

Catalytic amide-formation with α' -hydroxyenones as acylating reagents

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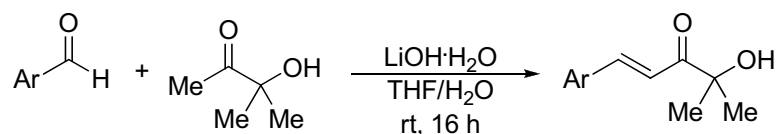
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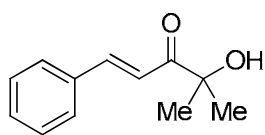
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General Methods. All reactions utilizing air- or moisture-sensitive reagents were performed in dried glassware under an atmosphere of dry N₂. CH₂Cl₂ was distilled from CaH₂. *N,N*-diisopropylethylamine (DIPEA) was purified by distillation from KOH prior to use. Triazolium salt **1** is commercially available from Sigma-Aldrich. Aniline and *o*-anisidine were distilled under vacuum, and tryptamine was purified by sublimation in vacuo. Other reagents were used without further purification. Thin layer chromatography (TLC) was performed on EMD precoated plates (silica gel 60 F₂₅₄, Art 5715, 0.25 mm) and were visualized by fluorescence quenching under UV light and by staining with phosphomolybdic acid or potassium permanganate, respectively. Preparative thin-layer chromatography (PTLC) was performed using plates prepared from silica gel EMD 60 PF₂₅₄ (Art 7749). Column chromatography was performed on EMD Silica Gel 60 (230–400 Mesh) using a forced flow of 0.5–1.0 bar. ¹H NMR (500 MHz) and ¹³C NMR (125 MHz) were measured on a Bruker Avance AVII-500 spectrometer. Chemical shifts are expressed in parts per million (ppm) downfield from residual solvent peaks and coupling constants are reported as Hertz (Hz). Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; quin, quintet; sext, sextet; m, multiplet; Infrared (IR) spectra were recorded on a JASCO FT/IR-4100 spectrophotometer and were reported as wavenumber (cm⁻¹).

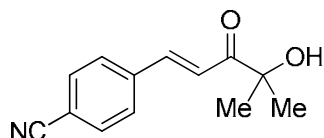
General Procedure for the Preparation of α' -Hydroxyenones



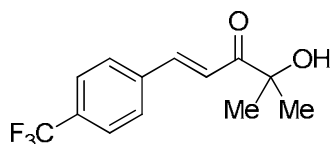
The α' -hydroxyenones were prepared according to modified literature procedures.¹ A mixture of 3-hydroxy-3-methyl-2-butanone (10 mmol, 1 equiv), the aldehyde (15 mmol, 1.5 equiv) and LiOH·H₂O (2 mmol, 0.2 equiv) in THF/H₂O (1:1 v/v, 0.08 M) was stirred at room temperature overnight. The THF was removed under reduced pressure, and the aqueous solution was extracted with CH₂Cl₂ (3×30 mL). The combined organic phase was dried over Na₂SO₄, filtered and concentrated. The residue was purified by column chromatography. All of characterization data of α' -hydroxyenones was published previously.²



(E)-4-Hydroxy-4-methyl-1-phenylpent-1-en-3-one (2). CAS RN: 63677-96-3.¹



(E)-4-(4-Hydroxy-4-methyl-3-oxopent-1-enyl)benzonitrile.²

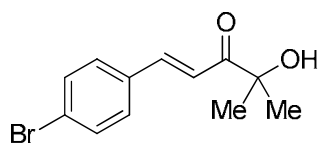


(E)-4-Hydroxy-4-methyl-1-(4-(trifluoromethyl)phenyl)pent-1-en-3-one. CAS RN: 1111644-46-2.²

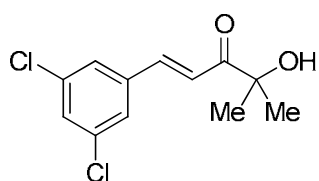
(1) (a) C. Palomo, M. Oiarbide, J. M. Garcia, A. Gonzalez and E. Arceo, *J. Am. Chem. Soc.*, 2003, **125**, 13942–13943. (b) M. Reiter, H. Turner, R. Mills-Webb and V. Gouverneur, *J. Org. Chem.*, 2005, **70**, 8478–8485.
(2) P.-C. Chiang, M. Rommel and J. W. Bode, *J. Am. Chem. Soc.*, 2009, DOI: 10.1021/ja902143w

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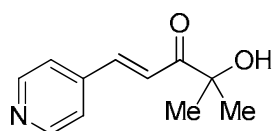
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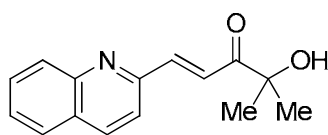
(E)-1-(4-Bromophenyl)-4-hydroxy-4-methylpent-1-en-3-one. CAS RN: 1111644-45-1.²



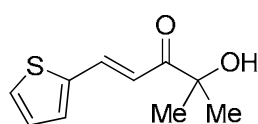
(E)-1-(3,5-Dichlorophenyl)-4-hydroxy-4-methylpent-1-en-3-one.²



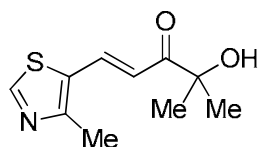
(E)-4-Hydroxy-4-methyl-1-(pyridin-4-yl)pent-1-en-3-one.²



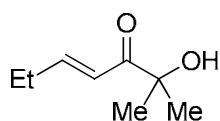
(E)-4-Hydroxy-4-methyl-1-(quinolin-2-yl)pent-1-en-3-one.²



(E)-4-Hydroxy-4-methyl-1-(thiophen-2-yl)pent-1-en-3-one.²



(E)-4-Hydroxy-4-methyl-1-(4-methylthiazol-5-yl)pent-1-en-3-one.²



(E)-2-Hydroxy-2-methylhept-4-en-3-one.¹

Optimization of the NHC-Catalyzed Amidation of α' -Hydroxyenones Conditions

The crude products were analyzed by NMR spectroscopy and the conversion of the benzylamine was determined by integration of the prominent signal for the methylene group in the starting material (δ =3.84 ppm, singlet) and in the product (δ = 4.38 ppm, doublet).

Table S-1. Co-catalysts survey of the amidation reaction of α' -hydroxyenone with benzylamine

Co-catalyst				
Conversion	77%	73%	76%	62%
Co-catalyst				NO co-catalyst
Conversion	36%	< 1%	< 1%	44%

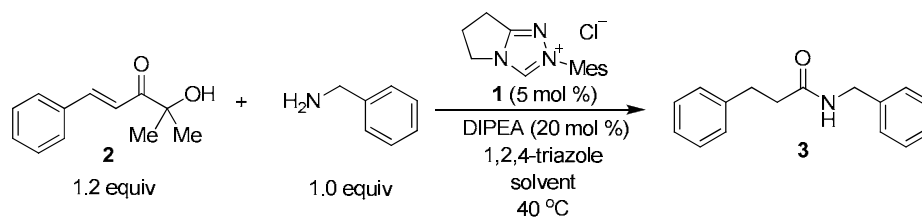
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Table S-2. Precatalyst survey of the amidation reaction of α' -hydroxyenone with benzylamine

68%	<1%	17%	15%
18%	<1%	<1%	<1%
< 1%	< 1%	<1%	

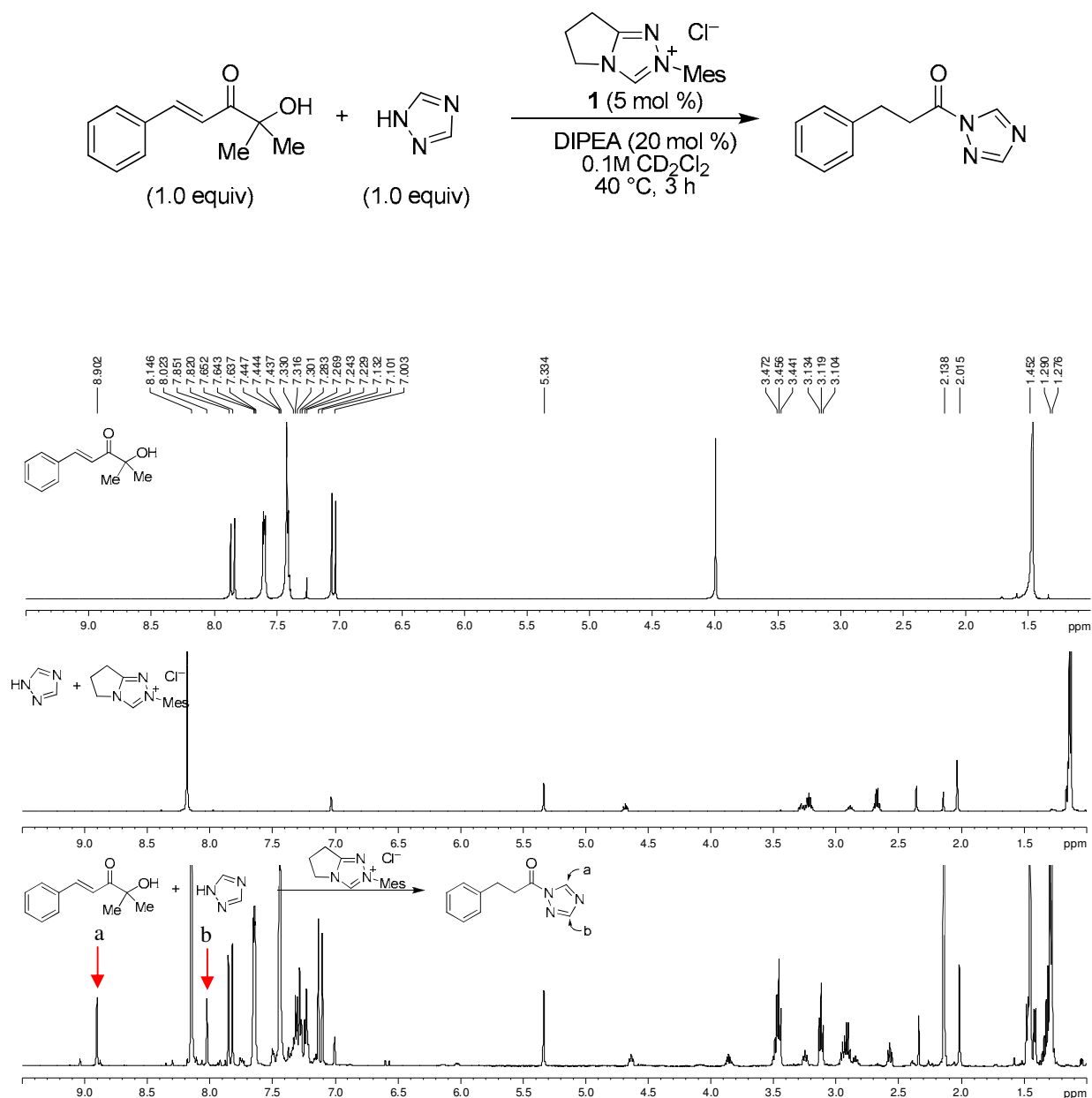
Table S-3. Optimization of the amidation reaction of α' -hydroxyenone with benzylamine



entry	mol % additive	solvent	time	% conversion
1	50	0.1 M CH ₂ Cl ₂	12 h	69
2	20	0.1 M CH ₂ Cl ₂	12 h	71
3	10	0.1 M CH ₂ Cl ₂	12 h	85
4	5	0.1 M CH ₂ Cl ₂	12 h	65
5	10	0.1M EtOAc	12 h	47
6	10	0.1M THF	12 h	52
8	50	0.2 M CH ₂ Cl ₂	12 h	34
9	50	0.5 M CH ₂ Cl ₂	12 h	79
10	50	1.0 M CH ₂ Cl ₂	12 h	66
11	10	0.5 M CH ₂ Cl ₂	1 h	68
12	10	0.5 M CH ₂ Cl ₂	2 h	79
13	10	0.5 M CH ₂ Cl ₂	3 h	82
14	10	0.5 M CH ₂ Cl ₂	4 h	86
15	10	0.5 M CH ₂ Cl ₂	5 h	82
16	10	0.5 M CH ₂ Cl ₂	24 h	87

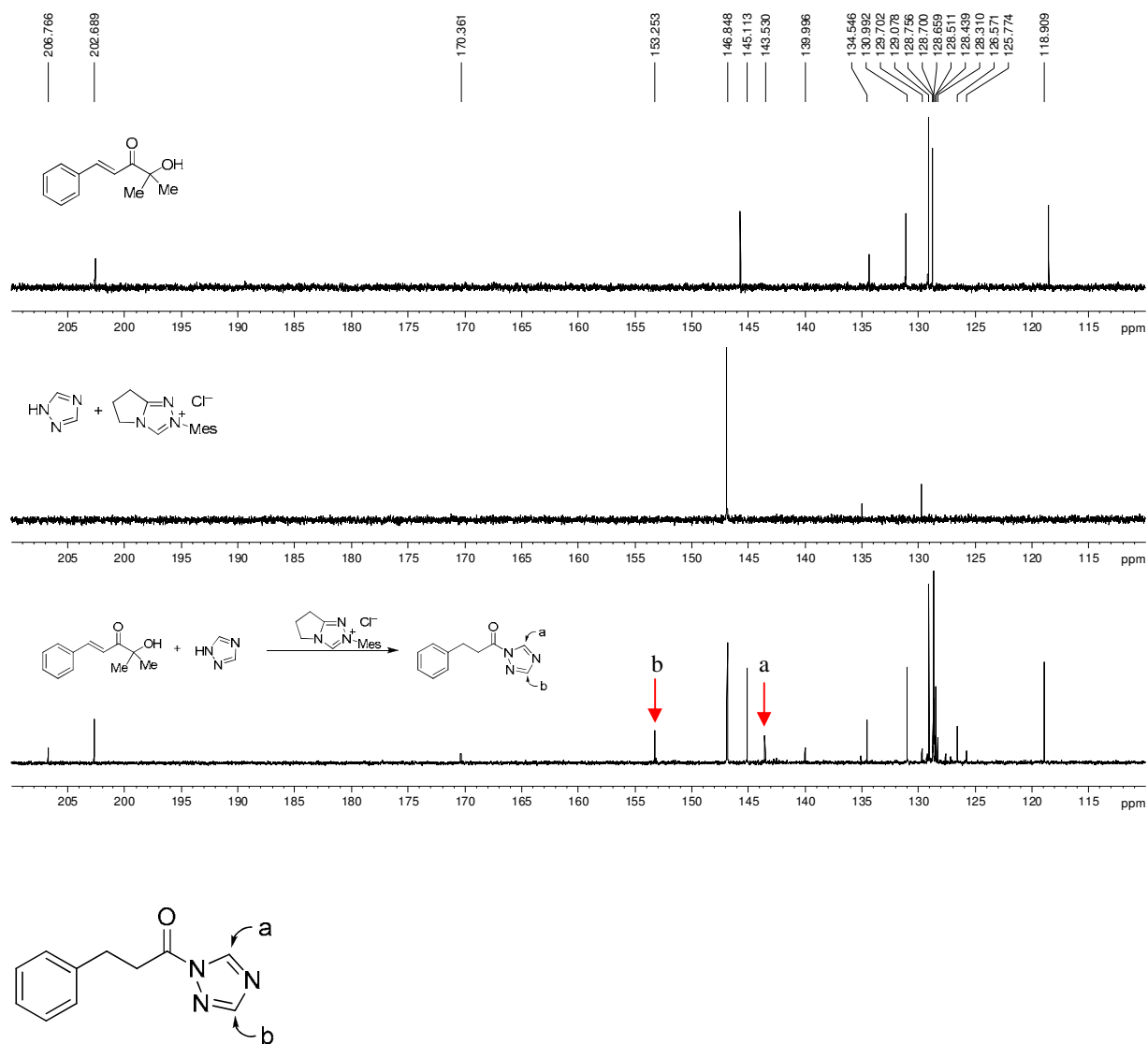
NMR Study of N-Acylation Intermediate

The reaction was carried out in the condition with 1 equiv of α' -hydroxyketone and 1 equiv of 1,2,4-triazole in 5 mol % precatalyst **1**, 20 mol % DIPEA, 0.1 M CDCl_2 at 40 °C for 3 hours. The regioselectivity of *N*-acylation was determined via the ^1H and ^{13}C NMR spectra comparison of reaction mixture and control experiment without α' -hydroxyketone.



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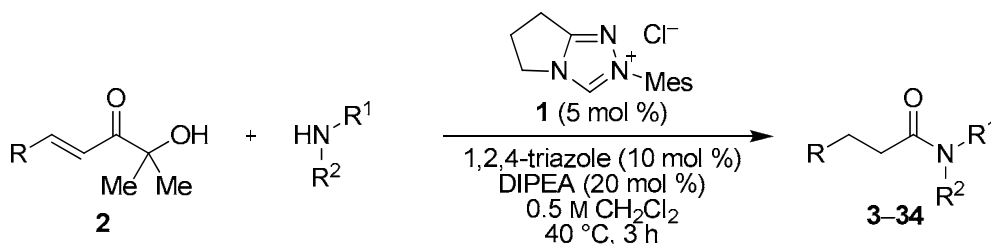
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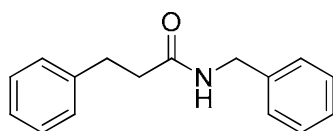
^1H NMR (500 MHz, CD_2Cl_2): H^{a} 8.90 ppm, H^{b} 8.02 ppm

^{13}C NMR (125 MHz, CD_2Cl_2): C^{a} 143.5 ppm, C^{b} 153.3 ppm

General Procedure for the Amidation of α -Hydroxyenones and Amines

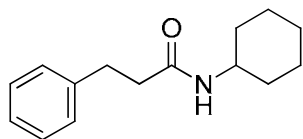


An oven-dried vial with a Teflon[®] coated screw cap and stir bar was charged with the triazolium precatalyst **1** (25 μ mol, 5 mol %), 1,2,4-triazole (50 μ mol, 10 mol %), α -hydroxyenone (0.60 mmol, 1.2 equiv), and amine (0.50 mmol, 1.0 equiv). It was purged with nitrogen, and the reactants were dissolved in dry CH_2Cl_2 (1.0 mL, 0.5 M). Finally, DIPEA (0.10 mmol, 20 mol %) was added, and the sealed vial was placed into an oil bath at 40 $^\circ\text{C}$ if not indicated otherwise. After 3 hours, the reaction mixture was concentrated, and the product isolated by column chromatography.

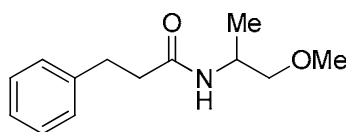


N-Benzyl-3-phenylpropanamide (3). CAS RN: 10264-10-5. Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 84% yield; ^1H NMR (500 MHz, CDCl_3) δ 7.31–7.26 (m, 5H), 7.22–7.19 (m, 3H), 7.14 (d, J = 7.3 Hz, 2H), 5.79 (brs, 1H), 4.38 (d, J = 5.5 Hz, 2H), 2.99 (t, J = 7.8 Hz, 2H), 2.51 (t, J = 7.8 Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.0, 140.9, 138.3, 128.7, 128.6, 128.5, 127.8, 127.5, 126.3, 43.6, 38.6, 31.8. Analytical data is consistent with published data.³

(3) (a) I. Shiina and Y. Kawakita, *Tetrahedron*, 2004, **60**, 4729–4733. (b) J. W. Bode and S. S. Sohn, *J. Am. Chem. Soc.*, 2007, **129**, 13798–13799.

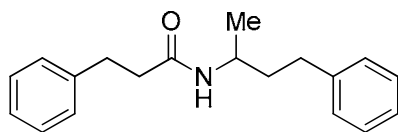


N-Cyclohexyl-3-phenylpropanamide (4). CAS RN: 10264-23-0. Prepared according to the general procedure; Purification using hexanes/acetone (6:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 92% yield; ^1H NMR (500 MHz, CDCl_3) δ 7.29–7.26 (m, 2H), 7.21–7.19 (m, 3H), 5.16 (brs, 1H), 3.76–3.71 (m, 1H), 2.95 (t, J = 7.7 Hz, 2H), 2.43 (t, J = 7.7 Hz, 2H), 1.84–1.81 (m, 2H), 1.66–1.63 (m, 2H), 1.60–1.57 (m, 1H), 1.37–1.29 (m, 2H), 1.15–1.08 (m, 1H), 1.04–0.97 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.2, 141.0, 128.54, 128.46, 126.3, 48.1, 38.8, 33.1, 32.0, 25.6, 24.9. Analytical data is consistent with published data.⁴

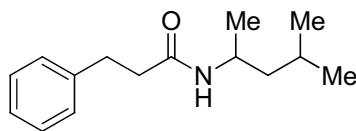


N-(1-Methoxypropan-2-yl)-3-phenylpropanamide (5). Prepared according to the general procedure; Purification using hexanes/EtOAc (1:1 v/v) as the eluent afforded the desired amidation product as a colorless oil in 73 % yield; ^1H NMR (500 MHz, CDCl_3) δ 7.26 (t, J = 7.0 Hz, 2H), 7.18 (d, J = 6.5 Hz, 3H), 5.65 (brs, 1H), 4.12 (brs, m, 1H), 3.29 (s, 3H), 3.26 (d, J = 3.1 Hz, 2H), 2.94 (t, J = 7.5 Hz, 2H), 2.44 (t, J = 7.5 Hz, 2H), 1.09 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.6, 141.0, 128.6, 128.5, 126.3, 77.5, 77.2, 76.9, 75.6, 59.1, 44.8, 38.7, 31.9, 17.7; IR (thin film) ν 3293, 3063, 3027, 2974, 2928, 1643, 1547, 1497, 1109 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{19}\text{NO}_2\text{Na}$: 244.1314, found 244.1322 $[\text{M}+\text{Na}]^+$.

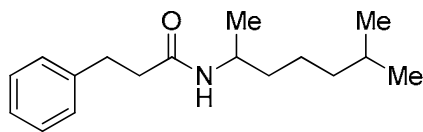
(4) H. Nambu, K. Hata, M. Matsugi, and Y. Kita, *Chem. Eur. J.*, 2005, **11**, 719–727.



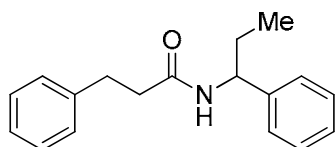
3-Phenyl-N-(4-phenylbutan-2-yl)propanamide (6). Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 69 % yield; mp: 67–68 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.28 (t, $J = 7.0$ Hz, 4H), 7.19 (dd, $J = 7.7, 6.9$ Hz, 4H), 7.13 (d, $J = 7.4$ Hz, 2H), 5.15 (d, $J = 7.4$ Hz, 1H), 4.03 (m, 1H), 2.96 (t, $J = 7.5$ Hz, 2H), 2.54 (m, 2H), 2.43 (t, $J = 7.5$ Hz, 2H), 1.66 (t, $J = 7.0$ Hz, 2H), 1.09 (d, $J = 5.6$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.4, 141.9, 141.0, 128.7, 128.5, 128.4, 126.4, 126.0, 45.2, 38.9, 38.7, 32.5, 31.9, 21.2; IR (thin film) ν 3287, 3084, 3062, 3026, 2965, 1640, 1550, 1496, 1454 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{24}\text{NO}$: 282.1853, found 282.1859 $[\text{M}+\text{H}]^+$.



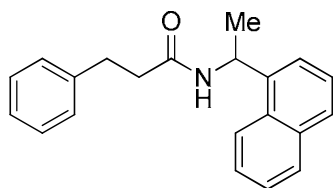
N-(4-Methylpentan-2-yl)-3-phenylpropanamide (7). Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 90 % yield. mp: 43–45 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.26 (t, $J = 7.5$ Hz, 2H), 7.19 (d, $J = 6.9$ Hz, 3H), 5.22 (d, $J = 7.4$ Hz, 1H), 4.02 (m, 1H), 2.94 (t, $J = 7.6$ Hz, 2H), 2.43 (t, $J = 7.6$ Hz, 2H), 1.45 (m, 1H), 1.24 (m, 1H), 1.16 (m, 1H), 1.02 (d, $J = 6.5$ Hz, 3H), 0.85 (t, $J = 6.8$ Hz, 6H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.4, 141.0, 128.6, 128.5, 127.5, 126.3, 46.4, 43.4, 38.9, 32.0, 25.0, 22.9, 22.6, 21.7; IR (thin film) ν 3290, 3065, 3029, 2957, 2927, 2363, 2342, 1638, 1559 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{24}\text{NO}$: 234.1853, found 234.1855 $[\text{M}+\text{H}]^+$.



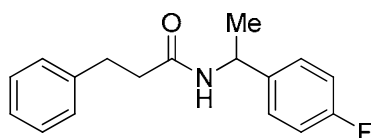
N-(6-Methylheptan-2-yl)-3-phenylpropanamide (8). Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless oil in 90 % yield; ^1H NMR (500 MHz, CDCl_3) δ 7.26 (d, $J = 7.4$ Hz, 2H), 7.18 (d, $J = 7.4$ Hz, 3H), 5.32 (d, $J = 7.3$ Hz, 1H), 3.92 (m, 1H), 2.94 (d, $J = 7.6$ Hz, 2H), 2.43 (m, 1H), 1.48 (m, 1H), 1.28 (m, 1H), 1.20 (m, 1H), 1.12 (m, 1H), 1.02 (d, $J = 6.5$ Hz, 3H), 0.84 (d, $J = 6.5$ Hz, 6H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.5, 141.0, 128.6, 128.5, 126.3, 77.5, 77.2, 77.0, 56.0, 45.3, 38.9, 38.8, 37.2, 32.0, 28.0, 23.9, 22.7, 22.7, 21.0; IR (thin film) ν 3285, 3064, 3028, 2955, 2930, 1640, 1550, 1454 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{27}\text{NONa}$: 284.1991, found 284.1978 $[\text{M}+\text{Na}]^+$.



3-Phenyl-N-(1-phenylpropyl)propamide (9). Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 84 % yield. mp: 74–77 $^{\circ}\text{C}$; ^1H NMR (500 MHz, CDCl_3) δ 7.30 (t, $J = 7.4$ Hz, 2H), 7.26 (d, $J = 7.4$ Hz, 4H), 7.19 (m, 4H), 5.53 (d, $J = 7.4$ Hz, 1H), 4.86 (q, $J = 7.6$ Hz, 1H), 2.96 (d, $J = 7.4$ Hz, 2H), 2.49 (d, $J = 7.4$ Hz, 1H), 1.73 (m, 1H), 0.81 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.4, 142.2, 140.9, 128.7, 128.6, 128.5, 127.4, 126.7, 126.4, 54.9, 38.7, 31.8, 29.1, 10.8; IR (thin film) ν 3287, 3062, 3028, 2965, 2930, 1641, 1545, 1495 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{18}\text{H}_{22}\text{O}$: 268.1701, found 268.1690 $[\text{M}+\text{H}]^+$.



***N*-(1-(Naphthalene-1-yl)ethyl)-3-phenylpropanamide (10).** Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 90 % yield; mp:134–135 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.07 (d, $J = 7.8$ Hz, 1H), 7.87 (d, $J = 7.8$ Hz, 1H), 7.78 (d, $J = 7.8$ Hz, 1H), 7.51(m, 2H), 7.40 (m, 2H), 7.24 (m, 3H), 7.17 (m, 3H), 5.91 (m, 1H), 5.60 (d, $J = 7.2$ Hz, 1H), 2.97 (m, 2H), 2.45 (t, $J = 7.5$ Hz, 2H), 1.58 (d, $J = 6.7$ Hz, 2H) ; ^{13}C NMR (125 MHz, CDCl_3) δ 171.1, 140.9, 138.4, 134.1, 131.2, 128.9, 128.6, 128.53, 128.47, 126.7, 126.4, 126.0, 125.3, 123.6, 122.7, 44.7, 38.6, 31.9, 20.8 ; IR (thin film) ν 3287, 3060, 2928, 1638, 1542, 1453 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{22}\text{NO}$ 304.1701, found 304.1707 $[\text{M}+\text{H}]^+$.

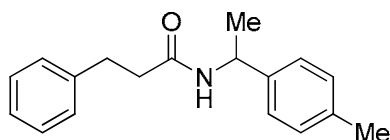


***N*-(1-(4-Fluorophenyl)ethyl)-3-phenylpropanamide (11).** Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 56 % yield;. mp:87–88 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.25 (d, $J = 6.5$ Hz, 2H), 7.21 (d, $J = 6.6$ Hz, 1H), 7.16 (d, $J = 7.8$ Hz, 2H), 7.12 (m, 1H), 6.96 (t, $J = 8.0$ Hz, 2H), 5.69 (s, 1H), 5.05(m, 1H), 2.95 (t, $J = 7.0$ Hz, 2H), 2.48 (q, $J = 6.5$ Hz, 2H), 1.36 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.2, 162.0 (d, $^1J_{\text{CF}} = 245.4$ Hz), 140.8, 139.0, 128.6 (d, $^3J_{\text{CF}} = 17.5$ Hz), 127.9 (d, $^4J_{\text{CF}} = 7.9$ Hz), 126.4, 115.5 (d, $^2J_{\text{CF}} = 21.6$ Hz), 48.1,

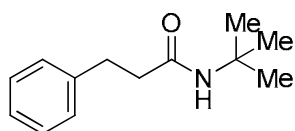
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38.7, 31.8, 21.8; IR (thin film) ν 3286, 3064, 2974, 2931, 1642, 1604, 1545, 1510, 1224 cm^{-1} ;
HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{19}\text{FNO}$: 272.1451, found 272.1451 $[\text{M}+\text{H}]^+$.

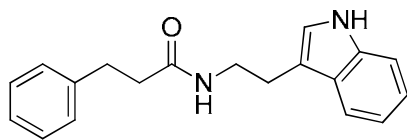


3-Phenyl-N-(1-*p*-tolylethyl)propanamide (12). Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 90 % yield; mp:78–79 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.28 (d, J = 7.2 Hz, 2H), 7.22 (d, J = 7.0 Hz, 1H), 7.18 (d, J = 7.7 Hz, 2H), 7.11 (m, 4H), 5.73 (d, J = 6.5 Hz, 1H), 5.07(m, 1H), 2.33 (s, 3H), 1.39 (d, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.2, 141.0, 140.3, 137.1, 129.4, 128.7, 128.6, 126.4, 126.3, 48.5, 38.7, 31.9, 21.8, 21.2; IR (thin film) ν 3283, 3926, 2971, 2925, 1639, 1545, 1453, 1374 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{18}\text{H}_{22}\text{NO}$: 268.1701, found 268.1697 $[\text{M}+\text{H}]^+$.

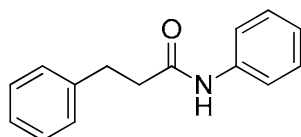


N-*tert*-Butyl-3-phenylpropanamide (13). CAS RN: 58680-45-8. Prepared according to the general procedure; Purification using hexanes/acetone (4:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 47% yield; ^1H NMR (500 MHz, CDCl_3) δ 7.29–7.27 (m, 2H), 7.20–7.18 (m, 3H), 5.13 (brs, 1H), 2.93 (t, J = 7.5 Hz, 2H), 2.38 (t, J = 7.5 Hz, 2H), 1.28 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.5, 141.2, 128.6, 126.3, 51.2, 39.6, 32.0, 28.9. Analytical data is consistent with published data.⁵

(5) Y. Saito, H. Ouchi and H. Takahata, *Tetrahedron*, 2008, **64**, 11129–11135.

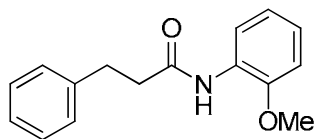


N-(2-(1H-Indol-3-yl)ethyl)-3-phenylpropanamide (14). CAS RN: 21803-90-7. Prepared according to the general procedure; Purification using hexanes/EtOAc (1:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 98% yield; ^1H NMR (500 MHz, CDCl_3) δ 8.51 (s, 1H), 7.57 (d, $J = 7.9$ Hz, 1H), 7.37 (d, $J = 8.1$ Hz, 1H), 7.29 (t, $J = 7.4$ Hz, 2H), 7.22 (t, $J = 7.4$ Hz, 2H), 7.18 (d, $J = 7.6$ Hz, 2H), 7.13 (t, $J = 7.4$ Hz, 1H), 5.61 (brs, 1H), 3.57 (dt, $J = 6.4, 6.4$ Hz, 2H), 2.95 (t, $J = 7.7$ Hz, 2H), 2.91 (t, $J = 6.7$ Hz, 2H), 2.40 (t, $J = 7.7$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.3, 140.9, 136.5, 128.6, 128.4, 127.4, 126.3, 122.2, 122.1, 119.4, 118.7, 112.7, 111.4, 39.8, 38.5, 31.8, 25.3. Analytical data is consistent with published data.⁶

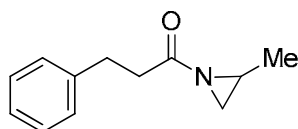


N,3-Diphenylpropanamide (15). CAS RN: 3271-81-6. Prepared according to the general procedure in 0.1 M CH_2Cl_2 for 12 h; Purification using hexanes/ Et_2O / CH_2Cl_2 (2:1:1 v/v/v) as the eluent afforded the desired amidation product as a colorless solid in 98% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.46–7.44 (m, 3H), 7.31–7.27 (m, 4H), 7.23–7.21 (m, 3H), 7.09 (t, $J = 7.3$ Hz, 1H), 3.04 (t, $J = 7.5$ Hz, 2H), 2.65 (t, $J = 7.8$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 170.7, 140.7, 137.9, 129.0, 128.7, 128.5, 126.5, 124.4, 120.2, 39.4, 31.7. Analytical data is consistent with published data.^{3,5}

(6) P. H. Kiviranta, H. S. Salo, J. Leppanen, V. M. Rinne, S. Kyrilenko, E. Kuusisto, T. Suuronen, A. Salminen, A. Poso, M. Lahtela-Kakkonen and E. A. A. Wallen, *Bioorg. Med. Chem.*, 2008, **16**, 8054–8062.



N-(2-Methoxyphenyl)-3-phenylpropanamide (16). CAS RN: 126545-09-3.⁷ Prepared according to the general procedure 0.1 M CH₂Cl₂ for 12 h; Purification using hexanes/Et₂O/CH₂Cl₂ (2:1:1 v/v/v) as the eluent afforded the desired amidation product as a colorless solid in 99% yield; mp: 46–47 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.41 (d, *J* = 7.9 Hz, 1H), 7.72 (brs, 1H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.27 (d, *J* = 6.8 Hz, 2H), 7.22 (t, *J* = 7.1 Hz, 1H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.97 (t, *J* = 7.7 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 3.83 (s, 3H), 3.08 (t, *J* = 7.8 Hz, 2H), 2.72 (t, *J* = 7.8 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 107.2, 147.8, 140.8, 128.6, 128.5, 126.3, 123.7, 121.1, 119.9, 109.9, 55.7, 39.7, 31.6; IR (thin film) ν 3414, 3317, 3062, 3026, 2935, 2836, 1680 s, 1600 s, 1527 s, 1484, 1460 s, 1252 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₆H₁₇NO₂Na: 278.1157, found 278.1148 [M+Na]⁺.



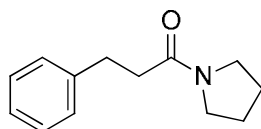
1-(2-Methylaziridin-1-yl)-3-phenylpropan-1-one (17). Prepared according to the general procedure; Purification using hexanes/acetone (4:1 v/v) as the eluent afforded the desired amidation product as a colorless liquid in 65% yield; ¹H NMR (500 MHz, CDCl₃) δ 7.30–7.27 (m, 2H), 7.21–7.19 (m, 3H), 2.97 (t, *J* = 7.7 Hz, 2H), 2.70 (t, *J* = 7.8 Hz, 2H), 2.33–2.31 (m, 1H), 2.20 (d, *J* = 5.8 Hz, 1H), 1.87 (brs, 1H), 1.26 (d, *J* = 5.4 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 184.9, 141.1, 128.6, 128.4, 126.3, 38.9, 32.7, 31.3, 31.2, 17.8; IR (thin film) ν 3584, 3062, 3027,

(7) Y. Kikugawa and M. Shimada, *J. Chem. Soc., Chem. Commun.*, 1989, 1450–1451.

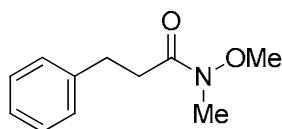
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2992, 2965, 2928, 1692 s, 1406, 1374 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{16}\text{NO}$: 190.1232, found 190.1224 $[\text{M}+\text{H}]^+$.

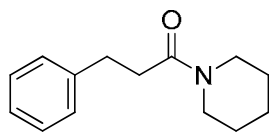


3-Phenyl-1-(pyrrolidin-1-yl)propan-1-one (18). CAS RN: 151647-54-0. Prepared according to the general procedure; Purification using hexanes/EtOAc (1:4 v/v) as the eluent afforded the desired amidation product as a pale yellow liquid in 96% yield; ^1H NMR (500 MHz, CDCl_3) δ 7.24 (t, $J = 7.3$ Hz, 2H), 7.19 (d, $J = 7.5$ Hz, 2H), 7.15 (t, $J = 7.0$ Hz, 1H), 3.42 (t, $J = 6.8$ Hz, 2H), 3.23 (t, $J = 6.6$ Hz, 2H), 2.95 (t, $J = 7.9$ Hz, 2H), 2.52 (t, $J = 7.9$ Hz, 2H), 1.86–1.74 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ 170.6, 141.4, 128.34, 128.32, 126.0, 46.4, 45.5, 36.6, 31.1, 26.0, 24.3. Analytical data is consistent with published data.⁵

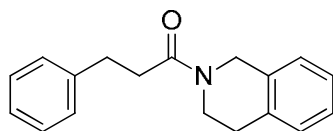


N-Methoxy-N-methyl-3-phenylpropanamide (19). CAS RN: 170646-96-5. Prepared according to the general procedure in 0.1 M CH_2Cl_2 for 12 h with the free amine by pre-treatment of weinreb's amine HCl salt with sodium bicarbonate; Purification using hexanes/EtOAc (3:2 v/v) as the eluent afforded the desired amidation product as a colorless liquid in 64% yield; ^1H NMR (500 MHz, CDCl_3) δ 7.30–7.27 (m, 2H), 7.24–7.18 (m, 3H), 3.59 (s, 3H), 3.17 (s, 3H), 2.96 (t, $J = 7.8$ Hz, 2H), 2.74 (t, $J = 7.3$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 173.7, 141.4, 128.48, 128.47, 126.1, 61.2, 33.8, 32.2, 30.7. Analytical data is consistent with published data.⁸

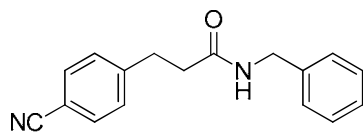
(8) J. A. Murphy, A. G. J. Commeureuc, T. N. Snaddon, T. M. McGuire, T. A. Khan, K. Hisler, M. L. Dewis, and R. Carling, *Org. Lett.*, 2005, **7**, 1427–1429.



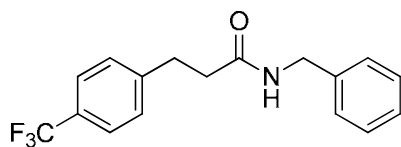
3-Phenyl-1-(piperidin-1-yl)propan-1-one (20). CAS RN: 21924-11-8. Prepared according to the general procedure; Purification using hexanes/EtOAc (2:1 v/v) as the eluent afforded the desired amidation product as a pale yellow liquid in 81% yield; ^1H NMR (500 MHz, CDCl_3) δ 7.28–7.25 (m, 2H), 7.21–7.16 (m, 3H), 3.54 (t, $J = 4.9$ Hz, 2H), 3.30 (t, $J = 4.9$ Hz, 2H), 2.95 (t, $J = 7.9$ Hz, 2H), 2.59 (t, $J = 7.9$ Hz, 2H), 1.58–1.43 (m, 6H); ^{13}C NMR (125 MHz, CDCl_3) δ 170.3, 141.4, 128.40, 128.38, 126.0, 46.5, 42.6, 35.1, 31.6, 26.3, 25.5, 24.5. Analytical data is consistent with published data.⁵



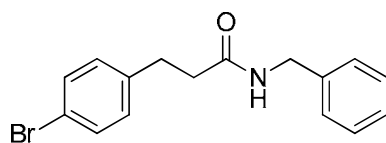
1-(3,4-Dihydroisoquinolin-2(1H)-yl)-3-phenylpropan-1-one (21). CAS RN: 349431-73-8. Prepared according to the general procedure; Purification using hexanes/EtOAc (4:1 v/v) as the eluent afforded the desired amidation product as a colorless liquid in 99% yield as a ~1.3:1 mixture of amide rotamers in CDCl_3 , 25 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$, 60 °C) δ 7.24–7.23 (m, 4H), 7.15 (m, 5H), 4.60 (s, 2H), 3.65 (brs, 2H), 2.86 (t, $J = 7.8$ Hz, 2H), 2.78 (brs, 2H), 2.70 (t, $J = 7.8$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.1, 171.0, 141.3, 135.1, 134.1, 133.5, 132.5, 128.9, 128.51, 128.48, 128.43, 128.41, 128.2, 126.9, 126.6, 126.5, 126.3, 126.2, 126.0, 47.2, 44.2, 43.1, 39.7, 35.8, 35.5, 31.42, 31.36, 29.4, 28.5; IR (thin film) ν 3061, 3025, 2929, 2860, 1646 s, 1495, 1452, 1207 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{18}\text{H}_{20}\text{NO}$: 266.1545, found 266.1537 $[\text{M}+\text{H}]^+$



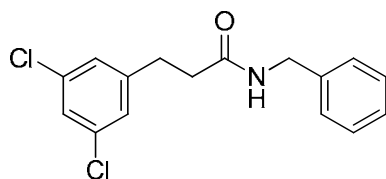
N-Benzyl-3-(4-cyanophenyl)propanamide (22). Prepared according to the general procedure in 0.1 M CH₂Cl₂ for 12 h; Purification using hexanes/EtOAc (1:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 97% yield; mp: 113–114 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.52 (d, *J* = 7.5 Hz, 2H), 7.30–7.27 (m, 5H), 7.14 (d, *J* = 6.5 Hz, 2H), 5.79 (brs, 1H), 4.38 (d, *J* = 5.5 Hz, 2H), 3.04 (t, *J* = 7.3 Hz, 2H), 2.51 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 171.0, 146.6, 138.1, 132.4, 129.4, 128.8, 127.8, 127.7, 119.1, 110.2, 43.7, 37.6, 31.6; IR (thin film) ν 3297, 3065, 3033, 2929, 2227, 1646, 1545, 1454 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₇H₁₇N₂O: 265.1341, found 265.1332 [M+H]⁺.



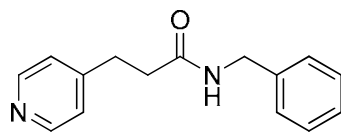
N-Benzyl-3-(4-(trifluoromethyl)phenyl)propanamide (23). Prepared according to the general procedure in 0.1 M CH₂Cl₂ for 12 h; Purification using hexanes/EtOAc (2:3 v/v) as the eluent afforded the desired amidation product as a colorless solid in 74% yield; mp: 117–118 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.51 (d, *J* = 7.5 Hz, 2H), 7.30–7.27 (m, 5H), 7.13 (d, *J* = 7.0 Hz, 2H), 5.78 (brs, 1H), 4.38 (d, *J* = 5.5 Hz, 2H), 3.04 (t, *J* = 7.3 Hz, 2H), 2.51 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 171.5, 145.0, 138.1, 128.8, 128.7, 128.6 (q, ²*J*_{CF} = 32.4 Hz), 127.7, 127.6, 125.5 (q, ³*J*_{CF} = 3.6 Hz), 124.4 (q, ¹*J*_{CF} = 272.0 Hz), 43.6, 37.8, 31.4; IR (thin film) ν 3260, 3086, 1645 s, 1573, 1323 s, 1266, 1115, 1065 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₇H₁₇F₃NO: 308.1262, found 308.1255 [M+H]⁺.



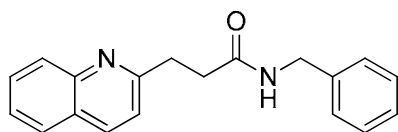
N-Benzyl-3-(4-bromophenyl)propanamide (24). Prepared according to the general procedure in 0.1 M CH₂Cl₂ for 12 h; Purification using hexanes/EtOAc (2:3 v/v) as the eluent afforded the desired amidation product as a colorless solid in 68% yield. mp: 140–141 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.38 (d, *J* = 8.0 Hz, 2H), 7.32–7.25 (m, 3H), 7.12 (d, *J* = 7.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 5.74 (brs, 1H), 4.37 (d, *J* = 5.5 Hz, 2H), 2.93 (t, *J* = 7.3 Hz, 2H), 2.47 (t, *J* = 7.3 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 171.6, 139.9, 138.2, 131.7, 130.3, 128.8, 127.8, 127.6, 120.2, 43.7, 38.3, 31.1; IR (thin film) ν 3293 s, 3031, 2926, 1635 s, 1538, 1486 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₆H₁₇BrNO: 318.0494, found 318.0491 [M+H]⁺.



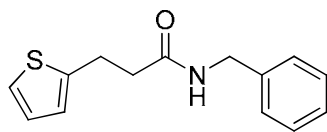
N-Benzyl-3-(3,5-dichlorophenyl)propanamide (25). Prepared according to the general procedure in 0.1 M CH₂Cl₂ for 12 h; Purification using hexanes/EtOAc (3:2 v/v) as the eluent afforded the desired amidation product as a colorless solid in 53% yield; mp: 103–104 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.33–7.30 (m, 2H), 7.28–7.26 (m, 1H), 7.21 (s, 1H), 7.18 (d, *J* = 7.0 Hz, 2H), 7.10 (s, 2H), 5.70 (brs, 1H), 4.41 (d, *J* = 5.5 Hz, 2H), 2.96 (t, *J* = 7.5 Hz, 2H), 2.48 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 171.0, 144.3, 138.1, 135.1, 128.9, 127.9, 127.7, 127.1, 126.7, 43.8, 37.8, 31.0; IR (thin film) ν 3291 s, 3086, 2936, 1640 s, 1568, 1429 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₆H₁₆Cl₂NO: 308.0609, found 308.0601 [M+H]⁺.



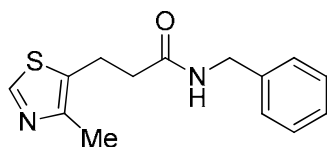
N-Benzyl-3-(pyridin-4-yl)propanamide (26). Prepared according to the general procedure in 0.1 M CH₂Cl₂ for 12 h; Purification using EtOAc/acetone (1:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 57% yield; mp: 33–35 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.36 (d, *J* = 5.5 Hz, 2H), 7.27–7.20 (m, 3H), 7.12 (d, *J* = 7.5 Hz, 2H), 7.05 (d, *J* = 5.0 Hz, 2H), 5.56 (brs, 1H), 4.35 (d, *J* = 6.0 Hz, 2H), 2.93 (t, *J* = 7.5 Hz, 2H), 2.48 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 171.3, 150.1, 149.6, 138.2, 128.7, 127.7, 127.5, 123.9, 43.6, 36.7, 30.8; IR (thin film) ν 3279 s, 3064, 2925, 1648 s, 1604, 1558, 1418 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₅H₁₇N₂O: 241.1341, found 241.1333 [M+H]⁺.



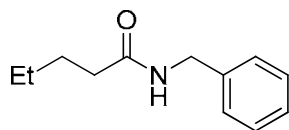
N-Benzyl-3-(quinolin-2-yl)propanamide (27). Prepared according to the general procedure; Purification using hexanes/EtOAc (1:4 v/v) as the eluent afforded the desired amidation product as a colorless solid in 78% yield; mp: 113–114 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.60–7.57 (m, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.33 (brs, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 7.18–7.17 (m, 3H), 7.12–7.11 (m, 2H), 4.37 (d, *J* = 5.5 Hz, 2H), 3.29 (t, *J* = 6.8 Hz, 2H), 2.81 (t, *J* = 7.0 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 172.5, 160.9, 147.5, 138.4, 136.5, 129.4, 128.52, 128.48, 127.6, 127.5, 127.2, 126.8, 125.9, 121.8, 43.5, 35.2, 34.0; IR (thin film) ν 3286, 3061, 2921, 1647 s, 1549, 1504, 1427 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₉H₁₉N₂O: 291.1497, found 291.1486 [M+H]⁺.



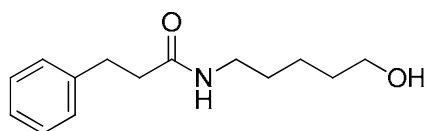
N-Benzyl-3-(thiophen-2-yl)propanamide (28). Prepared according to the general procedure; Purification using hexanes/EtOAc (3:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 48% yield; mp: 70–71 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.32–7.24 (m, 3H), 7.17 (d, J = 7.3 Hz, 2H), 7.12 (d, J = 5.1 Hz, 1H), 6.92–6.90 (m, 1H), 6.82–6.81 (m, 1H), 5.81 (brs, 1H), 4.41 (d, J = 5.5 Hz, 2H), 3.21 (t, J = 7.5 Hz, 2H), 2.56 (t, J = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 171.5, 143.4, 138.2, 128.8, 127.9, 127.6, 127.0, 125.0, 123.6, 43.7, 38.8, 26.0; IR (thin film) ν 3298 s, 3067, 3031, 2924, 1642 s, 1543, 1454 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{15}\text{NOSNa}$: 268.0772, found 268.0764 $[\text{M}+\text{Na}]^+$.



N-Benzyl-3-(4-methylthiazol-5-yl)propanamide (29). Prepared according to the general procedure; Purification using hexanes/acetone (3:2 v/v) as the eluent afforded the desired amidation product as a colorless solid in 59% yield; mp: 70–71 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.54 (s, 1H), 7.33–7.26 (m, 3H), 7.19 (d, J = 7.0 Hz, 2H), 5.71 (brs, 1H), 4.42 (d, J = 5.5 Hz, 2H), 3.16 (t, J = 7.3 Hz, 2H), 2.49 (t, J = 7.3 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 170.9, 149.5, 149.4, 138.1, 130.2, 128.9, 127.9, 127.8, 43.9, 38.2, 22.3, 15.0; IR (thin film) ν 3259, 2919, 2850, 1645, 1539, 1494, 1453, 1412, 1375 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{OS}$: 261.1062, found 261.1052 $[\text{M}+\text{H}]^+$.

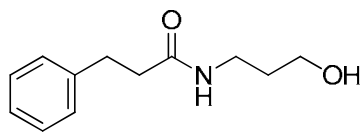


N-benzylpentanamide (30). CAS RN: 10264-05-8. Prepared according to the general procedure in 0.1 M CH₂Cl₂ for 12 h; Purification using hexanes/acetone (4:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 21% yield; ¹H NMR (500 MHz, CDCl₃) δ 7.35–7.27 (m, 5H), 5.67 (brs, 1H), 4.45 (d, *J* = 5.5 Hz, 2H), 2.22 (t, *J* = 7.5 Hz, 2H), 1.65 (quin, *J* = 7.5 Hz, 2H), 1.36 (sext, *J* = 7.5 Hz, 2H), 0.92 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 173.1, 138.5, 128.9, 128.0, 127.7, 43.8, 36.7, 28.0, 22.6, 13.9. Analytical data is consistent with published data.⁹

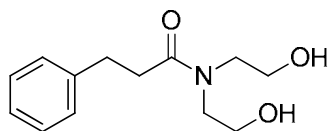


N-(5-Hydroxypentyl)-3-phenylpropanamide (31). Prepared according to the general procedure in 0.1 M CH₂Cl₂ solution; Purification using hexanes/EtOAc (1:4 v/v) as the eluent afforded the desired amidation product as a colorless solid in 51% yield; mp:44–46 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.26 (t, *J* = 7.4 Hz, 2H), 7.17 (d, *J* = 7.4 Hz, 3H), 5.74 (brs, 1H), 3.59 (t, *J* = 6.3 Hz, 2H), 3.18 (dd, *J* = 6.6, 12.9 Hz, 2H), 2.93 (t, *J* = 7.7 Hz, 2H), 2.44 (t, *J* = 7.7 Hz, 2H), 2.33 (brs, 1H), 1.52 (quintet, *J* = 7.0 Hz, 2H), 1.43 (quintet, *J* = 7.2 Hz, 2H), 1.29 (quintet, *J* = 7.5 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 172.5, 140.9, 128.5, 128.4, 126.2, 62.3, 39.4, 38.4, 32.2, 31.8, 29.2, 23.0; IR (thin film) ν 3297, 3086, 3028, 2935, 2862, 1647, 1557, 1496, 1454 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₄H₂₁NO₂Na: 258.1470, found 258.1462 [M+Na]⁺.

(9) Q. Liu, Z. Liu, Y.-L. Zhou, W. Zhang, L. Yang, Z.-L. Liu and W. Yu, *Synlett.*, 2005, 2510–2512.

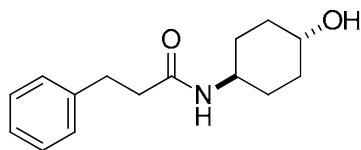


***N*-(3-Hydroxypropyl)-3-phenylpropanamide (32).** CAS RN: 401587-50-6. Prepared according to the general procedure in 0.1 M CH₂Cl₂ solution; Purification using hexanes/EtOAc (1:4 v/v) as the eluent afforded the desired amidation product as a colorless solid in 66% yield; ¹H NMR (500 MHz, CDCl₃) δ 7.28–7.25 (m, 2H), 7.20–7.17 (m, 3H), 6.24 (brs, 1H), 3.57 (brs, 1H), 3.50 (brs, 2H), 3.35–3.31 (m, 2H), 2.94 (t, *J* = 7.8 Hz, 2H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.61–1.57 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 173.5, 140.7, 128.6, 128.4, 126.4, 59.3, 38.4, 36.4, 32.1, 31.8. Analytical data is consistent with published data.¹⁰



***N,N*-bis(2-Hydroxyethyl)-3-phenylpropanamide (33).** Prepared according to the general procedure in 0.1 M CH₂Cl₂ solution; Purification using EtOAc/acetone (1:1 v/v) as the eluent afforded the desired amidation product as a colorless oil in 38% yield; ¹H NMR (500 MHz, CDCl₃) δ 7.28–7.26 (m, 2H), 7.20–7.19 (m, 3H), 3.82 (t, *J* = 4.6 Hz, 2H), 3.70 (t, *J* = 4.7 Hz, 2H), 3.54 (t, *J* = 4.5 Hz, 2H), 3.41 (t, *J* = 4.6 Hz, 2H), 2.95 (t, *J* = 7.7 Hz, 2H), 2.71 (t, *J* = 7.8 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 174.8, 141.1, 128.6, 128.5, 126.4, 61.4, 60.8, 52.2, 50.7, 35.5, 31.6; IR (thin film) ν 3366, 2932, 2876, 1618 s, 1454, 1048 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₃H₁₉NO₃Na: 260.1263, found 260.1254 [M+Na]⁺.

(10) A. Brizzi, G. Bruni, P. Massarelli, C. Nencini, R. Rauggi, R. Sirianni, V. Brizzi, *Bollettino Chimico Farmaceutico*, 2005, **144**, e1/1–e1/19.



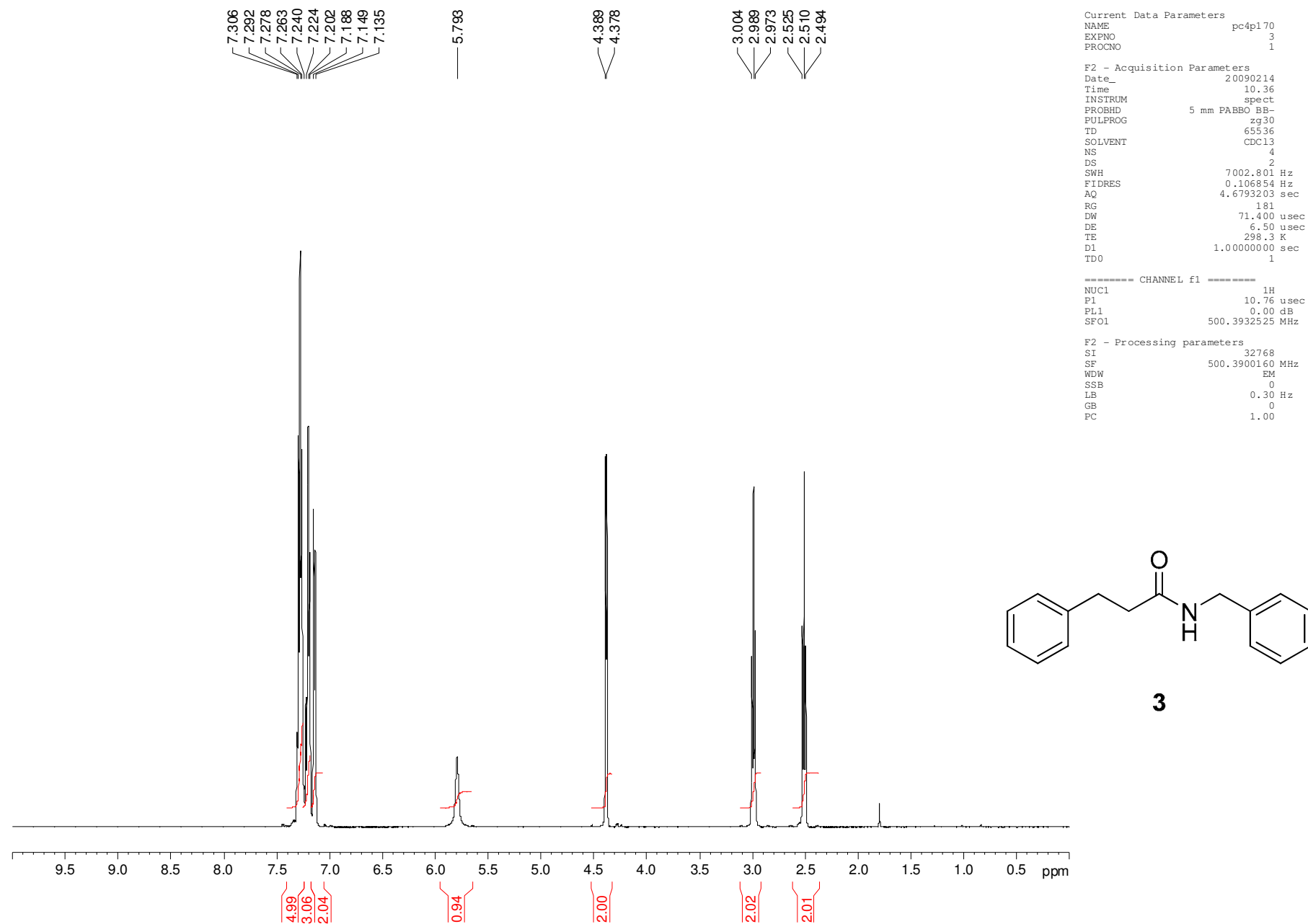
***N*-(*trans*-4-Hydroxycyclohexyl)-3-phenylpropanamide (34).** CAS RN: 713526-52-4. ¹¹

Prepared according to the general procedure in 0.1 M CH₂Cl₂ solution; Purification using EtOAc/acetone (4:1 v/v) as the eluent afforded the desired amidation product as a colorless solid in 74% yield; mp: 180–181 °C; ¹H NMR (500 MHz, Acetone-d₆) δ 7.25–7.15 (m, 5H), 6.81 (brs, 1H), 3.60 (brs, 2H), 3.47 (brs, 1H), 2.87 (t, *J* = 7.5 Hz, 2H), 2.39 (t, *J* = 7.5 Hz, 2H), 1.88–1.82 (m, 4H), 1.33–1.26 (m, 2H), 1.21–1.15 (m, 2H); ¹³C NMR (125 MHz, Acetone-d₆) δ 171.3, 142.6, 129.2, 129.1, 126.7, 69.8, 48.4, 38.6, 35.0, 32.4, 31.4; IR (thin film) ν 3295, 2935, 2861, 1637, 1544, 1064 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₅H₂₁NO₂Na: 270.1470, found 270.1462 [M+Na]⁺.

(11) M. Kawai, H. Nakamura, I. Sakurada, H. Shimokawa, H. Tanaka, M. Matsumizu, K. Ando, K. Hattori, A. Ohta, S. Nukui, A. Omura and M. Kawamura, *Bioorg. Med. Chem. Lett.*, 2007, **17**, 5533–5536.

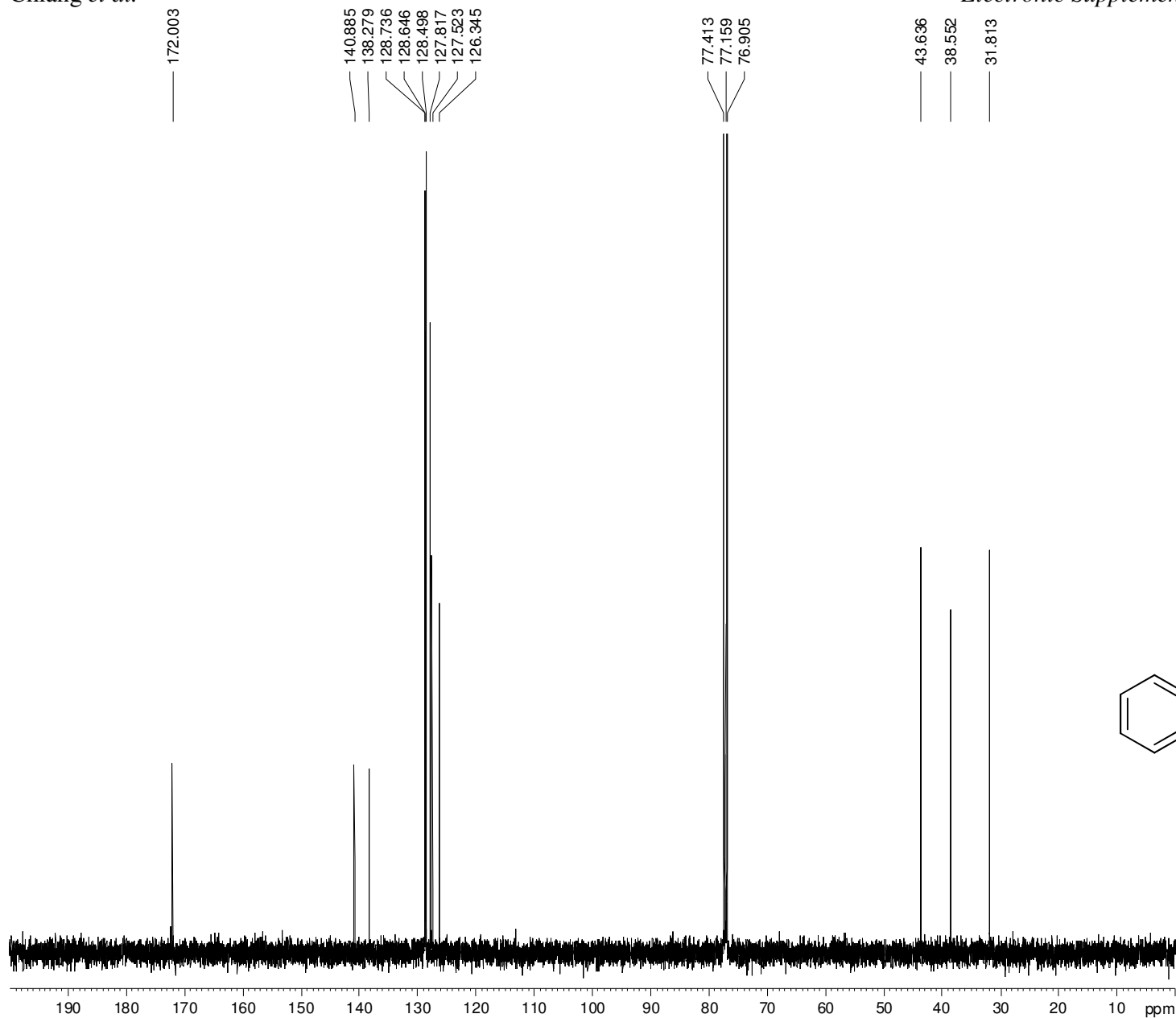
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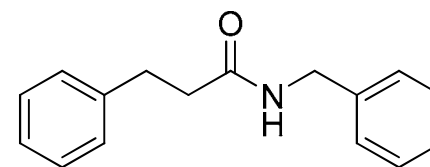
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DS                   4
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FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                   1150
DW                   16.800 usec
DE                   6.50 usec
TE                   298.5 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  13C
P1                    7.50 usec
PL1                   1.00 dB
SFO1                  125.8357479 MHz

===== CHANNEL f2 =====
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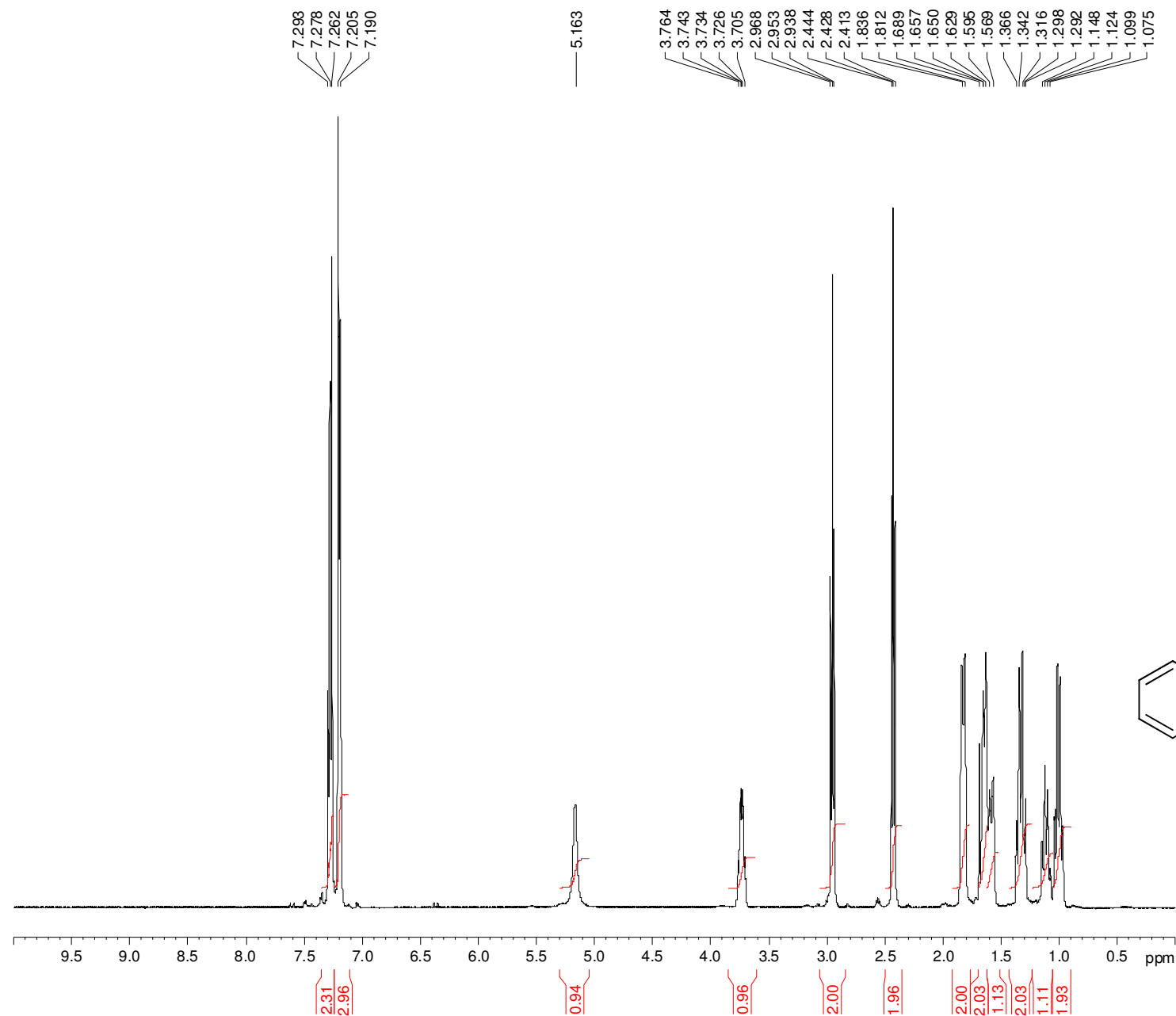
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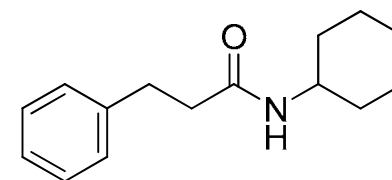


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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 228
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DE 6.50 usec
TE 297.1 K
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TD0 1

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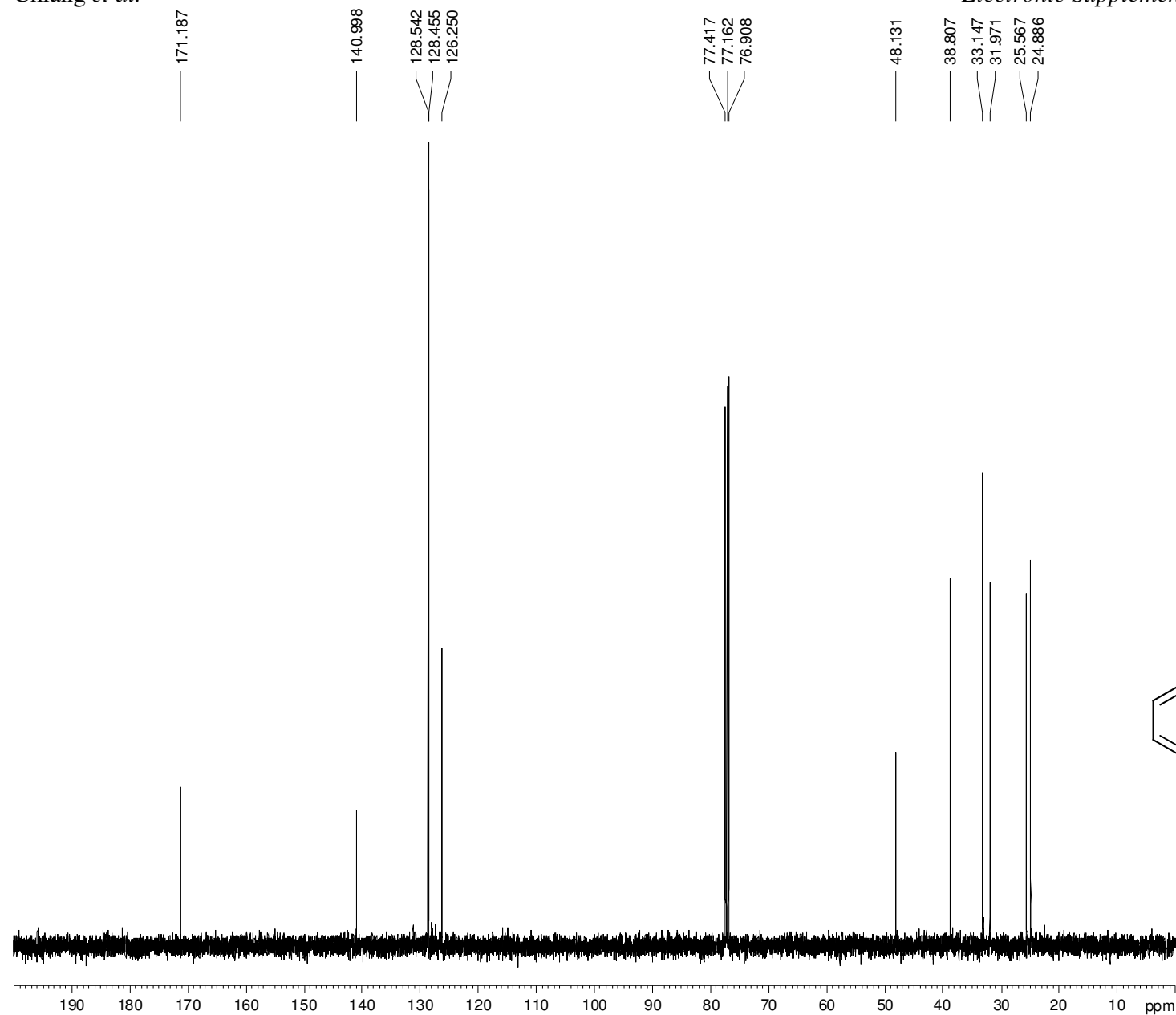
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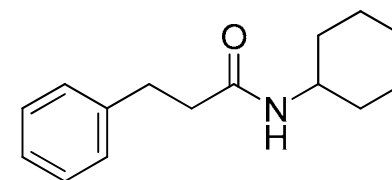
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TD                   65536
SOLVENT              CDCl3
NS                    17
DS                     4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                    2050
DW                   16.800 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                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
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PCPD2                 80.00 usec
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PL2                   0.00 dB
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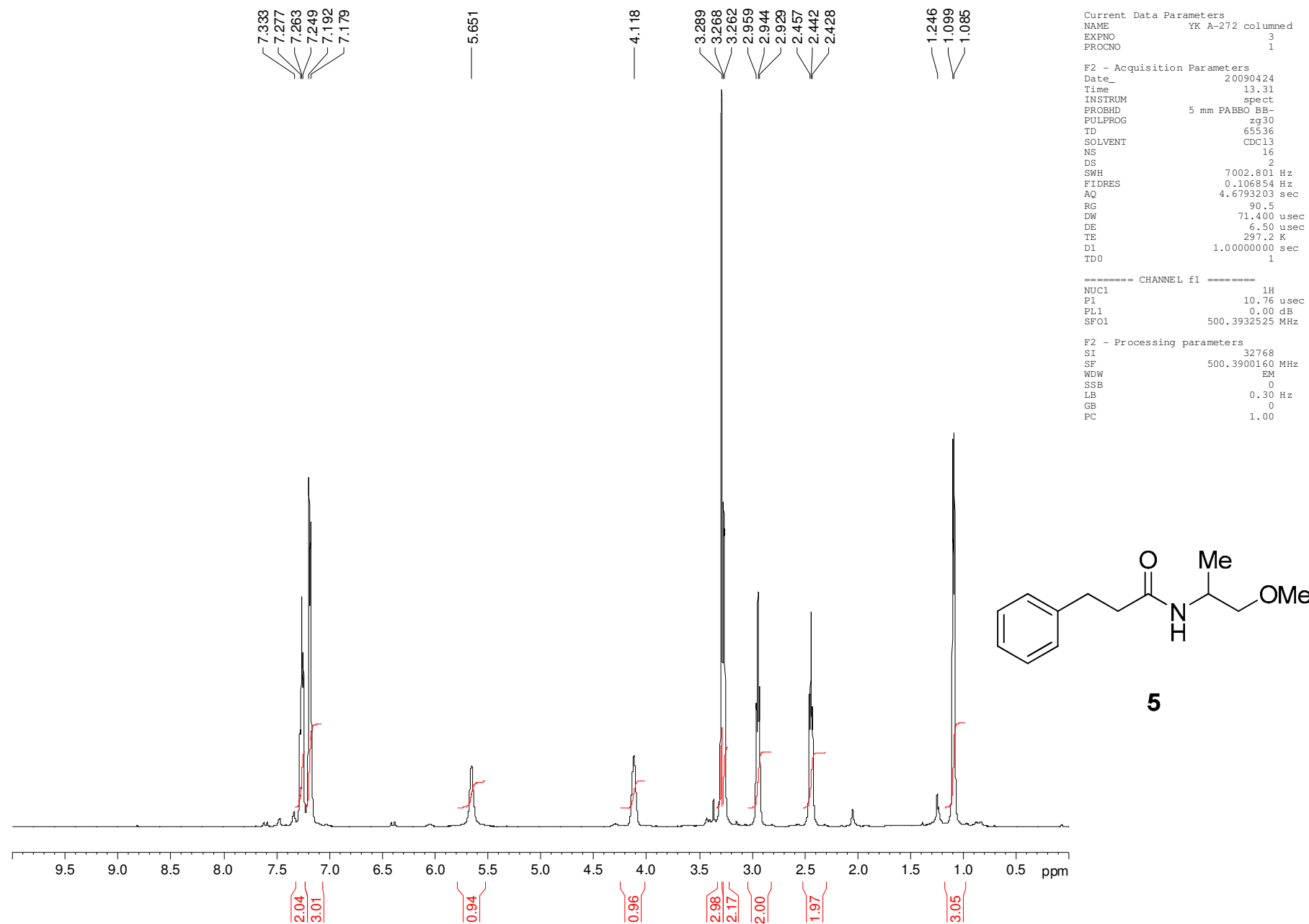
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4

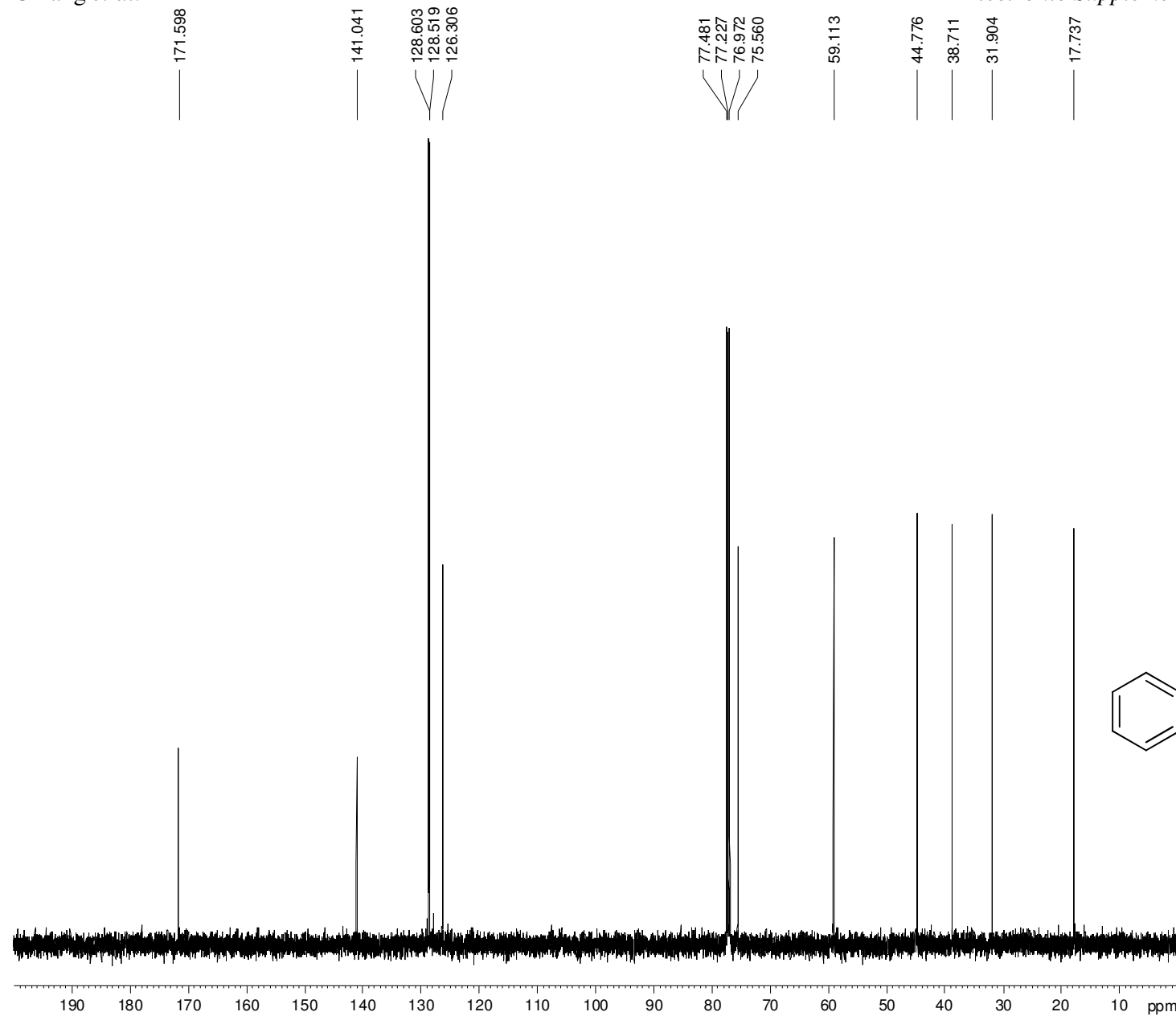
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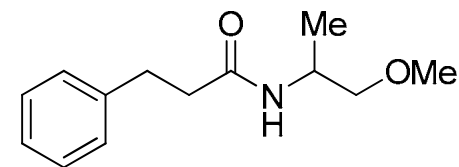
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PROCNO 1

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SOLVENT CDCl3
NS 37
DS 4
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FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
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PCPD2 80.00 usec
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PL2 0.00 dB
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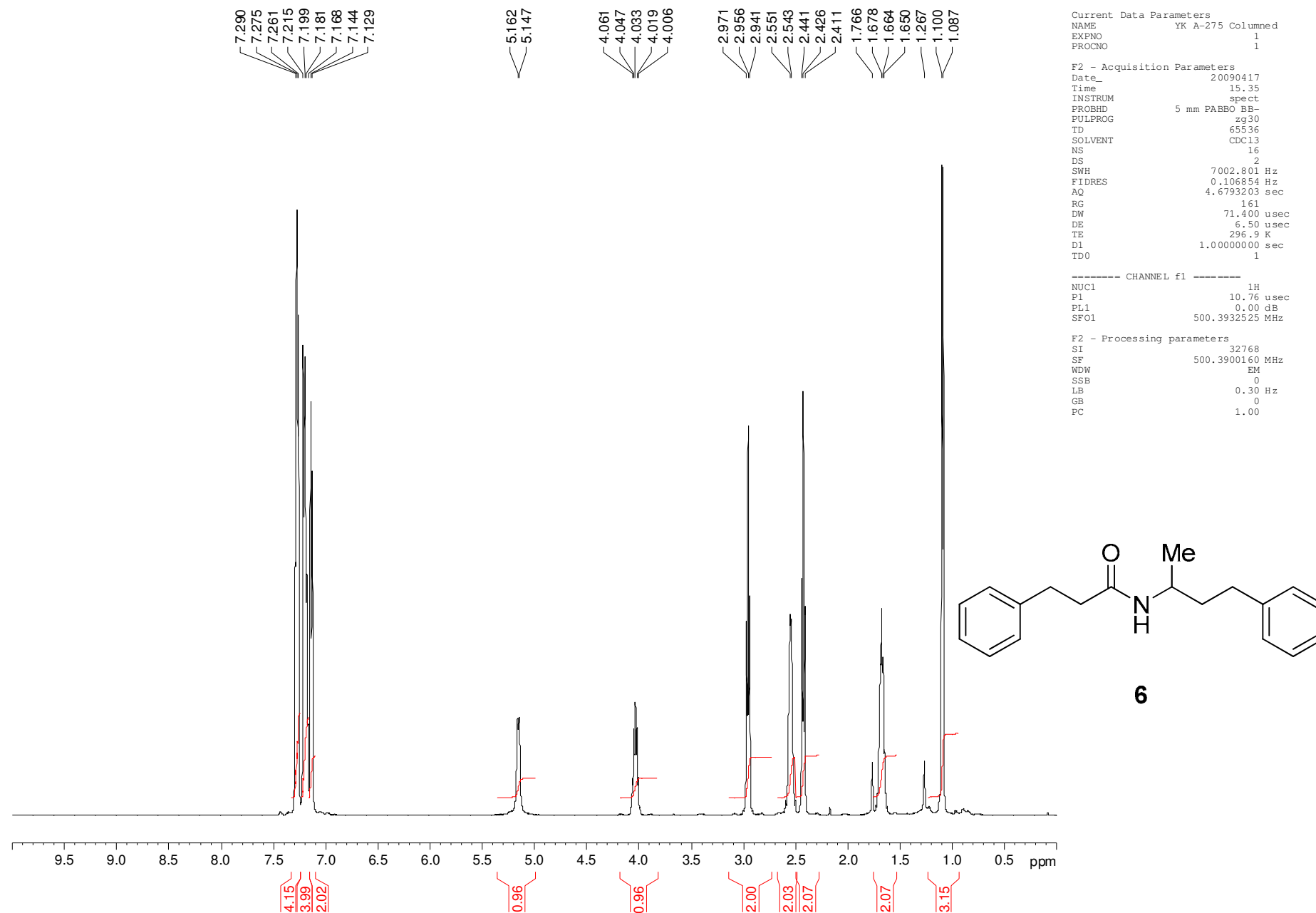
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PC 1.40



5

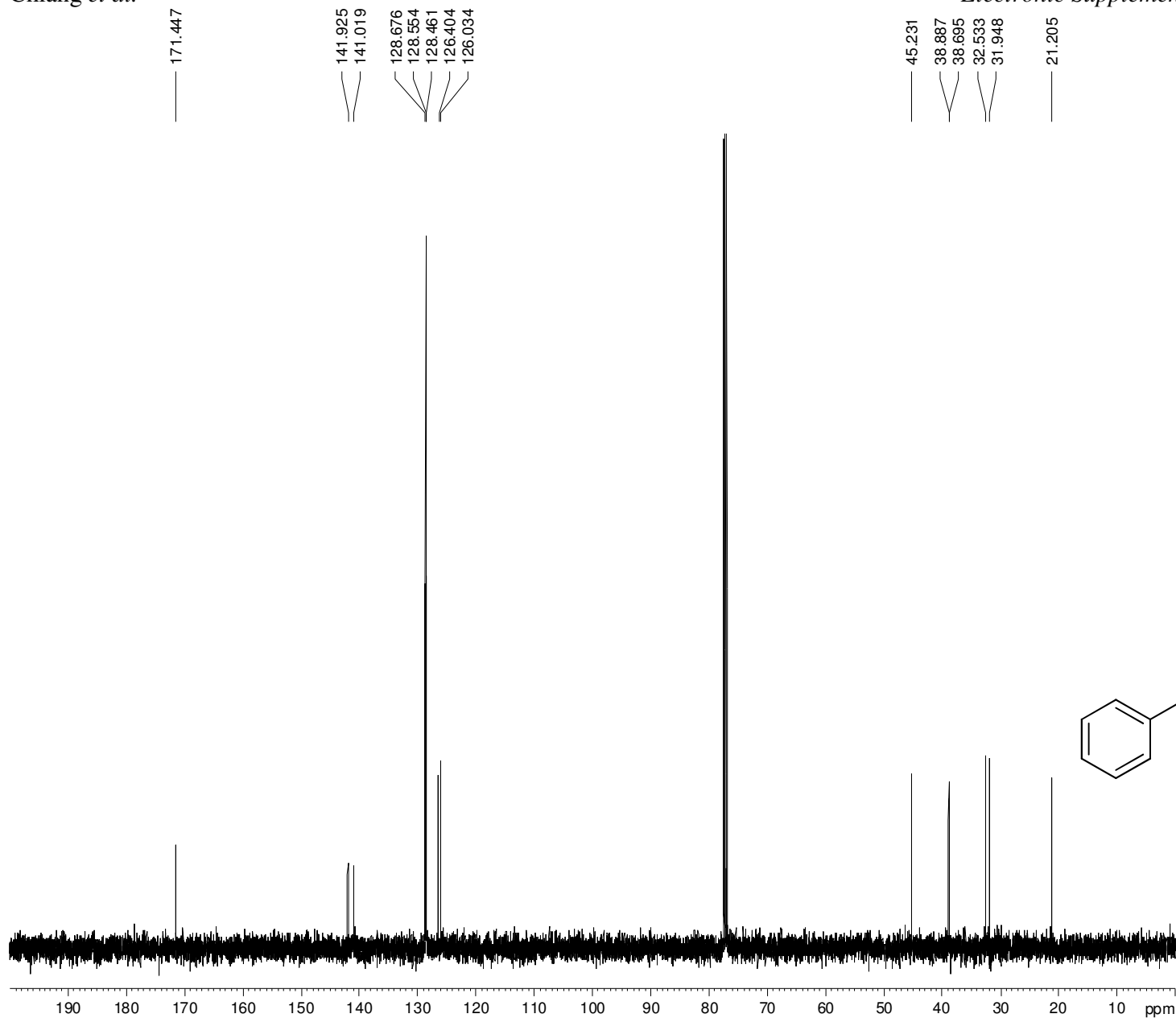
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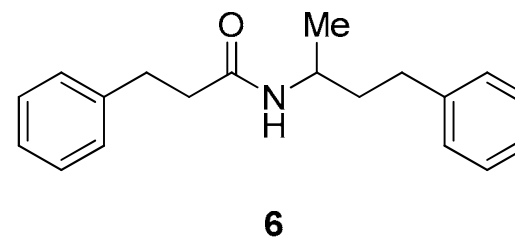
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AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 297.7 K
D1 2.0000000 sec
d11 0.0300000 sec
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===== CHANNEL f1 =====
NUC1 13C
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SFO1 125.8357479 MHz

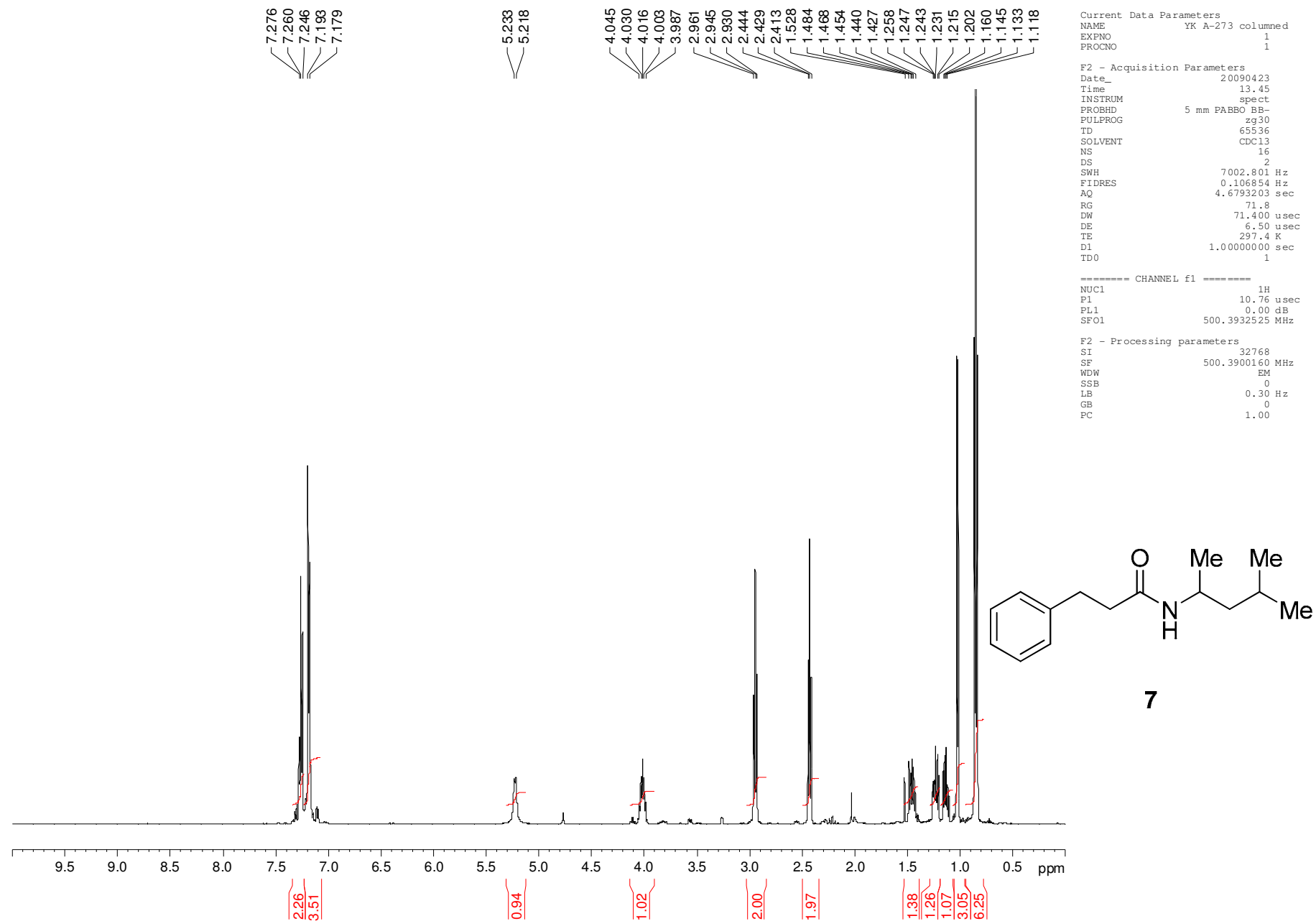
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F2 - Processing parameters
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LB 1.00 Hz
GB 0
PC 1.40



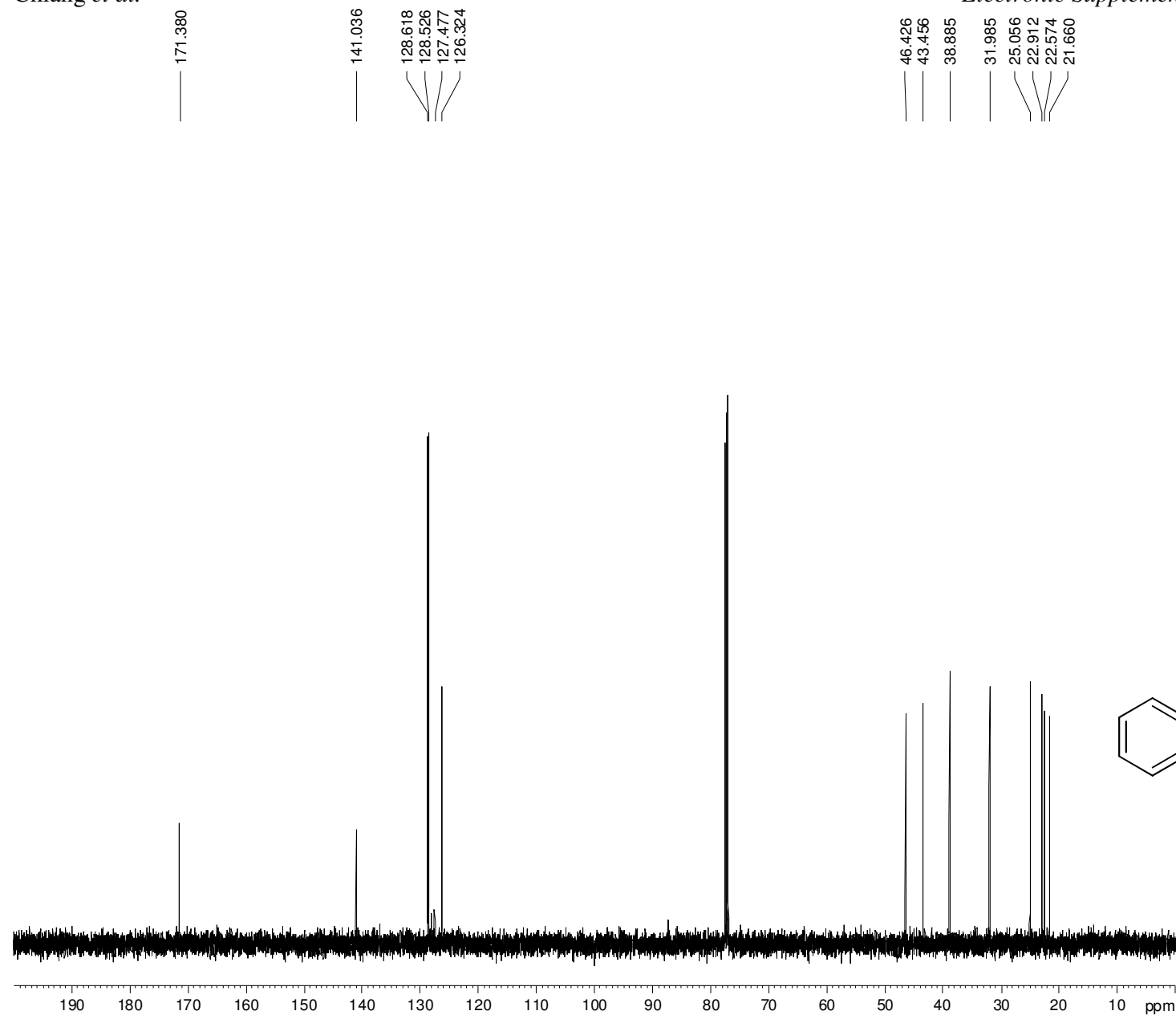
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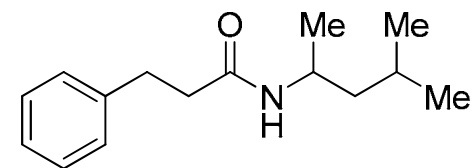
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SOLVENT CDCl3
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FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
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PCPD2 80.00 usec
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PL2 0.00 dB
SFO2 500.3920016 MHz

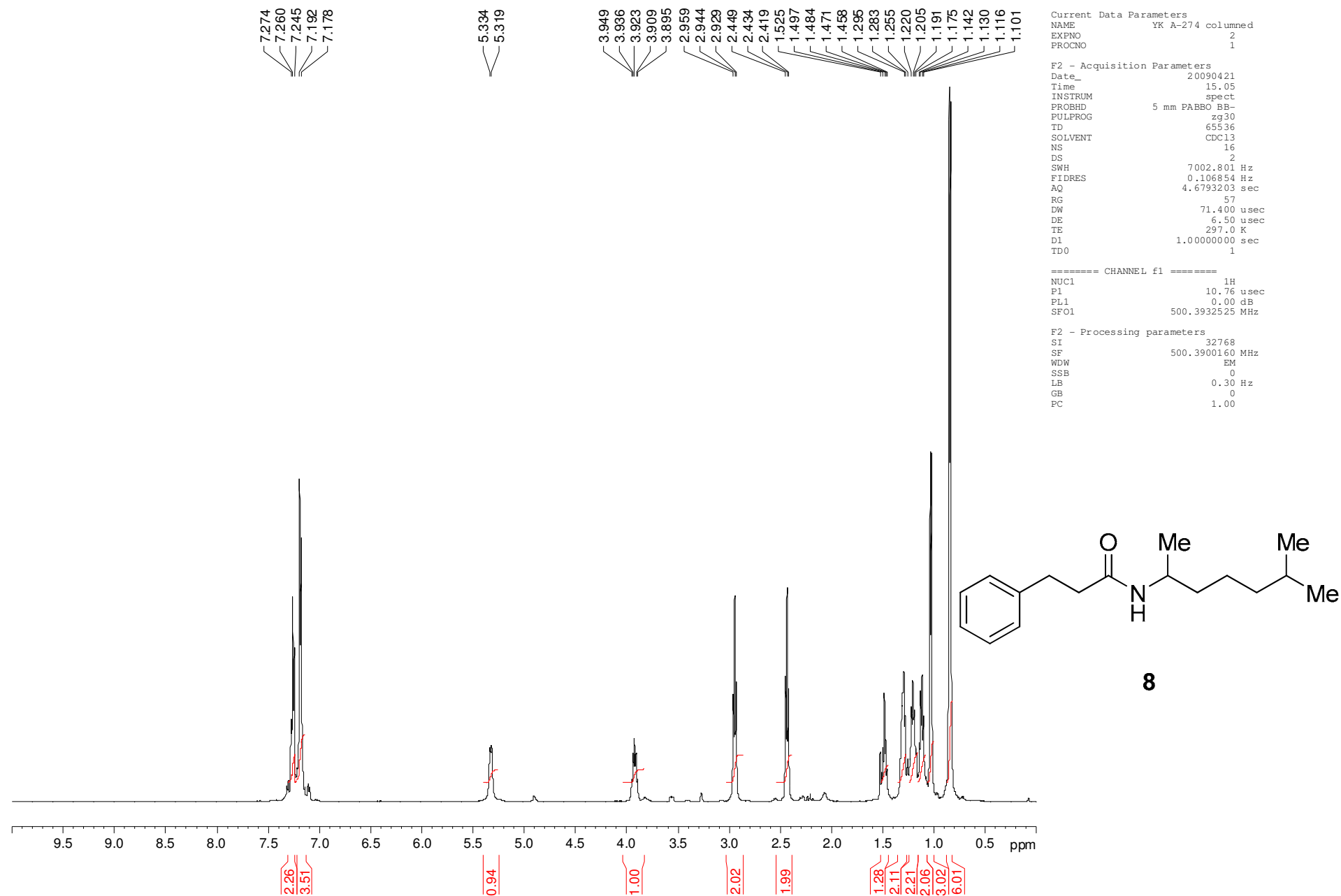
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7

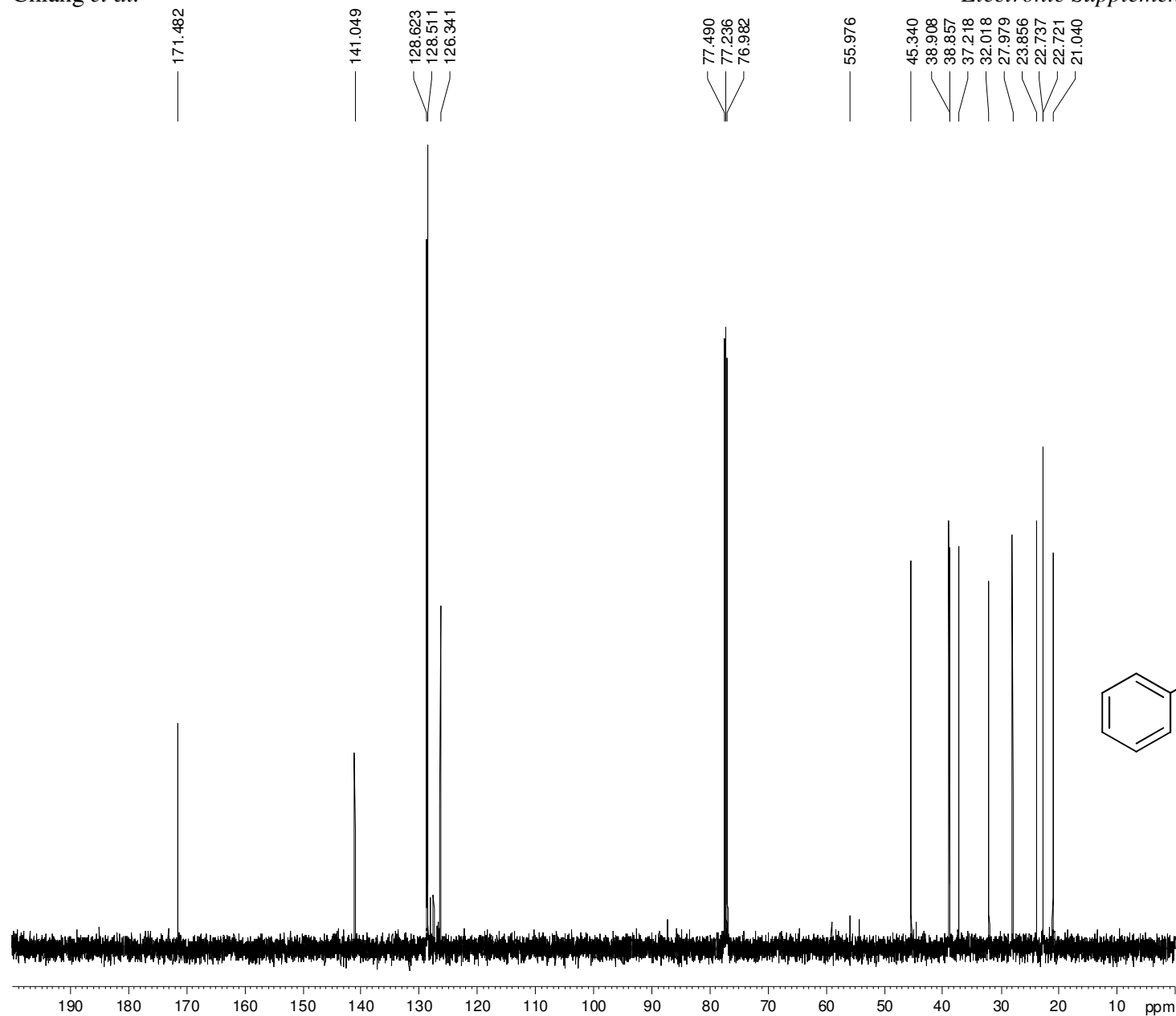
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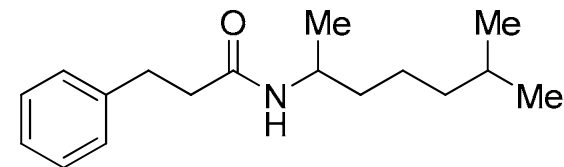
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PROCNO 1

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SOLVENT CDCl3
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DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
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PCPD2 80.00 usec
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PL13 18.43 dB
PL2 0.00 dB
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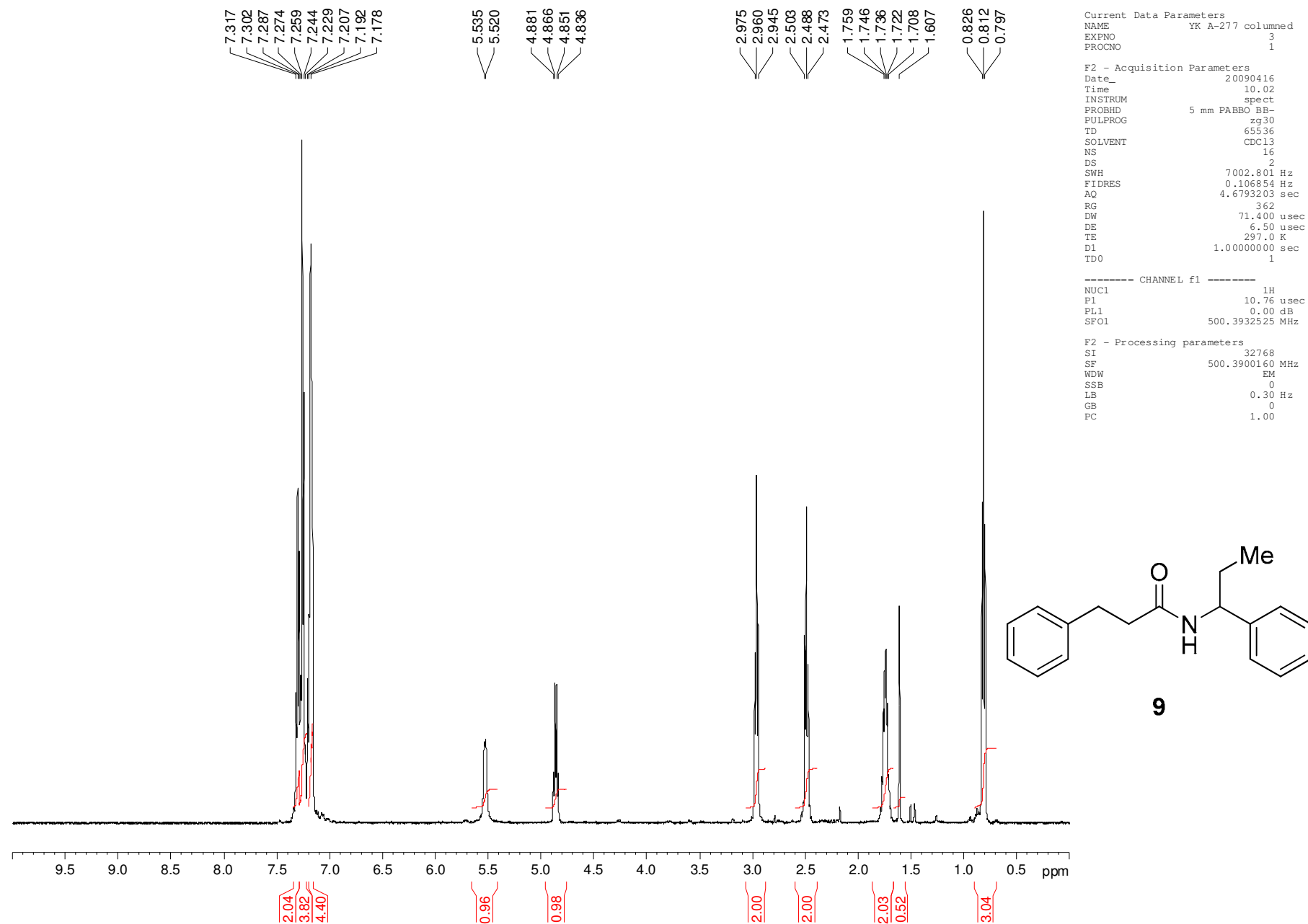
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8

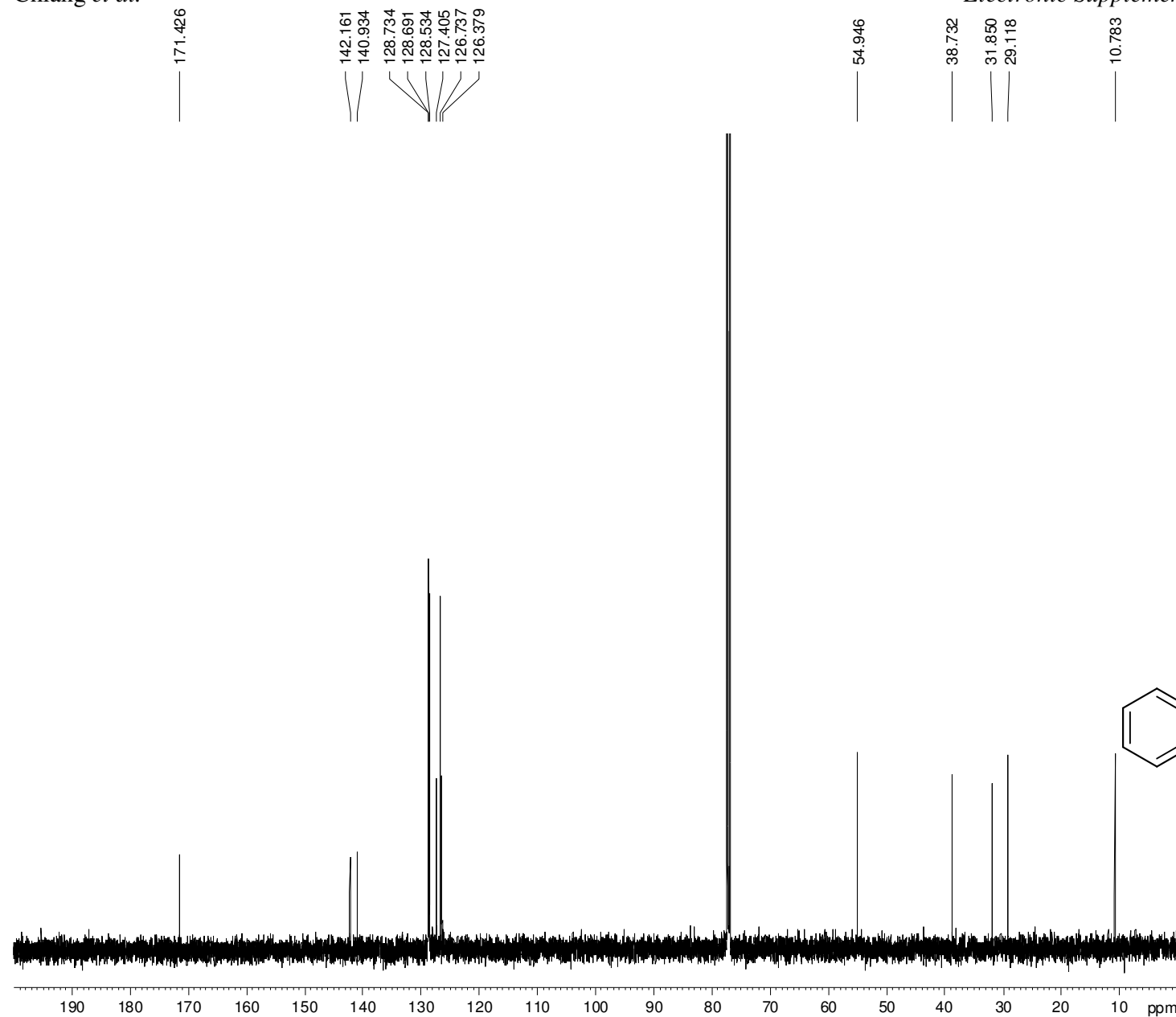
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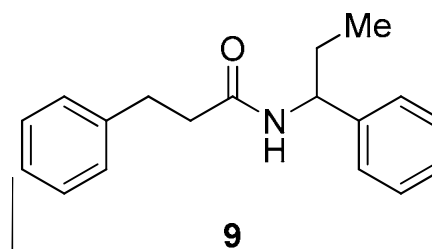
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AQ            1.1010548 sec
RG            456
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DE            6.50 usec
TE            297.6 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
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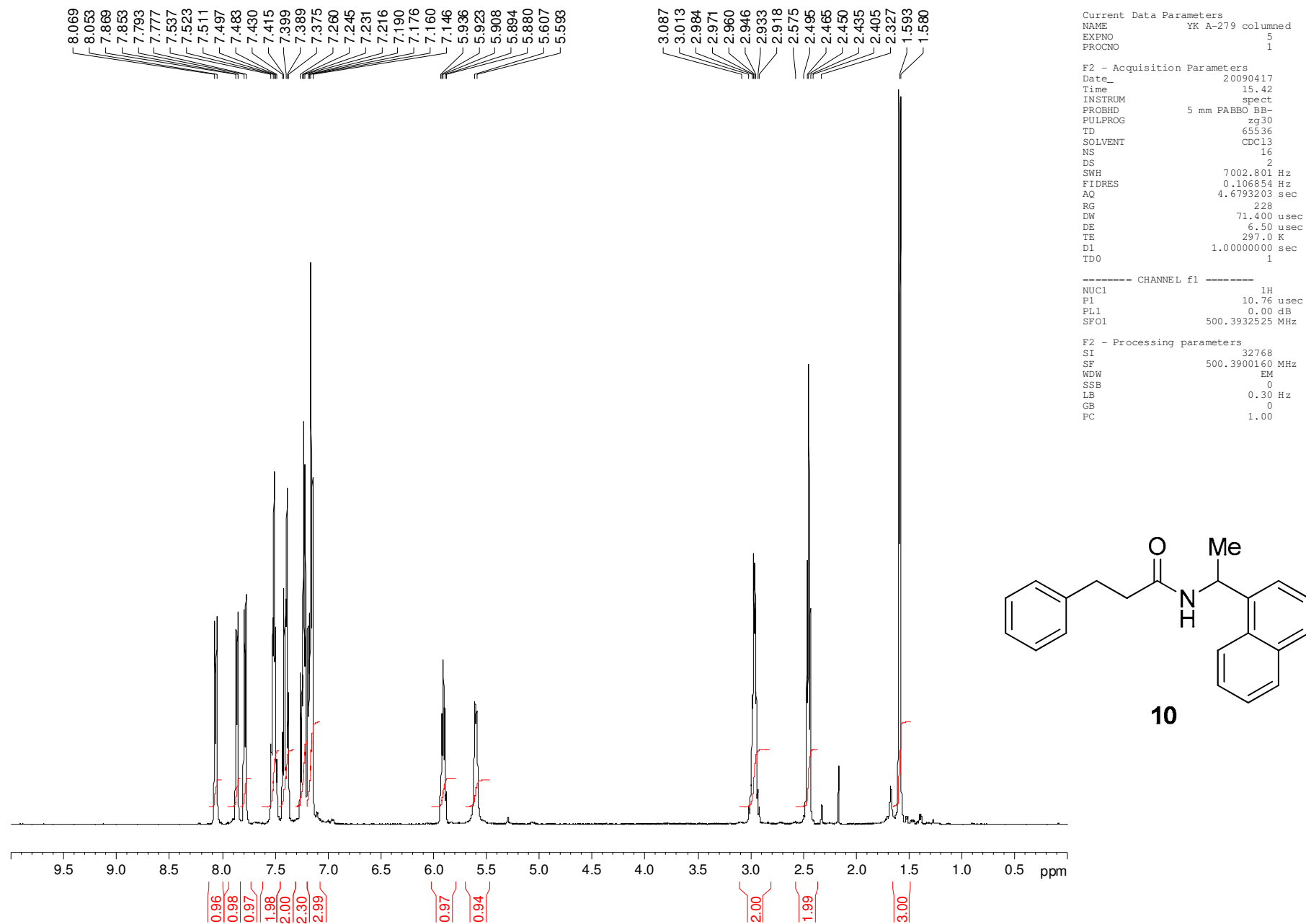
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PL13           18.43 dB
PL2            0.00 dB
SFO2          500.3920016 MHz

F2 - Processing parameters
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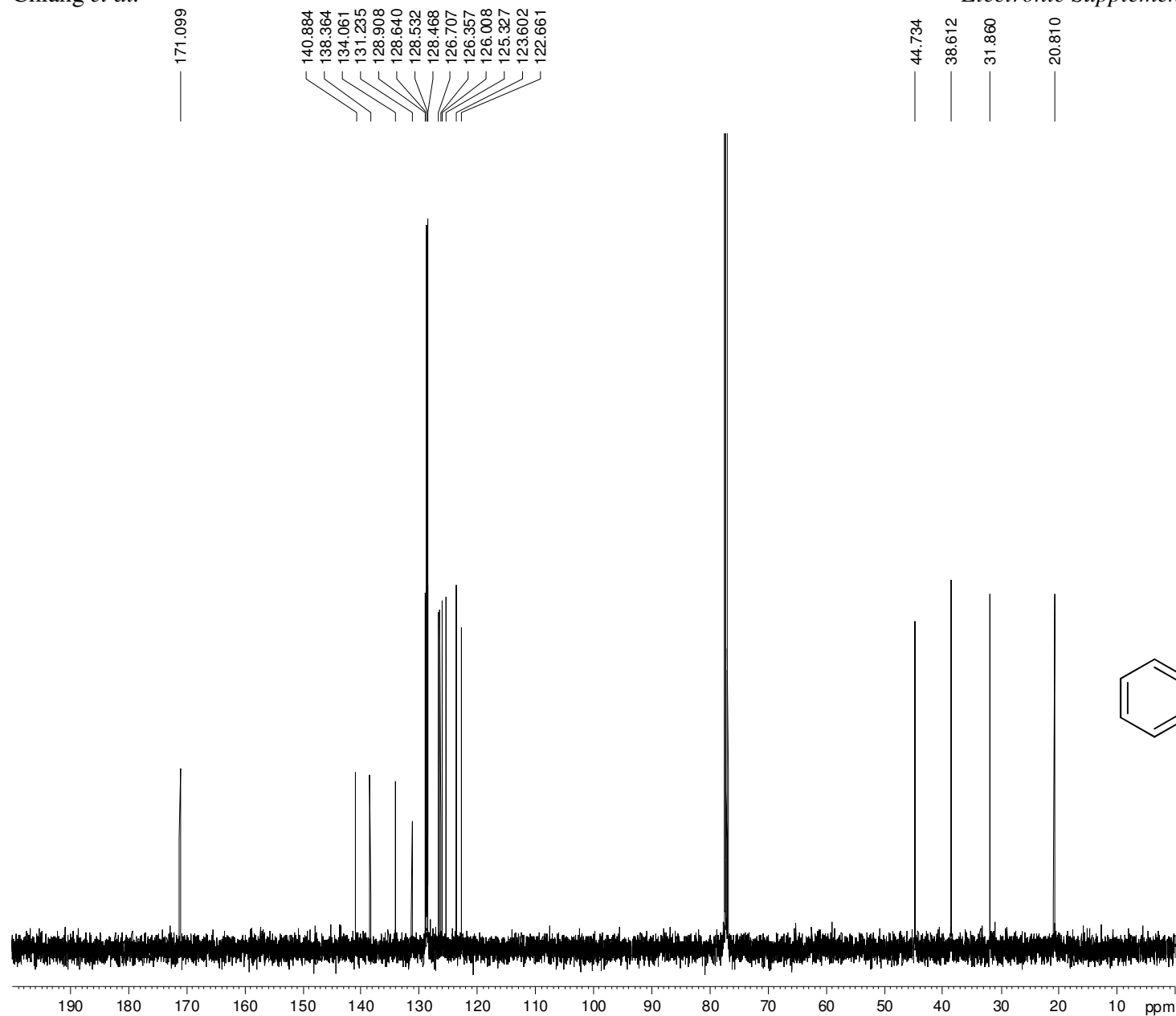
Chiang *et al.*

Electronic Supplementary Information



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Electronic Supplementary Information



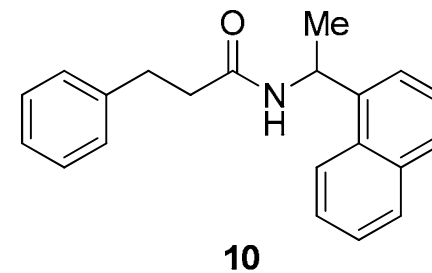
Current Data Parameters
NAME YK A-279 carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090429
Time 12.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 67
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1820
DW 16.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

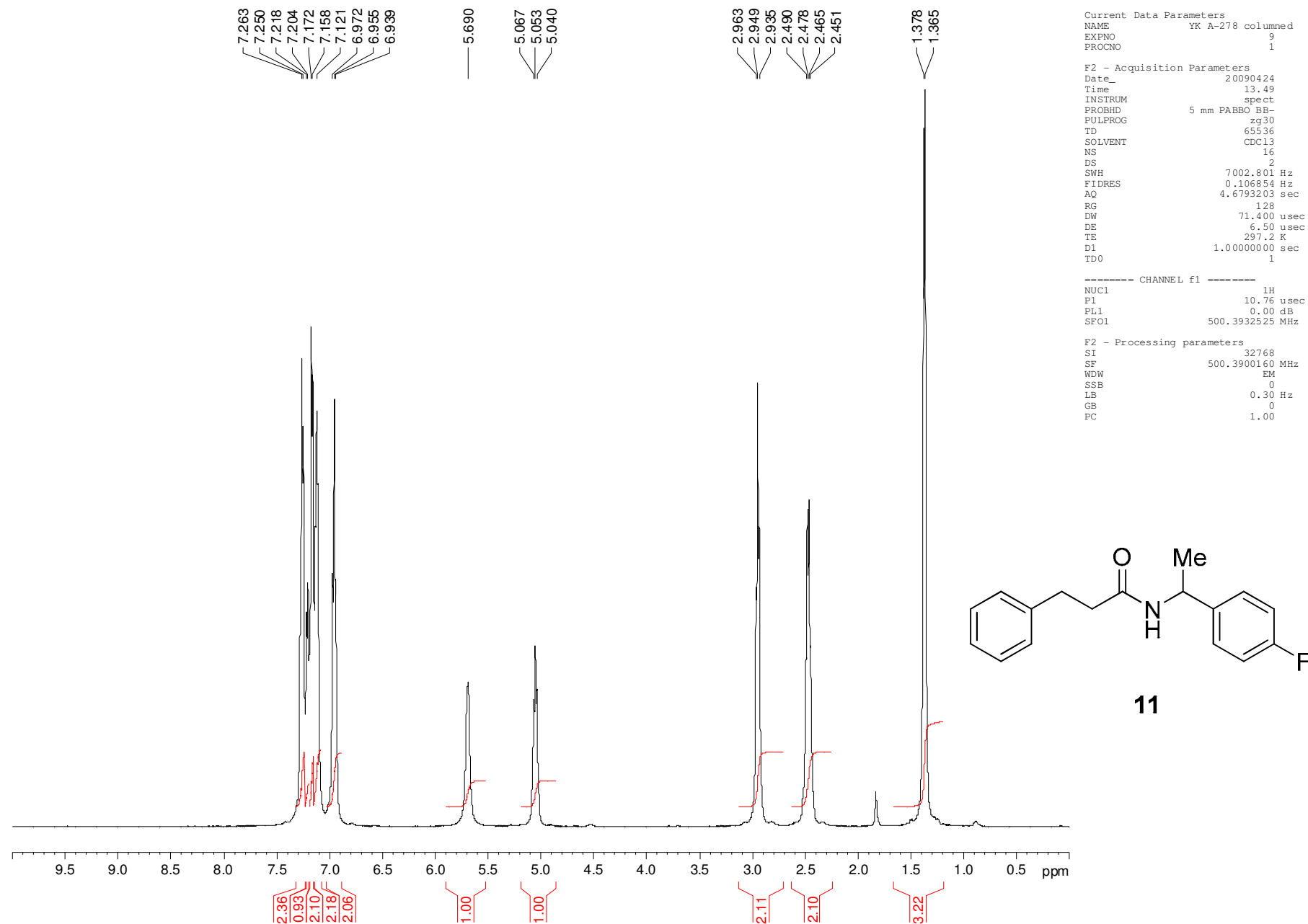
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 32768
SF 125.8231500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



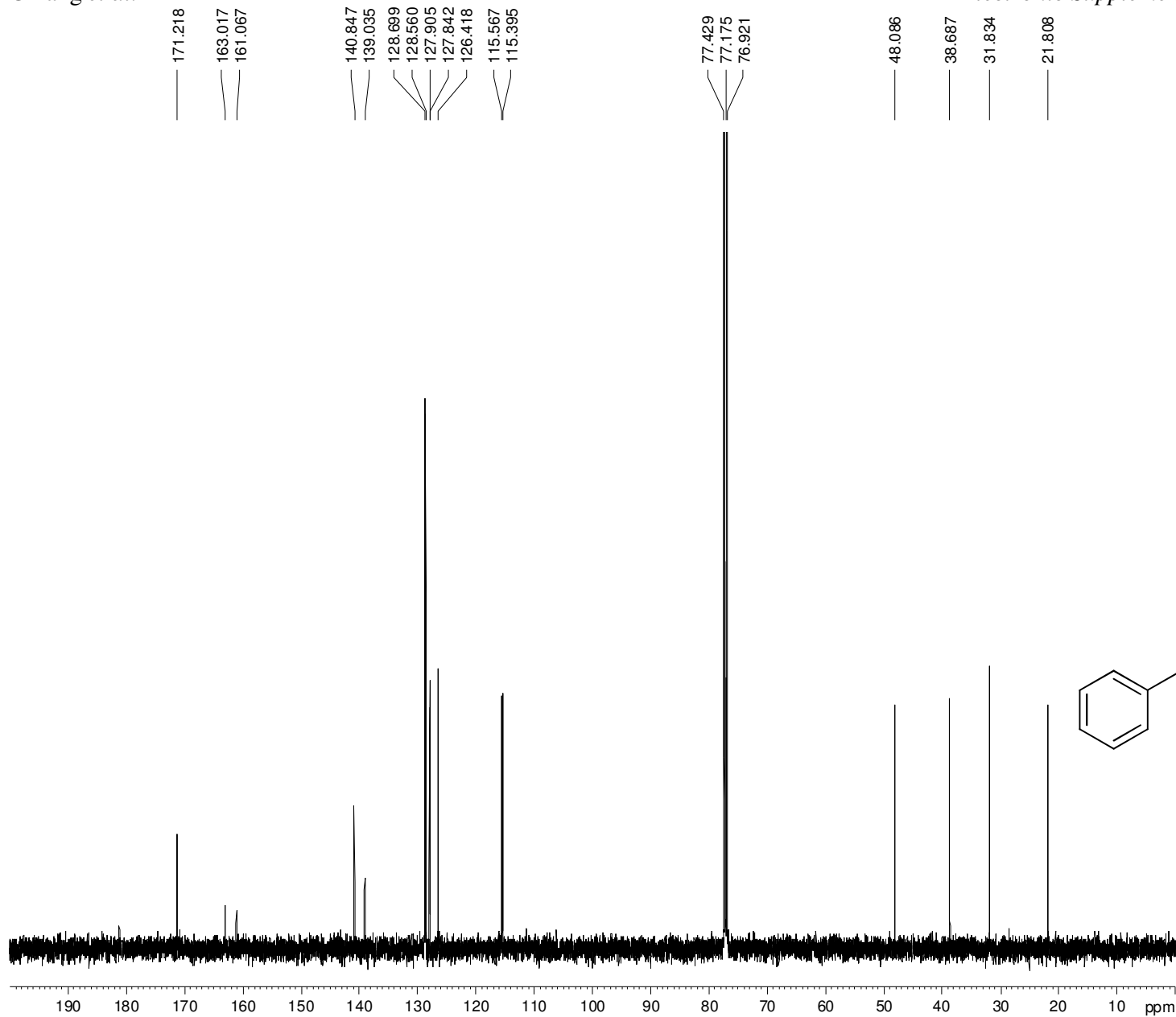
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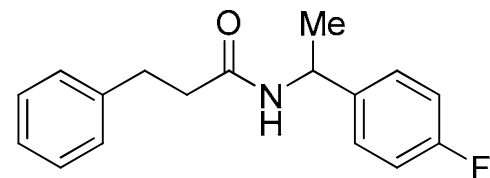
Current Data Parameters
NAME          YK A-278 carbon
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20090429
Time          17.40
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            118
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            456
DW            16.800 usec
DE            6.50 usec
TE            298.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

===== CHANNEL f1 =====
NUC1           13C
P1             7.50 usec
PL1            1.00 dB
SFO1          125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL12           17.43 dB
PL13           18.43 dB
PL2            0.00 dB
SFO2          500.3920016 MHz

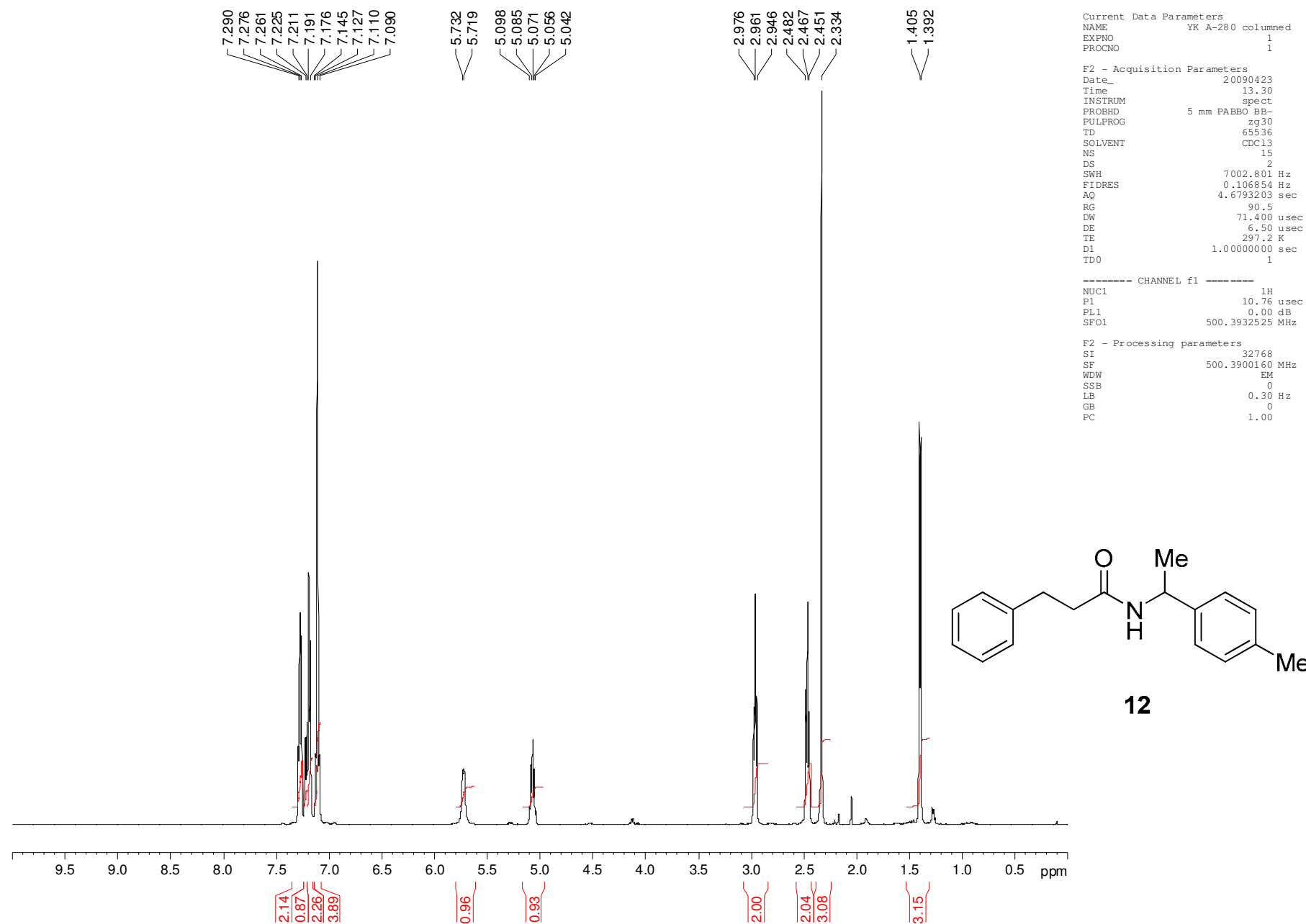
F2 - Processing parameters
SI             32768
SF            125.8231500 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
  
```



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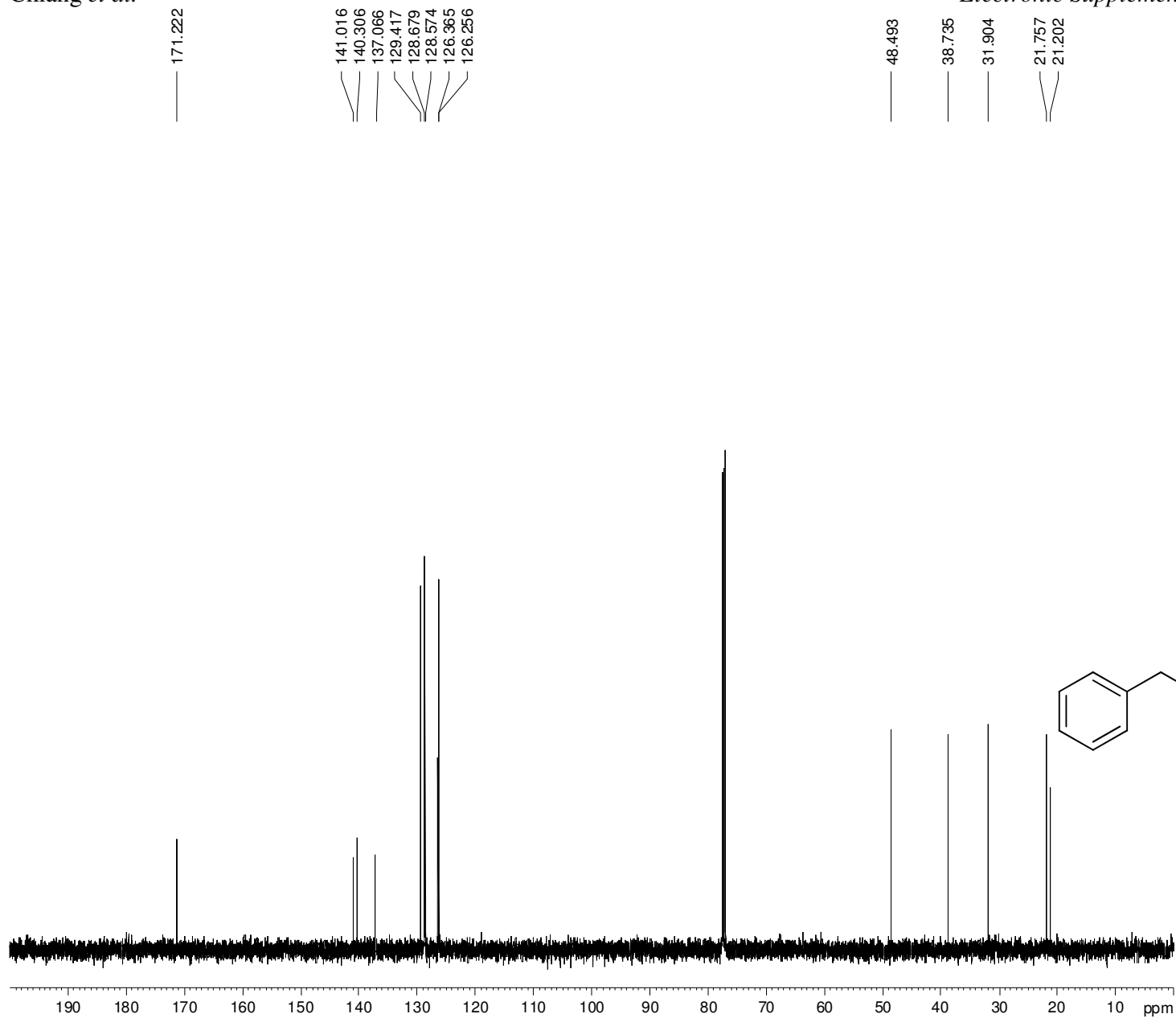
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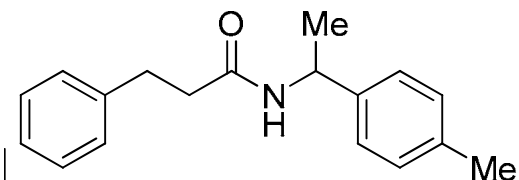
Current Data Parameters
NAME YK A-280 columned
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090423
Time 13.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 25
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

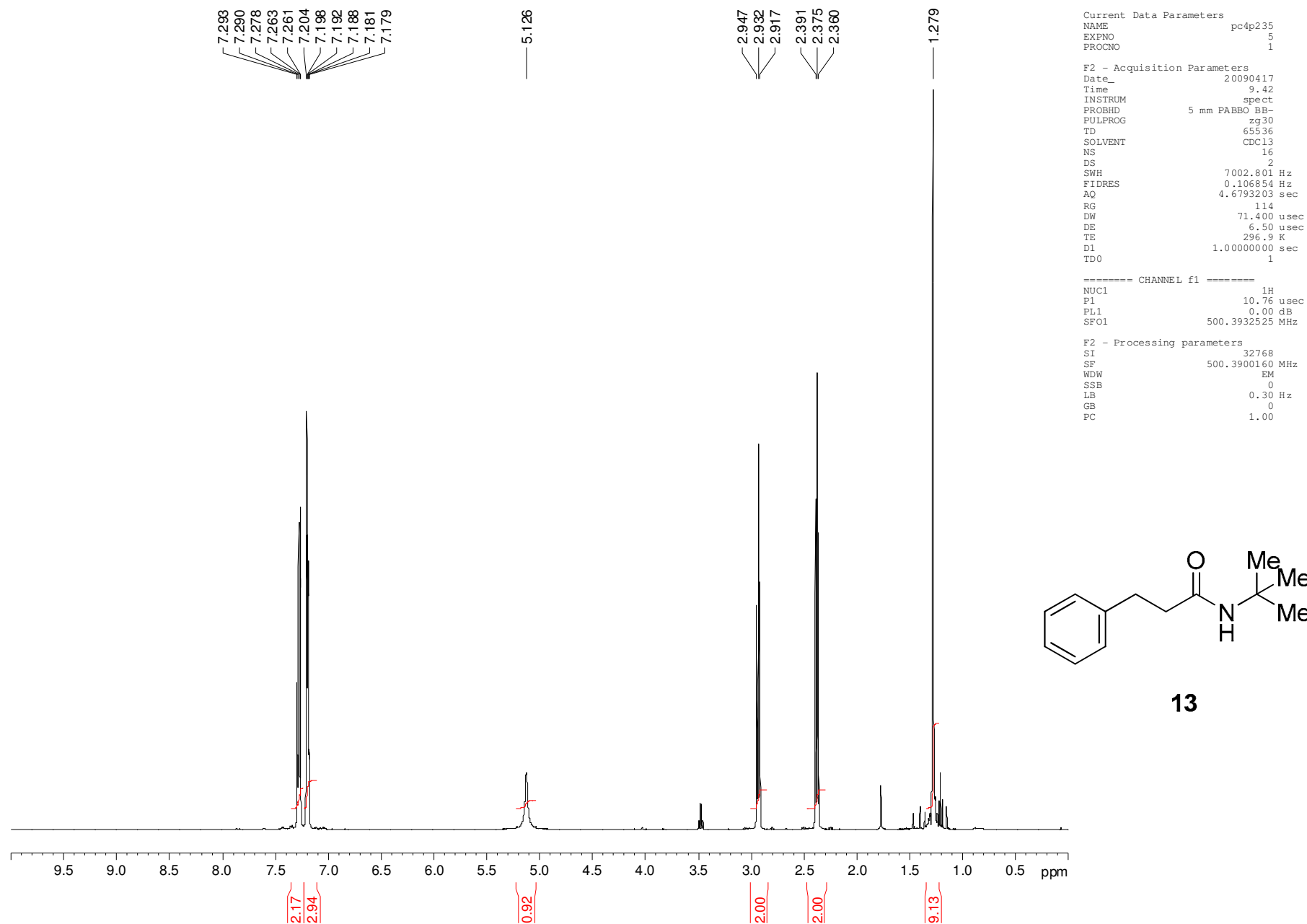
F2 - Processing parameters
SI 32768
SF 125.8231500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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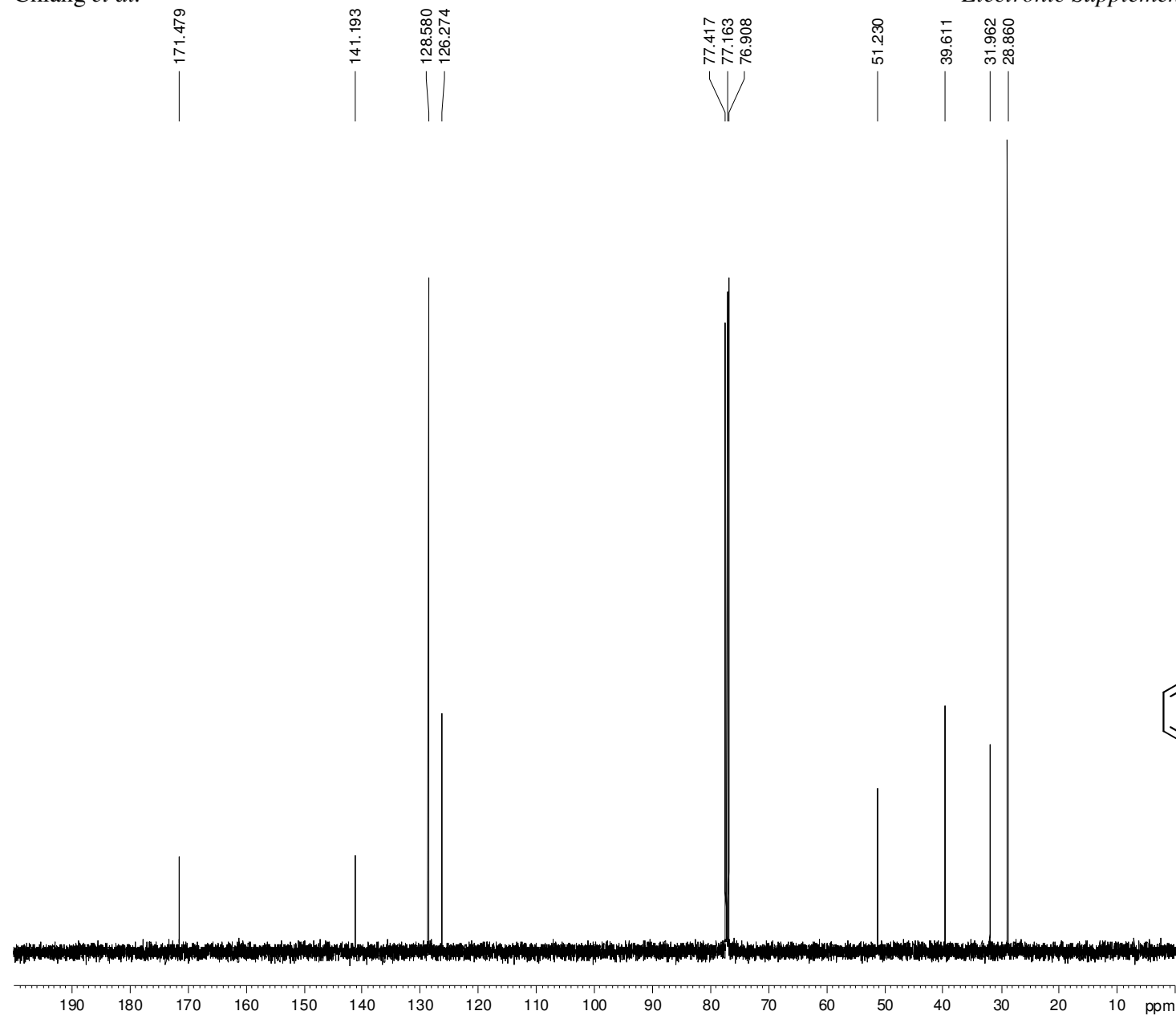
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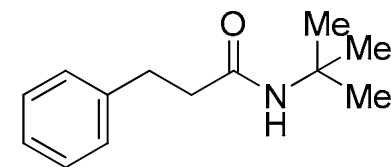
Current Data Parameters
NAME                pc4p235
EXPNO                6
PROCNO              1

F2 - Acquisition Parameters
Date_                20090417
Time                 9.46
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   64
DS                    4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                   1620
DW                   16.800 usec
DE                   6.50 usec
TE                   297.9 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  13C
P1                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                  1H
PCPD2                80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                   0.00 dB
SFO2                 500.3920016 MHz

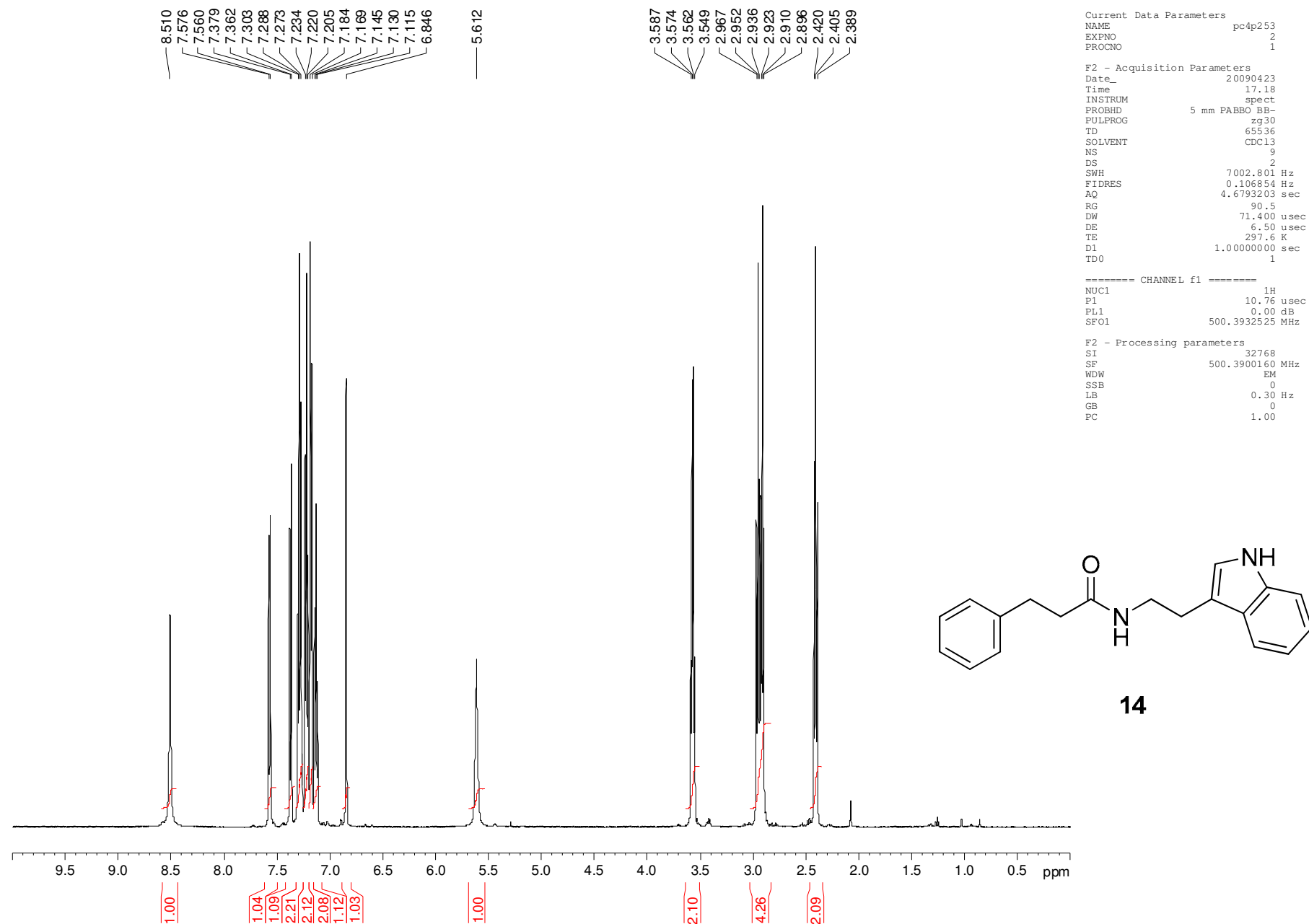
F2 - Processing parameters
SI                    32768
SF                   125.8231525 MHz
WDW                   EM
SSB                   0
LB                    1.00 Hz
GB                    0
PC                    1.40
  
```



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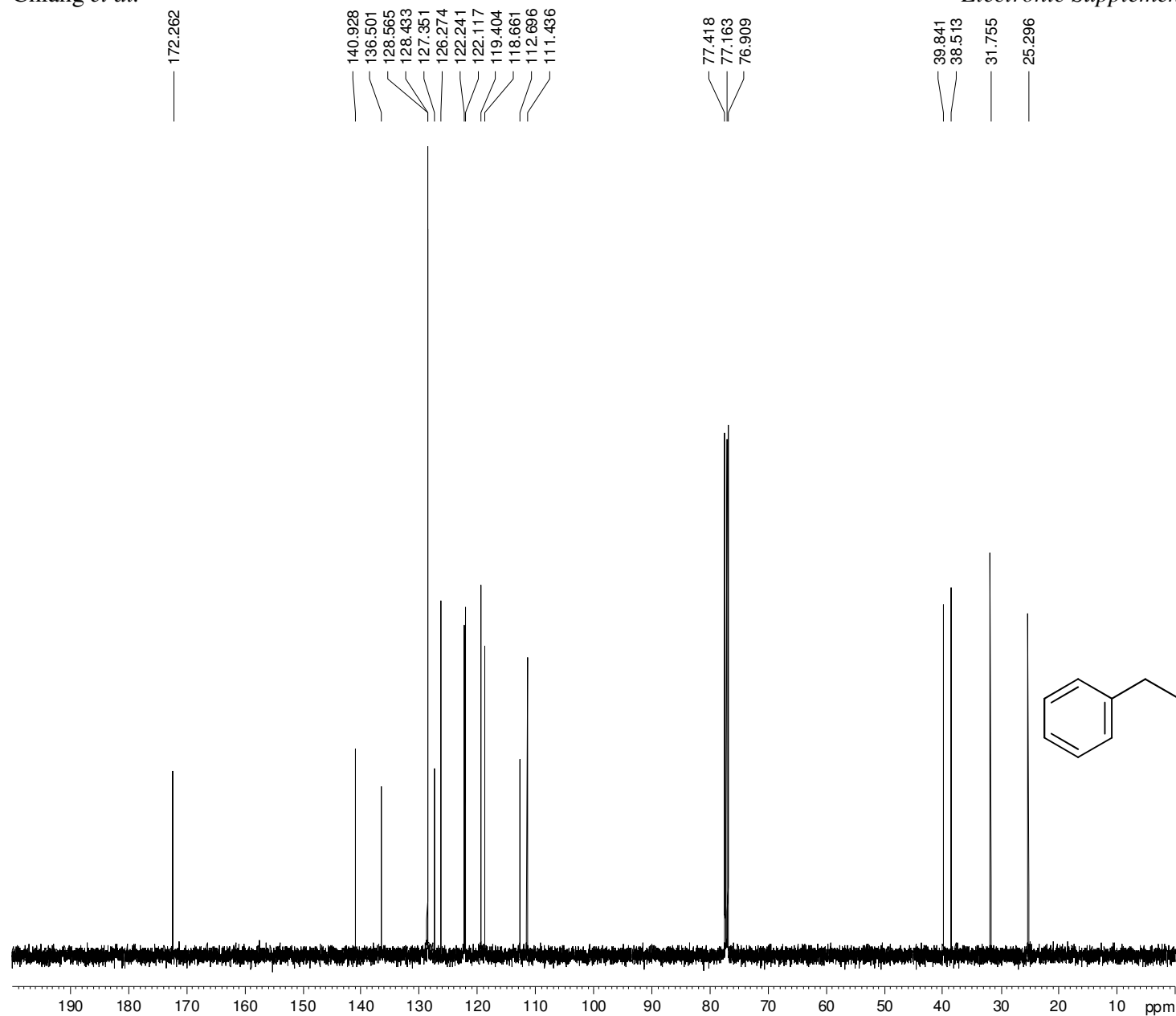
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Current Data Parameters
NAME                pc4p253
EXPNO                3
PROCNO              1

F2 - Acquisition Parameters
Date_                20090423
Time                 17.20
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   32
DS                    4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                   2050
DW                   16.800 usec
DE                   6.50 usec
TE                   298.3 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                  1

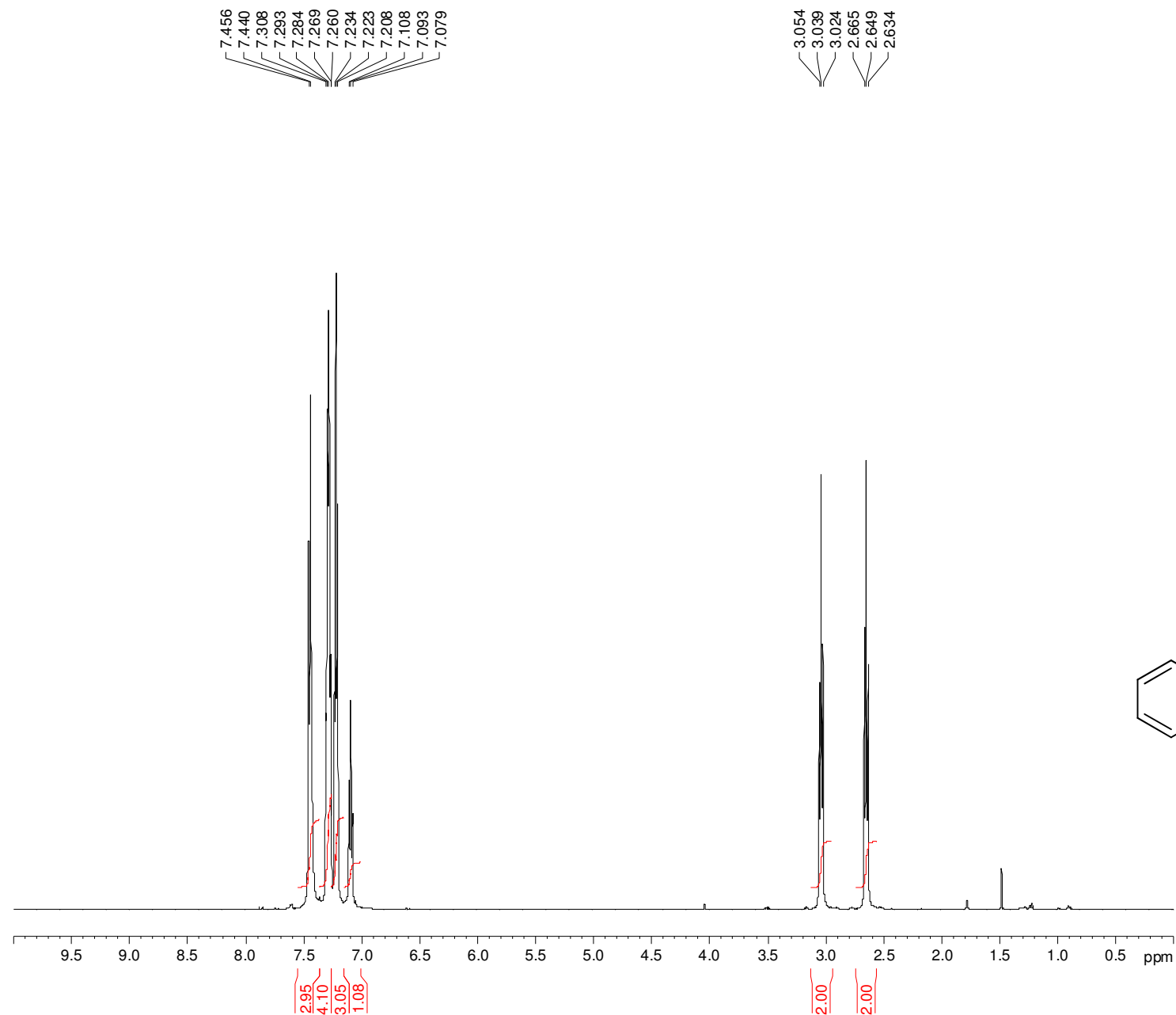
===== CHANNEL f1 =====
NUC1                  13C
P1                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                  1H
PCPD2                80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                   0.00 dB
SFO2                 500.3920016 MHz

F2 - Processing parameters
SI                    32768
SF                   125.8231670 MHz
WDW                   EM
SSB                   0
LB                    1.00 Hz
GB                    0
PC                    1.40
```

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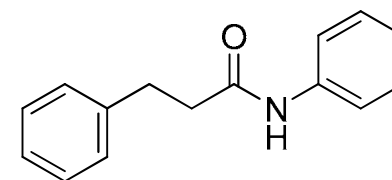


Current Data Parameters
NAME pc4p251
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090424
Time 9.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 144
DW 71.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

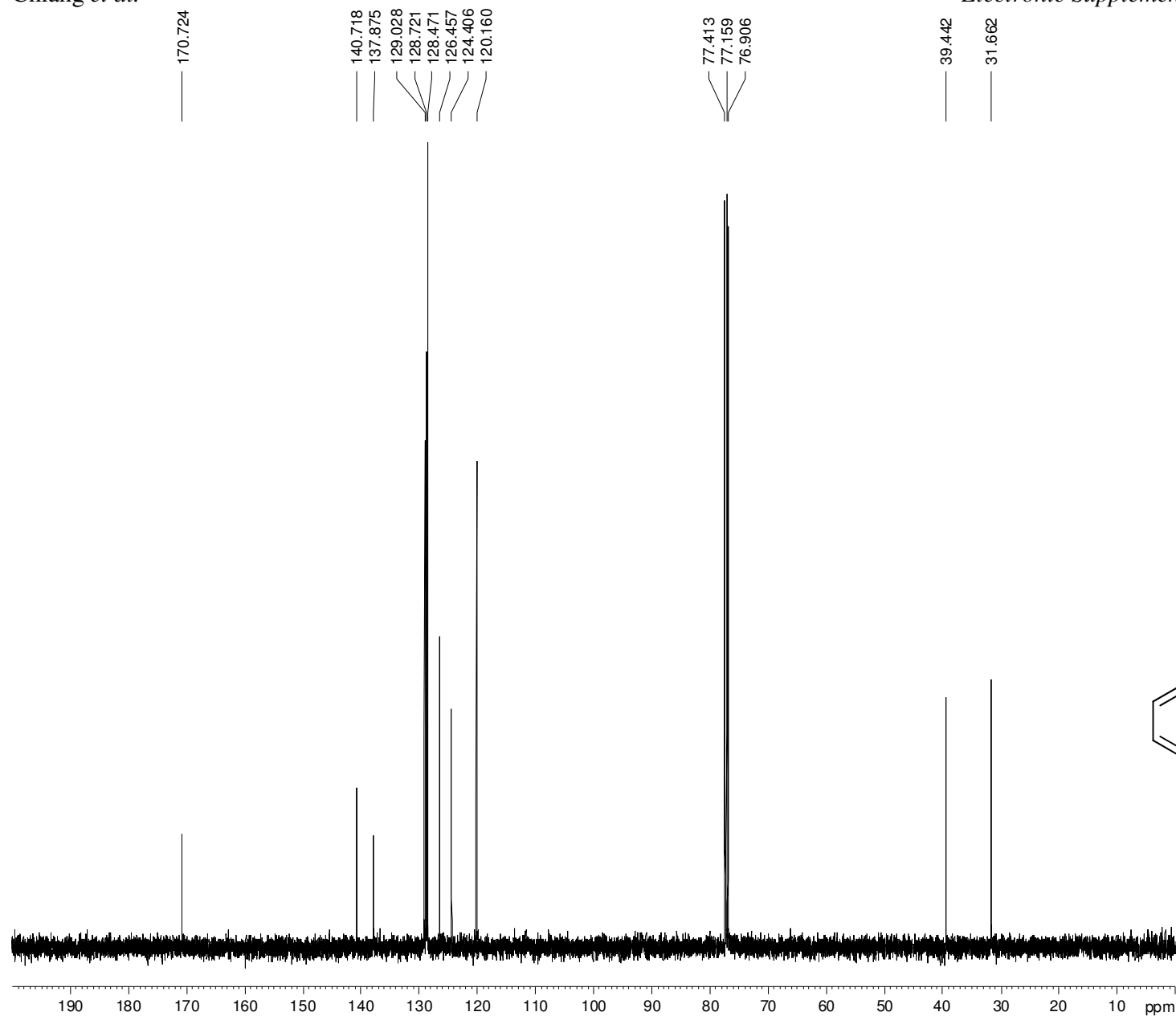
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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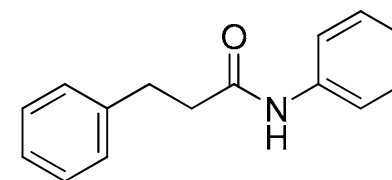
Current Data Parameters
NAME                pc4p251
EXPNO                3
PROCNO              1

F2 - Acquisition Parameters
Date_                20090423
Time                 17.08
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    36
DS                     4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                    2050
DW                   16.800 usec
DE                    6.50 usec
TE                   298.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  13C
P1                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                   1H
PCPD2                 80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                   0.00 dB
SFO2                 500.3920016 MHz

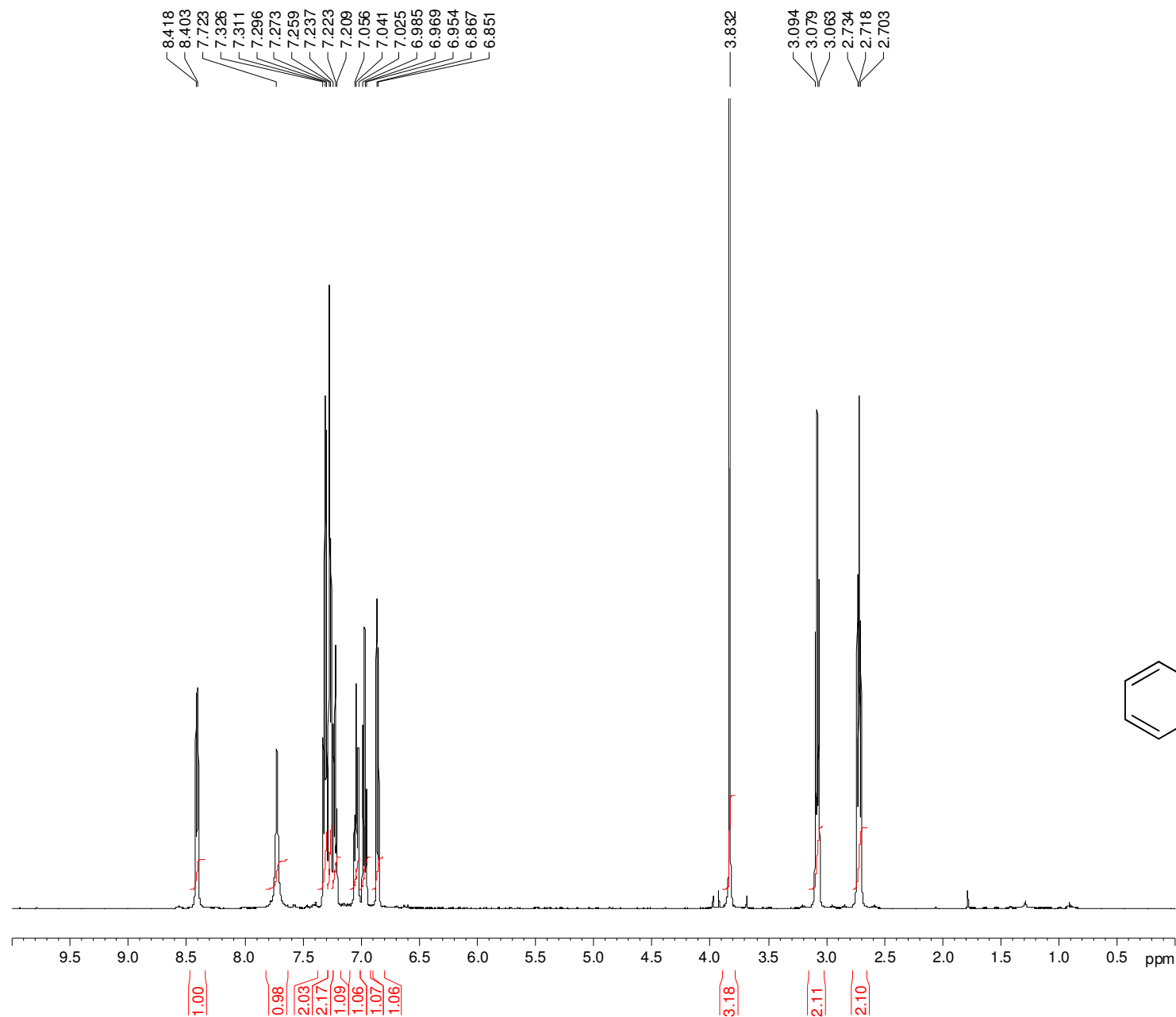
F2 - Processing parameters
SI                    32768
SF                   125.8231589 MHz
WDW                   EM
SSB                    0
LB                    1.00 Hz
GB                     0
PC                     1.40
  
```



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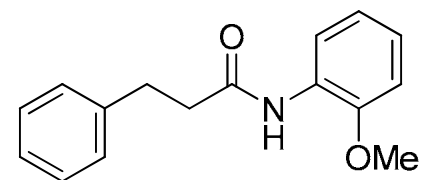


Current Data Parameters
NAME pc4p252
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090423
Time 17.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 114
DW 71.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

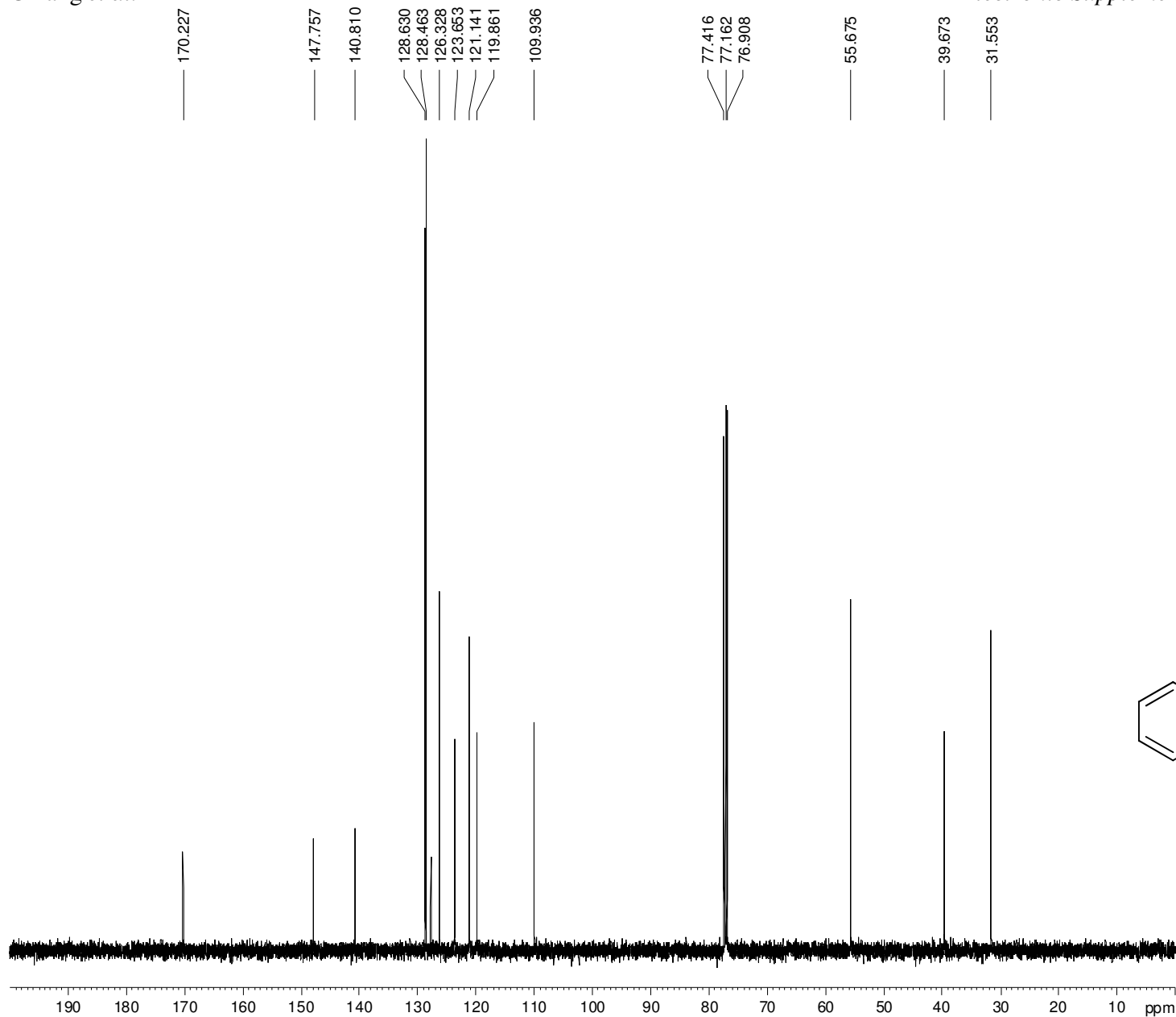
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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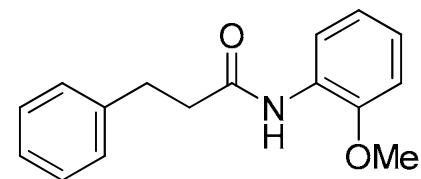
Current Data Parameters
NAME pc4p252
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090423
Time 17.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

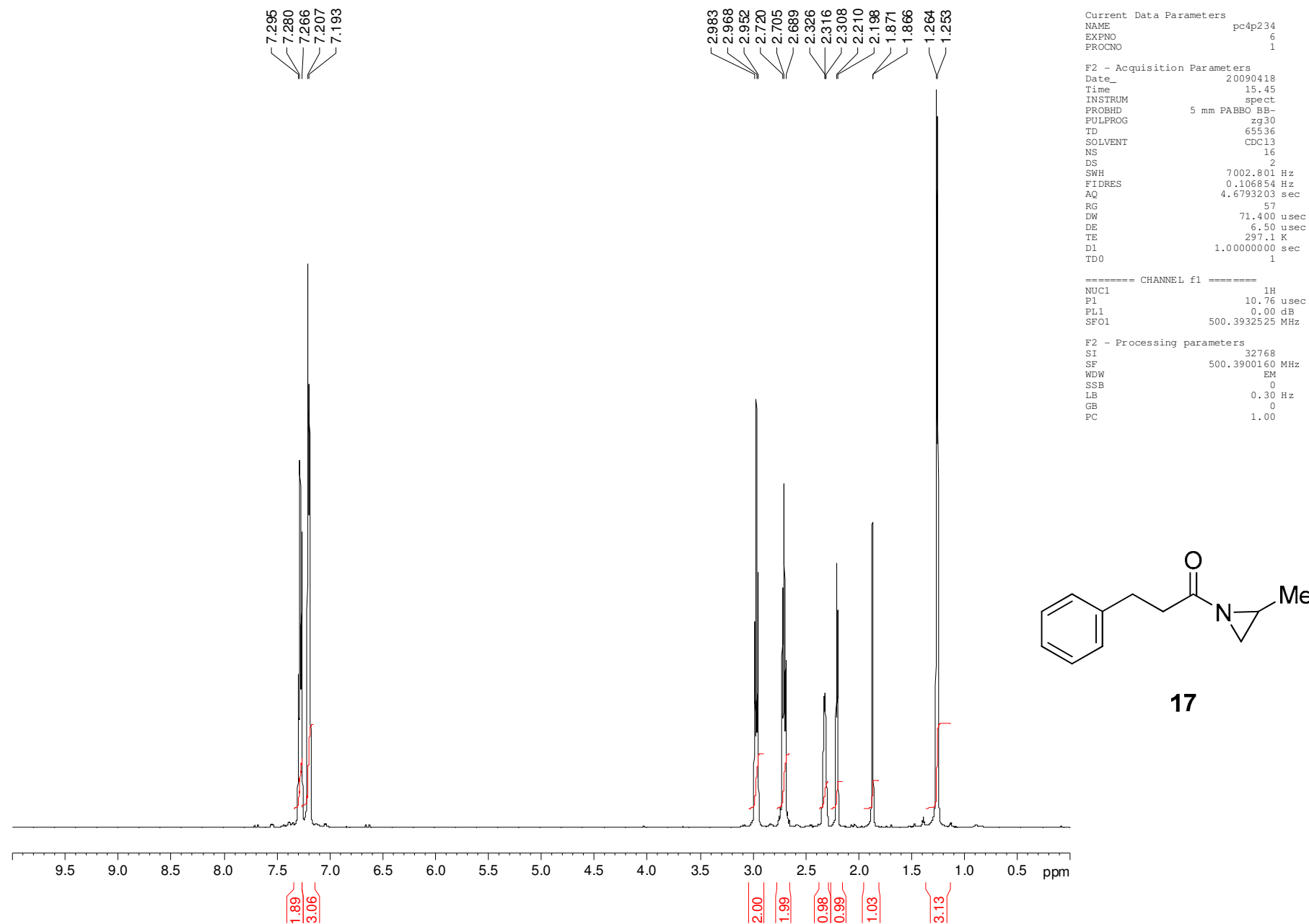
F2 - Processing parameters
SI 32768
SF 125.8231616 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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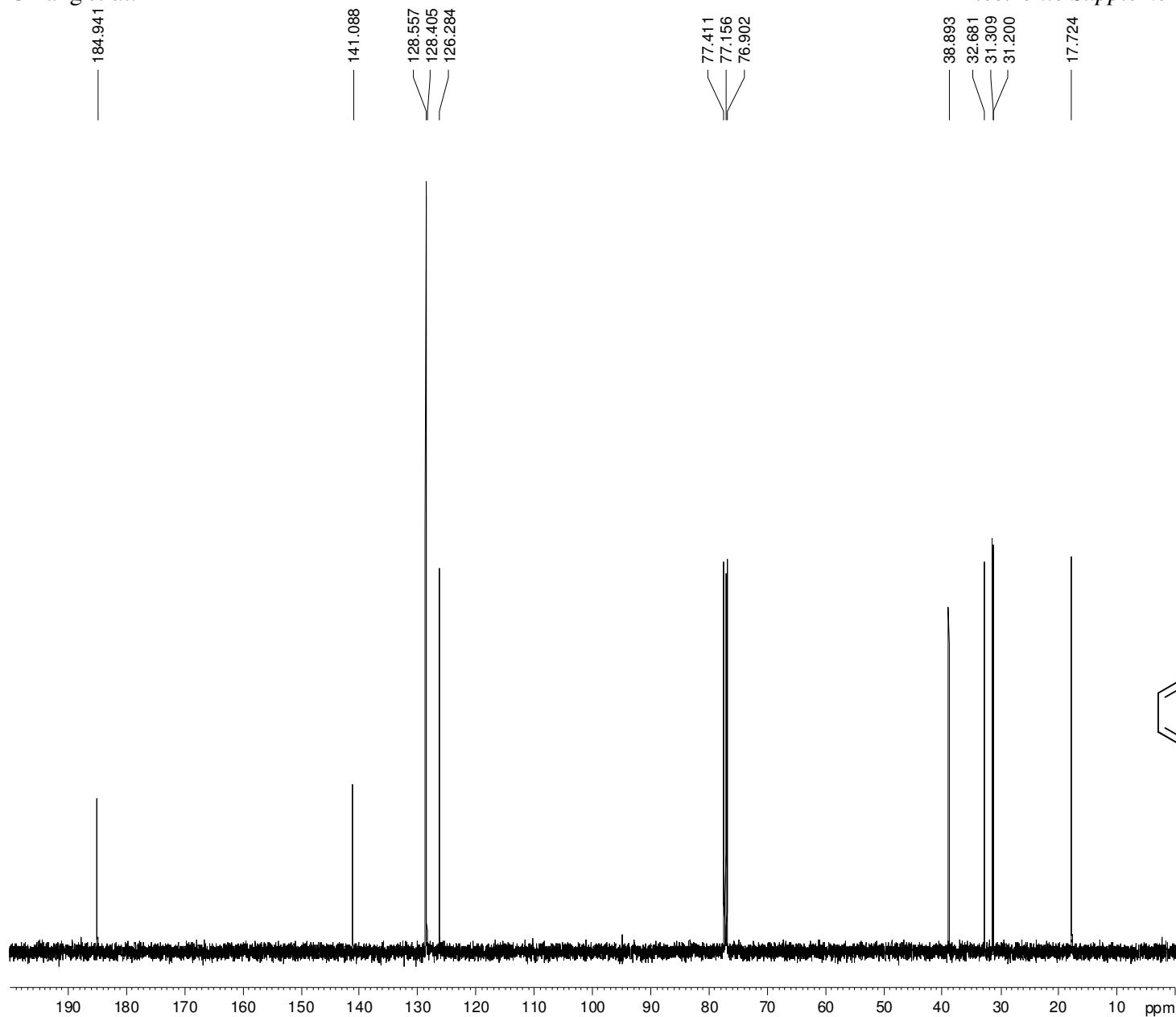
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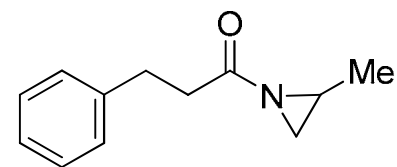
```
Current Data Parameters
NAME                pc4p234
EXPNO               7
PROCNO             1

F2 - Acquisition Parameters
Date_              20090418
Time               15.47
INSTRUM            spect
PROBHD             5 mm PABBO BB-
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 17
DS                  4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                 1620
DW                 16.800 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                  7.50 usec
PL1                 1.00 dB
SFO1                125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2            waltz16
NUC2                1H
PCPD2              80.00 usec
PL12                17.43 dB
PL13                18.43 dB
PL2                 0.00 dB
SFO2                500.3920016 MHz

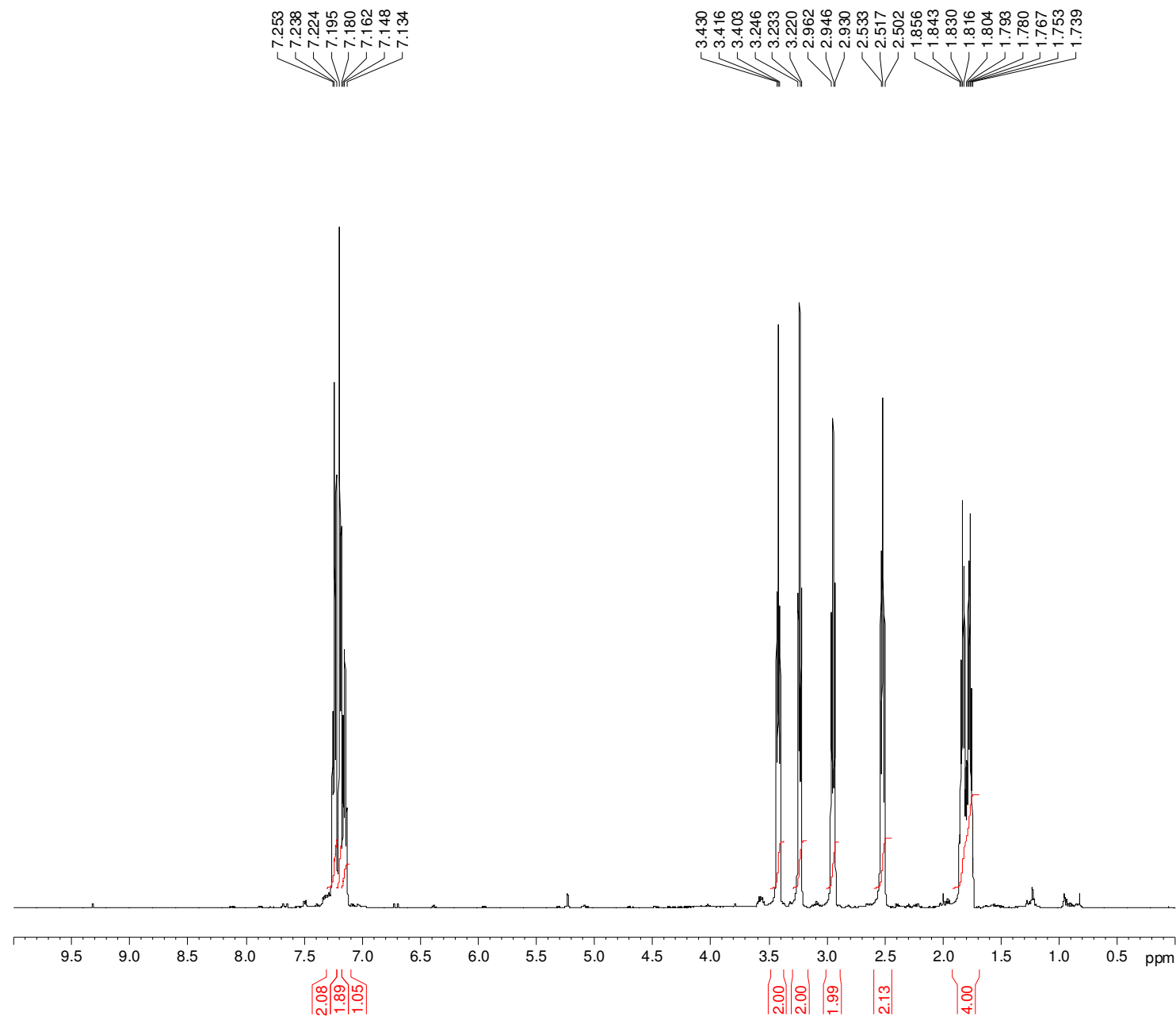
F2 - Processing parameters
SI                  32768
SF                  125.8231633 MHz
WDW                 EM
SSB                 0
LB                  1.00 Hz
GB                  0
PC                  1.40
```



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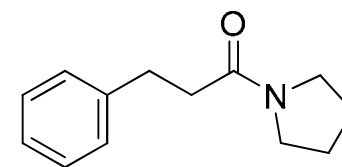


Current Data Parameters
NAME pc4p230
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090414
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 36
DW 71.400 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

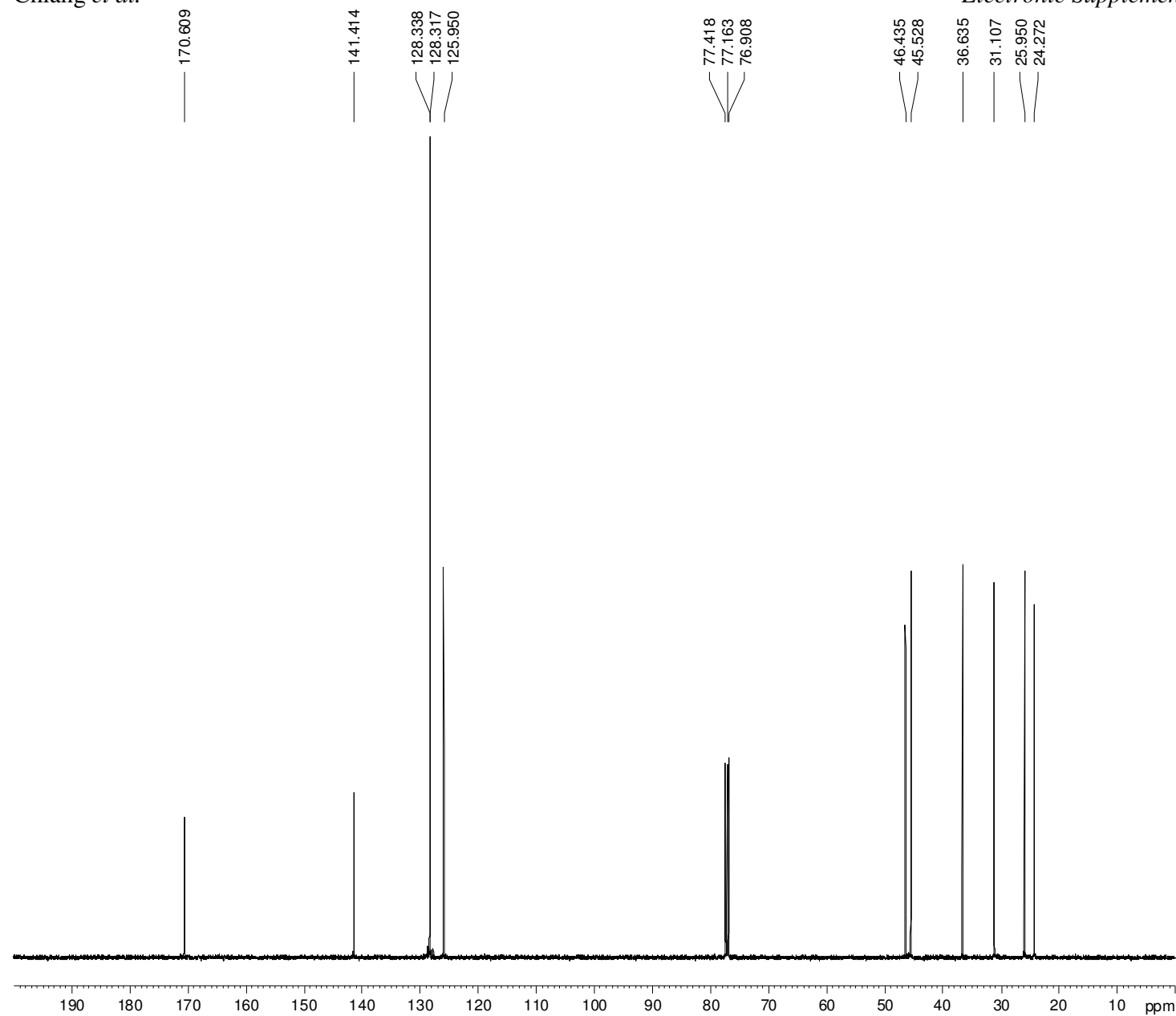
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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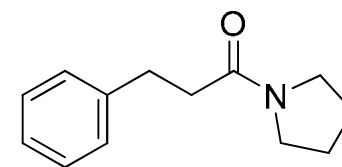
Current Data Parameters
NAME pc4p230
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090414
Time 10.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 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 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

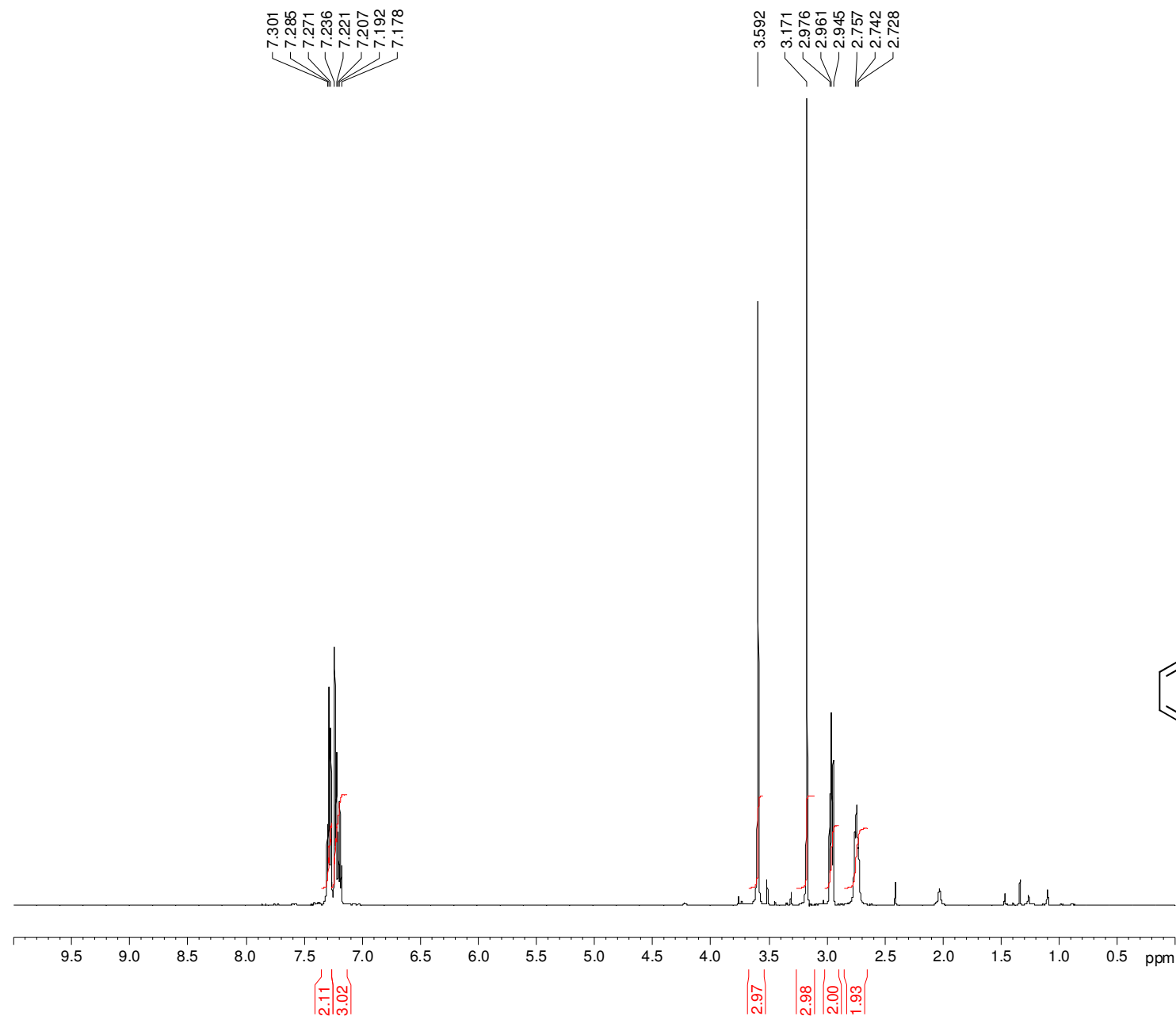
F2 - Processing parameters
SI 32768
SF 125.8231788 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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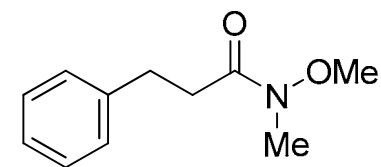
```

Current Data Parameters
NAME                pc4p256
EXPNO                3
PROCNO              1

F2 - Acquisition Parameters
Date_                20090427
Time                 9.10
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                    9
DS                     2
SWH                  7002.801 Hz
FIDRES               0.106854 Hz
AQ                   4.6793203 sec
RG                     50.8
DW                   71.400 usec
DE                     6.50 usec
TE                   298.0 K
D1                   1.00000000 sec
TD0                   1

===== CHANNEL f1 =====
NUC1                  1H
P1                   10.76 usec
PL1                    0.00 dB
SFO1                  500.3932525 MHz

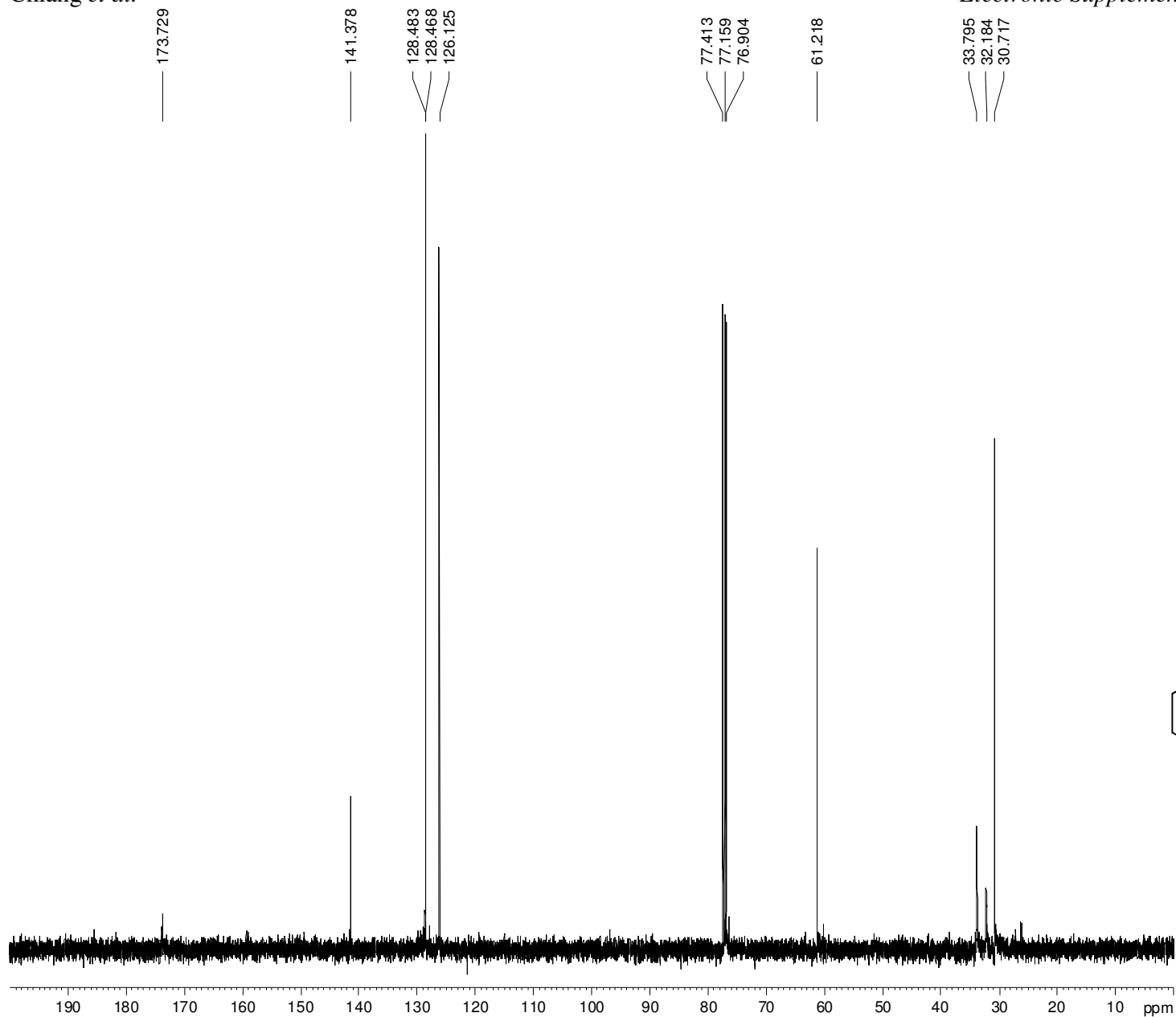
F2 - Processing parameters
SI                   32768
SF                   500.3900160 MHz
WDW                   EM
SSB                    0
LB                    0.30 Hz
GB                     0
PC                     1.00
  
```



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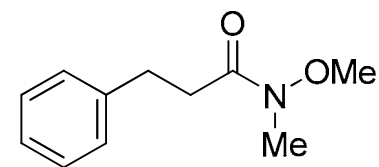
```
Current Data Parameters
NAME          pc4p256
EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
Date_         20090427
Time          9.12
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            2050
DW            16.800 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             7.50 usec
PL1            1.00 dB
SFO1          125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL12           17.43 dB
PL13           18.43 dB
PL2            0.00 dB
SFO2          500.3920016 MHz

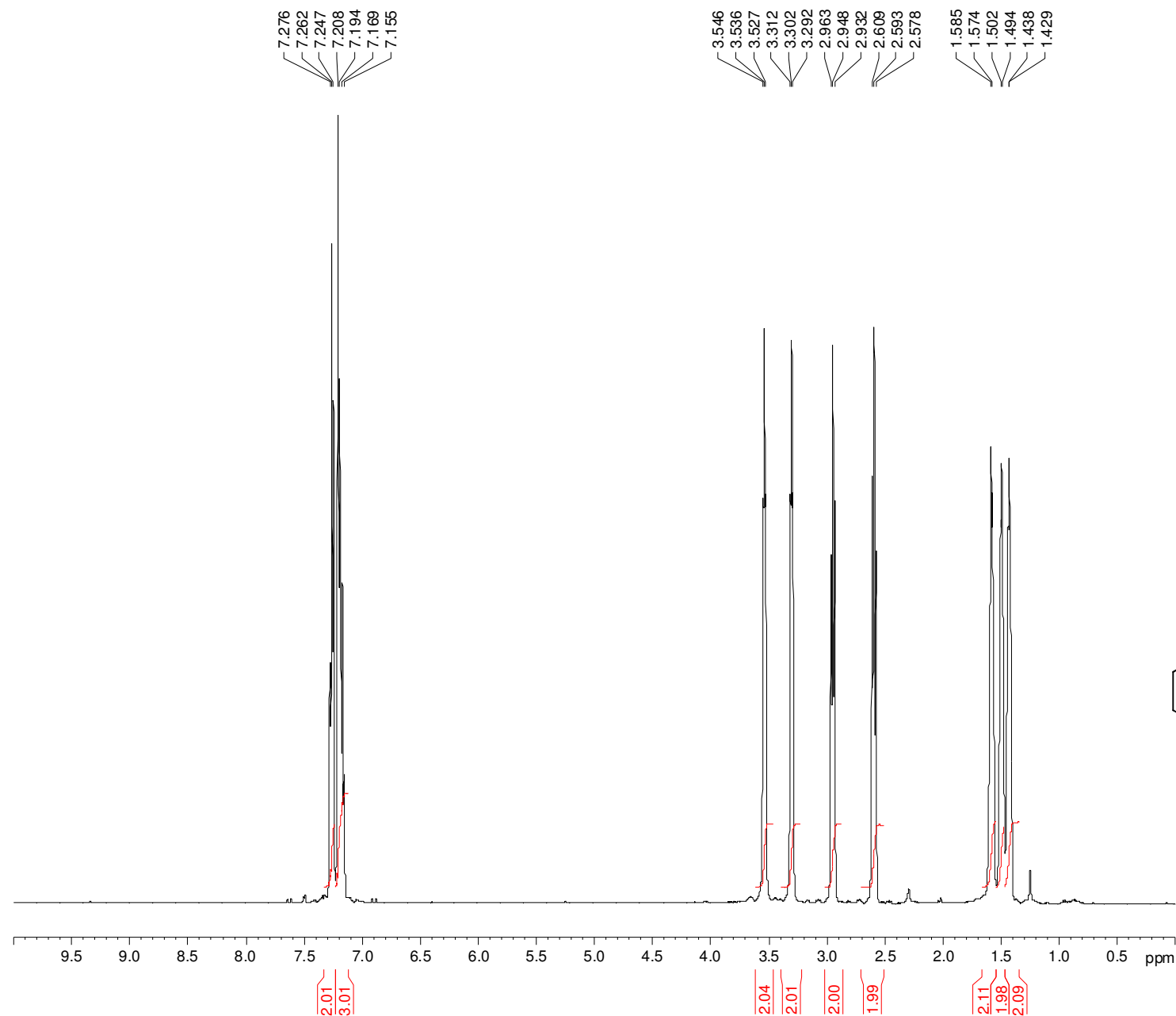
F2 - Processing parameters
SI             32768
SF            125.8231652 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
```



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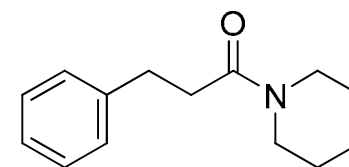


Current Data Parameters
NAME pc4p240
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090418
Time 16.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 36
DW 71.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

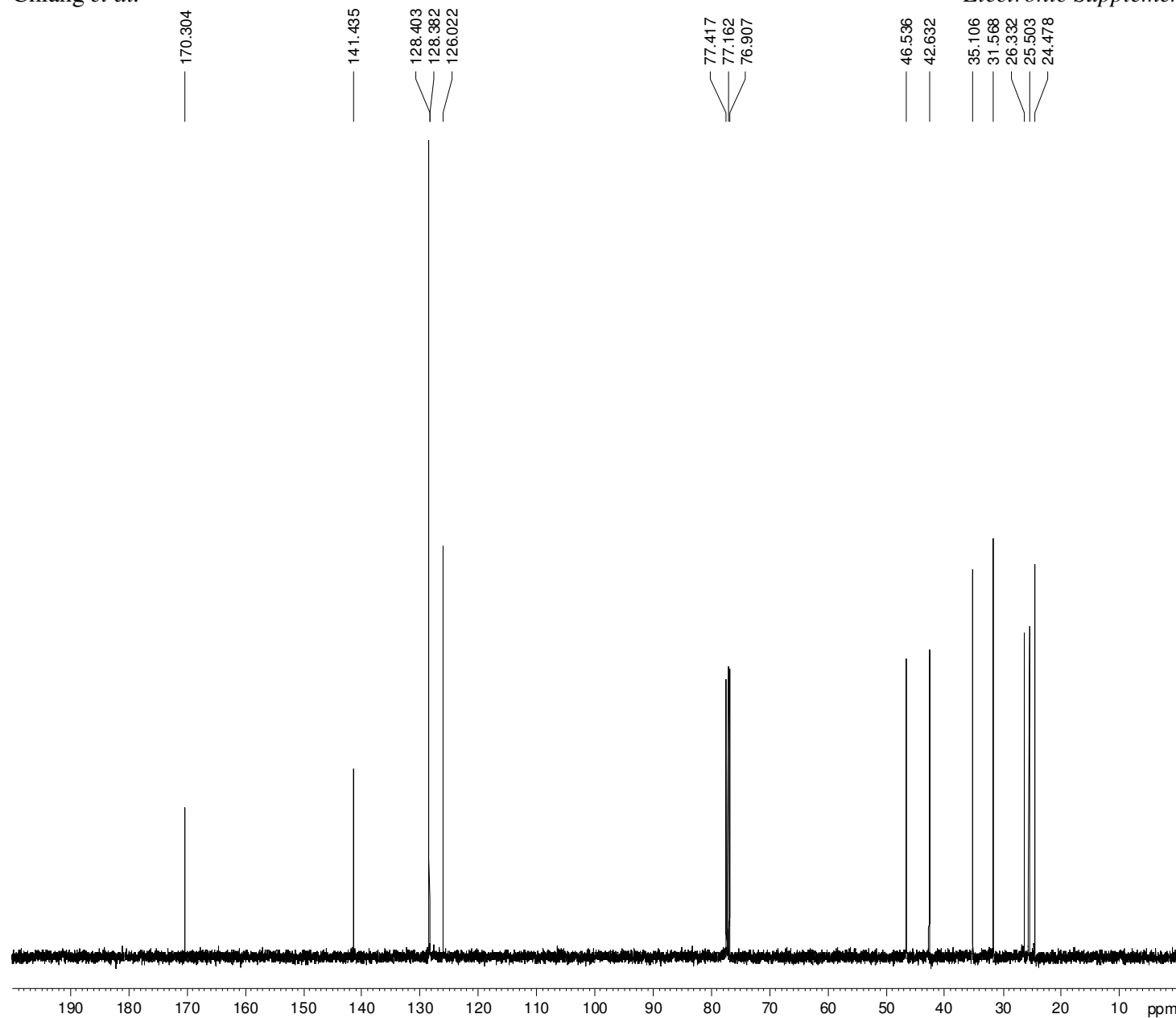
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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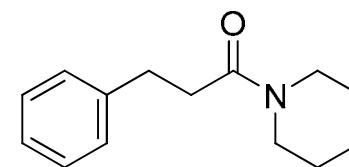
Current Data Parameters
NAME pc4p240
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090418
Time 16.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1820
DW 16.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

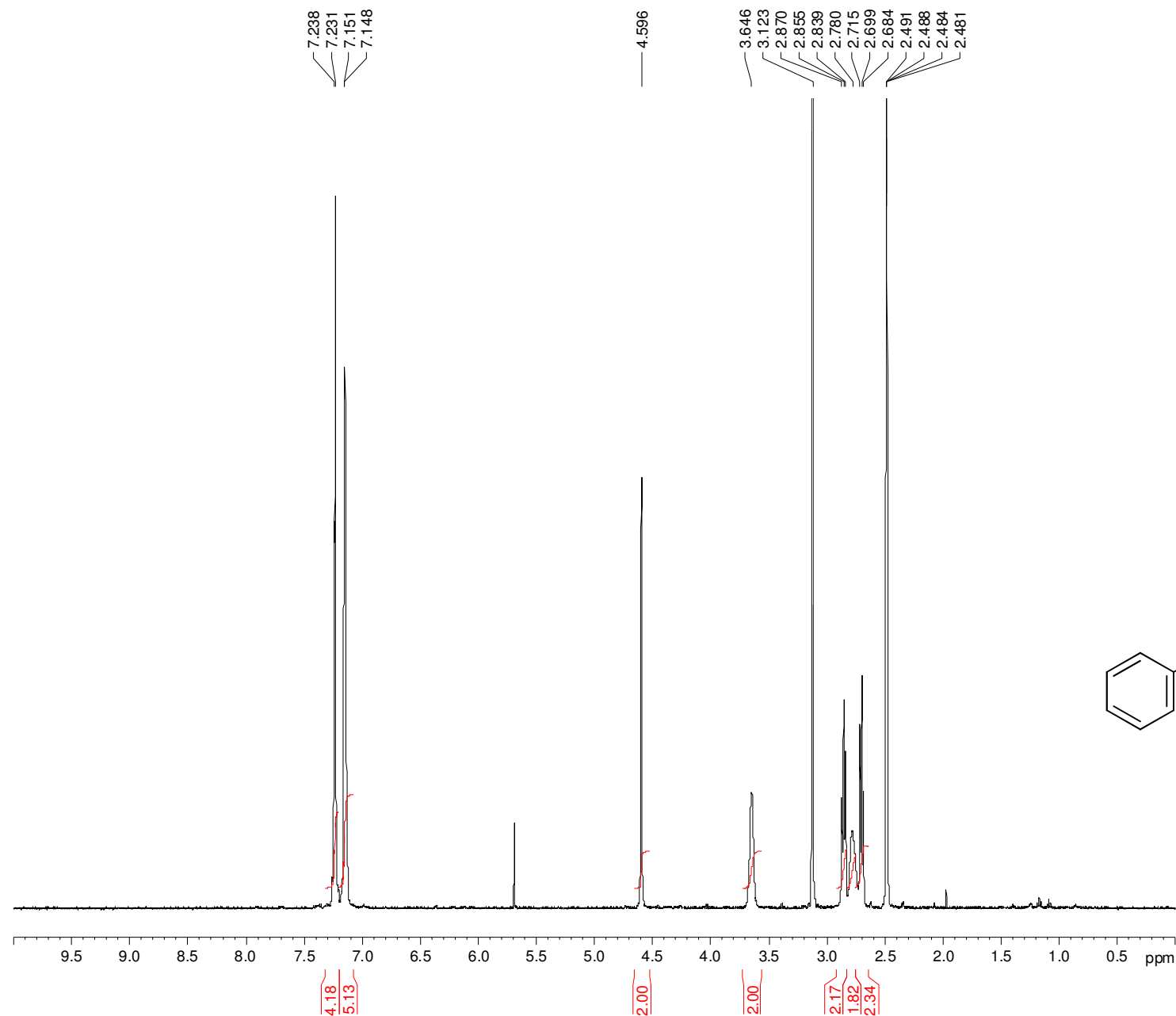
F2 - Processing parameters
SI 32768
SF 125.8231743 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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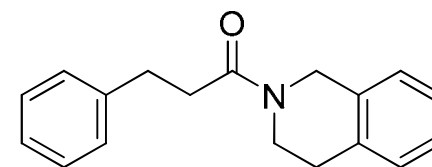


Current Data Parameters
NAME pc4p243
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090425
Time 11.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 575
DW 71.400 usec
DE 6.50 usec
TE 333.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

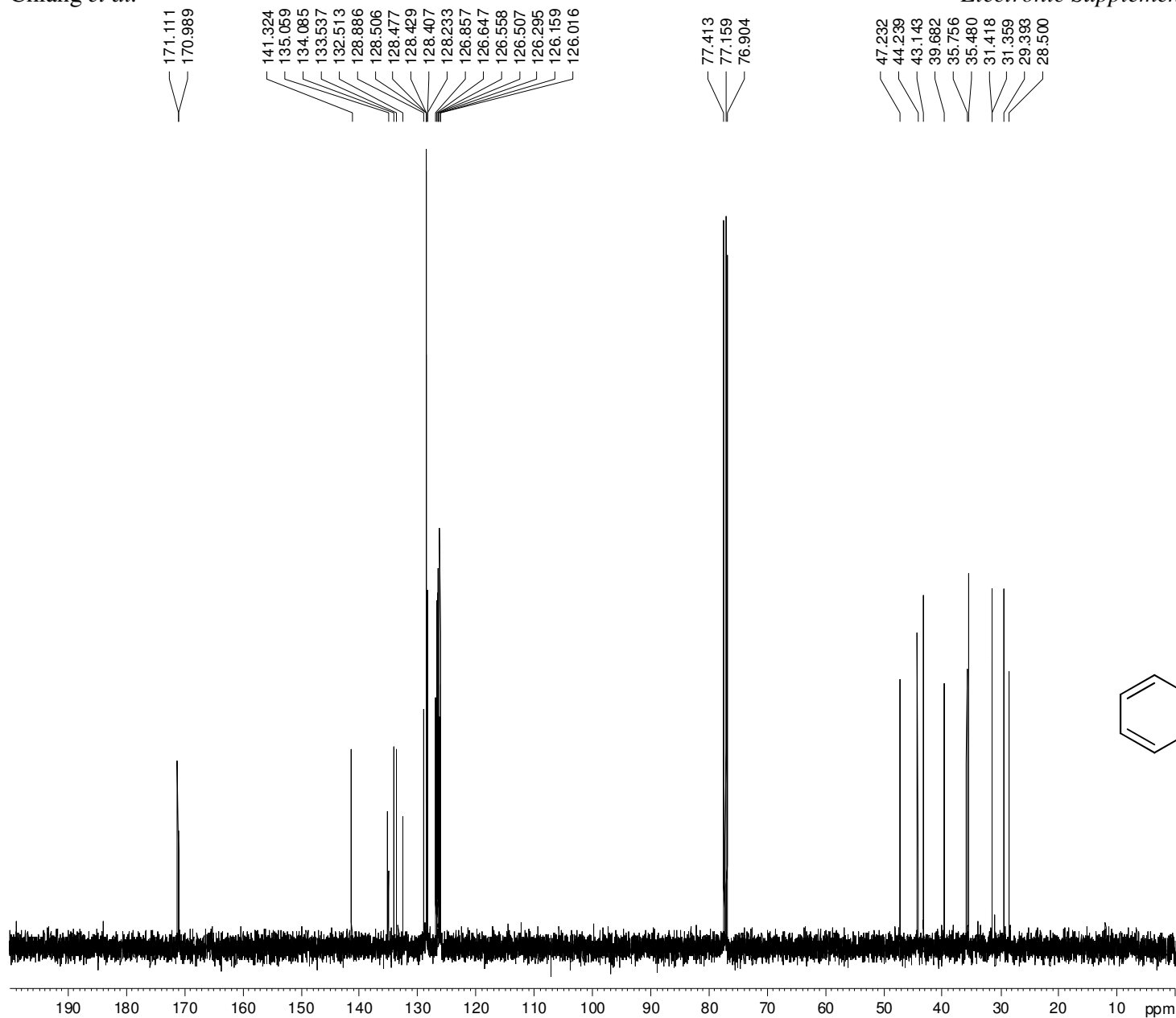
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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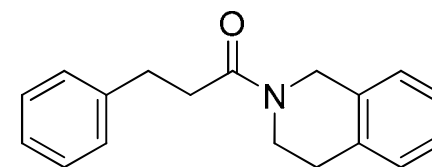
Current Data Parameters
NAME                pc4p243
EXPNO               7
PROCNO             1

F2 - Acquisition Parameters
Date_              20090422
Time               18.19
INSTRUM            spect
PROBHD             5 mm PABBO BB-
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 16
DS                 4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                1.1010548 sec
RG                 1820
DW                16.800 usec
DE                 6.50 usec
TE                297.6 K
D1                2.0000000 sec
d11               0.0300000 sec
DELTA              1.8999999 sec
TD0               1

===== CHANNEL f1 =====
NUC1                13C
P1                  7.50 usec
PL1                 1.00 dB
SFO1               125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2            waltz16
NUC2                1H
PCPD2              80.00 usec
PL12               17.43 dB
PL13               18.43 dB
PL2                 0.00 dB
SFO2               500.3920016 MHz

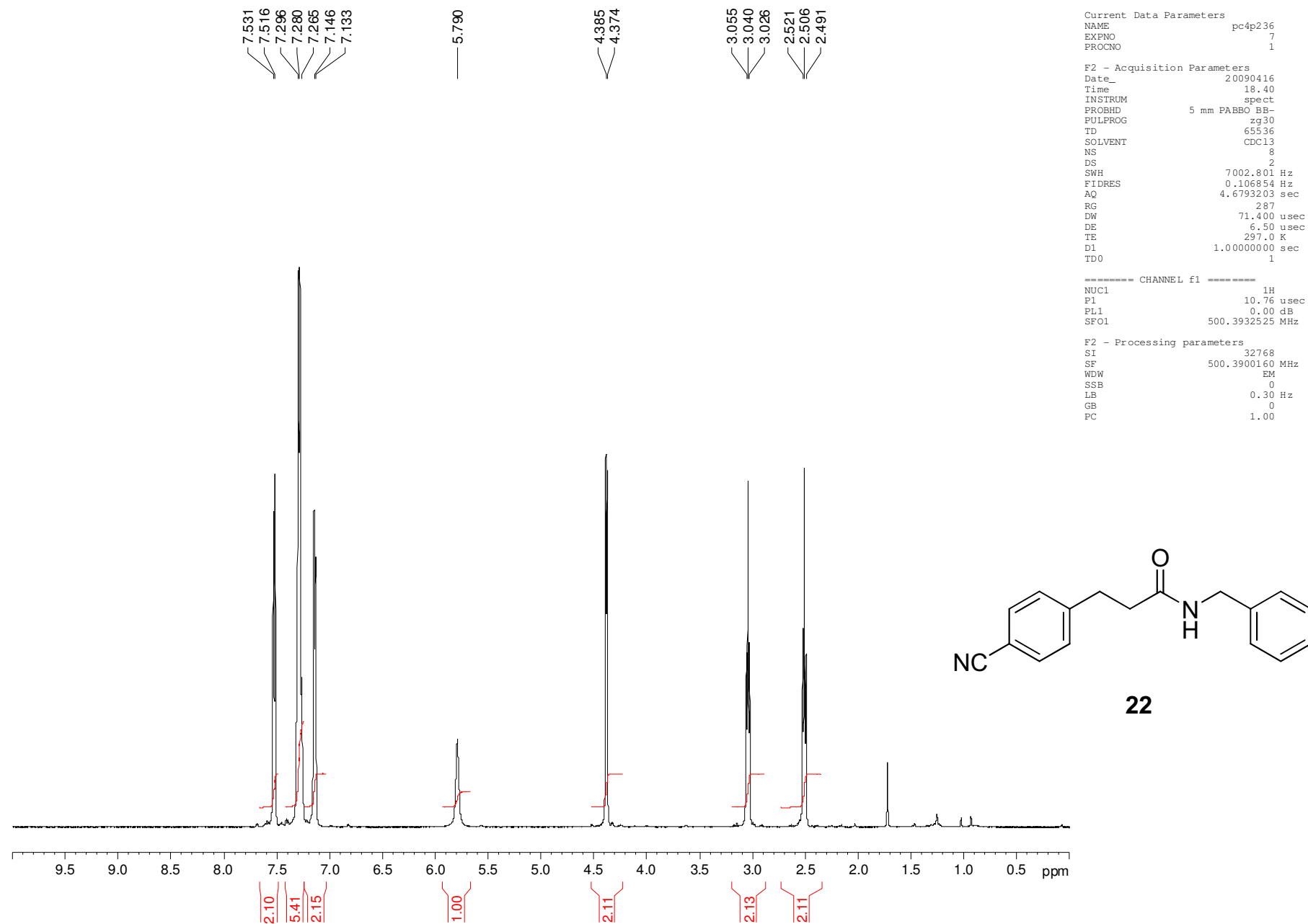
F2 - Processing parameters
SI                  32768
SF                 125.8231752 MHz
WDW                EM
SSB                 0
LB                  1.00 Hz
GB                  0
PC                  1.40
  
```



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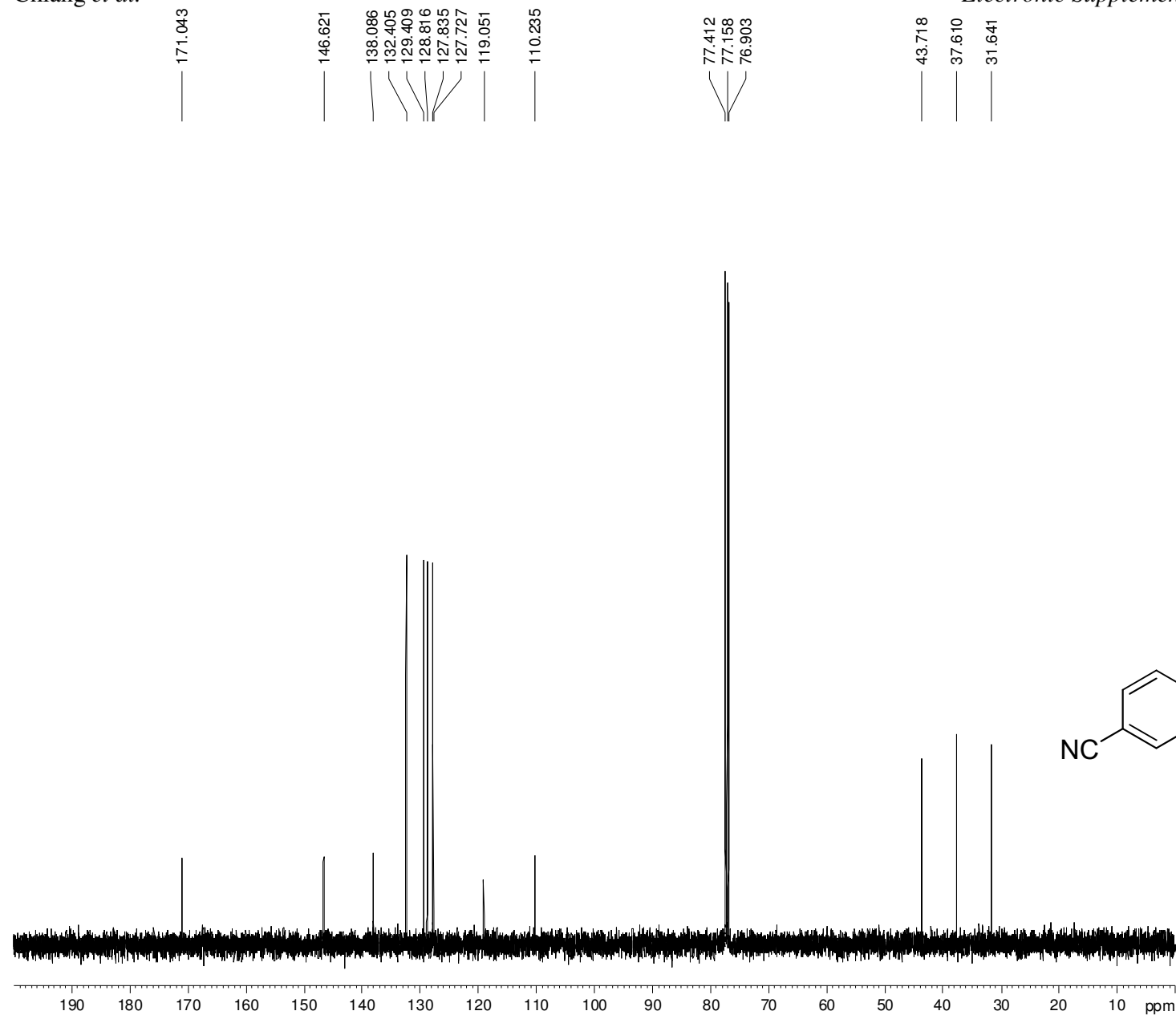
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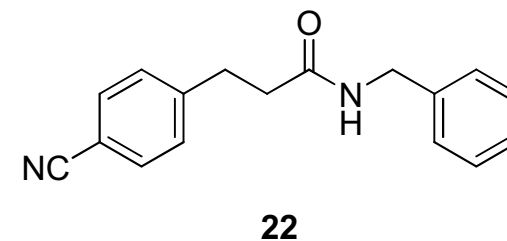
Current Data Parameters
NAME                pc4p236
EXPNO               8
PROCNO             1

F2 - Acquisition Parameters
Date_              20090416
Time               18.43
INSTRUM            spect
PROBHD             5 mm PABBO BB-
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 32
DS                 4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                1.1010548 sec
RG                 1030
DW                 16.800 usec
DE                 6.50 usec
TE                 297.9 K
D1                 2.00000000 sec
d11                 0.03000000 sec
DELTA              1.89999998 sec
TD0                1

===== CHANNEL f1 =====
NUC1                13C
P1                  7.50 usec
PL1                 1.00 dB
SFO1                125.8357479 MHz

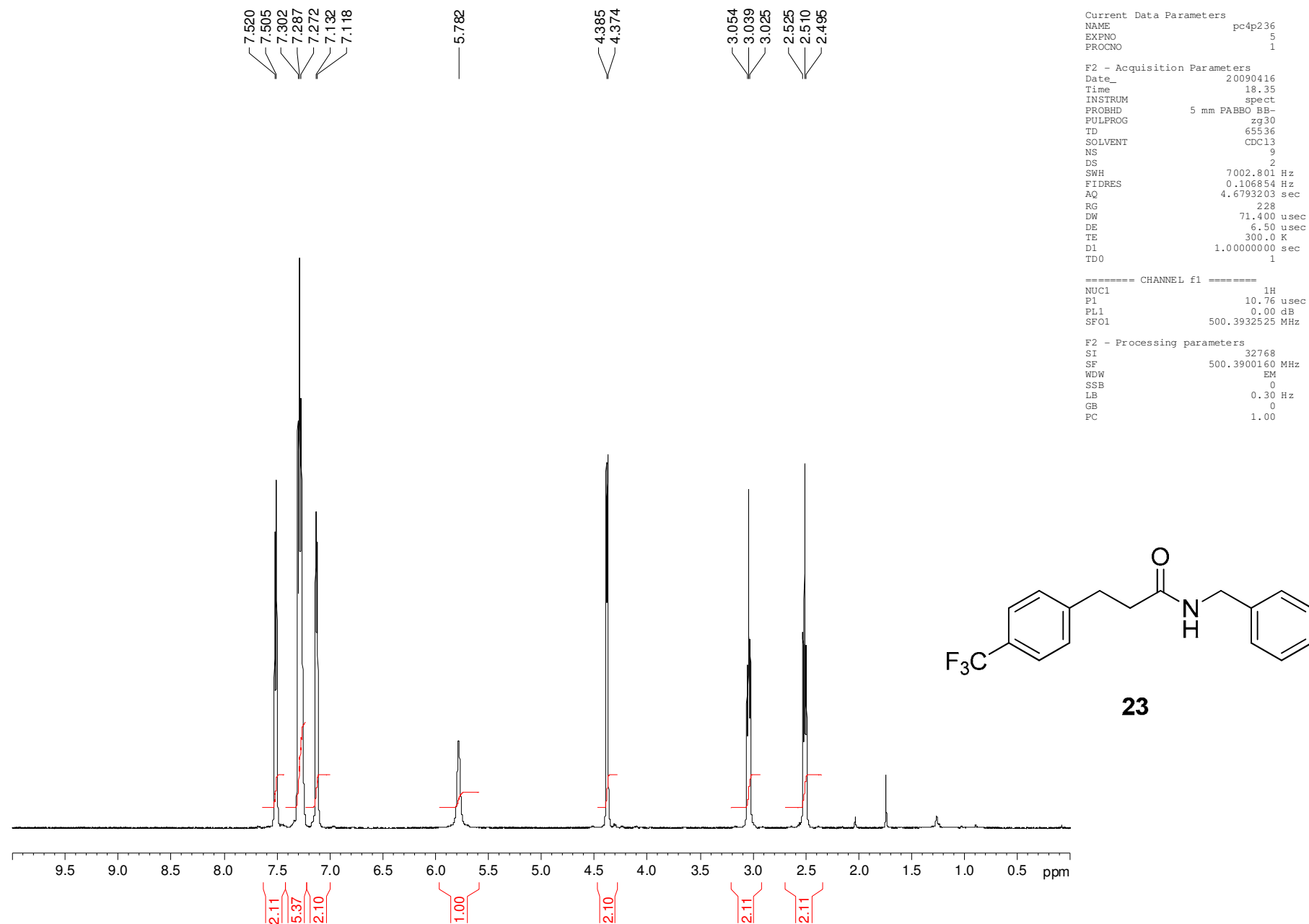
===== CHANNEL f2 =====
CPDPRG2            waltz16
NUC2                1H
PCPD2              80.00 usec
PL12                17.43 dB
PL13                18.43 dB
PL2                 0.00 dB
SFO2                500.3920016 MHz

F2 - Processing parameters
SI                  32768
SF                 125.8231552 MHz
WDW                 EM
SSB                 0
LB                  1.00 Hz
GB                  0
PC                  1.40
  
```



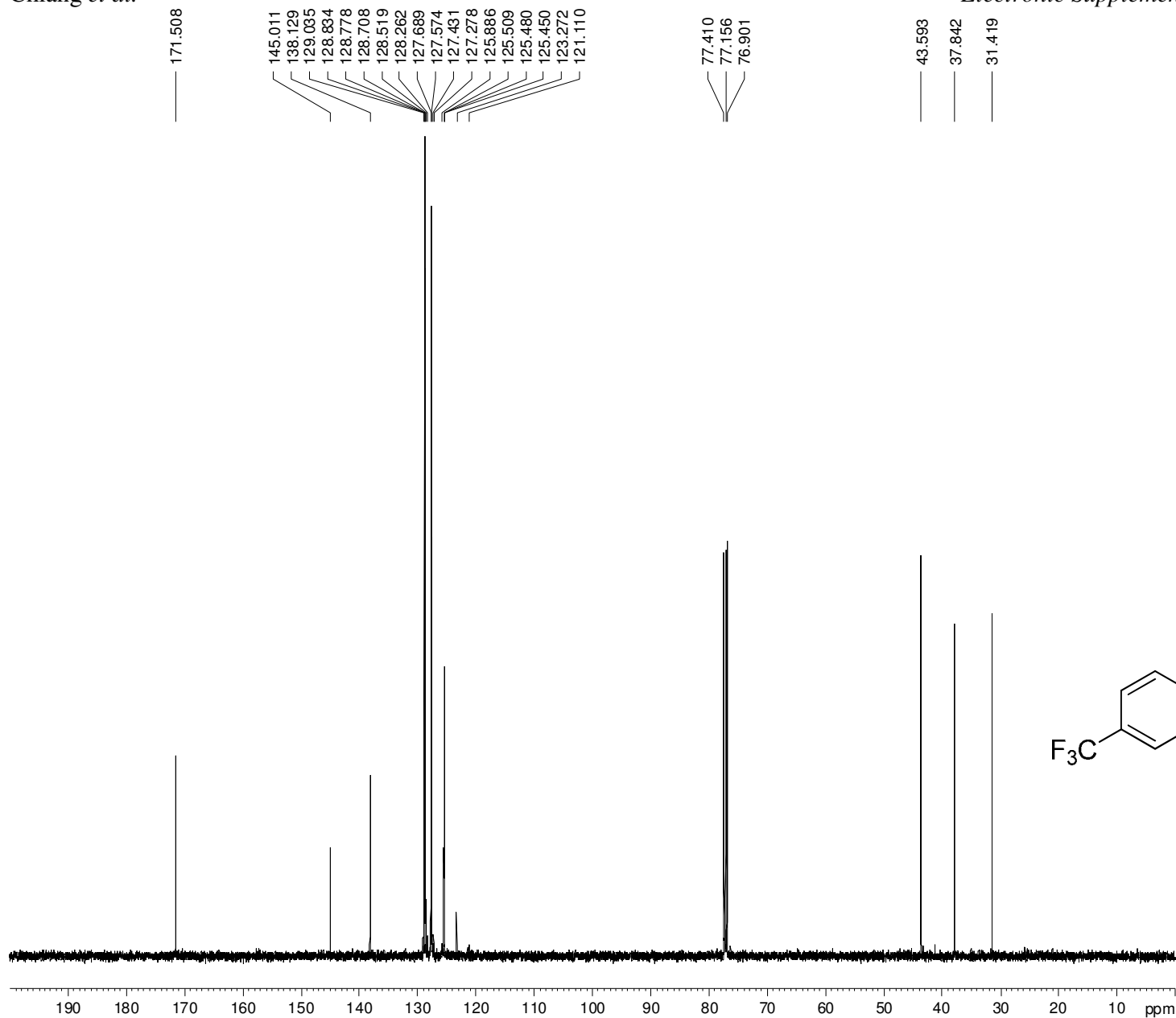
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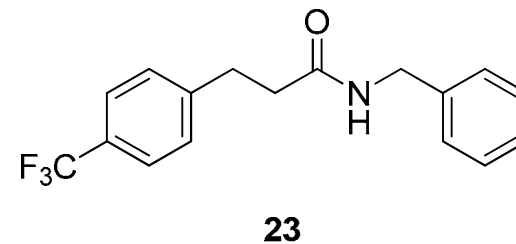
Current Data Parameters
NAME pc4p259
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090429
Time 15.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 89
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

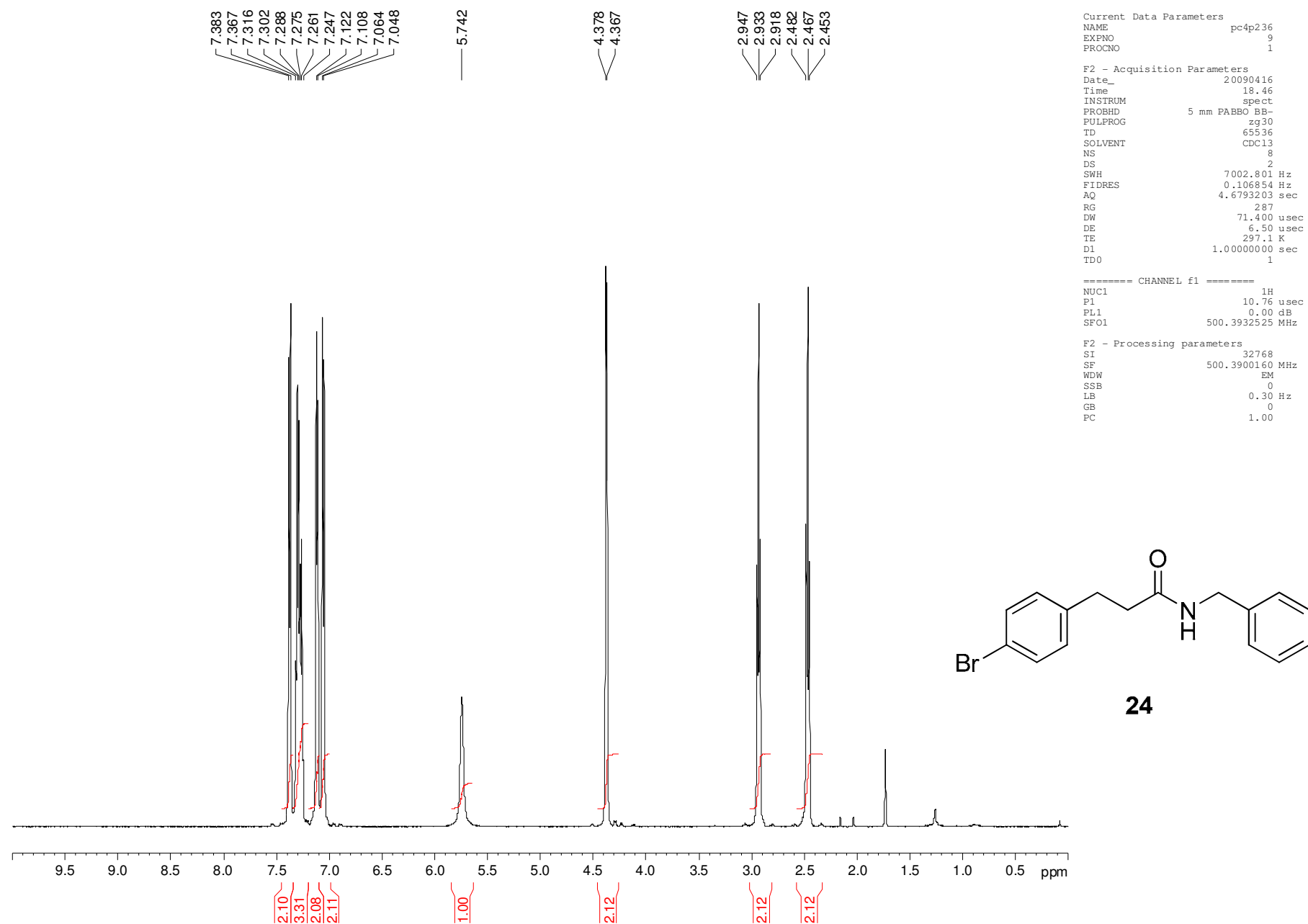
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 32768
SF 125.8231597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



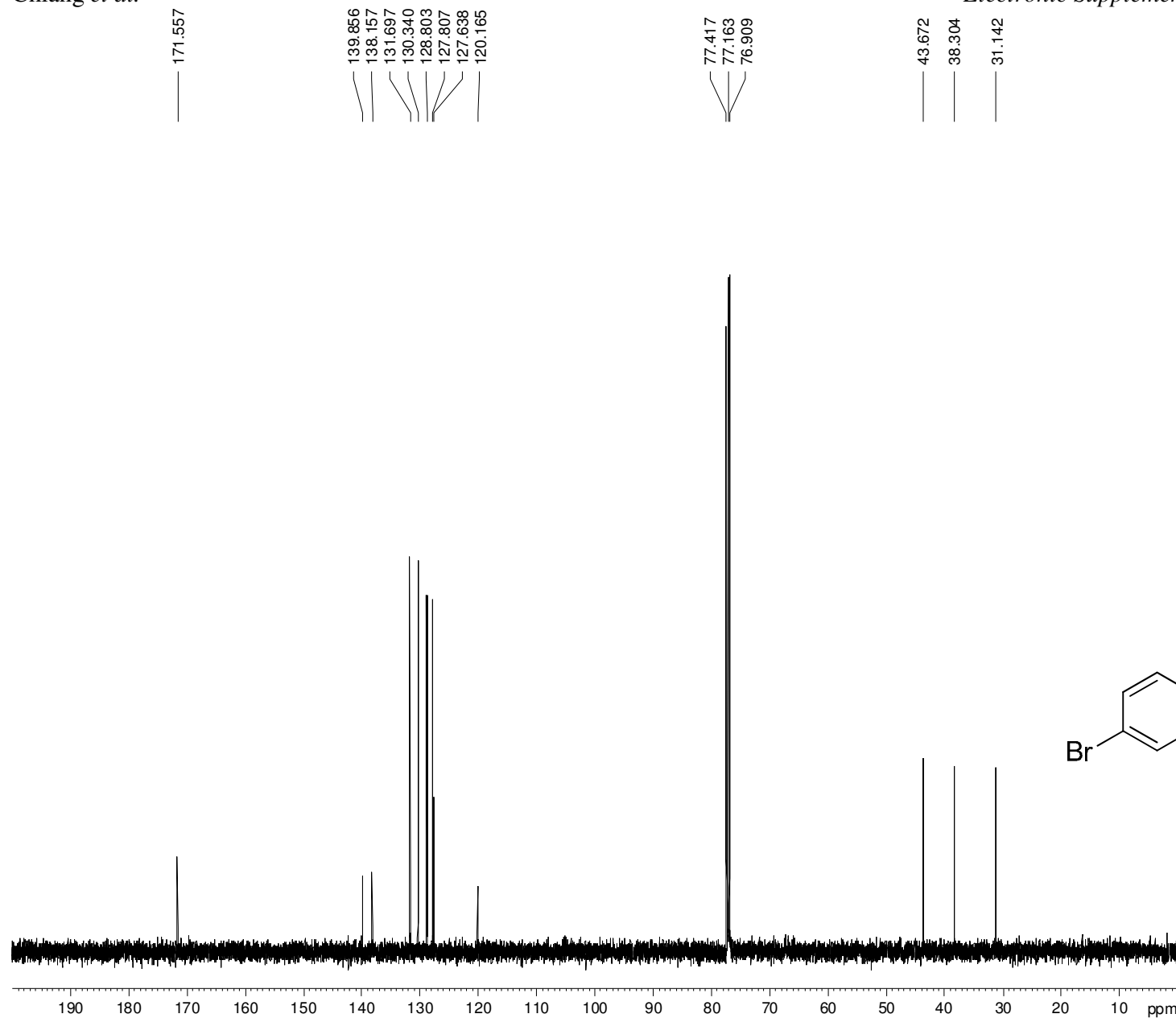
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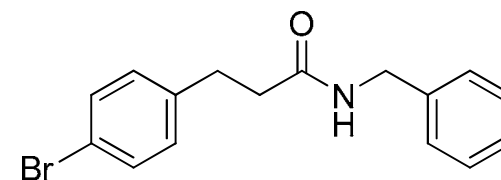
```
Current Data Parameters
NAME                pc4p236
EXPNO               10
PROCNO              1

F2 - Acquisition Parameters
Date_                20090416
Time                 18.47
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   32
DS                    4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                   1030
DW                   16.800 usec
DE                   6.50 usec
TE                   297.7 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  13C
P1                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                  1H
PCPD2                80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                   0.00 dB
SFO2                 500.3920016 MHz

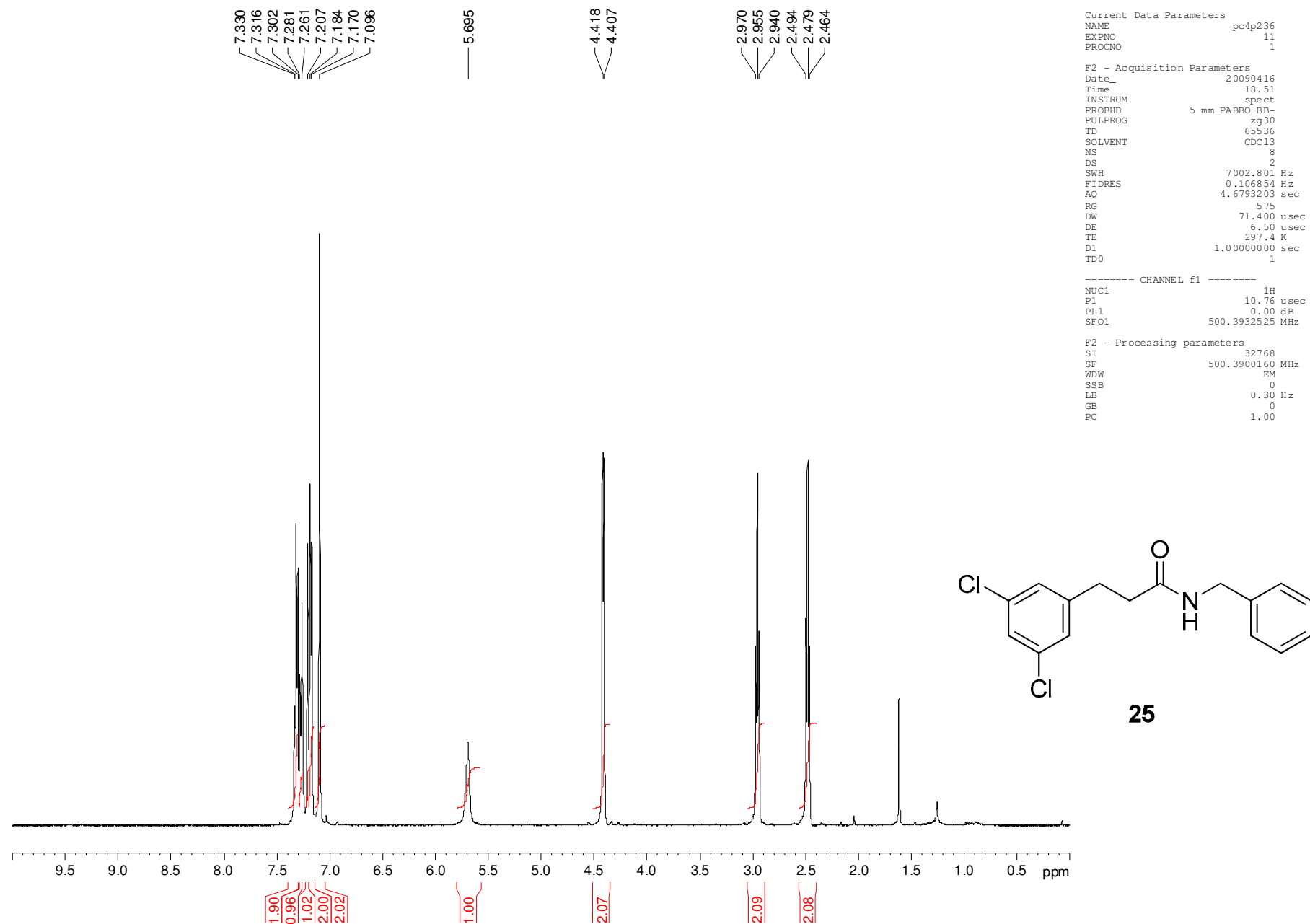
F2 - Processing parameters
SI                    32768
SF                   125.8231543 MHz
WDW                   EM
SSB                   0
LB                    1.00 Hz
GB                    0
PC                    1.40
```



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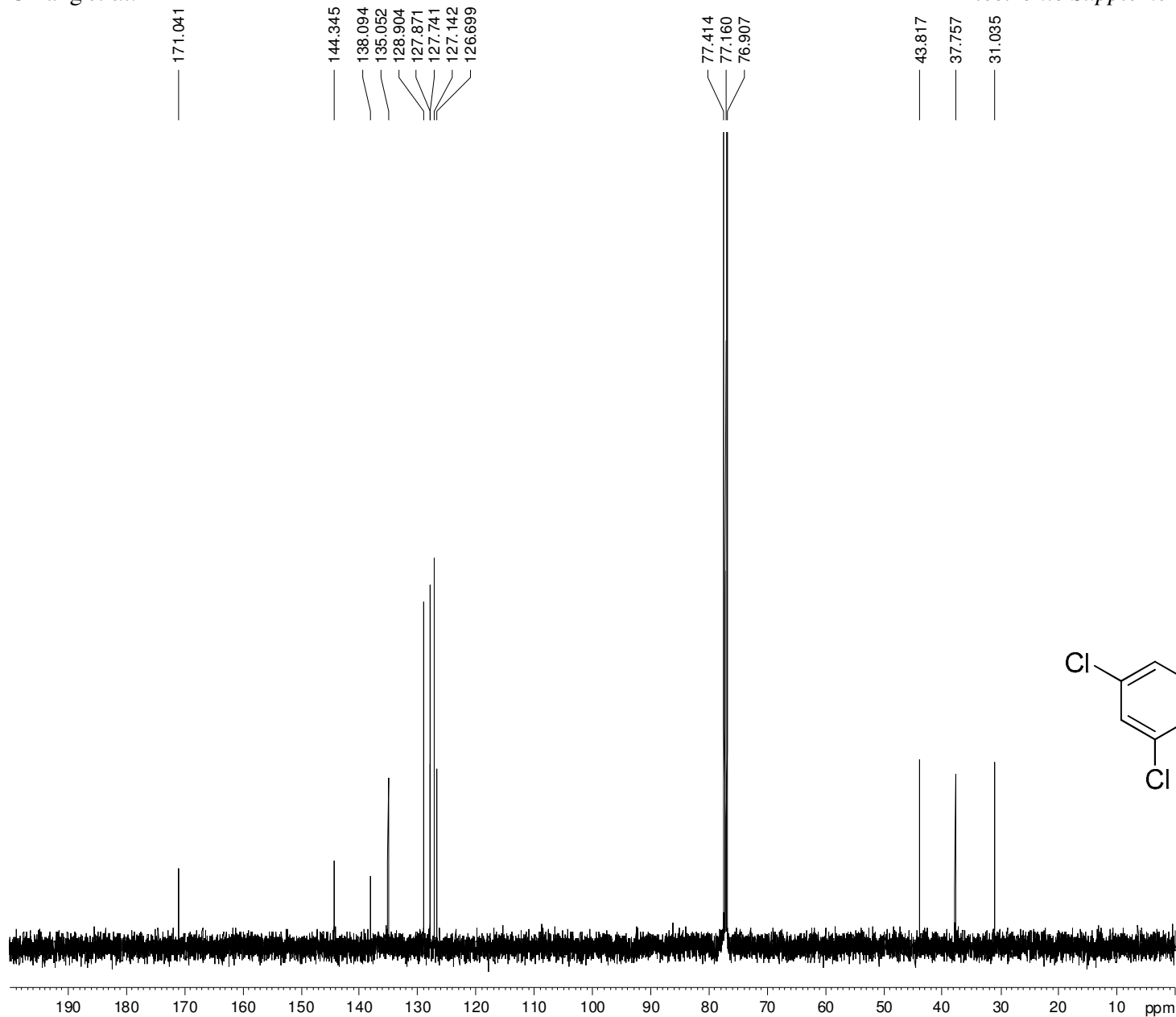
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Current Data Parameters
NAME                pc4p236
EXPNO               12
PROCNO              1

F2 - Acquisition Parameters
Date_                20090416
Time                 18.53
INSTRUM              spect
PROBHD                5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    128
DS                     4
SWH                 29761.904 Hz
FIDRES               0.454131 Hz
AQ                  1.1010548 sec
RG                   1820
DW                  16.800 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                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                   1H
PCPD2                 80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                   0.00 dB
SFO2                 500.3920016 MHz

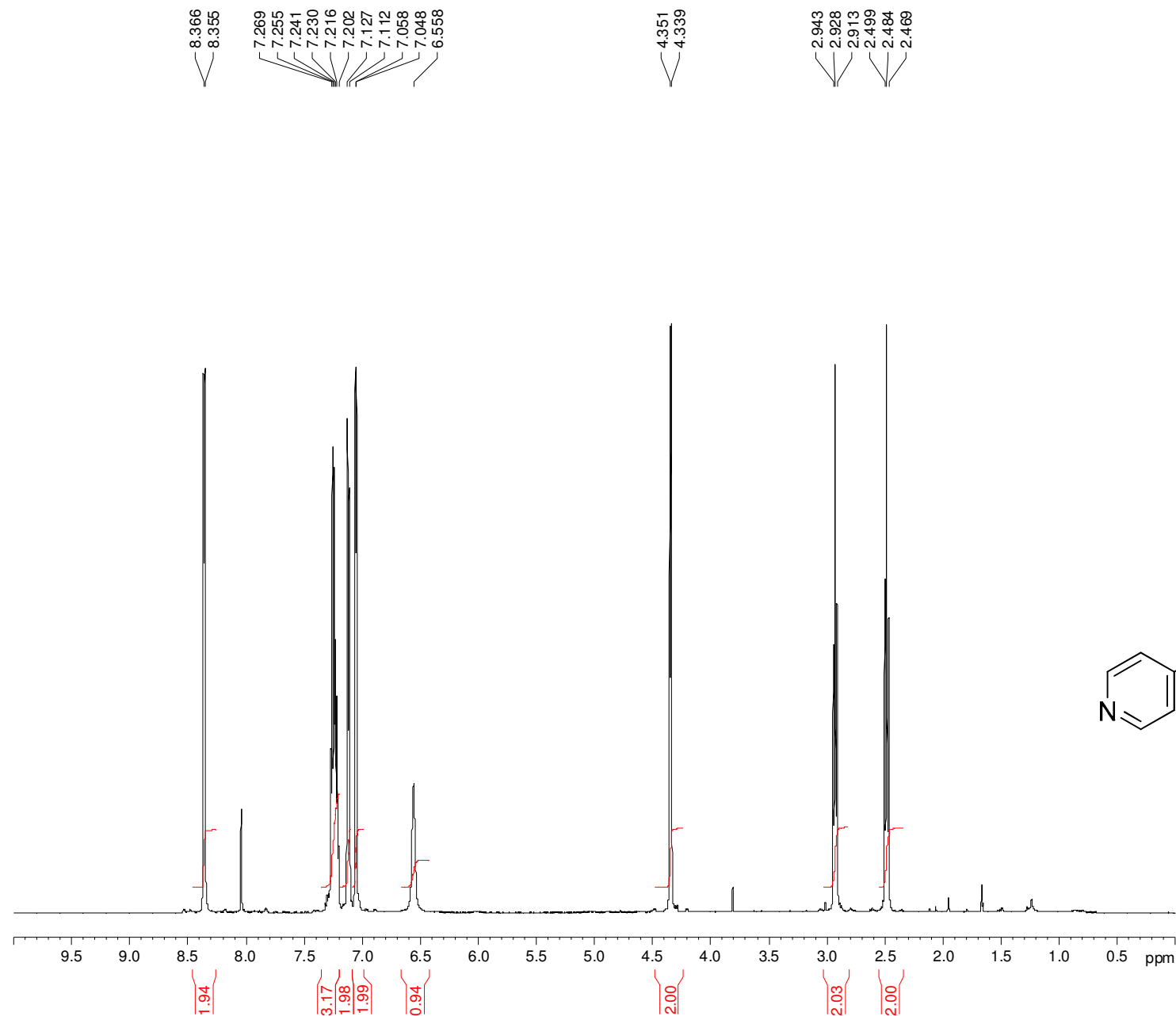
F2 - Processing parameters
SI                    32768
SF                   125.8231507 MHz
WDW                   EM
SSB                   0
LB                   1.00 Hz
GB                   0
PC                   1.40

```

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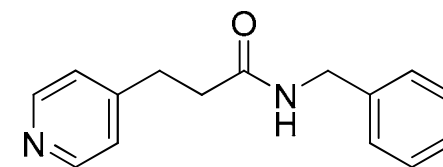


```
Current Data Parameters
NAME                pc4p254
EXPNO                6
PROCNO              1

F2 - Acquisition Parameters
Date_                20090427
Time                 9.05
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                    8
DS                    2
SWH                  7002.801 Hz
FIDRES               0.106854 Hz
AQ                   4.6793203 sec
RG                    114
DW                   71.400 usec
DE                    6.50 usec
TE                   298.1 K
D1                   1.00000000 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  1H
P1                    10.76 usec
PL1                   0.00 dB
SFO1                  500.3932525 MHz

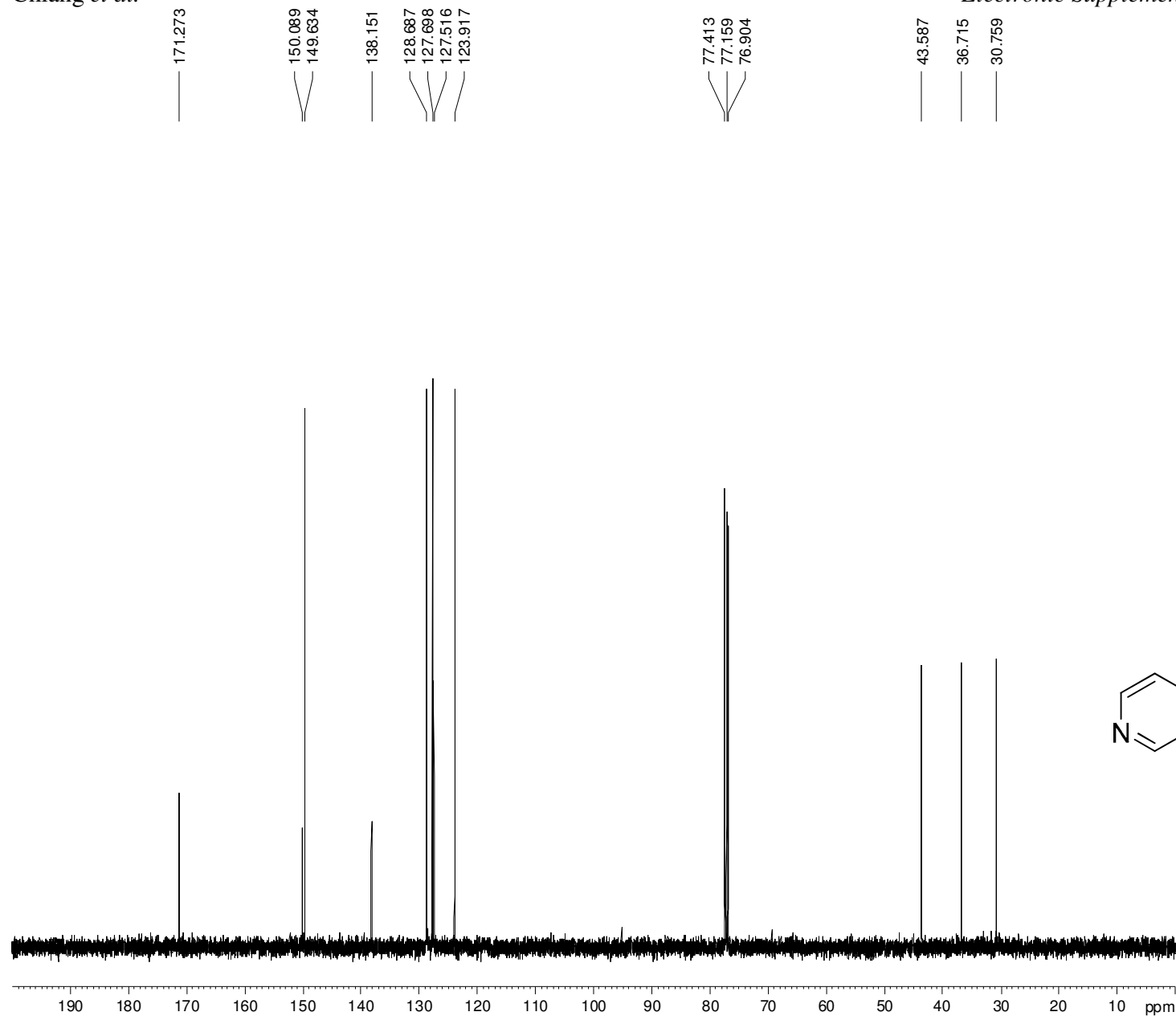
F2 - Processing parameters
SI                    32768
SF                    500.3900160 MHz
WDW                   EM
SSB                   0
LB                    0.30 Hz
GB                    0
PC                    1.00
```



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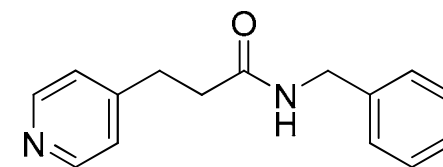
```
Current Data Parameters
NAME                pc4p254
EXPNO               8
PROCNO              1

F2 - Acquisition Parameters
Date_                20090427
Time                 9.07
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    16
DS                     4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                    2050
DW                   16.800 usec
DE                    6.50 usec
TE                   298.7 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  13C
P1                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                   1H
PCPD2                 80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                   0.00 dB
SFO2                 500.3920016 MHz

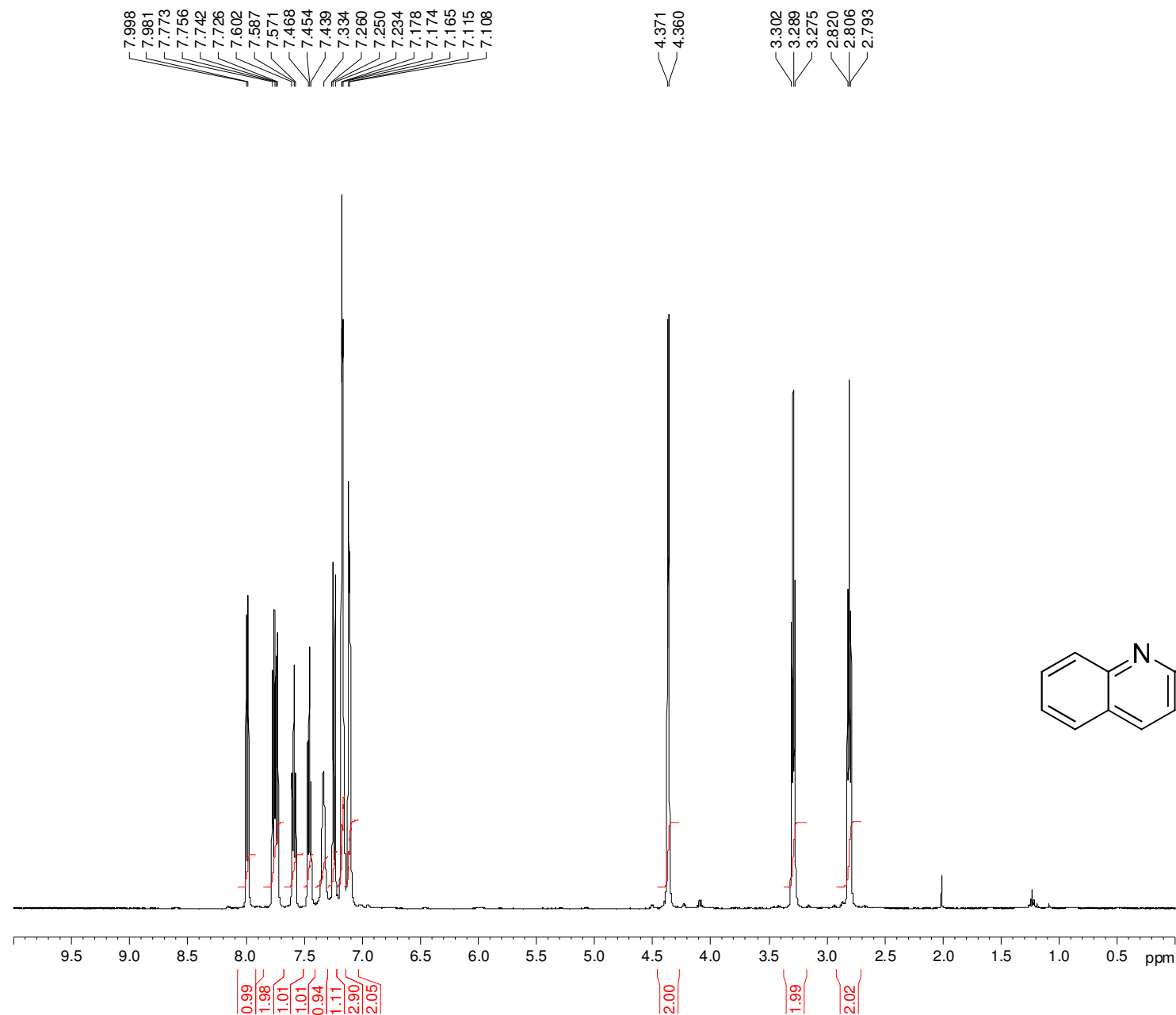
F2 - Processing parameters
SI                    32768
SF                   125.8231634 MHz
WDW                   EM
SSB                   0
LB                    1.00 Hz
GB                    0
PC                    1.40
```



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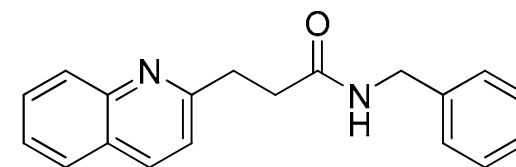


Current Data Parameters
NAME pc4p255
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090425
Time 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 45.2
DW 71.400 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

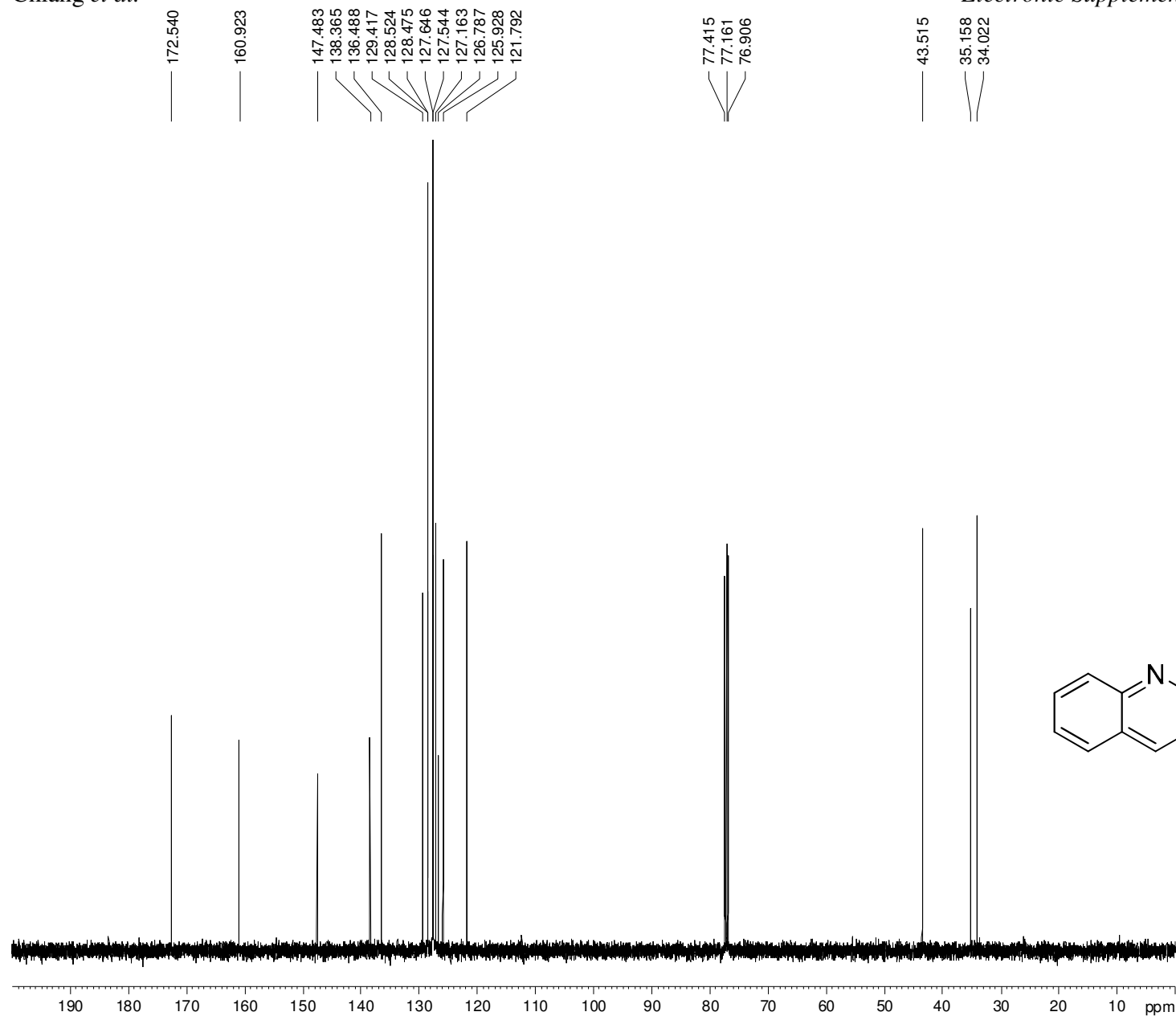
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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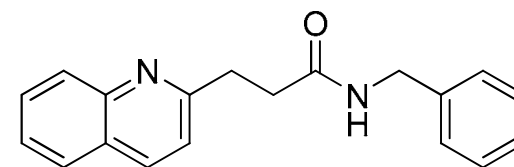
```
Current Data Parameters
NAME                pc4p255
EXPNO                3
PROCNO              1

F2 - Acquisition Parameters
Date_                20090425
Time                 10.04
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   17
DS                    4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                    2050
DW                   16.800 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                    7.50 usec
PL1                   1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                  1H
PCPD2                 80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                   0.00 dB
SFO2                 500.3920016 MHz

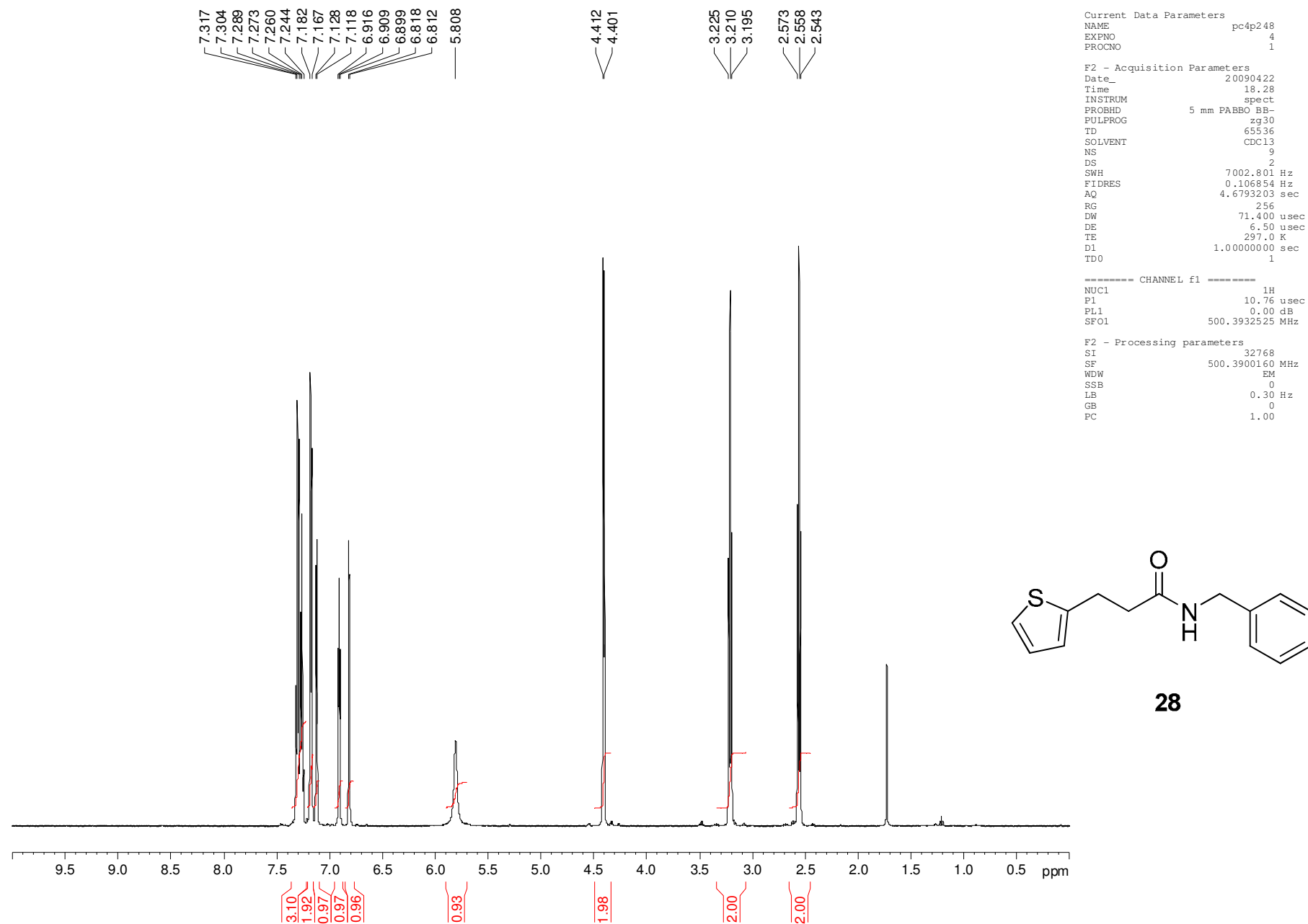
F2 - Processing parameters
SI                    32768
SF                   125.8231725 MHz
WDW                   EM
SSB                   0
LB                    1.00 Hz
GB                    0
PC                    1.40
```



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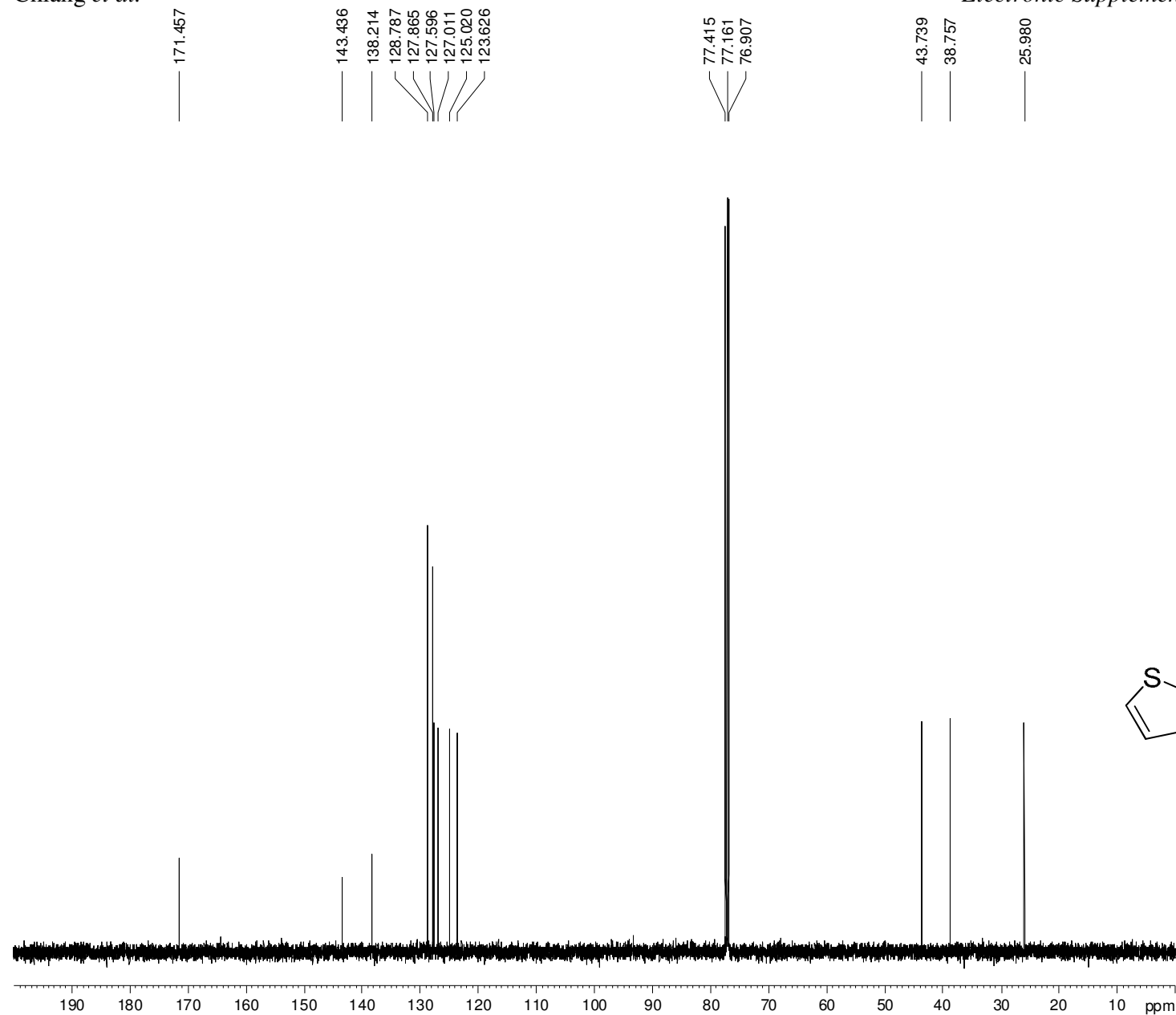
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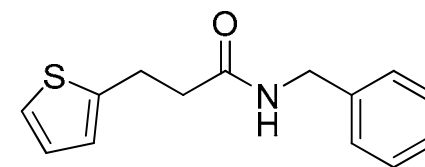
```
Current Data Parameters
NAME                pc4p248
EXPNO               5
PROCNO              1

F2 - Acquisition Parameters
Date_               20090422
Time                18.30
INSTRUM             spect
PROBHD              5 mm PABBO BB-
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   67
DS                   4
SWH                 29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010548 sec
RG                  1620
DW                  16.800 usec
DE                  6.50 usec
TE                  297.7 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                 1

===== CHANNEL f1 =====
NUC1                 13C
P1                   7.50 usec
PL1                  1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2             waltz16
NUC2                 1H
PCPD2                80.00 usec
PL12                 17.43 dB
PL13                 18.43 dB
PL2                  0.00 dB
SFO2                 500.3920016 MHz

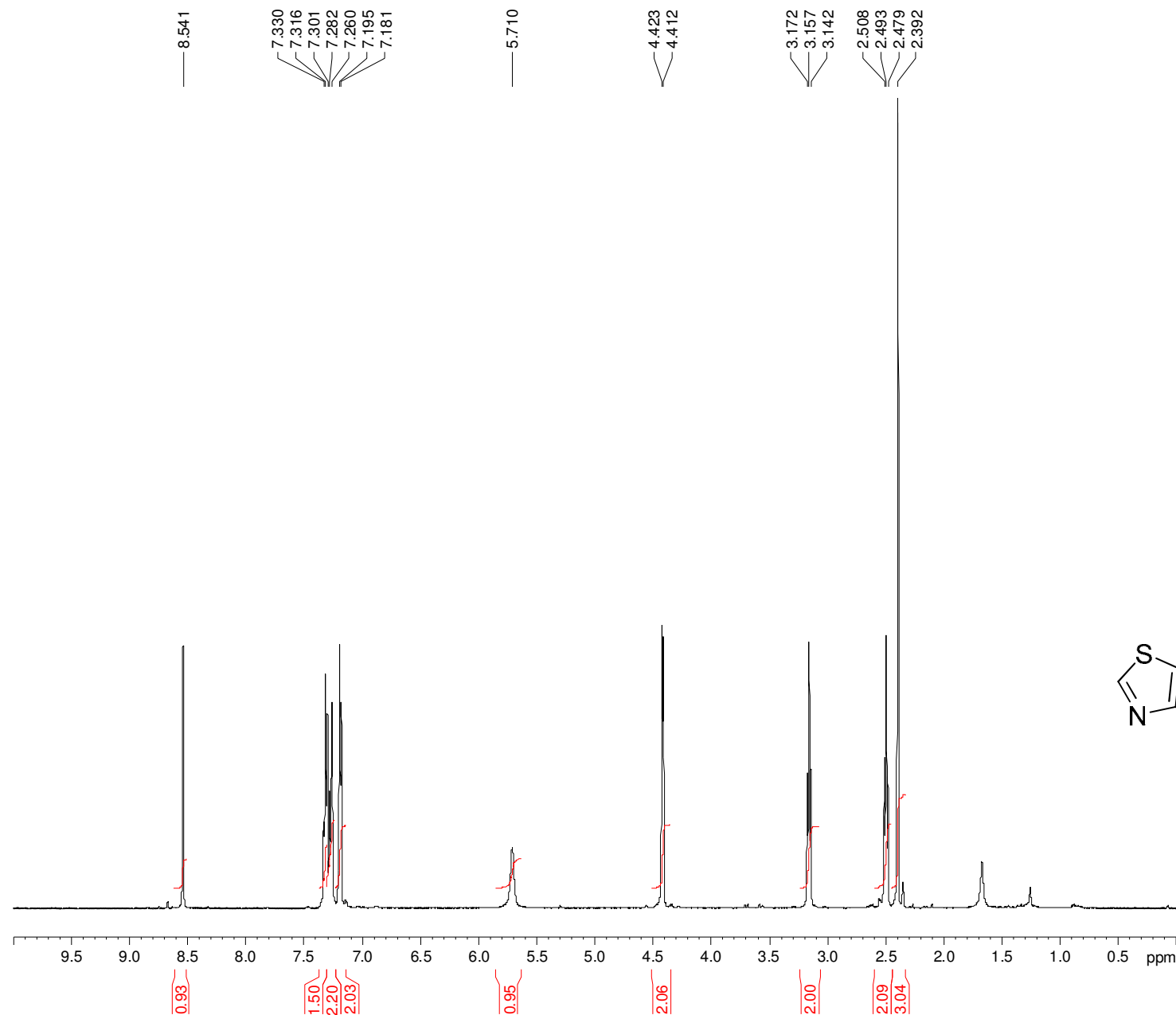
F2 - Processing parameters
SI                   32768
SF                   125.8231543 MHz
WDW                  EM
SSB                  0
LB                   1.00 Hz
GB                   0
PC                   1.40
```



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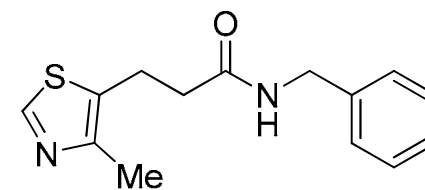
```

Current Data Parameters
NAME                pc4p241
EXPNO                2
PROCNO              1

F2 - Acquisition Parameters
Date_                20090418
Time                 16.24
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                   16
DS                   2
SWH                  7002.801 Hz
FIDRES               0.106854 Hz
AQ                   4.6793203 sec
RG                   645
DW                   71.400 usec
DE                   6.50 usec
TE                   297.1 K
D1                   1.00000000 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  1H
P1                   10.76 usec
PL1                   0.00 dB
SF01                  500.3932525 MHz

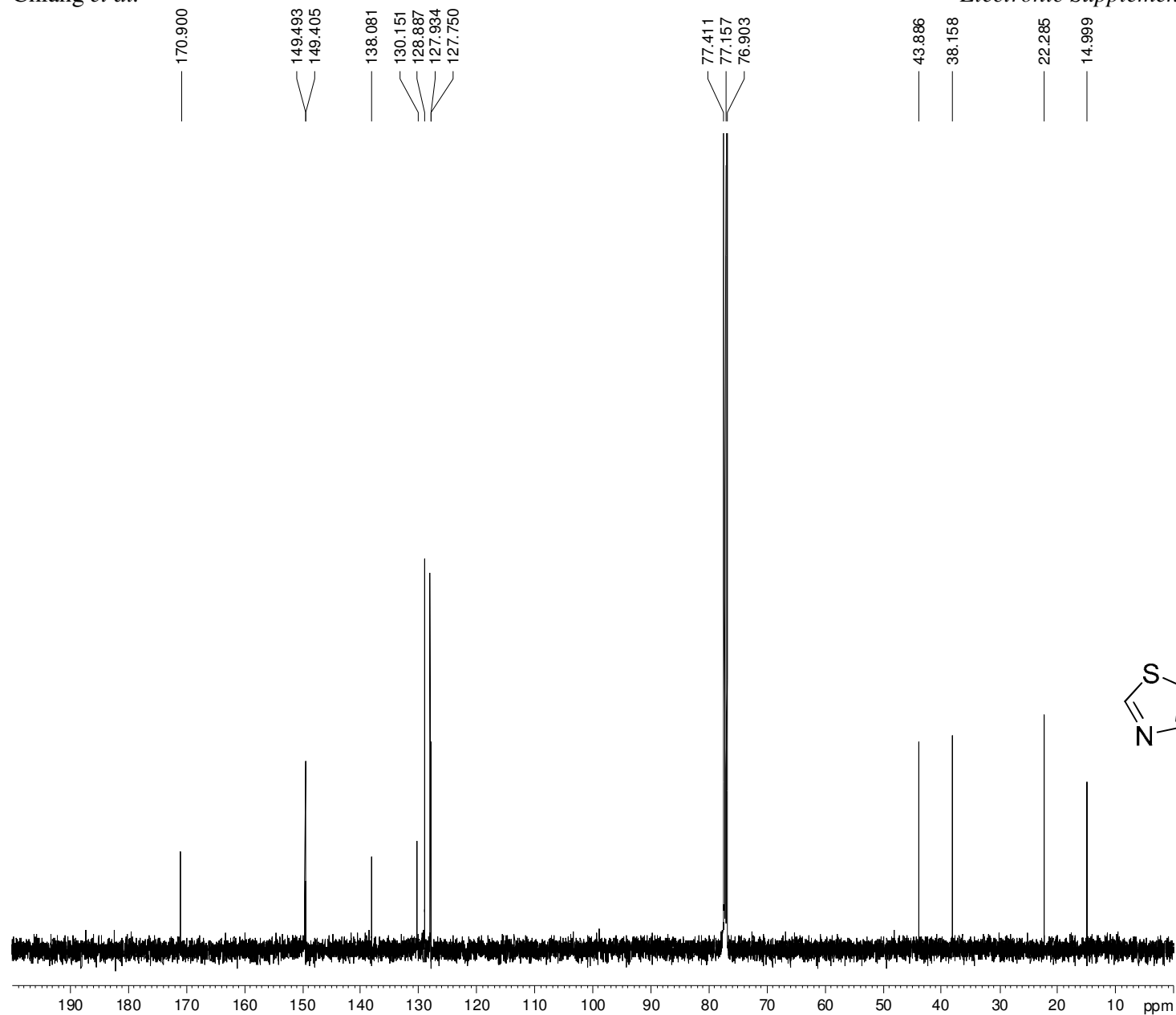
F2 - Processing parameters
SI                   32768
SF                   500.3900160 MHz
WDW                  EM
SSB                   0
LB                   0.30 Hz
GB                   0
PC                   1.00
    
```



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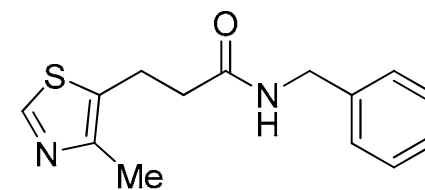
```
Current Data Parameters
NAME                pc4p241
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_                20090418
Time                 16.27
INSTRUM              spect
PROBHD               5 mm PABBO BB-
PULPROG              zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    512
DS                     4
SWH                  29761.904 Hz
FIDRES               0.454131 Hz
AQ                   1.1010548 sec
RG                    1620
DW                   16.800 usec
DE                    6.50 usec
TE                   297.9 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  13C
P1                     7.50 usec
PL1                    1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2              waltz16
NUC2                   1H
PCPD2                 80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                    0.00 dB
SFO2                 500.3920016 MHz

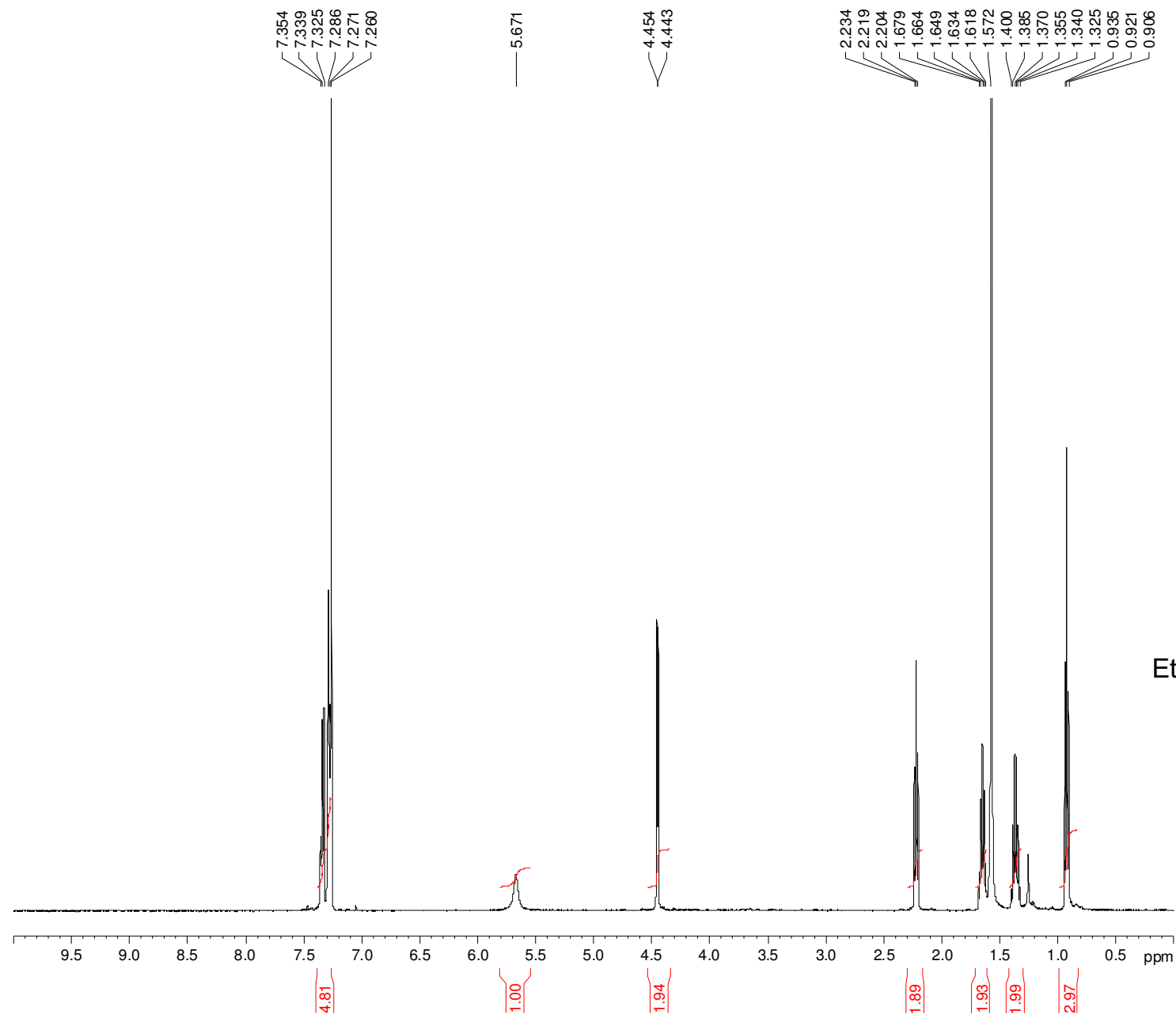
F2 - Processing parameters
SI                     32768
SF                  125.8231506 MHz
WDW                    EM
SSB                     0
LB                      1.00 Hz
GB                       0
PC                      1.40
```



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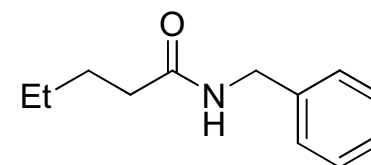


Current Data Parameters
NAME pc4p297
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090611
Time 13.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 1290
DW 71.400 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

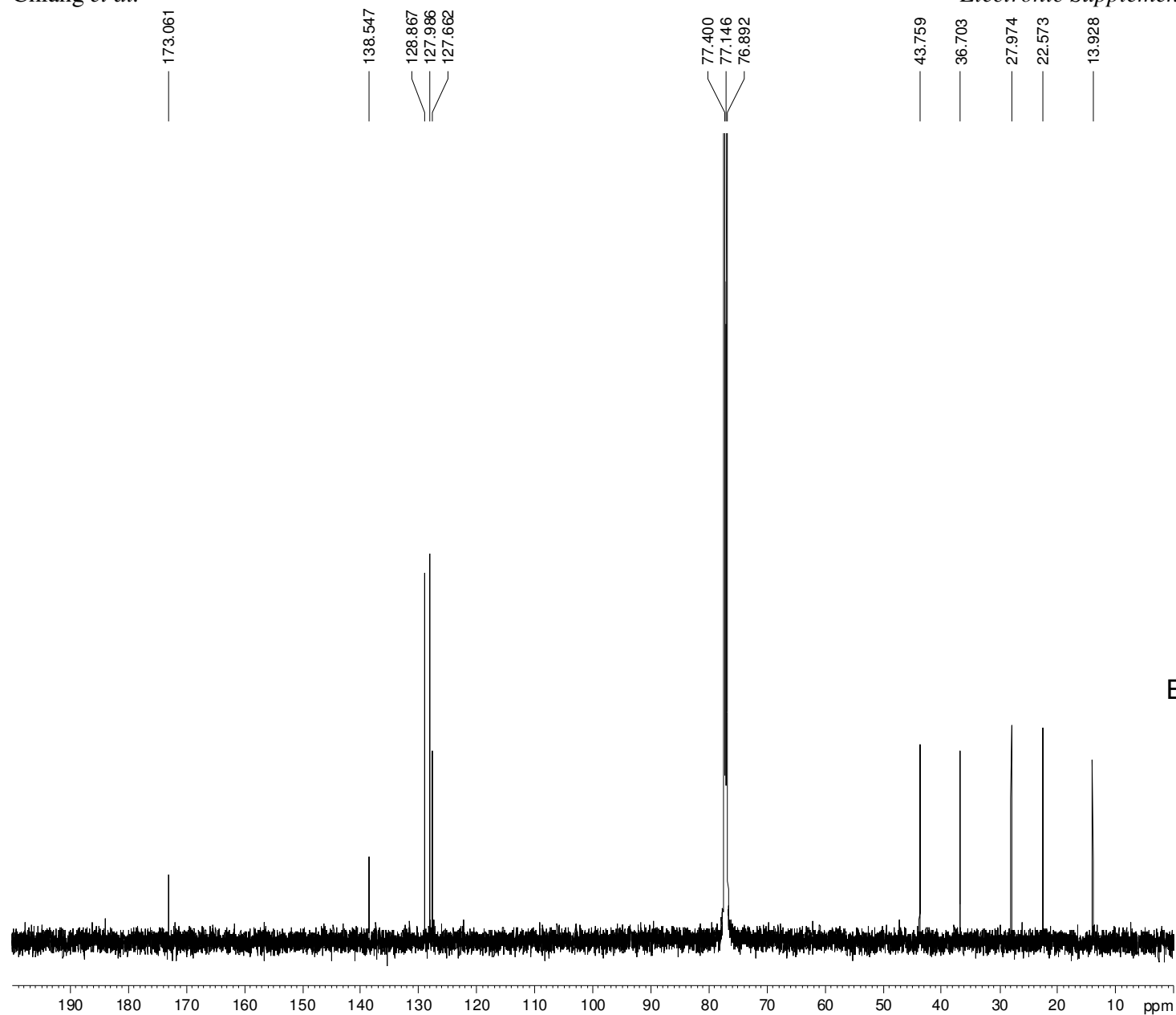
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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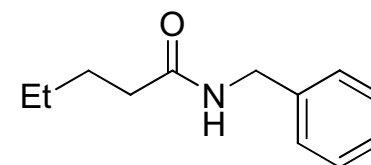
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Current Data Parameters
NAME          pc4p297
EXPNO         10
PROCNO        1

F2 - Acquisition Parameters
Date_         20090611
Time          21.34
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            12288
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            456
DW            16.800 usec
DE            6.50 usec
TE            297.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            7.50 usec
PL1           1.00 dB
SFO1          125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL12          17.43 dB
PL13          18.43 dB
PL2           0.00 dB
SFO2          500.3920016 MHz

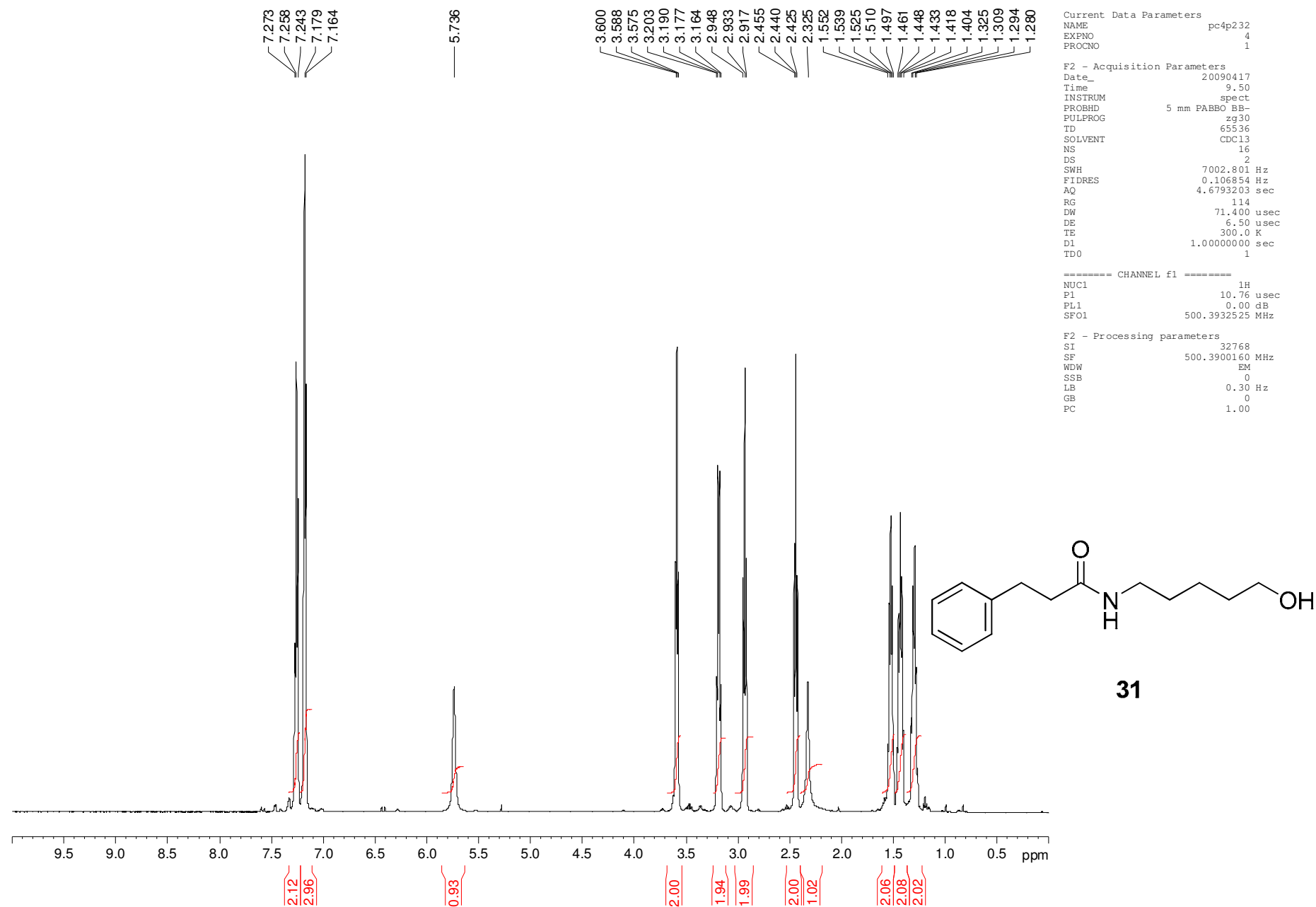
F2 - Processing parameters
SI            32768
SF            125.8231497 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



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Current Data Parameters
 NAME pc4p232
 EXPNO 4
 PROCNO 1

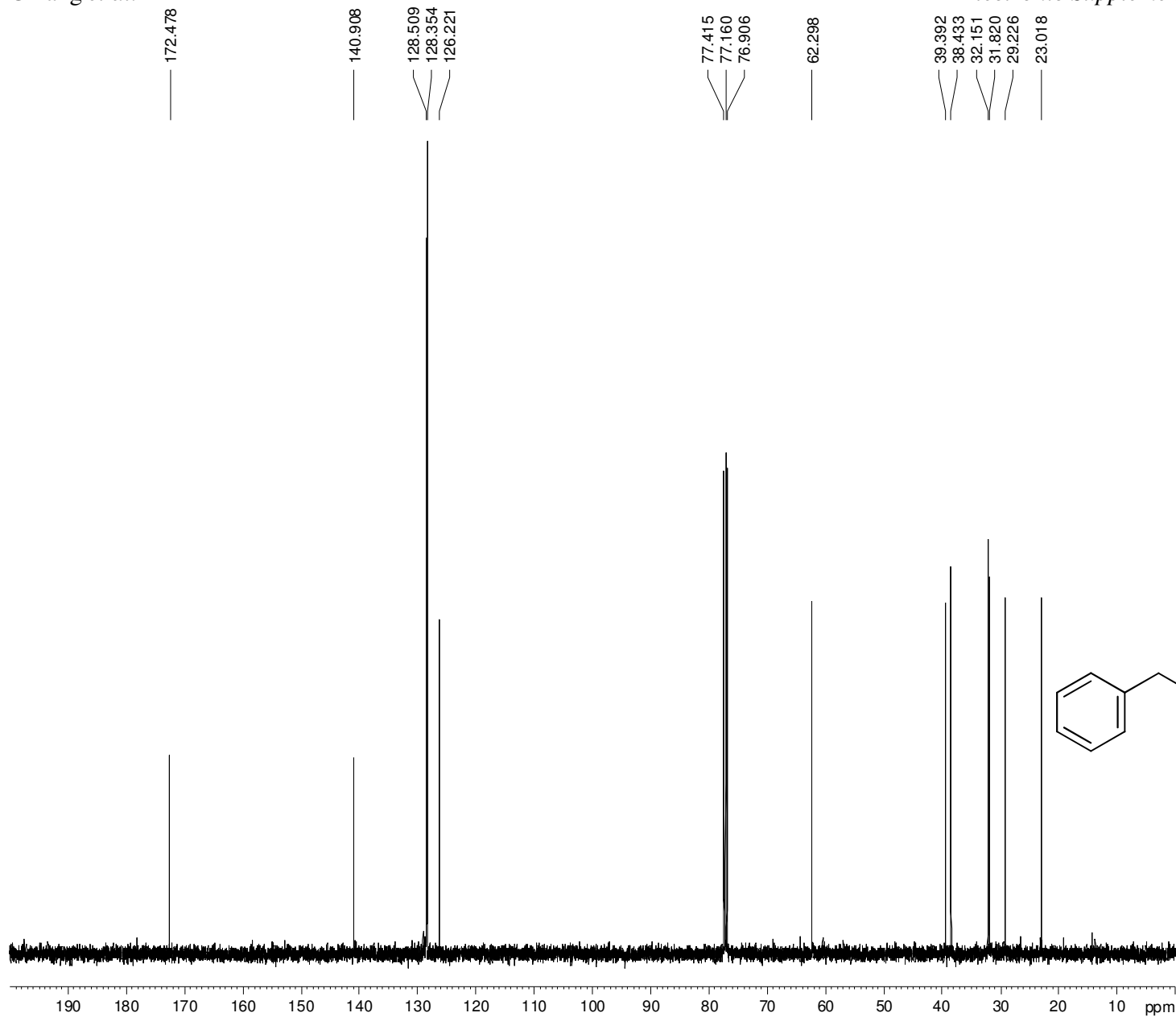
F2 - Acquisition Parameters
 Date_ 20090417
 Time 9.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 7002.801 Hz
 FIDRES 0.106854 Hz
 AQ 4.6793203 sec
 RG 114
 DW 71.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.76 usec
 PL1 0.00 dB
 SFO1 500.3932525 MHz

F2 - Processing parameters
 SI 32768
 SF 500.3900160 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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Current Data Parameters
NAME pc4p232
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090415
Time 10.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

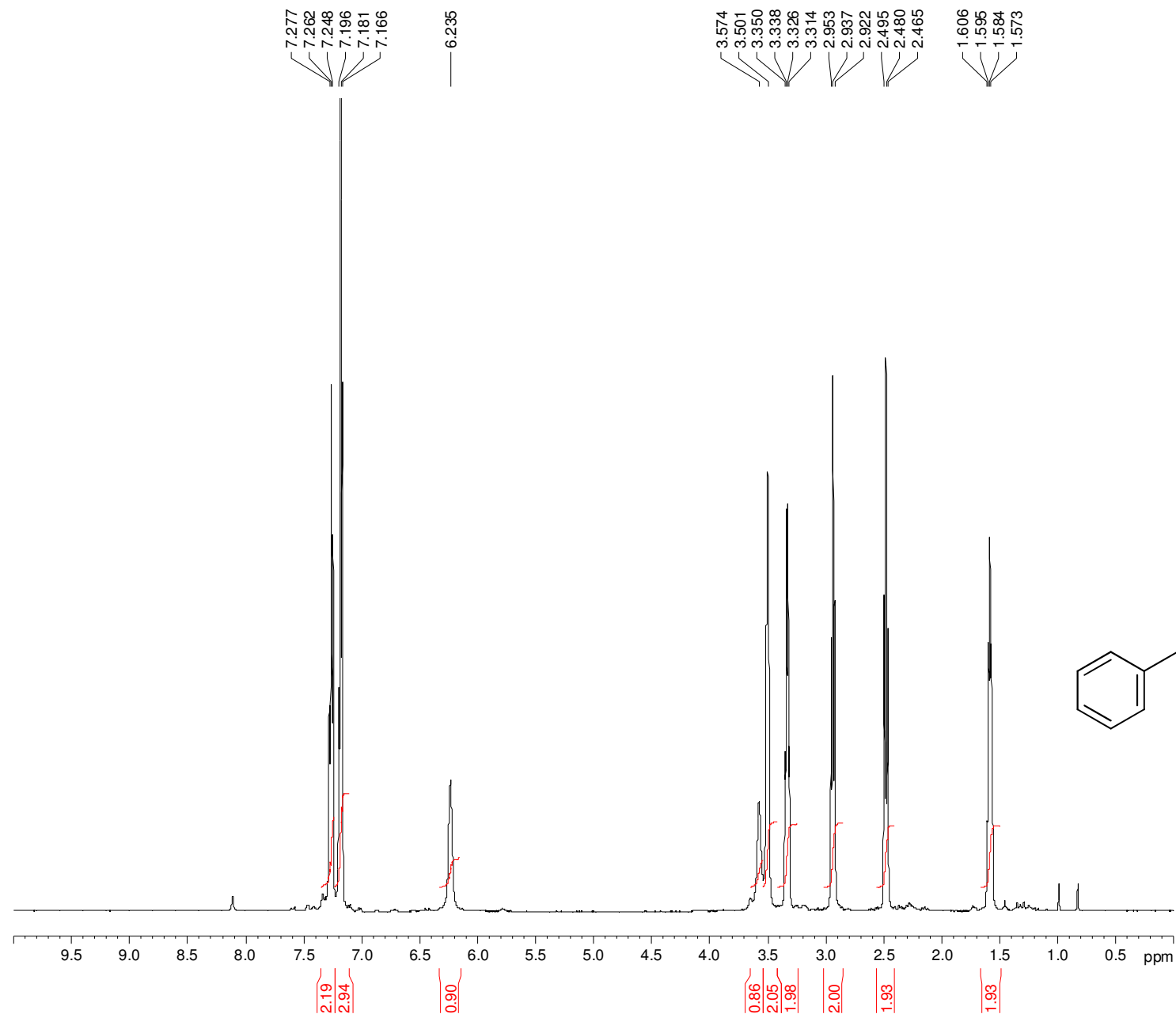
===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 32768
SF 125.8231643 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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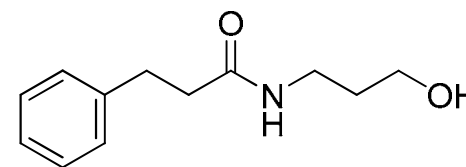


Current Data Parameters
NAME pc4p237
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090417
Time 9.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 101
DW 71.400 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

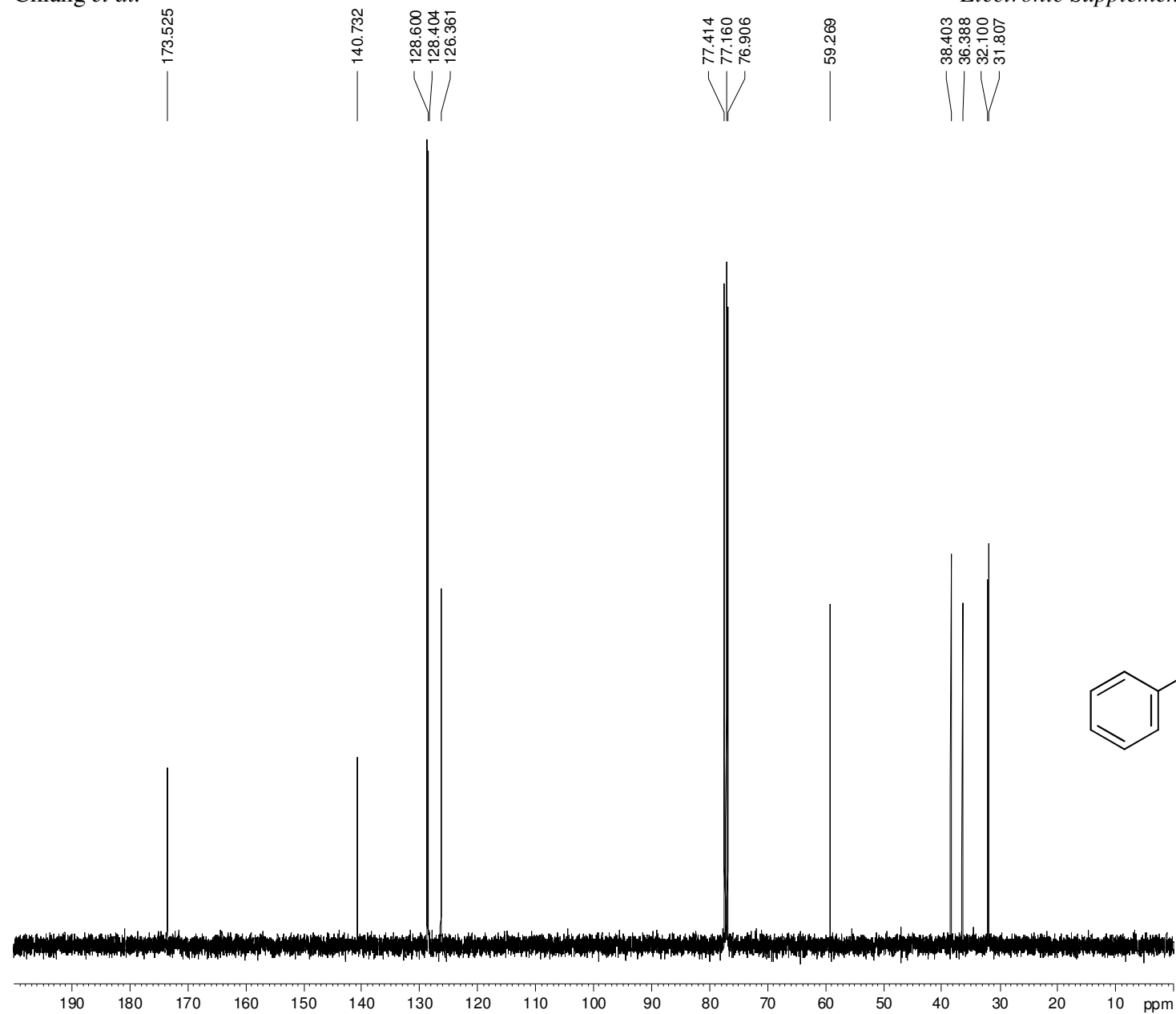
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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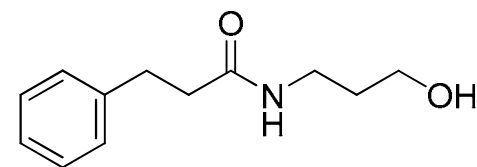
Current Data Parameters
NAME                pc4p237
EXPNO               5
PROCNO             1

F2 - Acquisition Parameters
Date_              20090417
Time               10.00
INSTRUM            spect
PROBHD             5 mm PABBO BB-
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 32
DS                 4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                 2050
DW                 16.800 usec
DE                 6.50 usec
TE                 297.9 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                1

===== CHANNEL f1 =====
NUC1                13C
P1                  7.50 usec
PL1                 1.00 dB
SFO1                125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2            waltz16
NUC2                1H
PCPD2              80.00 usec
PL12                17.43 dB
PL13                18.43 dB
PL2                 0.00 dB
SFO2                500.3920016 MHz

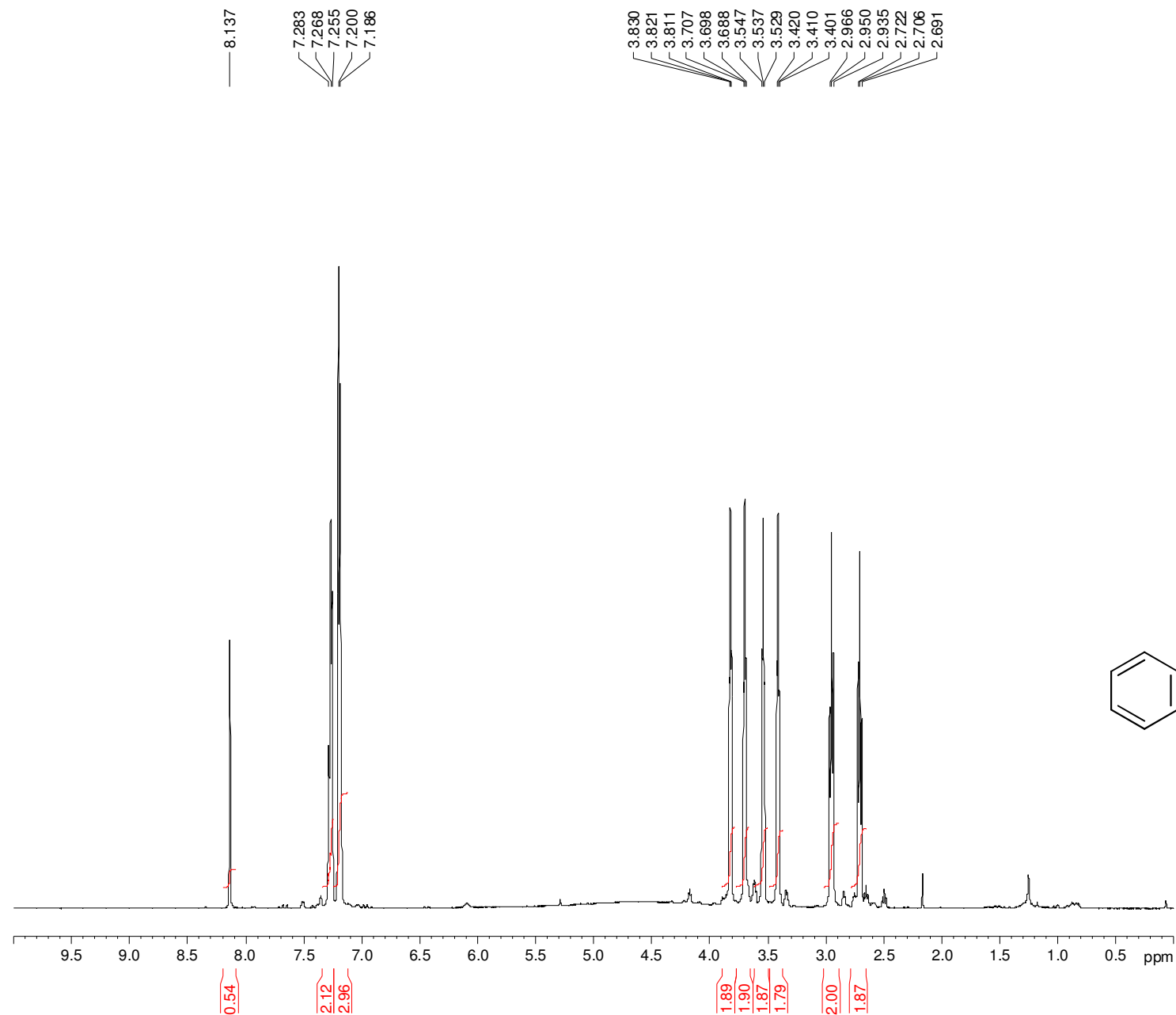
F2 - Processing parameters
SI                  32768
SF                  125.8231597 MHz
WDW                 EM
SSB                 0
LB                  1.00 Hz
GB                  0
PC                  1.40
  
```



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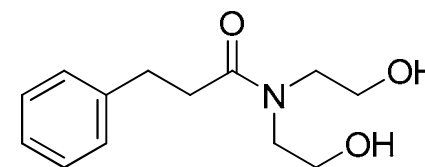


Current Data Parameters
NAME pc4p238
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090419
Time 11.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 161
DW 71.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz

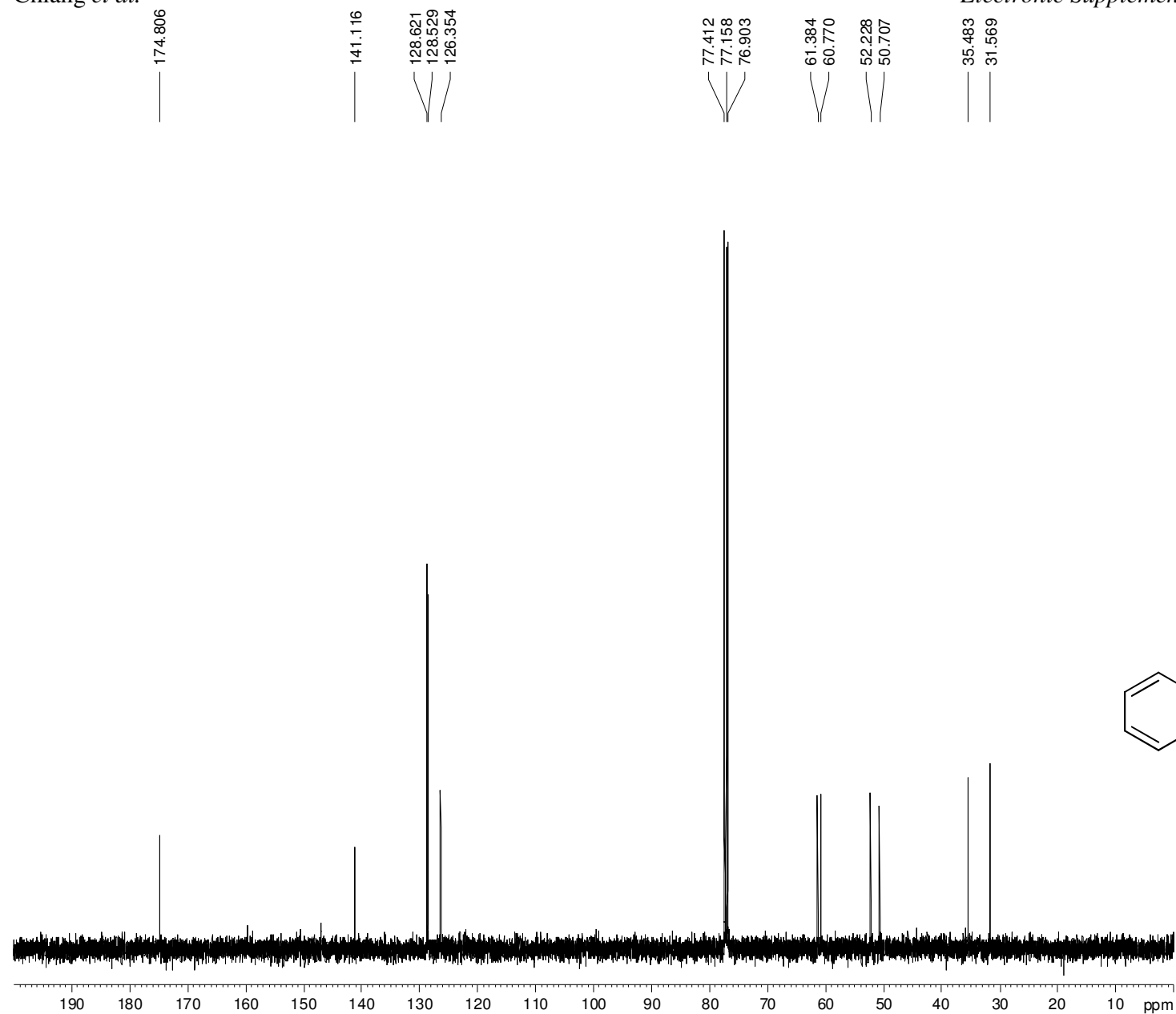
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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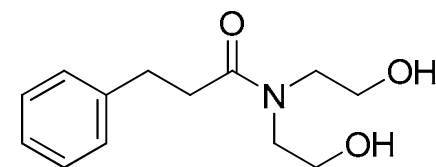
```
Current Data Parameters
NAME                pc4p238
EXPNO               7
PROCNO              1

F2 - Acquisition Parameters
Date_               20090419
Time                11.45
INSTRUM             spect
PROBHD              5 mm PABBO BB-
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   33
DS                   4
SWH                 29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010548 sec
RG                   1620
DW                  16.800 usec
DE                   6.50 usec
TE                  298.3 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                 1

===== CHANNEL f1 =====
NUC1                 13C
P1                   7.50 usec
PL1                  1.00 dB
SFO1                 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2             waltz16
NUC2                 1H
PCPD2                80.00 usec
PL12                 17.43 dB
PL13                 18.43 dB
PL2                  0.00 dB
SFO2                 500.3920016 MHz

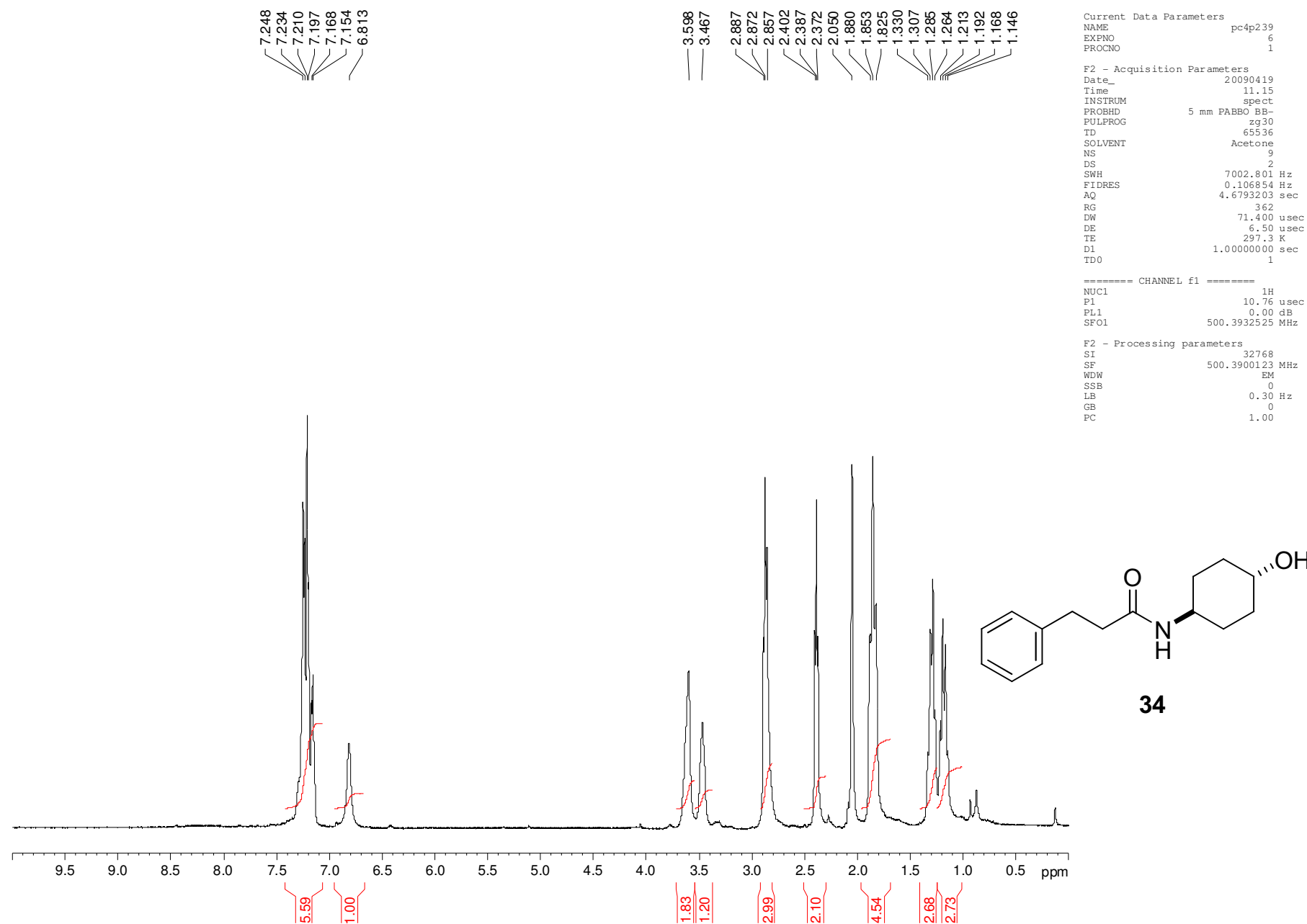
F2 - Processing parameters
SI                   32768
SF                   125.8231543 MHz
WDW                  EM
SSB                  0
LB                   1.00 Hz
GB                   0
PC                   1.40
```



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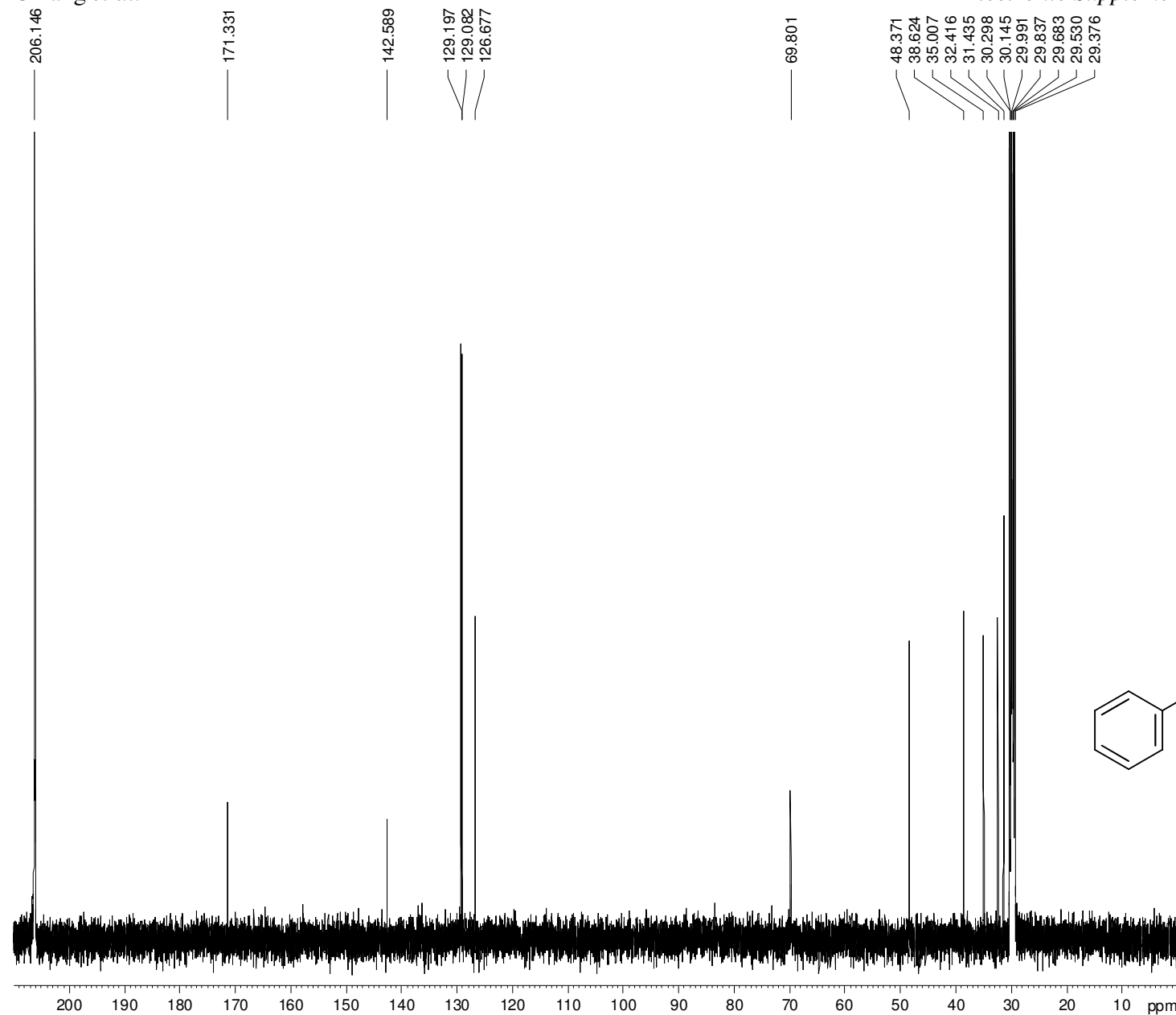
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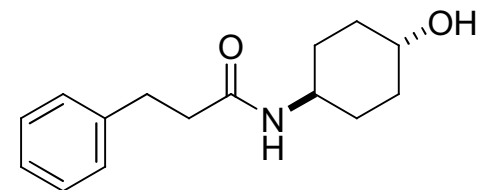
Current Data Parameters
NAME pc4p239
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090419
Time 11.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 297
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1440
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 32768
SF 125.8230547 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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