 4.03
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     11
DS                      0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                    645
DW                 83.200 usec
DE                  6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                 0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300086 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(thiophen-3-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9f**)



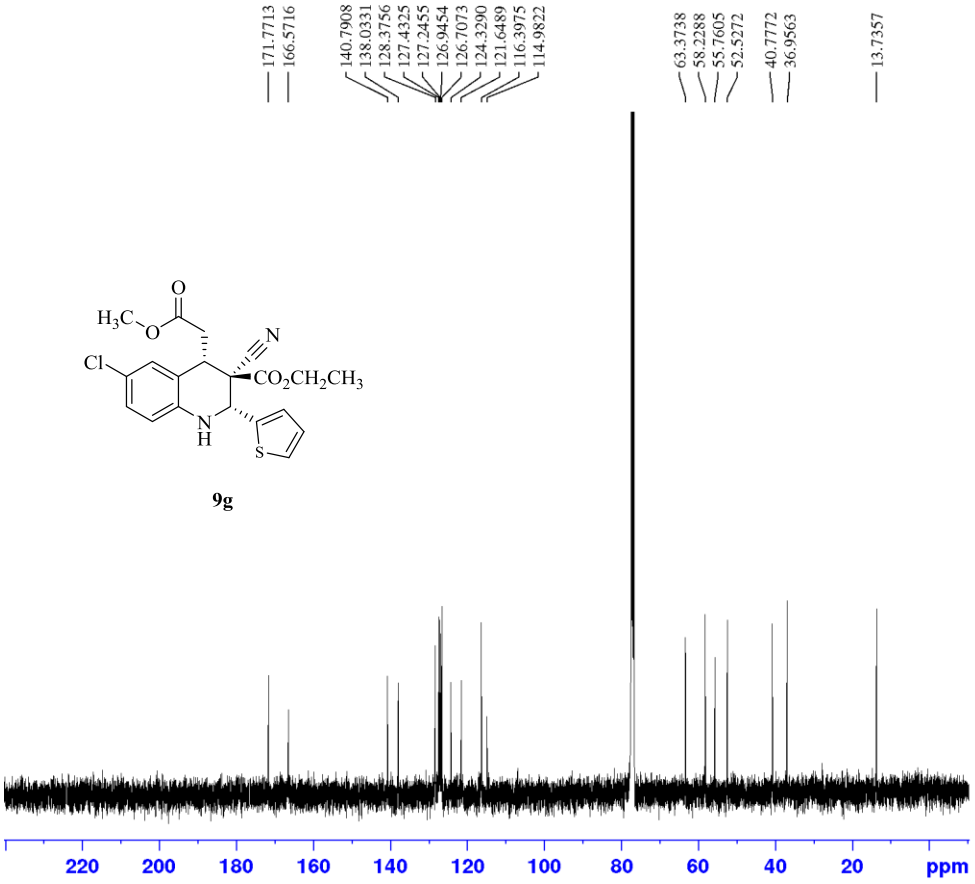

```
Current Data Parameters
NAME      ARN-II-CCP-046-1-C13
EXPNO              1129021
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171129
Time                 18.03
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2000
DS                      0
SWH             25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976128 sec
RG                   2050
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                 -0.40 dB
PL12                15.80 dB
PL13                18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(thiophen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9g**)



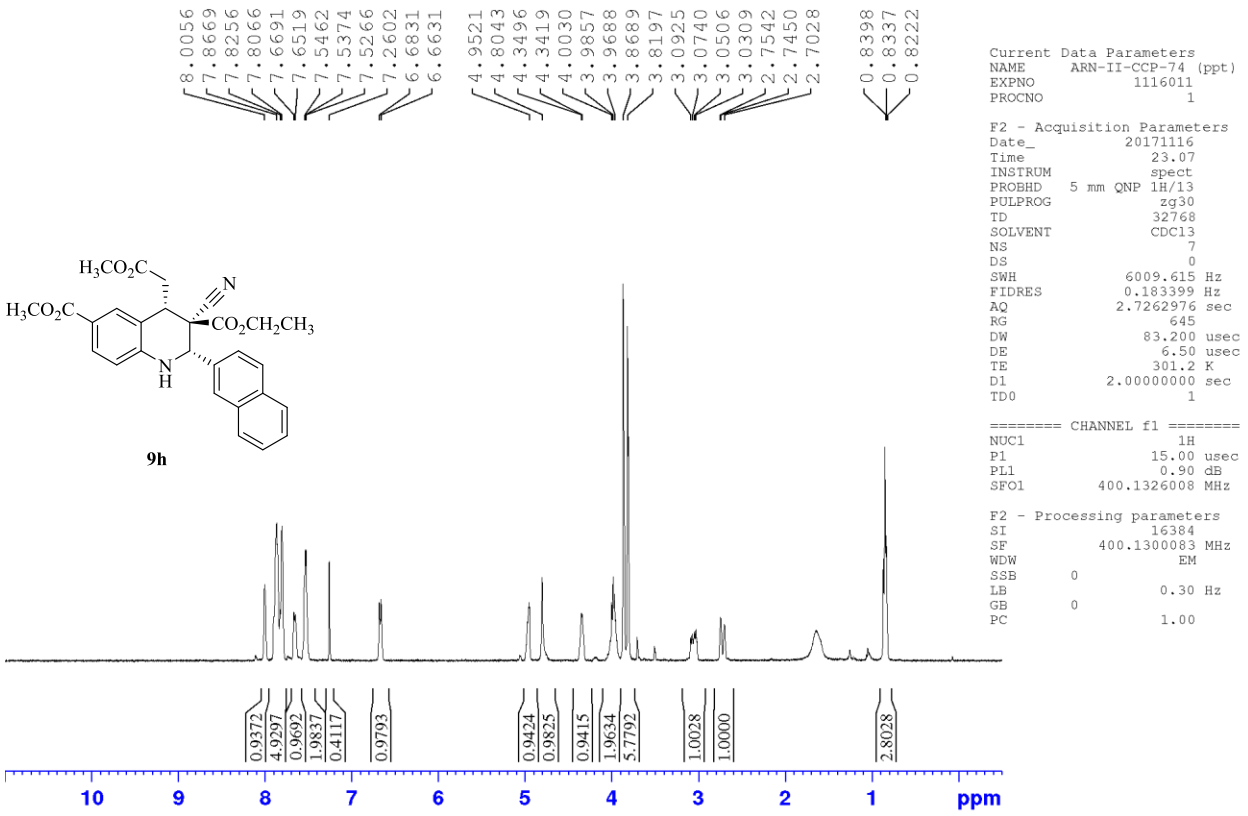

```
Current Data Parameters
NAME      ARN-II-CCP-45-ppt
EXPNO           1129011
PROCNO                1

F2 - Acquisition Parameters
Date_          20171129
Time               4.22
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   10
DS                    0
SWH            6009.615 Hz
FIDRES         0.183399 Hz
AQ             2.7262976 sec
RG                 1150
DW               83.200 usec
DE                6.50 usec
TE                298.6 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300101 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 6-chloro-3-cyano-4-(2-methoxy-2-oxoethyl)-2-(thiophen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9g**)

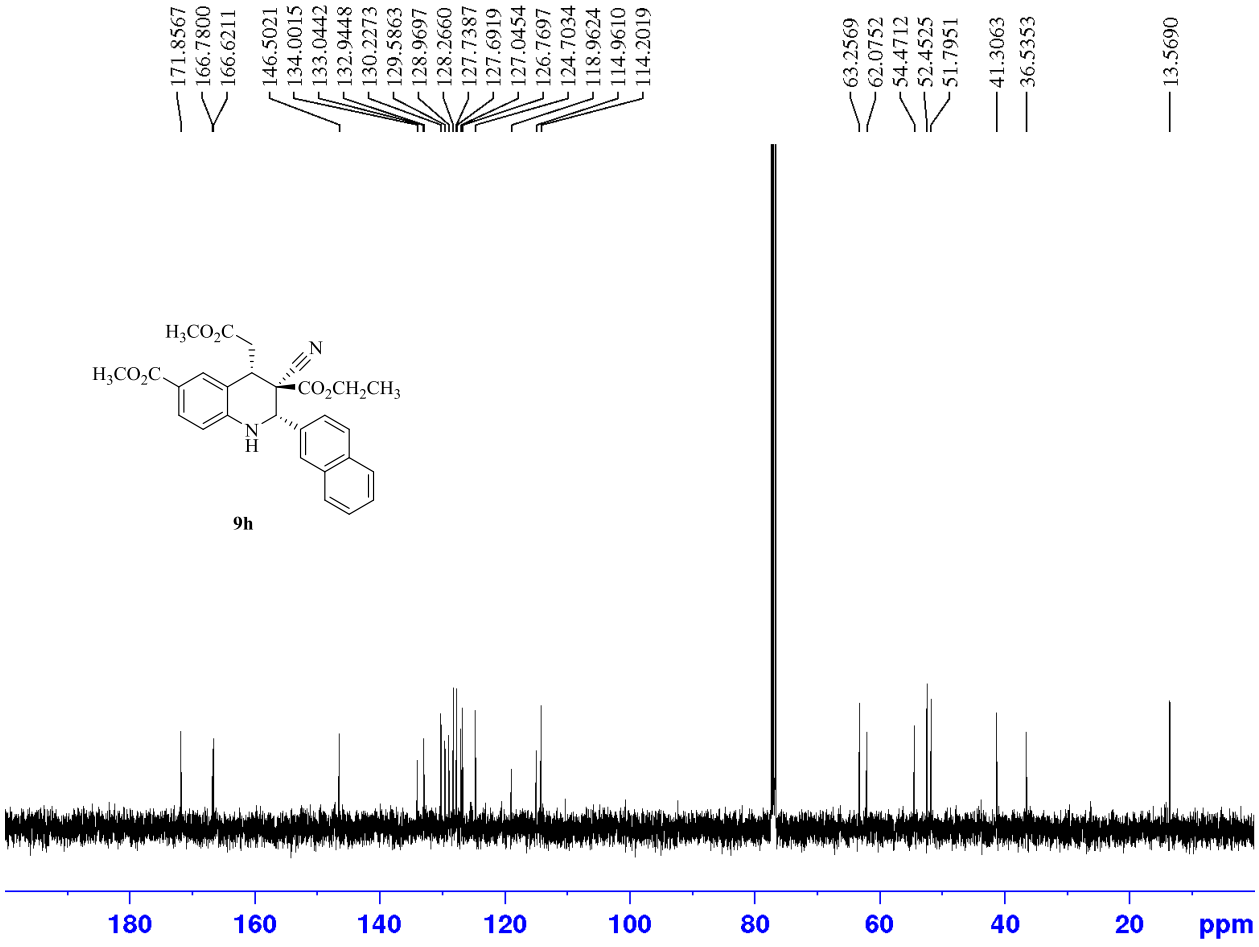



```
Current Data Parameters
NAME      ARN-II-CCP-045-1-C13
EXPNO              1129021
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171129
Time              16.06
INSTRUM           spect
PROBHD    5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1733
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE               296.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PL1               6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2              -0.40 dB
PL12             15.80 dB
PL13             18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

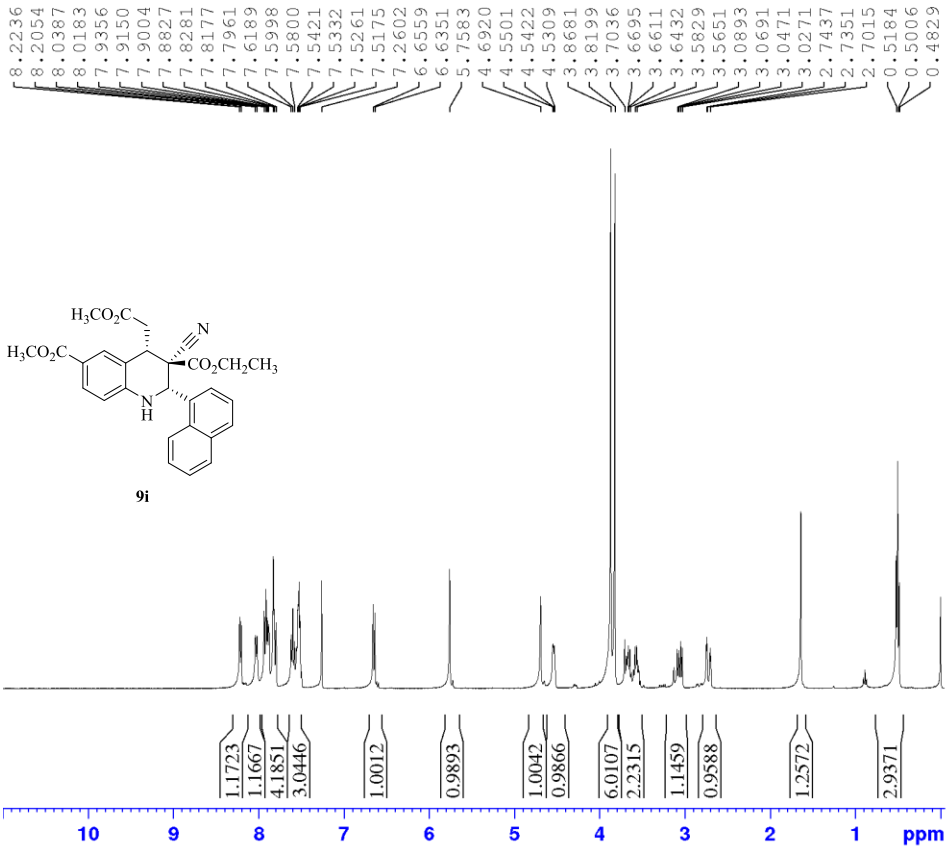
Racemate of 3-ethyl, 6-methyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-2-yl)-1,2,3,4-tetrahydroquinoline-3,6-dicarboxylate (**9h**)



Racemate of 3-ethyl, 6-methyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-2-yl)-1,2,3,4-tetrahydroquinoline-3,6-dicarboxylate (**9h**)

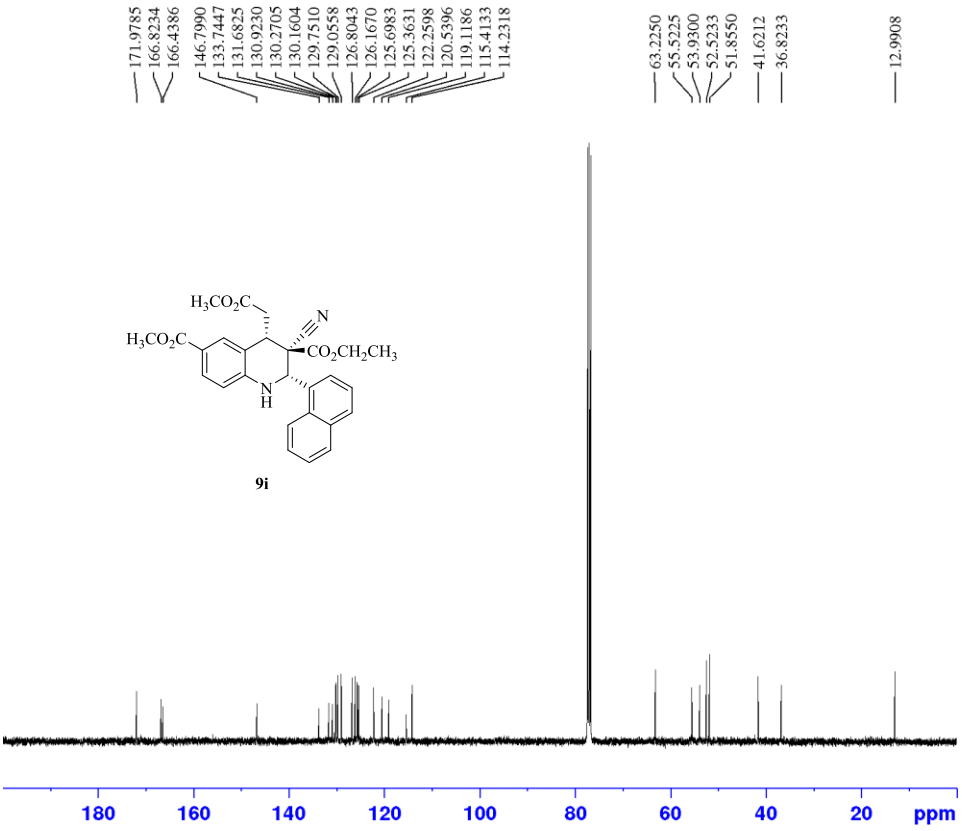


Racemate of 3-ethyl, 6-methyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-1-yl)-1,2,3,4-tetrahydroquinoline-3,6-dicarboxylate (**9i**).



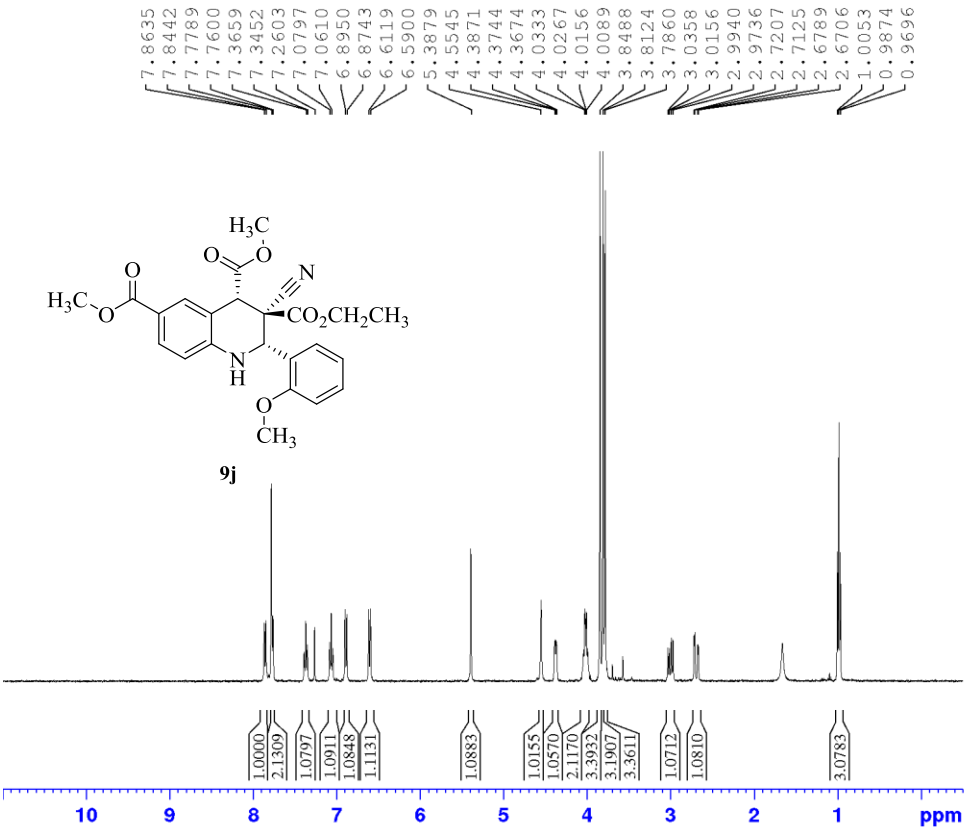

```
Current Data Parameters
NAME      ARN-II-CCP-73-2-ppt
EXPNO              411011
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180411
Time               15.59
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                   287
DW                83.200 usec
DE                 6.50 usec
TE                293.5 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300082 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of 3-ethyl 6-methyl 3-cyano-4-(2-methoxy-2-oxoethyl)-2-(naphthalen-1-yl)-1,2,3,4-tetrahydroquinoline-3,6-dicarboxylate (**9i**).



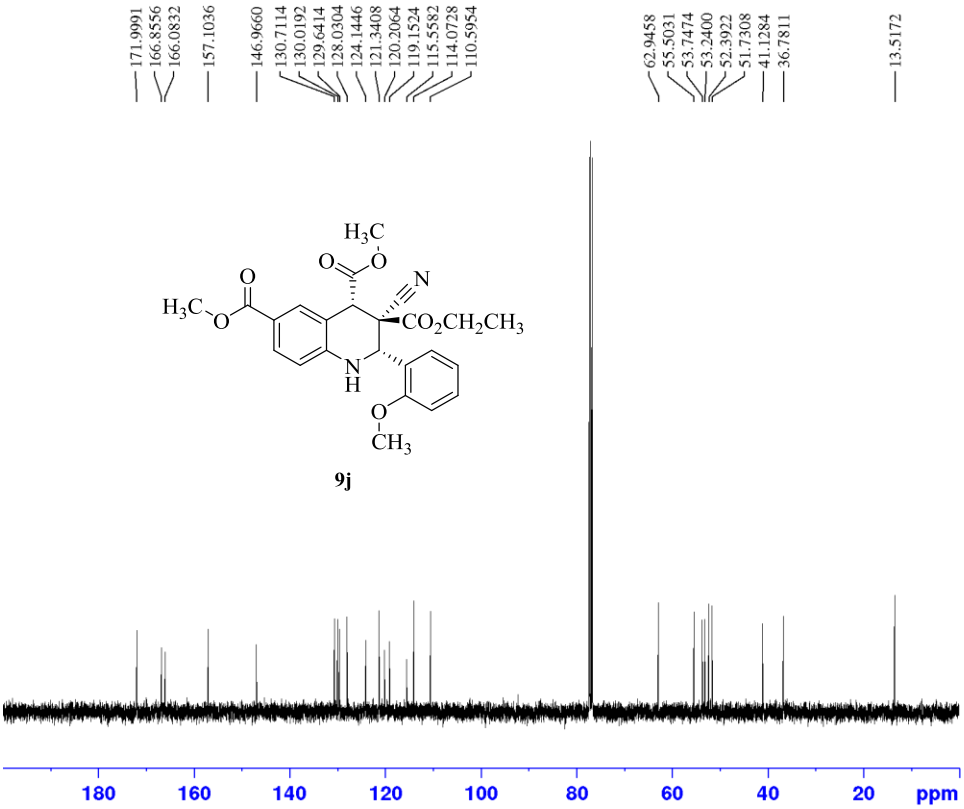

```
Current Data Parameters
NAME      ARN-II-CCP-73-2-ppt-c13
EXPNO               411011
PROCNO                   1

F2 - Acquisition Parameters
Date_            20180411
Time                16.09
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1107
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976128 sec
RG                   406
DW                19.800 usec
DE                 6.50 usec
TE                294.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Racemate of 3-ethyl, 4,6-dimethyl 3-cyano-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3,4,6-tricarboxylate (**9j**)




```
Current Data Parameters
NAME      ARN-II-CCP-075(ppt)
EXPNO           1116011
PROCNO                1

F2 - Acquisition Parameters
Date_          20171116
Time              23.40
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   1
DS                   0
SWH           6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG                 406
DW              83.200 usec
DE               6.50 usec
TE              301.2 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1              15.00 usec
PL1              0.90 dB
SFO1       400.1326008 MHz

F2 - Processing parameters
SI                16384
SF         400.1300080 MHz
WDW                  EM
SSB       0
LB               0.30 Hz
GB        0
PC               1.00
```

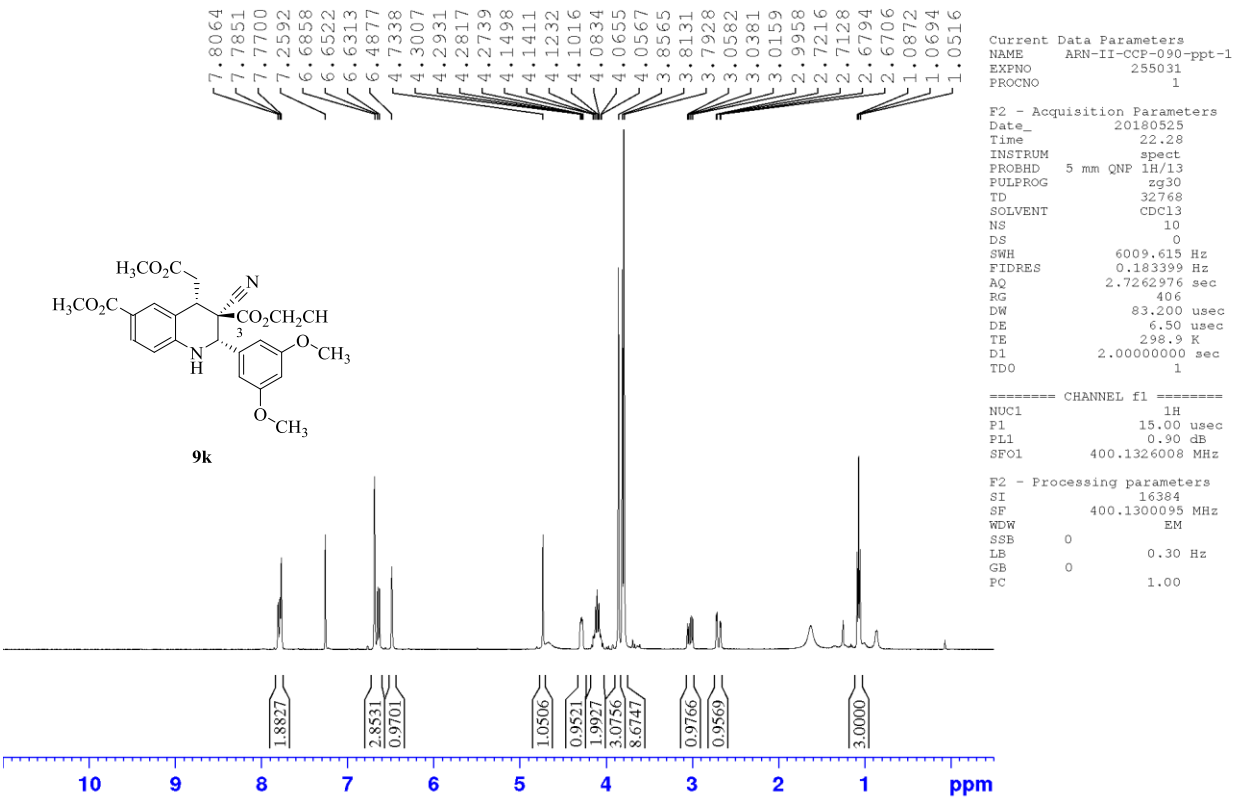
Racemate of 3-ethyl, 4,6-dimethyl 3-cyano-2-(2-methoxyphenyl)-1,2,3,4-tetrahydroquinoline-3,4,6-tricarboxylate (**9j**)



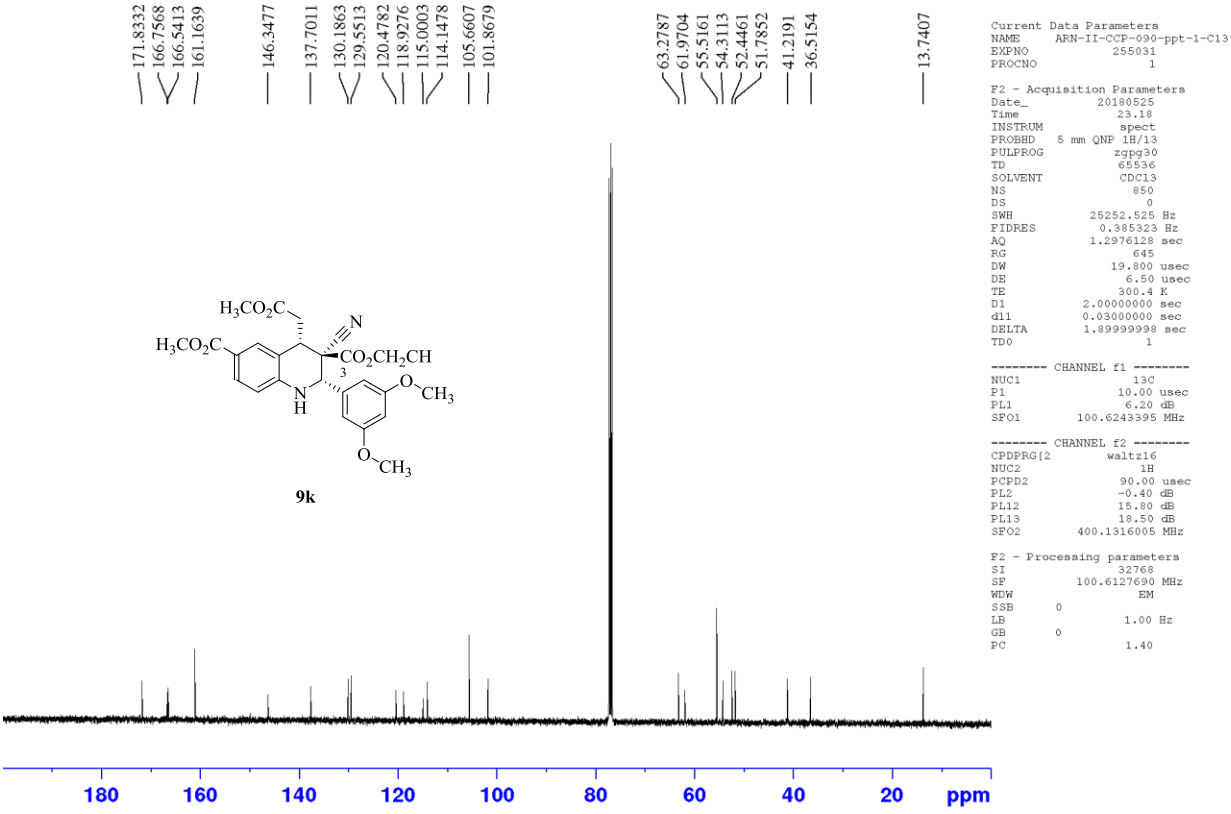
9j

```
Current Data Parameters
NAME      ARN-II-CCP-075(ppt)-C13
EXPNO              1116011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171116
Time              23.49
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   95
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE                301.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Racemate of 3-ethyl, 6-methyl 3-cyano-2-(3,5-dimethoxyphenyl)-4-(2-methoxy-2-oxoethyl)-1,2,3,4-tetrahydroquinoline-3,6-dicarboxylate (**9k**)

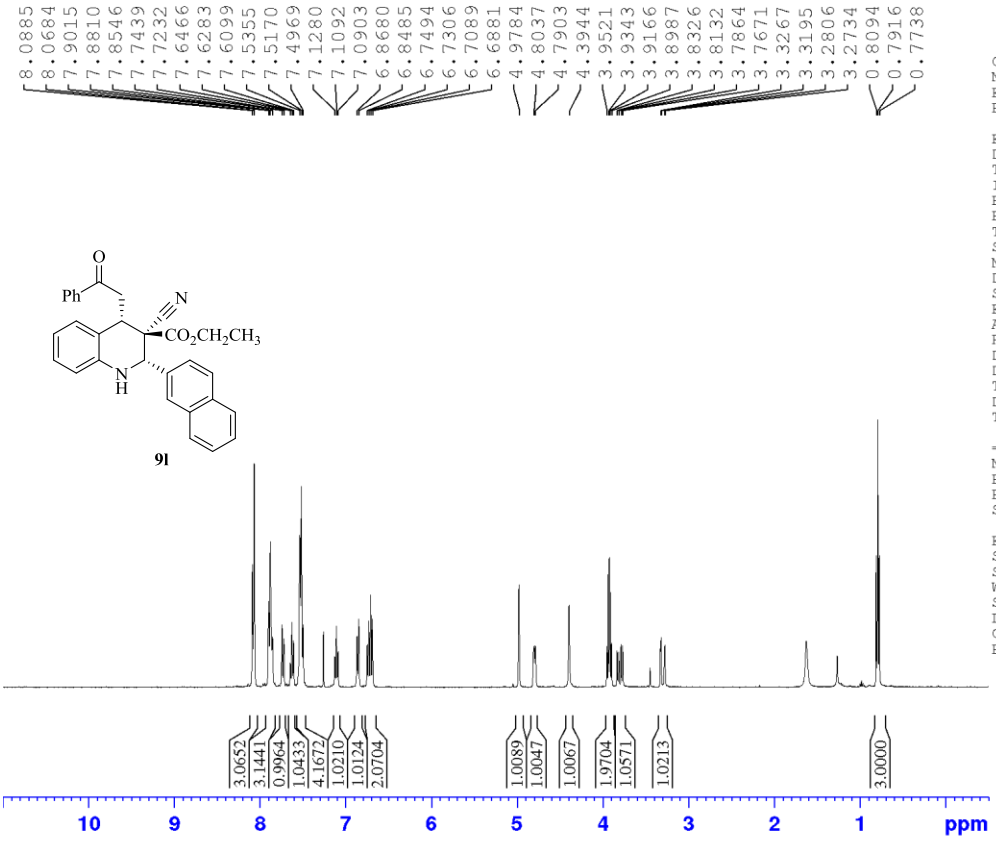


Racemate of 3-ethyl, 6-methyl 3-cyano-2-(3,5-dimethoxyphenyl)-4-(2-methoxy-2-oxoethyl)-1,2,3,4-tetrahydroquinoline-3,6-dicarboxylate (**9k**)



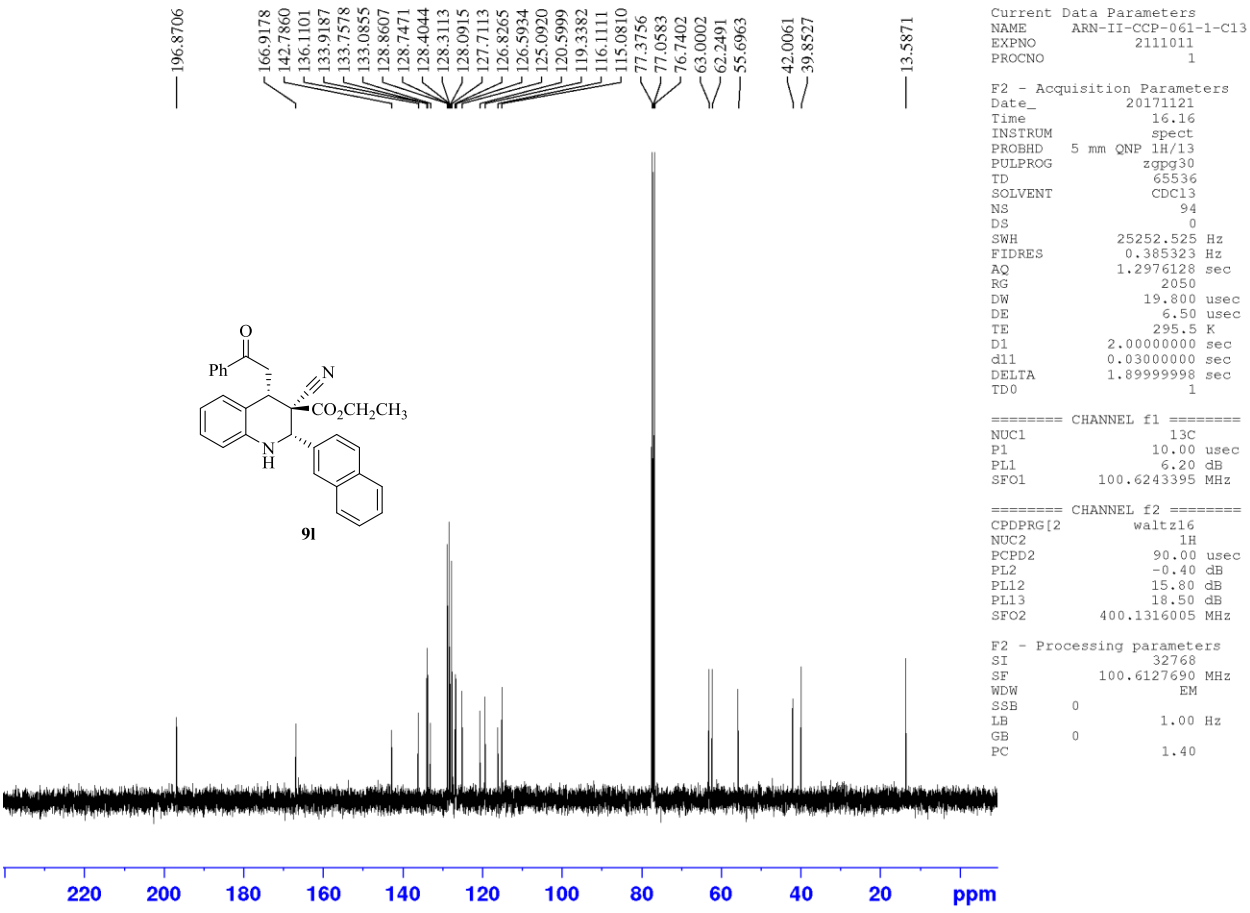

```
Current Data Parameters
NAME      ARN-II-CCP-090-ppt-1-C13
EXPNO              255031
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180525
Time                23.18
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    850
DS                      0
SWH             25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976128 sec
RG                    645
DW                19.800 usec
DE                 6.50 usec
TE                 300.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                     1

-------- CHANNEL f1 --------
NUC1                  13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

-------- CHANNEL f2 --------
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Racemate of ethyl 3-cyano-2-(naphthalen-2-yl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9l**)



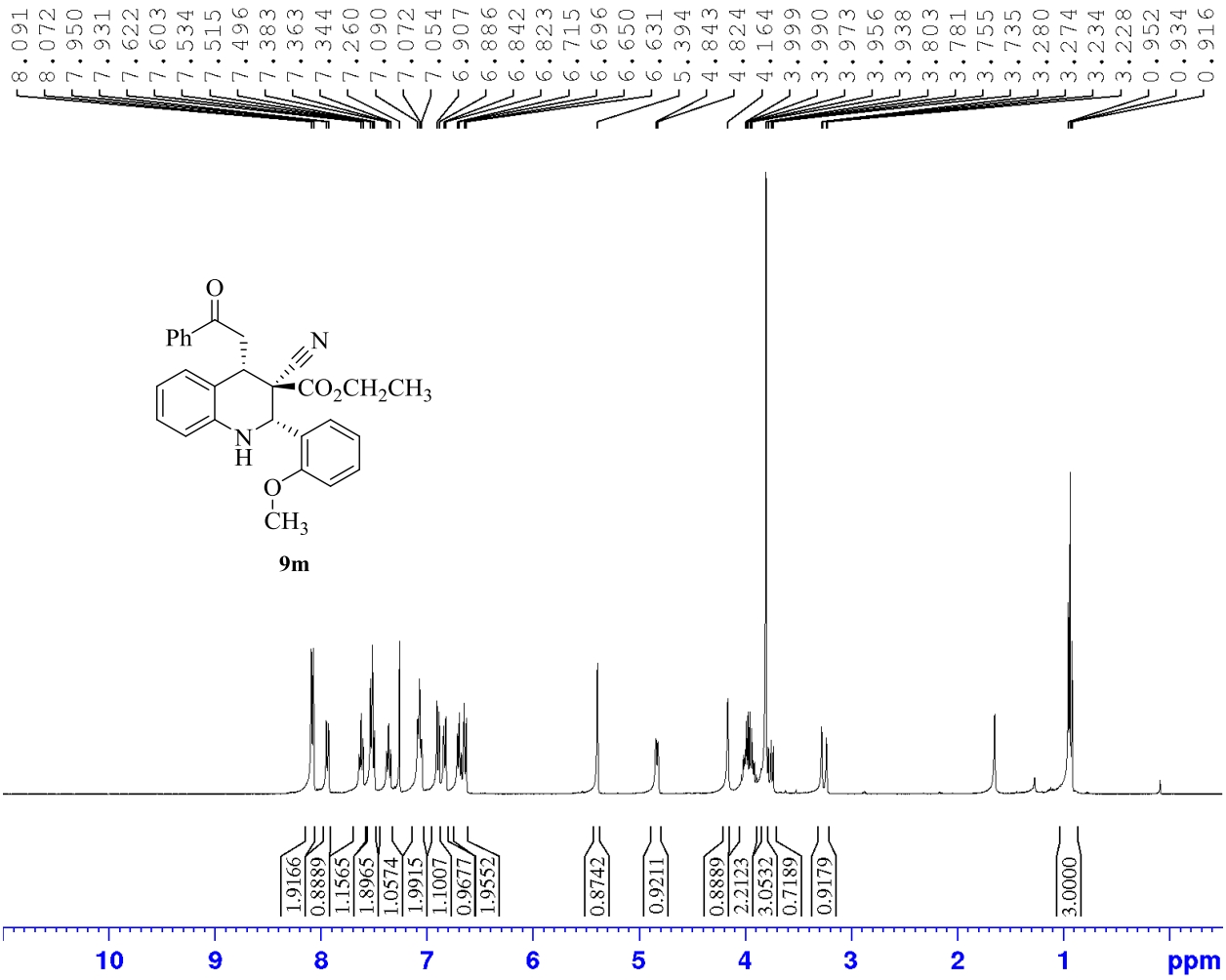

```
Current Data Parameters
NAME      ARN-II-CCP-061-1
EXPNO            2111011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171121
Time                16.07
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                   406
DW                83.200 usec
DE                 6.50 usec
TE                295.3 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300080 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 3-cyano-2-(naphthalen-2-yl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9l**)

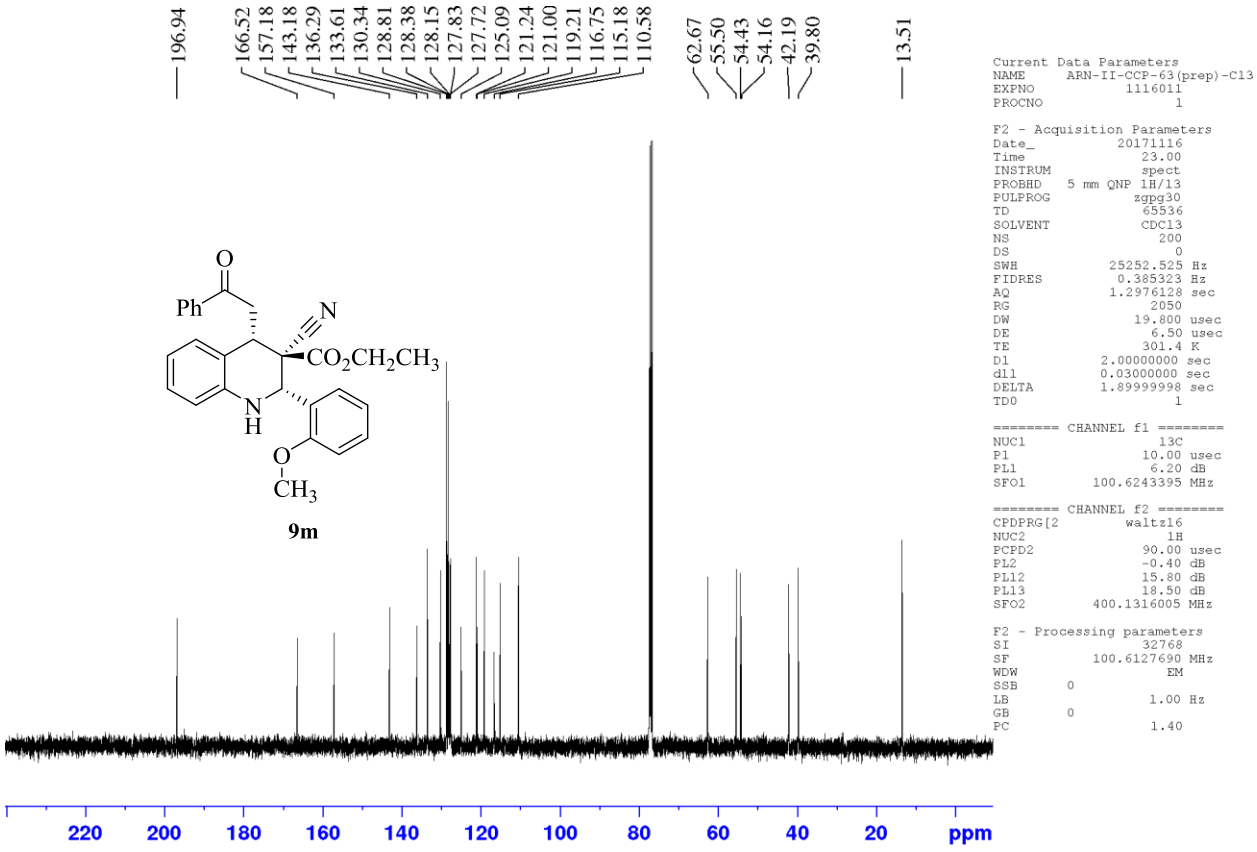



```
Current Data Parameters
NAME      ARN-II-CCP-061-1-C13
EXPNO              2111011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171121
Time              16.16
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   94
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE                295.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

Racemate of ethyl 3-cyano-2-(2-methoxyphenyl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9m**)

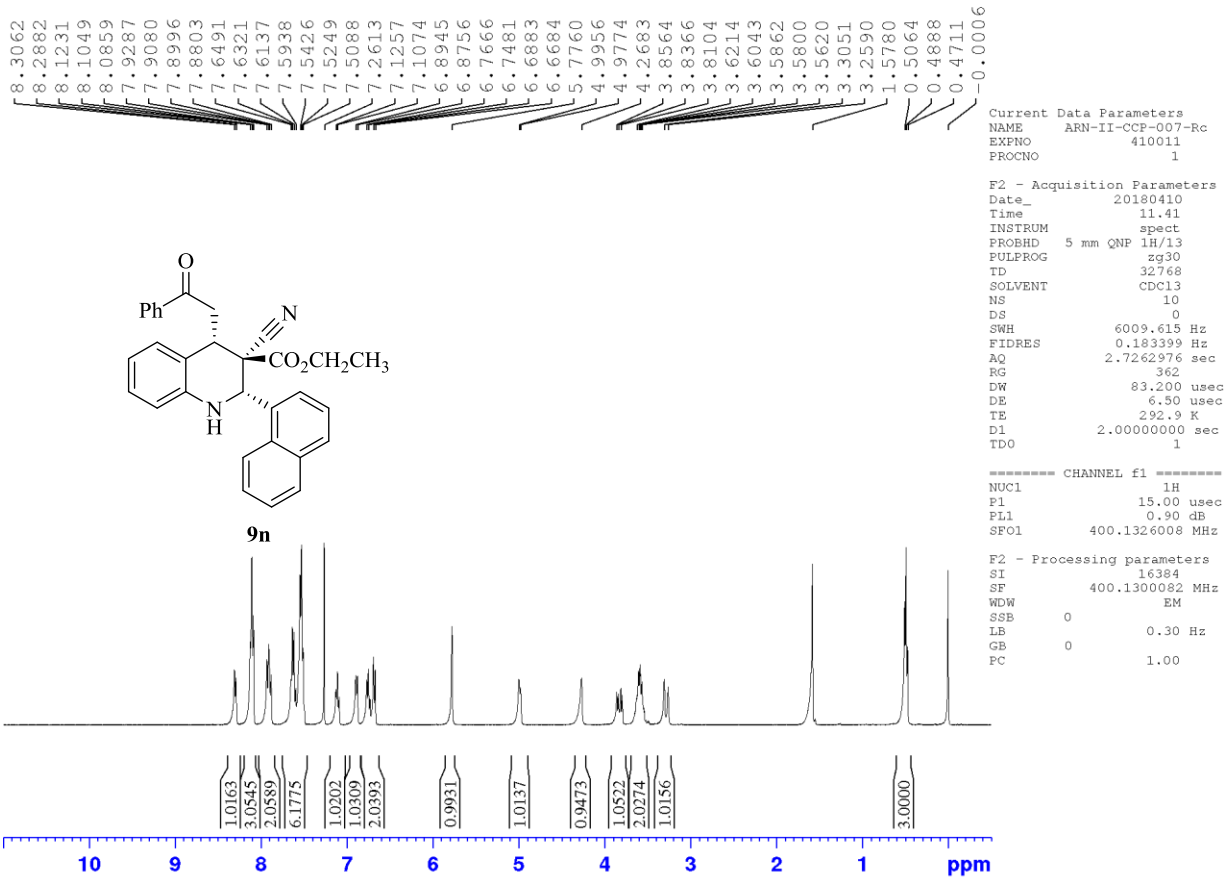


Racemate of ethyl 3-cyano-2-(2-methoxyphenyl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9m**)

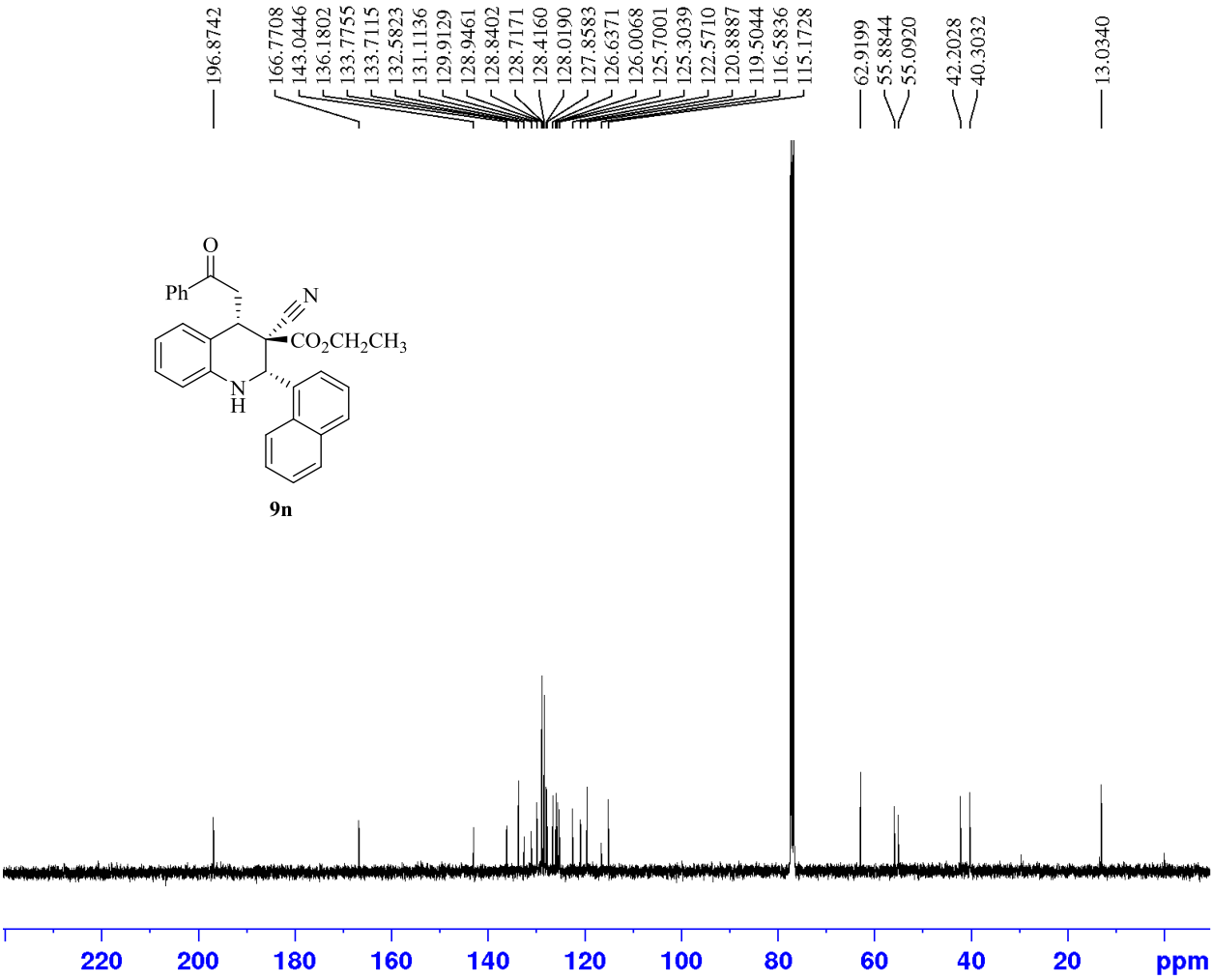



```
Current Data Parameters
NAME      ARN-II-CCP-63(prep)-C13
EXPNO            1116011
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171116
Time              23.00
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE                301.4 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                6.20 dB
SFO1        100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

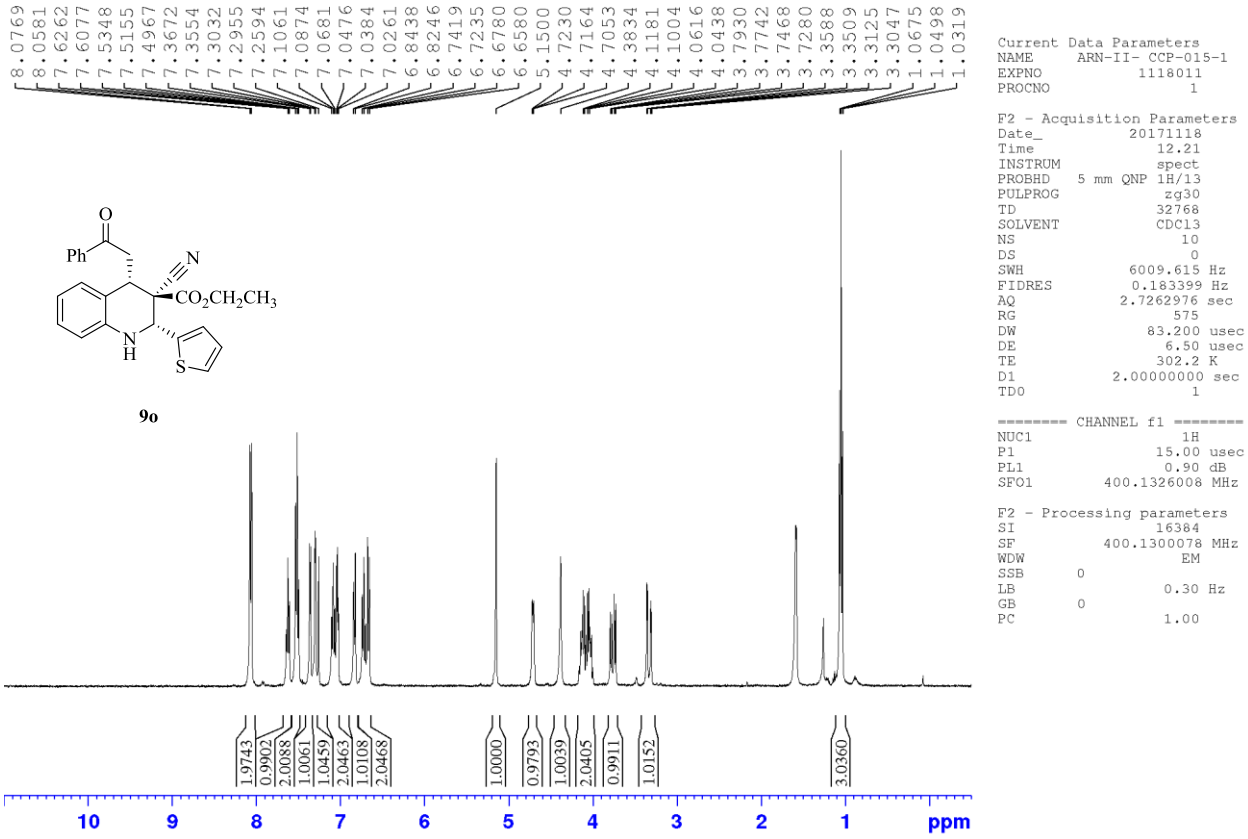
Racemate of ethyl 3-cyano-2-(naphthalen-1-yl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9n**)



Racemate of ethyl 3-cyano-2-(naphthalen-1-yl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9n**)

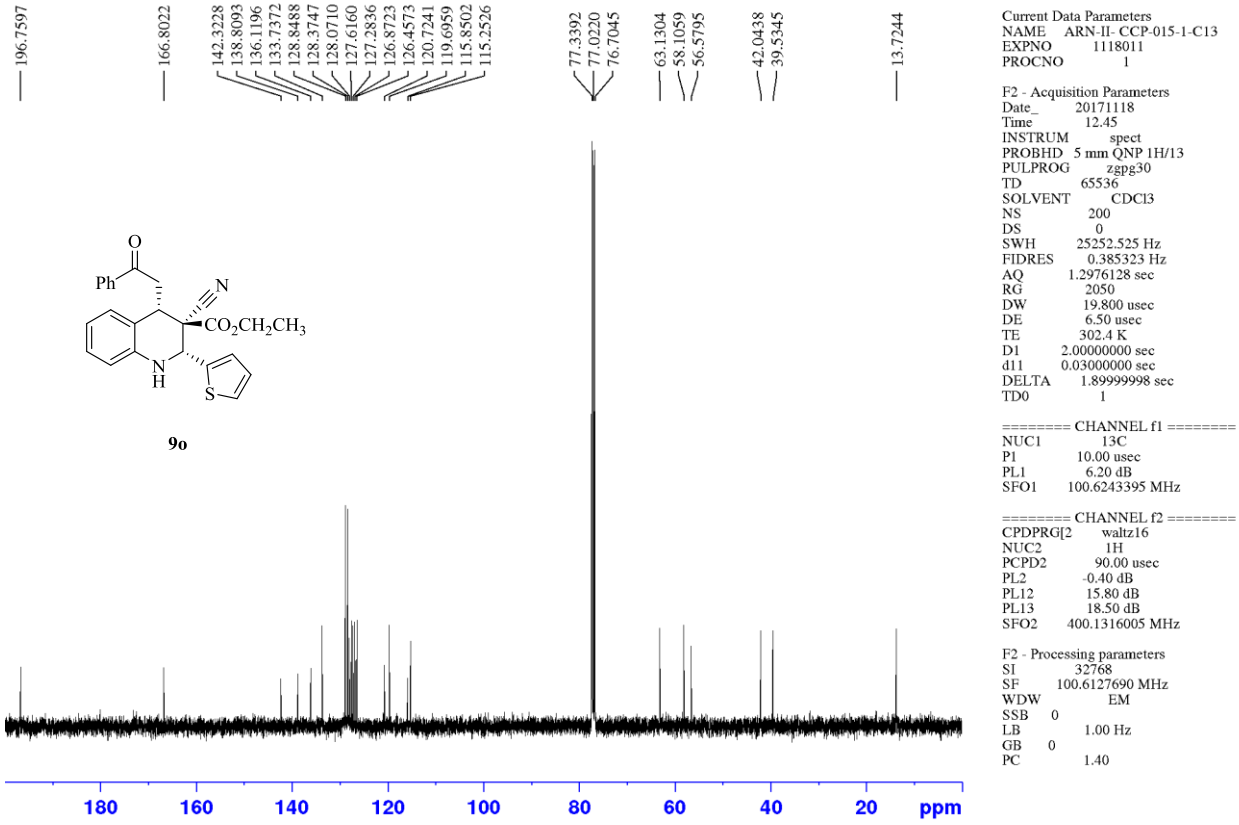


Racemate of (2R,3R,4S)-ethyl 3-cyano-4-(2-oxo-2-phenylethyl)-2-(thiophen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9o**)




```
Current Data Parameters
NAME      ARN-II- CCP-015-1
EXPNO              1118011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171118
Time               12.21
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   10
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG                  575
DW               83.200 usec
DE                6.50 usec
TE                302.2 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PL1                0.90 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300078 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 3-cyano-4-(2-oxo-2-phenylethyl)-2-(thiophen-2-yl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9o)**



Current Data Parameters
NAME ARN-II- CCP-015-1-C13
EXPNO 1118011
PROCNO 1

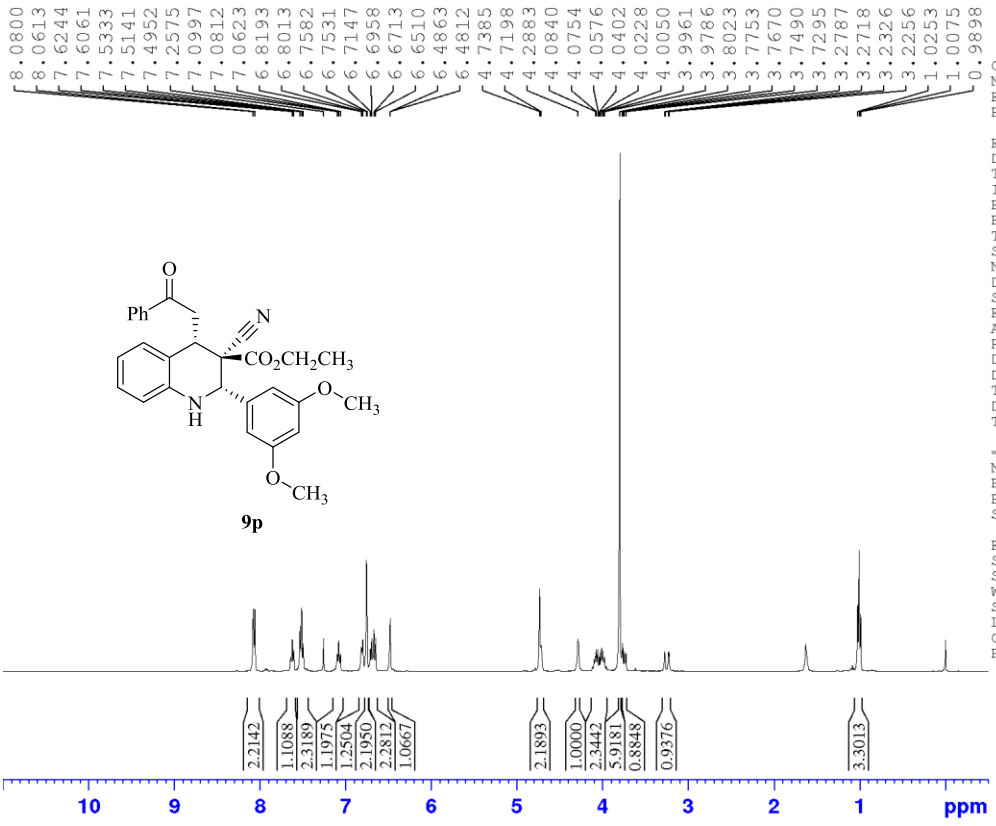
F2 - Acquisition Parameters
Date_ 20171118
Time 12.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 302.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.20 dB
SFO1 100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.40 dB
PL12 15.80 dB
PL13 18.50 dB
SFO2 400.1316005 MHz

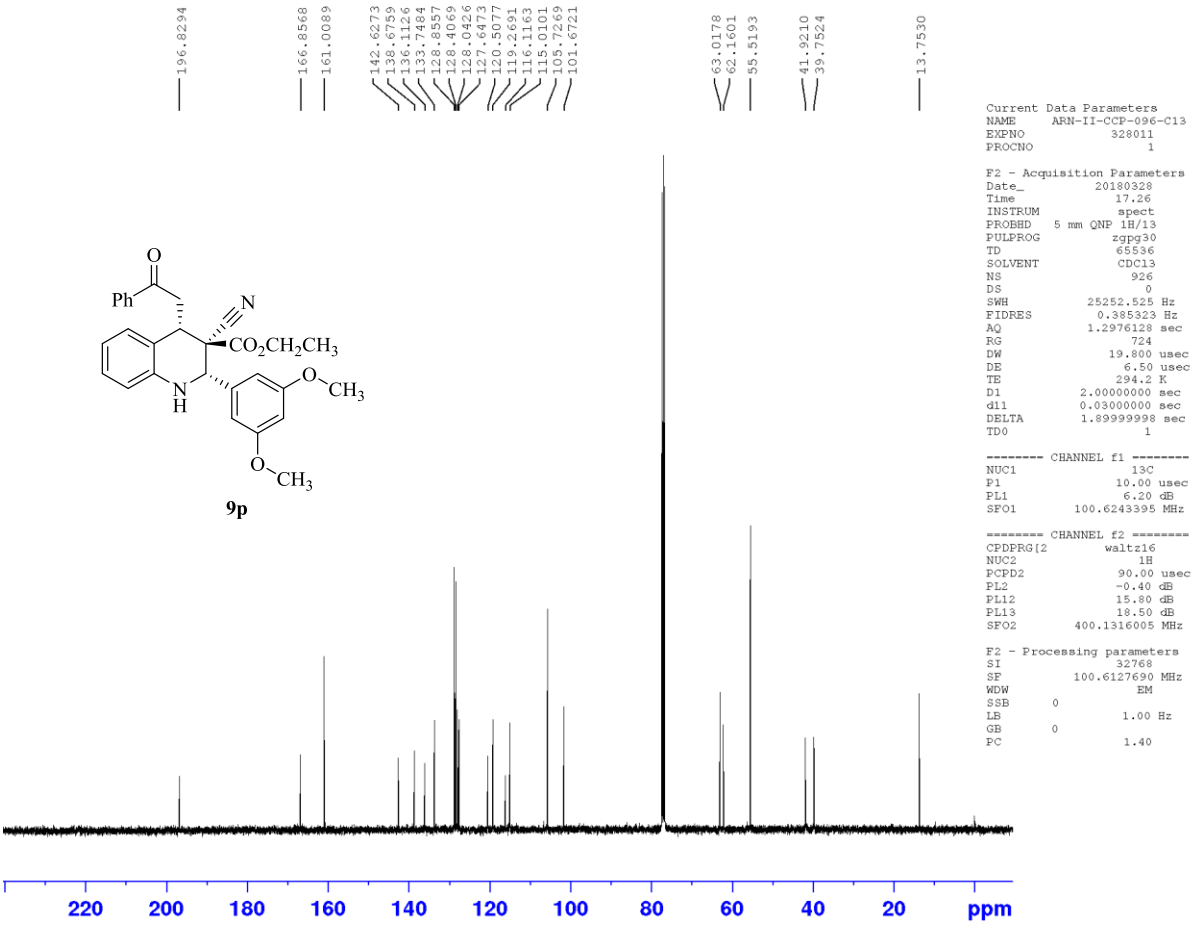
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Racemate of ethyl 4-benzoyl-3-cyano-2-(3,5-dimethoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9p**)



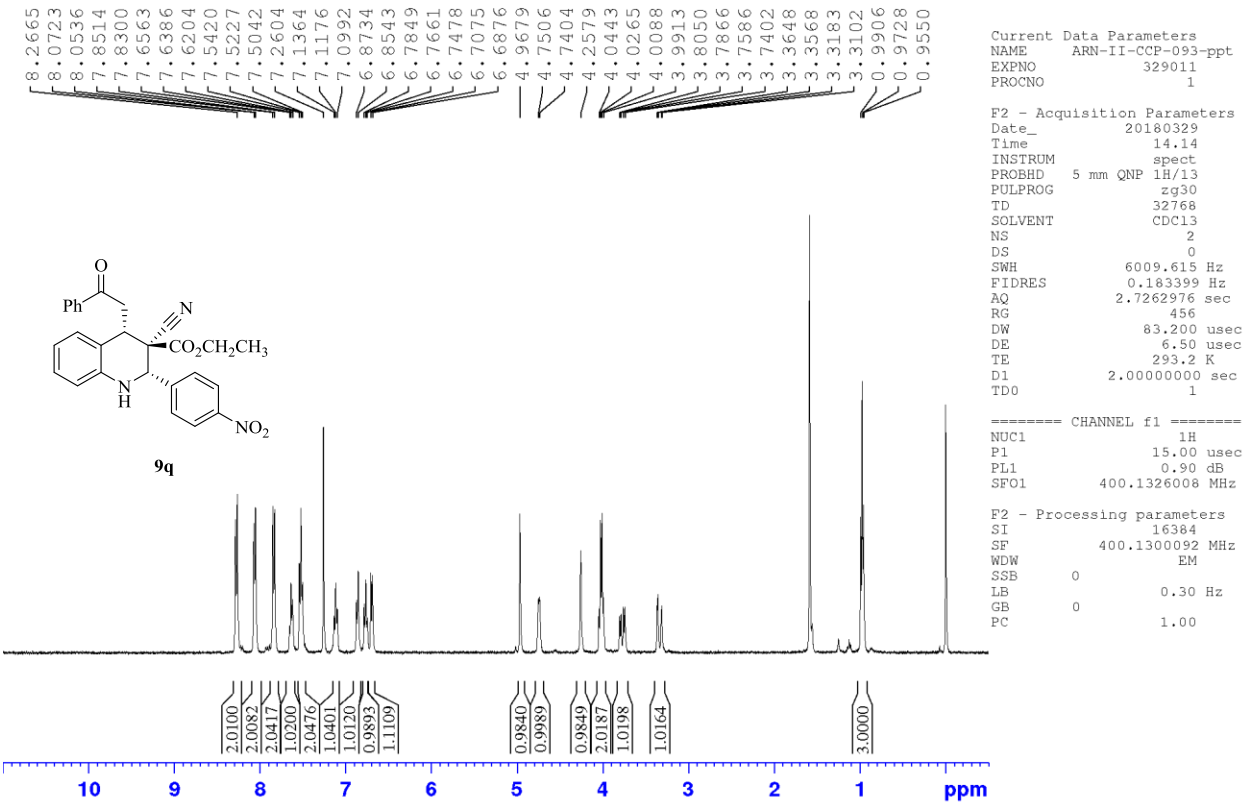

```
Current Data Parameters
NAME      ARN-II-CCP-096-ppt
EXPNO               327011
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180327
Time                10.56
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    10
DS                     0
SWH             6009.615 Hz
FIDRES           0.183399 Hz
AQ              2.7262976 sec
RG                   203
DW                83.200 usec
DE                 6.50 usec
TE                295.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300097 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemate of ethyl 4-benzoyl-3-cyano-2-(3,5-dimethoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9p**)



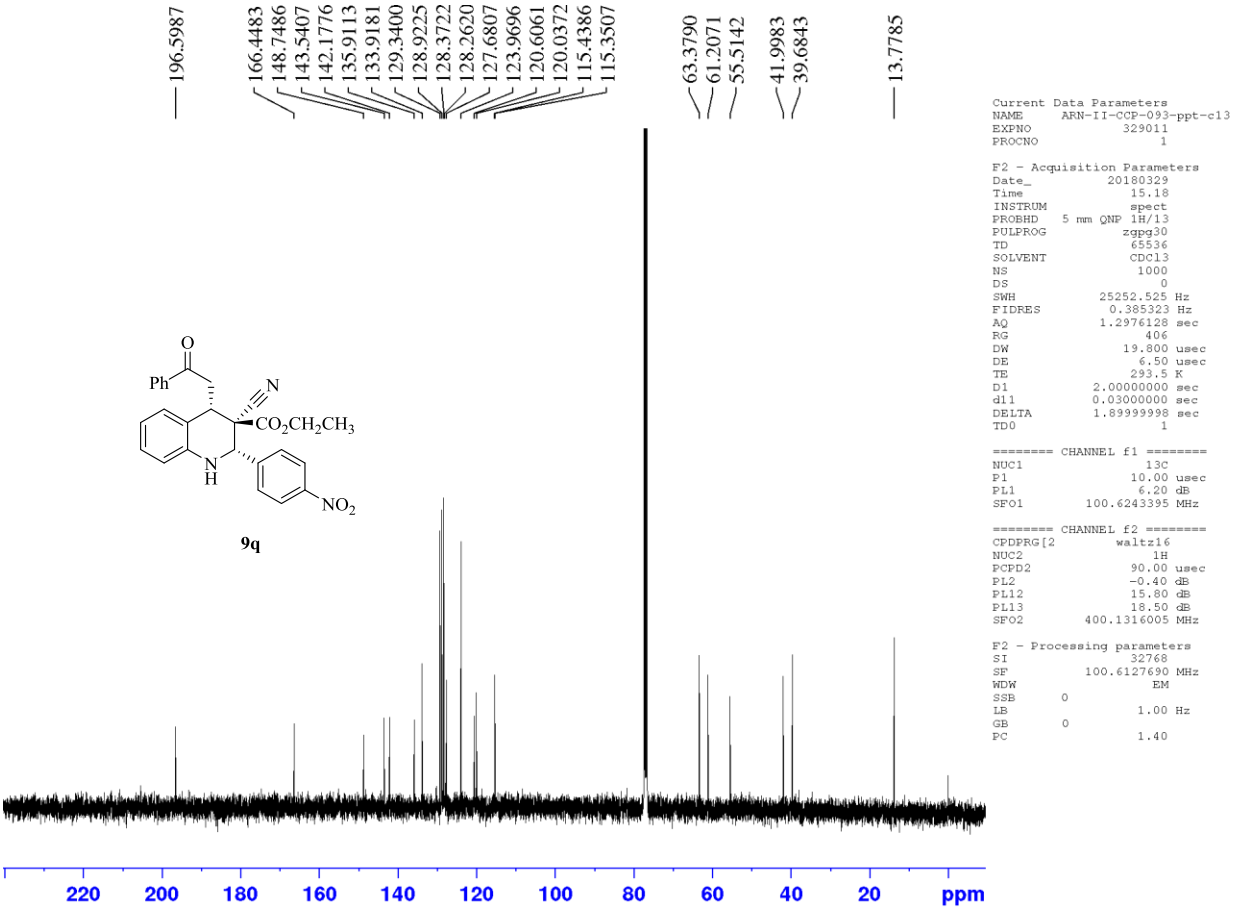

```
Current Data Parameters
NAME      ARN-II-CCP-096-C13
EXPNO              328011
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180328
Time              17.26
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  926
DS                    0
SWH           25252.525 Hz
FIDRES            0.385323 Hz
AQ             1.2976128 sec
RG                  724
DW               19.800 usec
DE                6.50 usec
TE                294.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -0.40 dB
PL12              15.80 dB
PL13              18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Racemate of ethyl 3-cyano-2-(4-nitrophenyl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9q**)



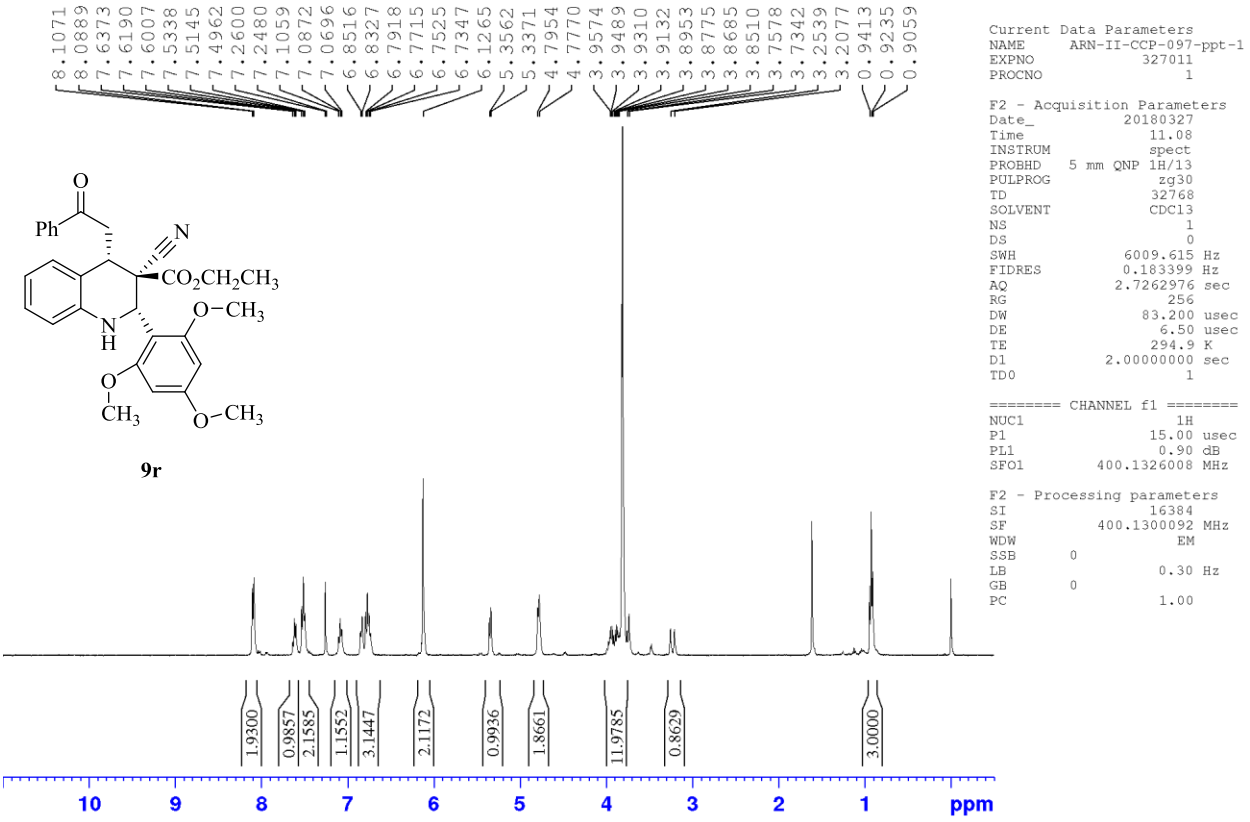

```
Current Data Parameters
NAME      ARN-II-CCP-093-ppt
EXPNO              329011
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180329
Time                14.14
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                     2
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                   456
DW                83.200 usec
DE                 6.50 usec
TE                293.2 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300092 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemic of ethyl 3-cyano-2-(4-nitrophenyl)-4-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydroquinoline-3-carboxylate (**9q**)



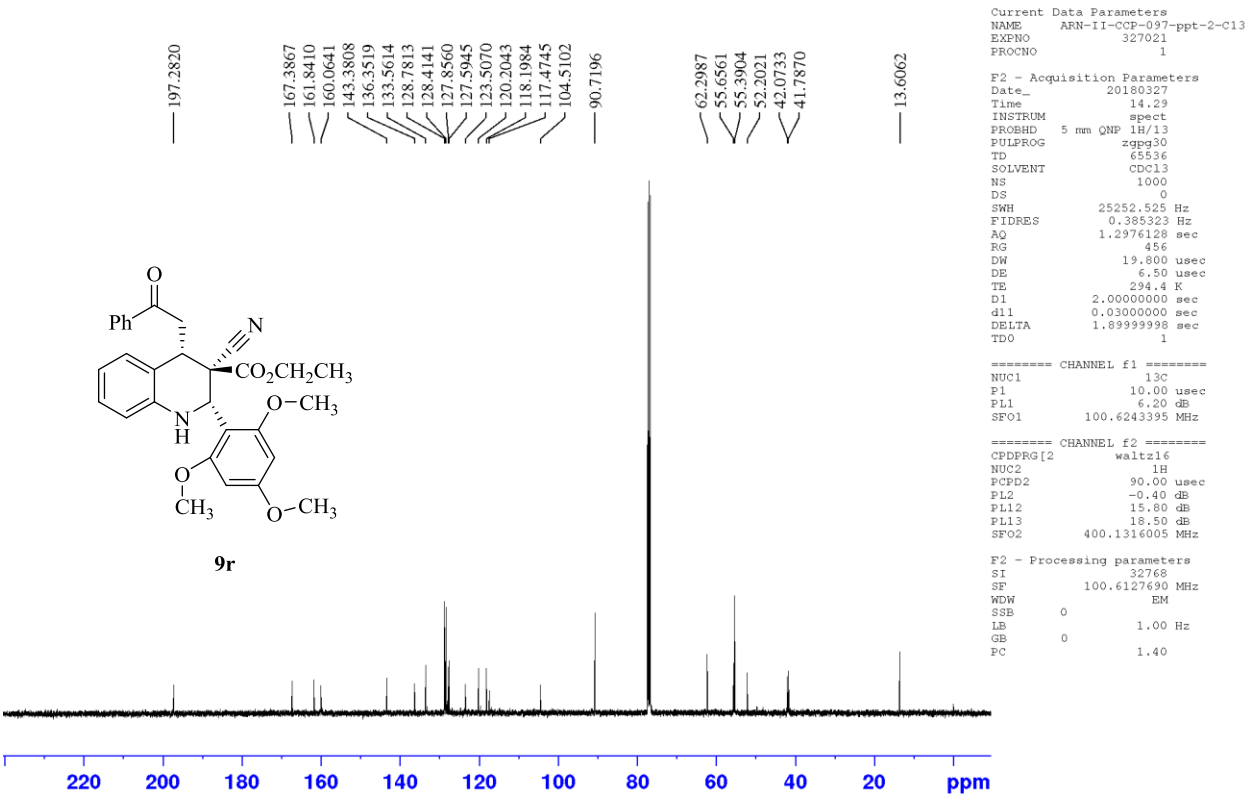

```
Current Data Parameters
NAME      ARN-II-CCP-093-ppt-c13
EXPNO                329011
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180329
Time                 15.18
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1000
DS                       0
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976128 sec
RG                     406
DW                19.800 usec
DE                 6.50 usec
TE                 293.5 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PL1                  6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                 -0.40 dB
PL12                15.80 dB
PL13                18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF           100.6127690 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

Racemic of 3-((ethylperoxy)-l2-methyl)-4-(2-oxo-2-phenylethyl)-2-(2,4,6-trimethoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carbonitrile (**9r**)




```
Current Data Parameters
NAME      ARN-II-CCP-097-ppt-1
EXPNO               327011
PROCNO                   1

F2 - Acquisition Parameters
Date_            20180327
Time                11.08
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     1
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                   256
DW                83.200 usec
DE                 6.50 usec
TE                294.9 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 0.90 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300092 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Racemic of 3-((ethylperoxy)-l2-methyl)-4-(2-oxo-2-phenylethyl)-2-(2,4,6-trimethoxyphenyl)-1,2,3,4-tetrahydroquinoline-3-carbonitrile (**9r**)




```
Current Data Parameters
NAME      ARN-II-CCP-097-ppt-2-C13
EXPNO              327021
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180327
Time                14.29
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1000
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976128 sec
RG                   456
DW                19.800 usec
DE                 6.50 usec
TE                294.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 6.20 dB
SFO1         100.6243395 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -0.40 dB
PL12               15.80 dB
PL13               18.50 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```