Supplementary Material for Organic & Biomolecular Chemistry

Supporting Materials

New, versatile synthesis of 4,6-disubstituted pyridazin-3(2*H*)-ones

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Characterization data for compounds **7b,c,e,f,h,j,k**, **9a,b,d,f-k** and **10b,c**

4-Diethoxyphosphorylo-6-ethylpyridazin-3(2*H*)-one 7b (0.44 g, 95%) colorless oil (Found: C, 45.9; H, 7.2. $C_{10}H_{19}N_2O_4P$ requires C, 45.8; H, 7.3%); ν_{max}(film)/cm^{-1} 1600, 1232 and 1024; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.14 (3H, t, *J* 7.4, C*H*$_3$), 1.29-1.38 (6H, m, 2 x C*H*$_3$CH$_2$O), 2.37 (2H, q, *J* 7.4, C*H*$_2$), 2.55-3.25 (3H, m, C*H*$_2$, C*H*), 4.13-4.22 (4H, m, 2 x CH$_3$C*H*$_2$O) and 8.50 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 9.78 (s, *C*H$_3$), 16.05 (d, *J* 5.9 2 x *C*H$_3$CH$_2$O), 25.81 (d, *J* 5.2 *C*-5), 29.51 (s, *C*H$_2$), 34.24 (d, *J* 135.0, *C*-4), 62.77 (d, *J* 7.5, CH$_3$*C*H$_2$O), 62.89 (d, *J* 6.9, CH$_3$*C*H$_2$O), 155.14 (d, *J* 5.0, *C*-6) and 162.54 (d, *J* 4.3, *C*-3); δ_P(101 MHz; $CDCl_3$; H_3PO_4) 21.59.

4-Diethoxyphosphorylo-6-pentylpyridazin-3(2*H*)-one 7c (0.58 g, 86%) colorless crystal, mp 55 ^oC (from Et_2O) (Found: C, 51.5; H, 8.2. $C_{13}H_{25}N_2O_4P$ requires C, 51.3; H, 8.3%); ν_{max}(film)/cm^{-1} 1684, 1240, and 1024; δ_H(250 MHz; $CDCl_3$; Me_4Si) 0.90 (3H, t, *J* 7.5, C*H*$_3$), 1.24-1.41 (8H, m, 2 x C*H*$_3$CH$_2$O, C*H*$_2$), 1.55-1.65 (3H, m, C*H*$_2$, C*H*), 2.33 (2H, dd, *J* 7.5, C*H*$_2$), 2.70-3.25 (4H, m, 2 x C*H*$_2$), 4.14-4.25 (4H, m, 2 x CH$_3$C*H*$_2$O) and 8.31 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 11.94 (s, *C*H$_3$), 14.32 (d, *J* 6.0, 2 x *C*H$_3$CH$_2$O), 20.39 (s, *C*H$_2$), 23.39 (s, *C*H$_2$), 24.18 (d, *J* 5.3, *C*-5), 29.43 (s, *C*H$_2$), 34.47 (d, *J* 137.4, *C*-4), 34.57 (s, *C*H$_2$), 60.45 (d, *J* 6.5, CH$_3$*C*H$_2$O), 61.12 (d, *J* 6.9, CH$_3$*C*H$_2$O), 151.51 (d, *J* 5.1, *C*-6) and 160.80 (d, *J* 5.0, *C*-3); δ_P(101 MHz; $CDCl_3$; H_3PO_4) 21.59.

6-(3,4-Dimethoxybenzyl)-4-diethoxyphosphorylopyridazin-3(2*H*)-one 7e (0.71 g, 85%) yellow oil (Found: C, 53.3; H, 6.8. $C_{17}H_{25}N_2O_6P$ requires C, 53.1; H, 6.6%); ν_{max}(film)/cm^{-1} 1684, 1516, 1240, 1028 and 972; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.28 (6H, t, *J* 7.5, 2 x C*H*$_3$CH$_2$O), 2.52-3.05 (3H, m, C*H*$_2$, C*H*), 3.56, 3.62 (2H, AB, *J* 15.0, C*H*$_2$), 3.87 (3H, s, C*H*$_3$O), 3.88 (3H, s, C*H*$_3$O), 4.09-4.21 (4H, m, 2 x CH$_3$C*H*$_2$O), 6.75-6.85 (3H, m, 3 x C*H*$_{Ar}$) and 8.42 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 16.14 (d, *J* 5.6, *C*H$_3$CH$_2$O), 16.23 (d, *J* 5.6, *C*H$_3$CH$_2$O), 25.52 (d, *J* 5.6, *C*-5), 36.46 (d, *J* 135.8, *C*-4), 42.61 (s, *C*H$_2$Ph), 55.81 (s, 2 x CH$_3$O), 62.78 (d, *J* 6.8 CH$_3$*C*H$_2$O), 63.16 (d, *J* 6.8, CH$_3$*C*H$_2$O), 111.27 (s, 2 x *C*-Ar), 112.15 (s, 2 x *C*-Ar), 121.21 (s, *C*-Ar), 127.88 (s, *C*-Ar), 148.13 (s, *C*-Ar), 149.08 (s, *C*-Ar), 153.42 (d, *J* 5.6, *C*-6) and 162.47 (d, *J* 4.3, *C*-3); δ_P(101 MHz; $CDCl_3$; H_3PO_4) 21.34.

4-Diethoxyphosphorylo-6-phenylpyridazin-3(2*H*)-one 7f[1] (0.57 g, 92%) yellow oil (Found: C, 54.3; H, 6.4. $C_{14}H_{19}N_2O_4P$ requires C, 54.2; H, 6.2%); ν_{max}(film)/cm^{-1} 1684, 1616, 1256 and 1004; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.23 (3H, t, *J* 7.0, C*H*$_3$CH$_2$O), 1.34 (3H, t, *J* 7.0, C*H*$_3$CH$_2$O), 3.04-3.28 (2H, m, C*H*$_2$), 3.41-3.58 (1H, m, C*H*), 4.05-4.26 (4H, m, 2 x CH$_3$C*H*$_2$O), 7.29-7.47 (3H, m, 3 x C*H*$_{Ar}$), 7.72-7.77 (2H, m, 2 x C*H*$_{Ar}$) and 8.82 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 16.19 (d, *J* 5.6, *C*H$_3$CH$_2$O), 16.23 (d, *J* 5.6, *C*H$_3$CH$_2$O), 24.16

(d, *J* 5.6, *C*-5), 36.64 (d, *J* 134.5, *C*-4), 63.08 (d, *J* 5.6, CH_3CH_2O), 63.18 (d, *J* 5.6, CH_3CH_2O), 125.99 (s, 2 x *C*-Ar), 128.57 (s, 2 x *C*-Ar), 129.90 (s, *C*-Ar), 135.18 (s, *C*-Ar), 149.57 (d, *J* 4.9, *C*-6) and 162.77 (d, *J* 4.3, *C*-3); δ_P(101 MHz; $CDCl_3$; H_3PO_4) 21.35.

4-Diethoxyphosphorylo-6-(4-methoxyphenyl)-pyridazin-3(2*H*)-one 7h (0.44 g, 65%) yellow oil (Found: C, 52.6; H, 6.5. $C_{15}H_{21}N_2O_5P$ requires C, 52.9; H, 6.2%); ν_{max}(film)/cm^{-1} 1680, 1512, 1248, and 1032; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.22 (3H, t, *J* 7.0, CH_3CH_2O), 1.34 (3H, t, *J* 7.0, CH_3CH_2O), 3.00-3.26 (2H, m, CH_2), 3.37-3.55 (1H, m, C*H*), 4.04-4.26 (4H, m, 2 x $CH_3CH_2OP(O)$), 6.84-6.96 (2H, m, 2 x CH_{Ar}), 7.66-7.72 (2H, m, 2 x CH_{Ar}) and 8.54 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 16.01 (d, *J* 5.6, 2 x CH_3CH_2O), 23.82 (d, *J* 4.9, *C*-5), 36.42 (d, *J* 135.1, *C*-4), 55.22 (s, OCH_3), 62.98 (d, *J* 6.8, CH_3CH_2O), 63.10 (d, *J* 6.8, CH_3CH_2O), 113.12 (s, 2 x *C*-Ar), 127.41 (s, *C*-Ar), 127.58 (s, 2 x *C*-Ar), 149.17 (s, *C*-6), 160.84 (s, *C*-Ar) and 162.72 (s, *C*-3); δ_P(101 MHz; $CDCl_3$; H_3PO_4) 21.40.

4-Diethoxyphosphorylo-2,6-diphenylpyridazin-3(2*H*)-one 7j (0.53 g, 69%) yellow oil (Found: C, 62.4; H, 6.1. $C_{20}H_{23}N_2O_4P$ requires C, 62.2; H, 6.0%); ν_{max}(film)/cm^{-1} 1676, 1324, 1254 and 1020; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.24 (3H, dt, *J* 7.0 and 0.5, CH_3CH_2O), 1.34 (3H, dt, *J* 7.0 and 0.5, CH_3CH_2O), 3.12-3.49 (2H, m, CH_2), 3.51-3.70 (1H, m, C*H*), 4.02-4.29 (4H, m, 2 x CH_3CH_2O), 7.28-7.32 (1H, m, CH_{Ar}), 7.38-7.48 (2H, m, 2 x CH_{Ar}), 7.54-7.62 (5H, m, 5 x CH_{Ar}) and 7.78-7.90 (2H, m, 2 x CH_{Ar}); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 14.57 (d, *J* 6.0, 2 x CH_3CH_2O), 22.85 (d, *J* 5.1, *C*-5), 36.34 (d, *J* 136.2, *C*-4), 61.36 (d, *J* 7.2, CH_3CH_2O), 61.48 (d, *J* 7.9, CH_3CH_2O), 123.30 (s, *C*-Ar), 124.54 (s, *C*-Ar), 125.11 (s, *C*-Ar), 126.80 (s, 2 x *C*-Ar), 126.88 (s, 2 x *C*-Ar), 128.35 (s, *C*-Ar), 133.41 (s, *C*-Ar), 139.45 (s, *C*-Ar), 148.40 (d, *J* 5.8, *C*-6) and 159.24 (d, *J* 4.6, *C*-3); δ_P(101 MHz; $CDCl_3$; H_3PO_4) 22.02.

6-(4-Bromophenyl)-4-diethoxyphosphorylo-2-phenylpyridazin-3(2*H*)-one 7k (0.72 g, 78%) orange oil (Found: C, 51.4; H, 4.9. $C_{20}H_{22}BrN_2O_4P$ requires C, 51.6; H, 4.8%); ν_{max}(film)/cm^{-1} 1680, 1492, 1260 and 1020; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.21 (3H, t, *J* 7.0, CH_3CH_2O), 1.34 (3H, t, *J* 7.0, CH_3CH_2O), 3.10-3.65 (3H, m, CH_2, C*H*), 4.02-4.28 (4H, m, 2 x CH_3CH_2O), 6.60-6.82 (2H, m, 2 x CH_{Ar}), 7.12-7.20 (2H, m, 2 x CH_{Ar}), 7.38-7.58 (4H, m, 4 x CH_{Ar}) and 7.66-7.72 (1H, m, CH_{Ar}); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 14.58 (d, *J* 5.7, 2 x CH_3CH_2O), 22.69 (d, *J* 5.1, *C*-5), 36.26 (d, *J* 135.4, *C*-4), 61.44 (d, *J* 5.0, CH_3CH_2O), 61.53 (d, *J* 6.5, CH_3CH_2O), 113.37 (s, *C*-Ar), 116.77 (s, *C*-Ar), 122.83 (s, 2 x *C*-Ar), 123.32 (s, *C*-Ar), 125.27 (s, *C*-Ar), 126.09 (s, *C*-Ar), 126.86 (s, *C*-Ar), 127.49 (s, 2 x *C*-Ar), 130.09 (s, *C*-Ar), 132.33 (s, *C*-Ar), 147.25 (d, *J* 5.3, *C*-6) and 159.15 (d, *J* 4.6, *C*-3); δ_P(101 MHz; $CDCl_3$; H_3PO_4) 21.44.

4,6-Dimethylpyridazin-3(2*H*)-one 9a[2, 3] (0.093 g, 75%) colorless oil (Found: C, 58.3; H, 6.3. $C_6H_8N_2O$ requires C, 58.05; H, 6.5%); ν_{max}(film)/cm^{-1} 1628, 1608, 952 and 912; δ_H(250 MHz; $CDCl_3$; Me_4Si) 2.19 (3H, s, CH_3), 2.28 (3H, s, CH_3), 7.00 (1H, s, C*H*) and 10.56 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 12.48 (s, *C*H_3), 16.20 (s, *C*H_3), 131.82 (s, *C*-5), 140.80 (s, *C*-4), 145.33 (s, *C*-6) and 162.82 (s, *C*-3).

6-Ethyl-4-methylpyridazin-3(2*H*)-one 9b[4] (0.117 g, 85%) colorless crystal, mp 78 ^oC (from Et_2O) (Found: C, 61.0; H, 7.2. $C_7H_{10}N_2O$ requires C, 60.85; H, 7.3%); ν_{max}(film)/cm^{-1} 1660, 1608 and 784; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.23 (3H, t, *J* 7.5, CH_3), 2.21 (3H, d, *J* 1.2, CH_3), 2.59 (2H, q, *J* 7.5, CH_2), 7.03 (1H, q, *J* 1.2, C*H*) and 10.56 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 15.96 (s, *C*H_3), 20.42 (s, *C*H_3), 27.78 (s, *C*H_2), 130.94 (s, *C*-5), 140.38 (s, *C*-4), 150.02 (s, *C*-6) and 162.72 (s, *C*-3).

6-Benzyl-4-methylpyridazin-3(2*H*)-one 9d[2] (0.140 g, 70%) colorless crystal, mp 130 ^oC (from Et_2O) (Found: C, 72.1; H, 5.9. $C_{12}H_{12}N_2O$ requires C, 72.0; H, 6.0%); ν_{max}(film)/cm^{-1} 1656, 1612, 1460, 1232, 1008 and 952; δ_H(250 MHz; $CDCl_3$; Me_4Si) 2.15 (3H, s, CH_3), 3.89 (2H, s, CH_2), 6.91 (1H, s, C*H*), 7.21-7.37 (5H, m, 5 x CH_{Ar}) and 11.71 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 15.26 (s, *C*H_3), 39.92 (s, *C*H_2Ph), 125.96 (s, *C*-5), 127.82 (s, 2 x *C*-Ar), 127.90 (s, 2 x *C*-Ar), 130.18 (s, *C*-Ar), 133.02 (s, *C*-Ar), 139.76 (s, *C*-4), 147.03 (s, *C*-6) and 161.71 (s, *C*-3).

4-Methyl-6-phenylpyridazin-3(2*H*)-one 9f [3] (0.163 g, 88%) yellow oil (Found: C, 71.2; H, 5.3. $C_{11}H_{10}N_2O$ requires C, 70.95; H, 5.4%); ν_{max}(film)/cm^{-1} 1648, 1576, 1532, 1260 and 1008; δ_H(250 MHz; $CDCl_3$; Me_4Si) 2.04 (3H, s, CH_3), 7.12 (1H, s, C*H*), 7.44-7.46 (3H, m, 3 x CH_{Ar}) and 7.58-7.82 (2H, m, 2 x CH_{Ar}); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 13.98 (s, CH_3), 124.97 (s, 2 x *C*-Ar), 125.06 (s, *C*-Ar), 127.99 (s, *C*-5), 128.60 (s, 2 x *C*-Ar), 130.69 (s, *C*-Ar), 133.48 (s, *C*-4), 144.65 (s, *C*-6) and 160.71 (s, *C*-3).

6-(4-Bromophenyl)-4-methylpyridazin-3(2*H*)-one 9g[5] (0.235 g, 89%) colorless oil (Found: C, 49.6; H, 3.6. $C_{11}H_9BrN_2O$ requires C, 49.8; H, 3.4%); ν_{max}(film)/cm^{-1} 1648, 1576, 1532, 1260 and 1008; δ_H(250 MHz; $CDCl_3$; Me_4Si) 2.30 (3H, s, CH_3), 7.56-7.67 (5H, m, C*H*, 4 x CH_{Ar}) and 10.60 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 16.61 (s, *C*H_3), 123.79 (s, *C*-Ar), 127.52 (s, 2 x *C*-Ar), 128.41 (s, *C*-5), 132.01 (s, 2 x *C*-Ar), 133.81 (s, *C*-4), 144.40 (s, *C*-6), 140.91 (s, *C*-Ar) and 162.78 (s, *C*-3).

6-(4-Methoxyphenyl)-4-methylpyridazin-3(2*H*)-one 9h[2, 5] (0.129 g, 60%) dark orange oil (Found: C, 66.4; H, 5.8. $C_{12}H_{12}N_2O_2$ requires C, 66.65; H, 5.6%); ν_{max}(film)/cm^{-1} 1660, 1608,

1512, 1252, 1176 and 1000; δ_H(250 MHz; $CDCl_3$; Me_4Si) 2.30 (3H, s, CH_3), 3.86 (3H, s CH_3O), 6.96-6.99 (2H, m, 2 x CH_{Ar}), 7.56 (1H, s, C*H*) and 7.69-7.73 (2H, m, 2 x CH_{Ar}); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 13.10 (s, *C*H_3), 54.38 (s, O*C*H_3), 113.30 (s, 2 x *C*-Ar), 124.50 (s, *C*-Ar), 126.34 (s, 2 x *C*-Ar), 127.72 (s, C-4), 139.83 (s, *C*-Ar), 144.50 (s, *C*-5), 159.70 (s, *C*-6) and 160.78 (s, *C*-3).

6-Ethyl-4-methyl-2-phenylpyridazin-3(2*H*)-one 9i[6] (0.104 g, 49%) orange oil (Found: C, 72.7; H, 6.5. $C_{13}H_{14}N_2O$ requires C, 72.8; H, 6.6%); ν_{max}(film)/cm^{-1} 1660, 1620, 1456 and 1288; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.23 (3H, t, *J* 7.5 CH_3CH_2), 2.24 (3H, s, CH_3), 2.62 (2H, t, *J* 7.5 CH_3CH_2), 7.04 (1H, s, C*H*) 7.32-7.50 (3H, m, 3 x CH_{Ar}) and 7.56-7.65 (2H, m, 2 x CH_{Ar}); δ_C (62.9 MHz; $CDCl_3$; Me_4Si) 11.69 (s, *C*H_3CH$_2$), 15.96 (s, *C*H_3), 27.16 (s, CH$_3$*C*H$_2$), 124.54 (s, 2 x *C*-Ar), 126.76 (s, *C*-5), 127.61 (s, 2 x *C*-Ar), 128.53 (s, *C*-Ar), 140.67 (s, *C*-4), 141.09 (s, *C*-Ar), 148.18 (s, *C*-6) and 159.67 (s, *C*-3).

2,6-Diphenyl-4-methylpyridazin-3(2*H*)-one 9j[7] (0.175 g, 67%) orange crystal mp 184 ^oC (from Et_2O) (Found: C, 77.6; H, 5.7. $C_{17}H_{14}N_2O$ requires C, 77.8; H, 5.4%); ν_{max}(film)/cm^{-1} 1652, 1616, 1592, 1200 and 1008; δ_H(250 MHz; $CDCl_3$; Me_4Si) 2.37 (3H, s, CH_3), 7.34-7.58 (6H, m, 6 x CH_{Ar}), 7.64-7.74 (4H, m, 4 x CH_{Ar}) and 7.86 (1H, s, C*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 16.34 (s, *C*H_3), 124.57 (s, 2 x *C*-Ar), 125.07 (s, 2 x *C*-Ar), 126.48 (s, *C*-5), 126.92 (s, *C*-Ar), 127.59 (s, 2 x *C*-Ar), 127.83 (s, 2 x *C*-Ar), 128.33 (s, *C*-Ar), 134.02 (s, *C*-Ar), 140.56 (s, *C*-4), 141.10 (s, *C*-Ar), 143.48 (s, *C*-6) and 159.59 (s, *C*-3).

6-(4-Bromophenyl)-4-methyl-2-phenylpyridazin-3(2*H*)-one 9k (0.170 g, 50%) orange crystal mp 147 ^oC (from Et_2O) (Found: C, 60.0; H, 3.65. $C_{17}H_{13}BrN_2O$ requires C, 59.8; H, 3.8%); ν_{max}(film)/cm^{-1} 1652, 1524 and 1344; δ_H(250 MHz; $CDCl_3$; Me_4Si) 2.35 (3H, d, *J* 1.2 CH_3), 7.35-7.62 (6H, m, C*H*, 5 x CH_{Ar}) and 7.64-7.75 (4H, m, 4 x CH_{Ar}); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 17.41 (s, *C*H_3), 123.81 (s, *C*-Ar), 125.55 (s, 2 x *C*-Ar), 127.02 (s, *C*-Ar), 127.59 (s, 2 x *C*-Ar), 128.09 (s, *C*-5), 128.67 (s, 2 x *C*-Ar), 132.03 (s, 2 x *C*-Ar), 133.91 (s, *C*-4), 141.87 (s, *C*-Ar), 141.92 (s, *C*-Ar), 143.41 (s, *C*-6) and 160.50 (s, *C*-3).

4-Isobutyl-6-pentylpyridazin-3(2*H*)-one 10b (0.133 g, 60%) colorless oil (Found: C, 70.3; H, 9.8. $C_{13}H_{22}N_2O$ requires C, 70.2; H, 10.0%); ν_{max}(film)/cm^{-1} 1656, 1608 and 1464; δ_H(250 MHz; $CDCl_3$; Me_4Si) 0.81-1.05 (9H, m, 3 x CH_3), 1.25-1.40 (2H, m, CH_2), 1.55-1.68 (6H, m, 3 x CH_2), 2.31-2.60 (3H, m, CH_2, C*H*), 7.23 (1H, s, C*H*) and 11.46 (1H, s, N*H*); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 13.86 (s, *C*H_3), 22.35 (s, 2 x *C*H_3), 26.53 (s, *C*H(CH$_3$)$_2$), 28.19 (s, *C*H$_2$), 31.16 (s, *C*H$_2$), 31.49 (s, *C*H$_2$), 34.49 (s, *C*H$_2$), 38.84 (s, *C*H$_2$), 130.95 (s, *C*-5), 142.88 (s, *C*-4), 149.10 (s, *C*-6) and 162.75 (s, *C*-3).

4-Benzyl-2,6-diphenylpyridazin-3(2*H*)-one 10c (0.253 g, 75%) yellow crystal mp 118 ^{o}C (from Et_2O) (Found: C, 81.7; H, 5.6. $C_{23}H_{18}N_2O$ requires C, 81.6; H, 5.4%); ν_{max}(film)/cm^{-1} 1660, 1616 and 1280; δ_H(250 MHz; $CDCl_3$; Me_4Si) 4.27 (2H, d, *J* 1.2, CH_2), 7.55-7.76 (12H, m, 11 x CH_{Ar}, C*H*), 7.90-8.10 (4H, m, 4 x CH_{Ar}); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 36.39 (s, *C*H_2Ph) 125.47 (s, 2 x *C*-Ar), 125.64 (s, 2 x *C*-Ar), 126.81 (s, 2 x *C*-Ar), 127.86 (s, *C*-5), 128.50 (s, 2 x *C*-Ar), 128.82 (s, 4 x *C*-Ar), 128.99 (s, *C*-Ar), 129.22 (s, *C*-Ar), 129.40 (s, *C*-Ar), 129.55 (s, *C*-Ar), 134.86 (s, *C*-Ar) 137.14 (s, *C*-4), 141.94 (s, *C*-Ar), 144.46 (s, *C*-6) and 159.85 (s, *C*-3).

2,6-Diphenyl-4-isobutylpyridazin-3(2*H*)-one 10d (0.231 g, 76%) orange crystal mp 62 ^{o}C (from Et_2O) (Found: C, 79.1; H, 6.4. $C_{20}H_{20}N_2O$ requires C, 78.9; H, 6.6%); ν_{max}(film)/cm^{-1} 1660, 1616, 1492, 1440, 1296 and 1196; δ_H(250 MHz; $CDCl_3$; Me_4Si) 1.00 (6H, d, *J* 7.0, (CH_3)$_2$CH), 2.05-2.30 (1H, m, (CH_3)$_2$C*H*), 2.58 (2H, d, *J* 7.0, CH_2), 7.34-7.55 (6H, m, 5 x CH_{Ar}, C*H*), 7.67-7.74 (3H, m, 3 x CH_{Ar}) and 7.82-7.86 (2H, m, 2 x CH_{Ar}); δ_C(62.9 MHz; $CDCl_3$; Me_4Si) 22.55 (s, 2 x *C*H_3), 26.88 (s, (CH_3)$_2$*C*H), 40.02 (s, (CH_3)$_2$CH*C*H_2) 125.55 (s, 2 x *C*-Ar), 126.06 (s, 2 x *C*-Ar), 127.30 (s, *C*-5), 127.84 (s, *C*-Ar), 128.51 (s, 2 x *C*-Ar), 128.81 (s, 2 x *C*-Ar), 129.30 (s, *C*-Ar), 135.10 (s, *C*-Ar), 142.10 (s, *C*-4), 144.23 (s, *C*-Ar), 144.41 (s, *C*-6) and 160.30 (s, *C*-3).

References for supporting information:

(1) S.Touil and H. Zantour, *Phosphorus, Sulfur Silicon Relat. Elem.* 1998, **134**, 493

(2) C-G. Wermuth, G. Schlewer, J-J. Bourguignon, G. Maghiros, M-J. Bouchet, C. Moire, J-P. Kan, P. Worms and K. Biziere, K. *J. Med. Chem.* 1989, **32**, 528.

(3) W. Hu, H.R. Ranaivo, S.M. Roy, H.A. Behanna, L.K. Wing, L. Munoz, L. Guo, L.J. Van Eldik and D.M. Watterson, *Bioorg.Med.Chem. Lett* 2007, **17**, 414

(4) P.G. Baraldi, A. Bigoni, B. Cacciari, C. Caldari, S. Manfredini and G. Spalluto, *Synthesis*, 1994, 1158.

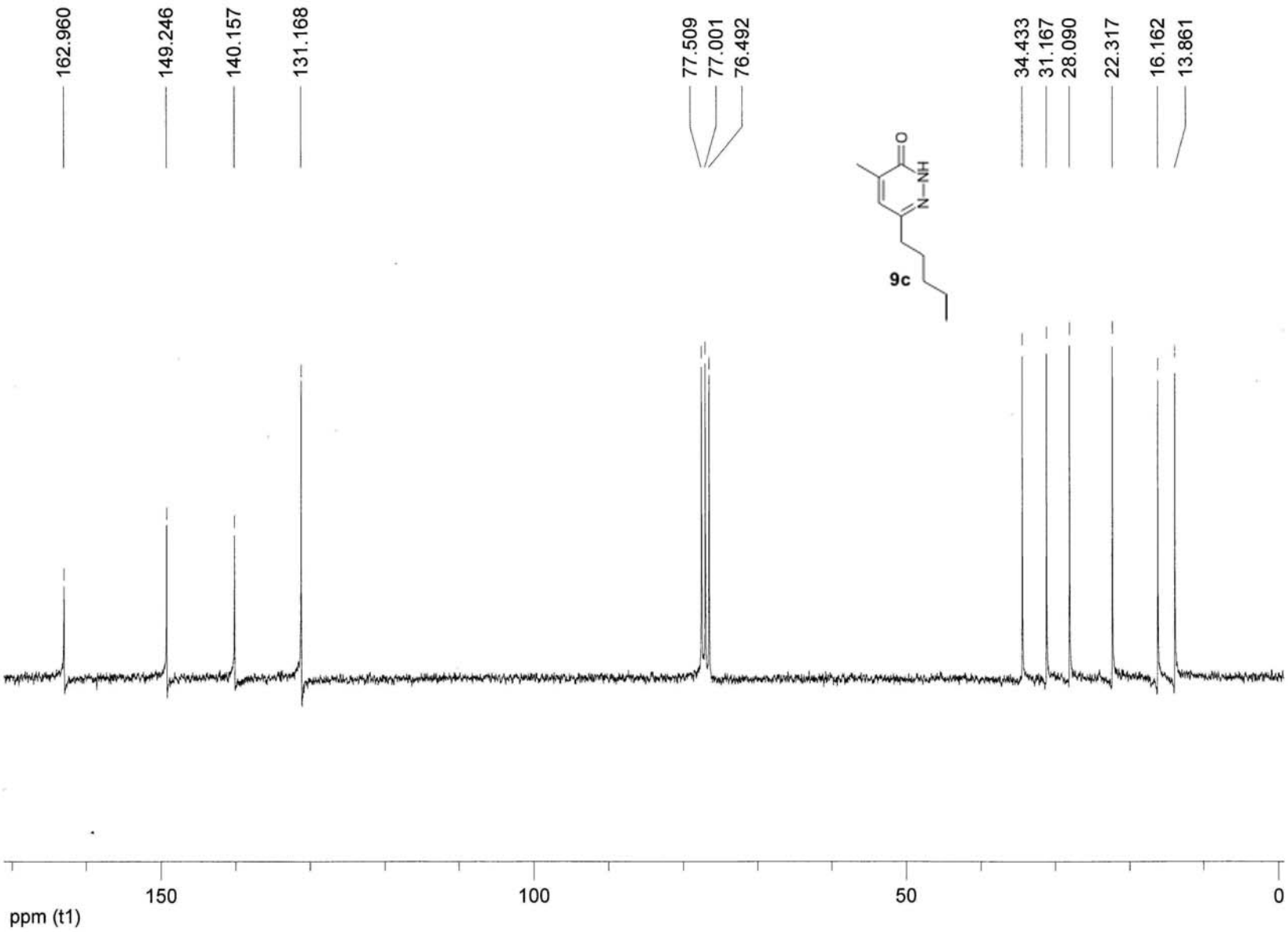
(5) A.A. Siddiqui and S.M. Wani, *Indian. J. Chem. Sect. B*, 2004, **43B**, 1574.

(6) Hoffman-La Roche *US Pat*. US 2783232, 1955

(7) G. Leclerc, C-G. Wermuth, *C.R. Hebd. Seances Acad. Sci. Ser. C*, 1968, **267**, 1242

^{13}C, ^{1}H NMR spectra of **9c**, **9e**, **9k**, **9l**, **10a**, **10b**, **10c** and **10d**.

Graphic data.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140.157
131.168
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77.001
76.492
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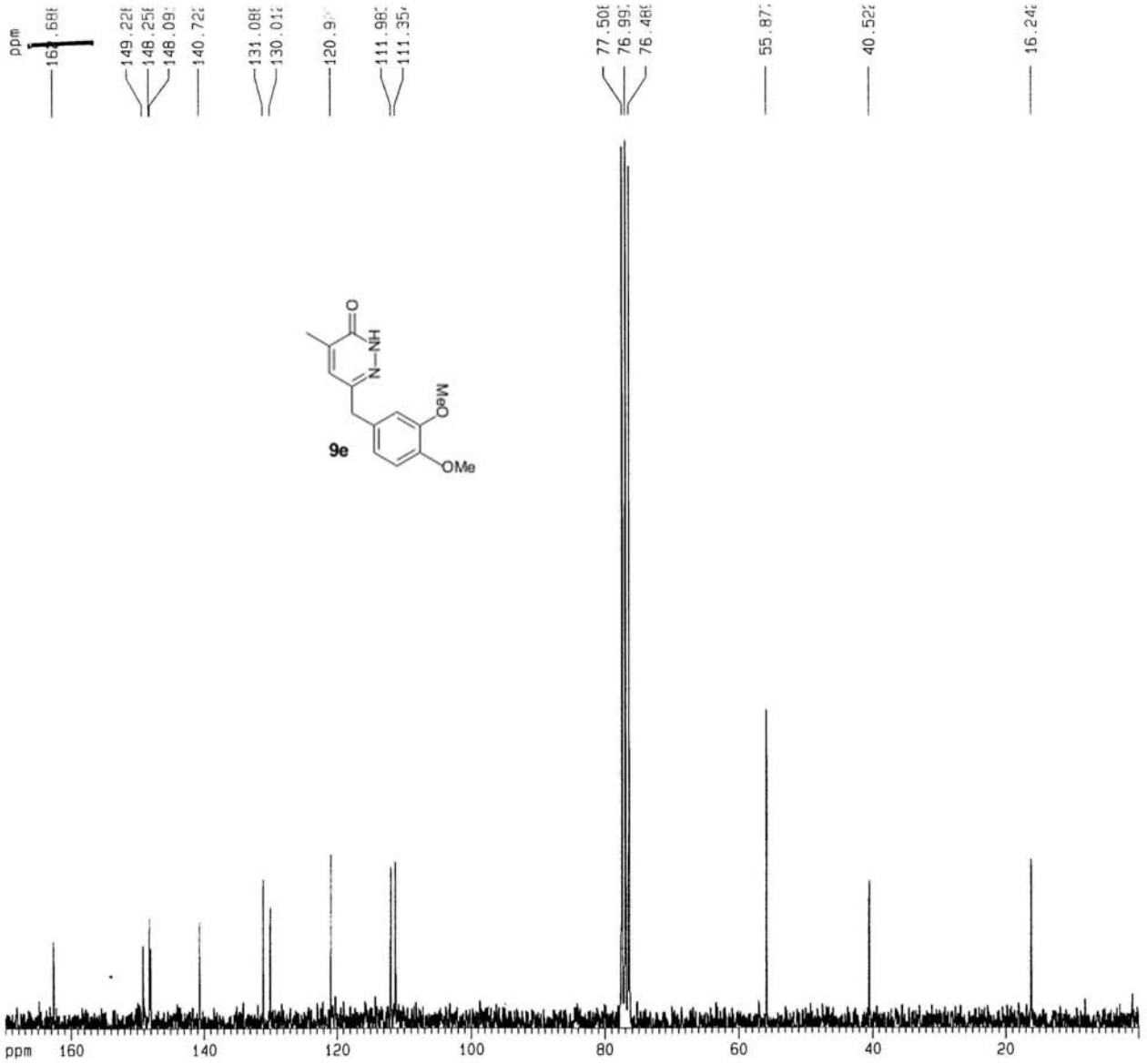
31.167
28.090
22.317
16.162
13.861
O
HN–N
9c
150
100
50
0
ppm (t1)

1.296
1.310
1.324
1.338
1.353
1.376
1.597
1.603
1.624
1.645
1.650
1.655
2.172
2.199
2.204
2.503
2.535
2.565
HN–N
O
9c
3.84
5.66
3.53
3.22
2.14
7.008
7.013
7.263
1.00
10.691
10.697
10.700
10.703
10.706
10.713
0.68
5.0
10.0
ppm (t1)



A. ALBRECHT

Current Data Parameters

NAME	AA-38-A
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

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PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	800
DS	4
SWH	19960.080 Hz
FIDRES	0.609133 Hz
AQ	0.8208884 sec
RG	11585.2
DW	25.050 usec
DE	30.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

******** CHANNEL f1 ********

NUC1	13C
P1	15.60 usec
PL1	-6.00 dB
SFO1	62.9025098 MHz

******** CHANNEL f2 ********

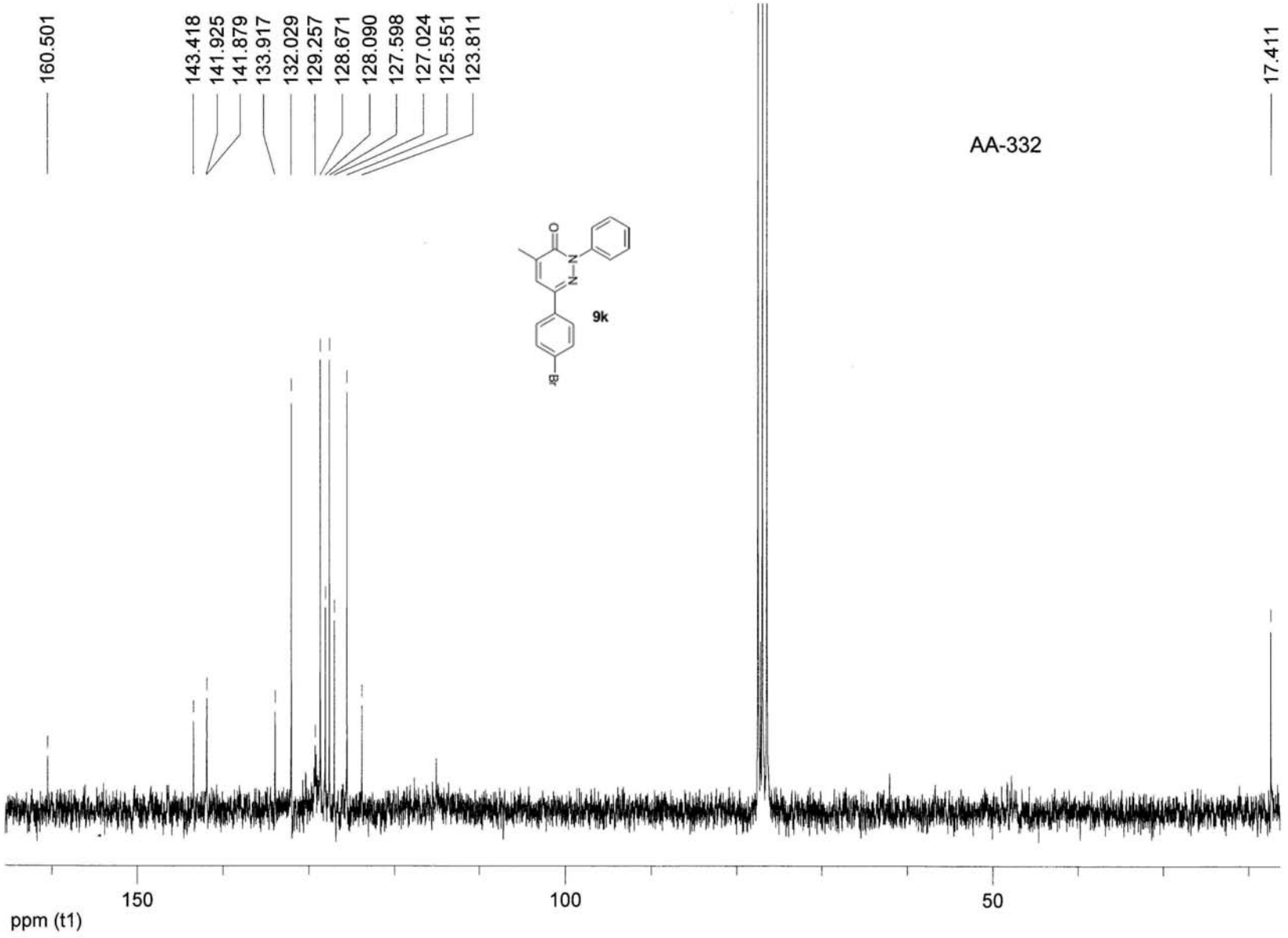
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-4.00 dB
PL12	16.09 dB
PL13	18.00 dB
SFO2	250.1310005 MHz

F2 - Processing parameters

SI	65536
SF	62.8952423 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	21.50 cm
CY	16.50 cm
F1P	170.000 ppm
F1	10692.19 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	7.90698 ppm/cm
HZCM	497.31119 Hz/cm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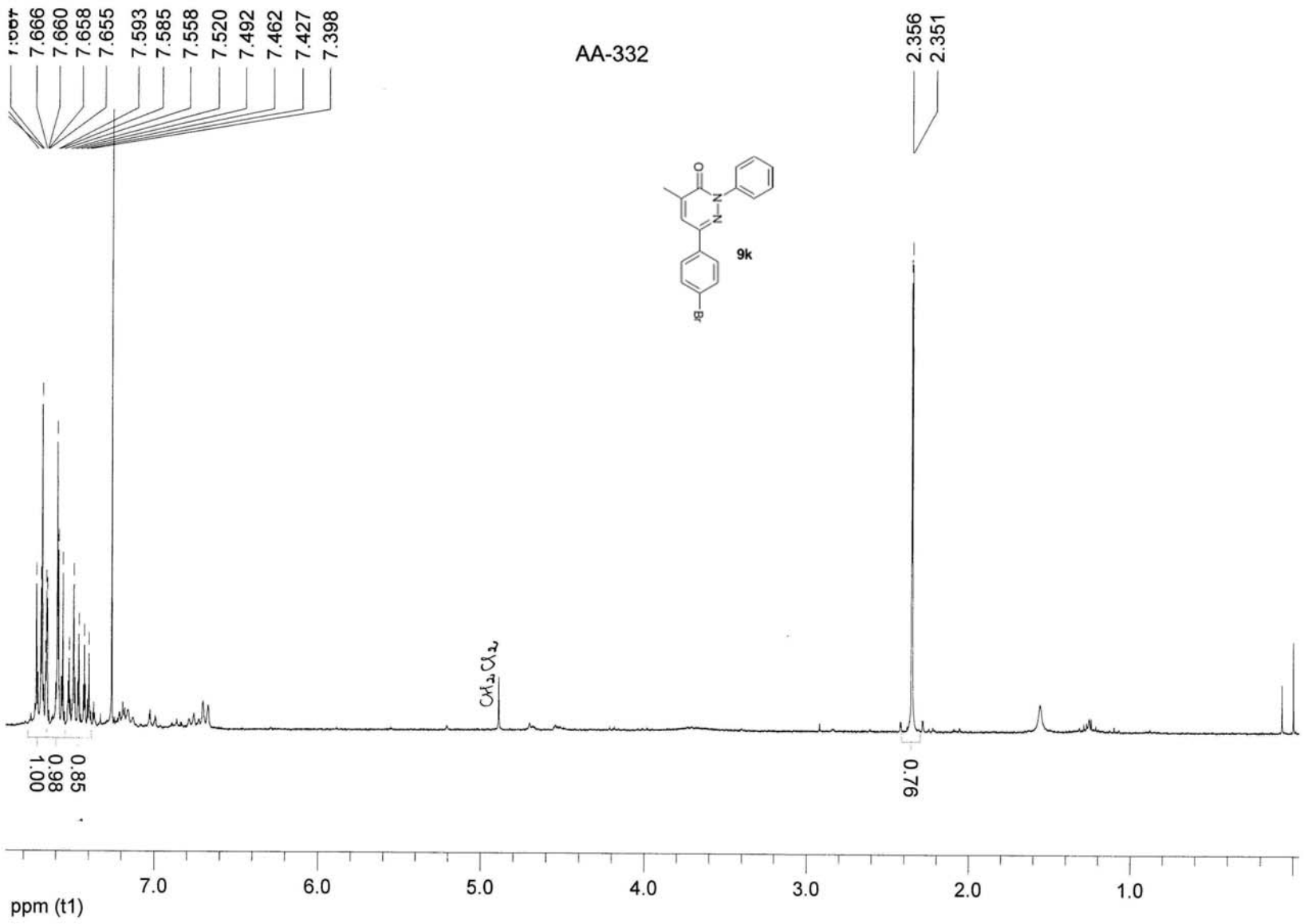
143.418
141.925
141.879
133.917
132.029
129.257
128.671
128.090
127.598
127.024
125.551
123.811
17.411
AA-332
9k
Br
150
100
50
ppm (t1)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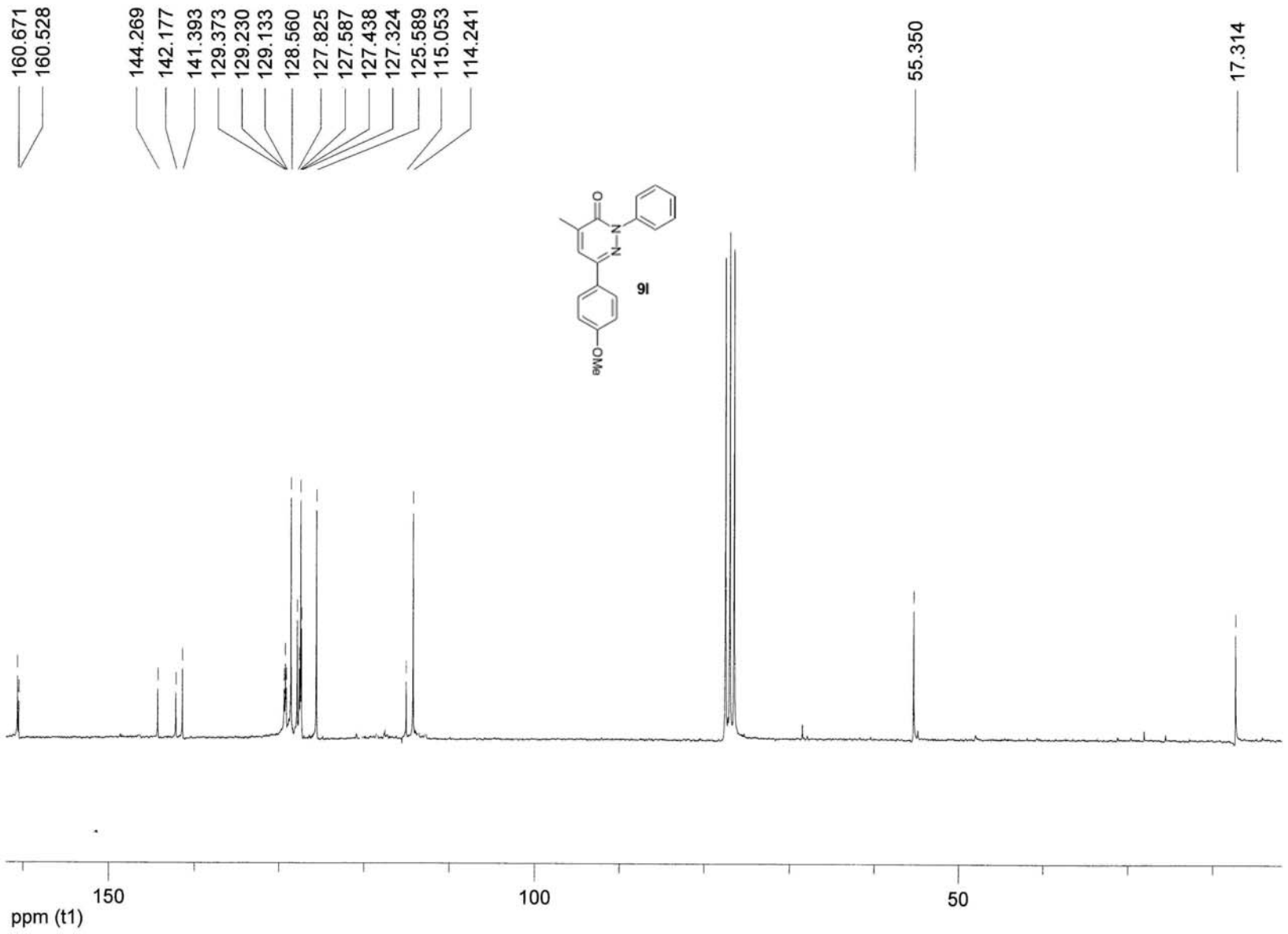
7.658
7.655
7.593
7.585
7.558
7.520
7.492
7.462
7.427
7.398
2.356
2.351
9k
CH2Cl2
1.00
0.98
0.85
0.76
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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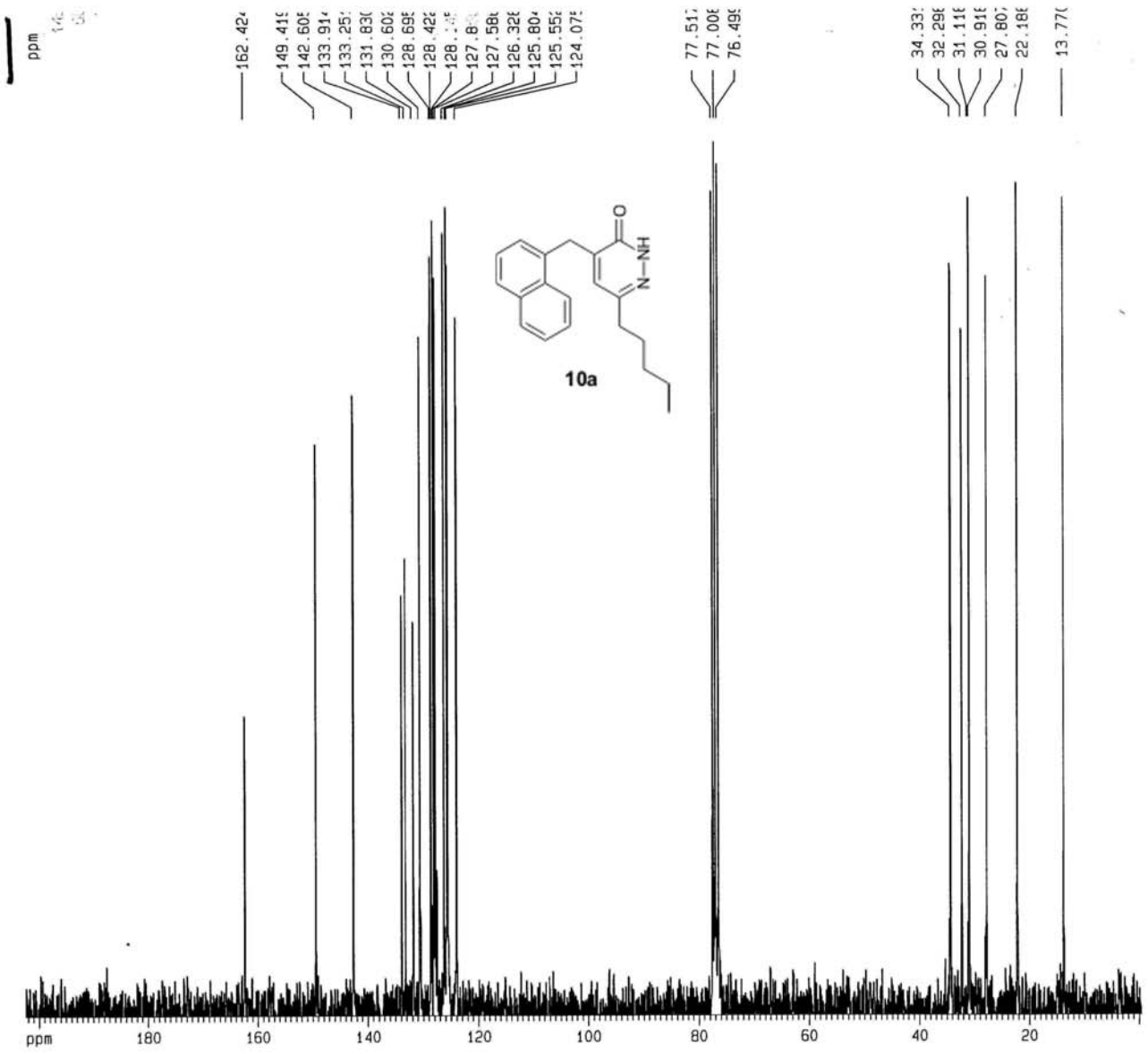
141.393
129.373
129.230
129.133
128.560
127.825
127.587
127.438
127.324
125.589
115.053
114.241
55.350
17.314
OMe
9l
150
100
50
ppm (t1)

AA-335B
1.493
2.191
2.361
2.366
3.869
4.910
6.715
6.972
6.981
6.999
7.008
7.017
7.021
7.052
7.057
7.180
7.209
7.217
7.237
7.243
7.278
7.407
7.430
7.436
7.441
7.479
7.485
7.503
7.510
7.513
7.538
7.543
7.595
7.600
7.605
7.715
7.718
7.723
7.738
0.16
0.68
0.94
1.34
0.71
1.12
1.00
2.0
3.0
4.0
5.0
6.0
7.0
ppm (t1)
OMe



A.Albrecht

Current Data Parameters

NAME	AA-40-C
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20050128
Time	11.57
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	141
DS	4
SWH	19960.080 Hz
FIDRES	0.609133 Hz
AQ	0.8208884 sec
RG	4000
DW	25.050 usec
DE	30.00 usec
TE	299.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	7.00 usec
PL1	-6.00 dB
SFO1	62.9025098 MHz

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

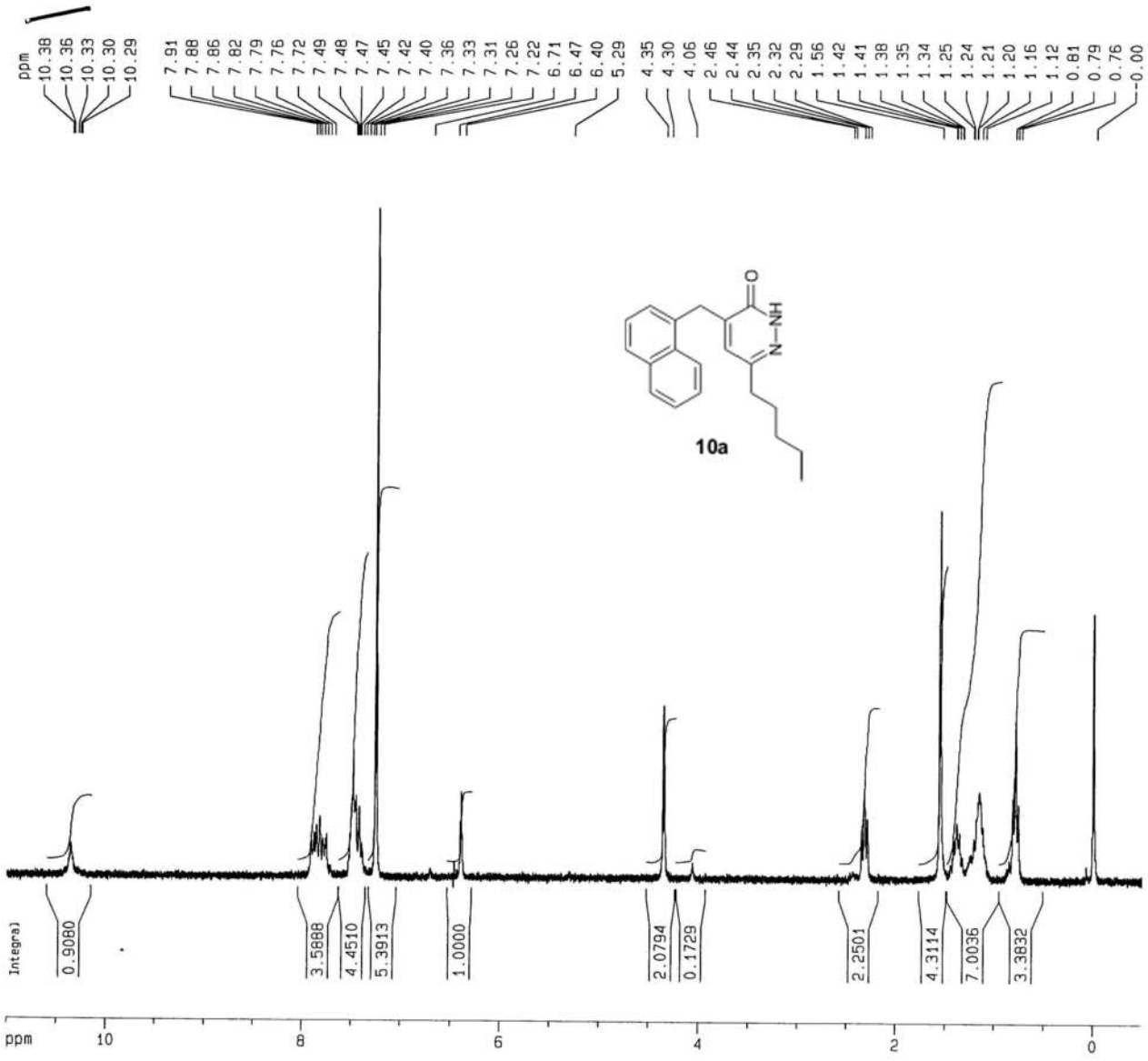
CPDPRG2	waltz16
NUC2	1H
PCPD2	120.00 usec
PL2	-6.00 dB
PL12	16.00 dB
PL13	16.00 dB
SFO2	250.1310005 MHz

F2 - Processing parameters

SI	65536
SF	62.8952465 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	21.50 cm
CY	16.50 cm
F1P	202.431 ppm
F1	12731.94 Hz
F2P	-0.449 ppm
F2	-28.26 Hz
PPMCM	9.43629 ppm/cm
HZCM	593.49750 Hz/cm



A.ALBRECHT

Current Data Parameters

NAME	AA-40C
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

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Time	16.38
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PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	4
SWH	3742.515 Hz
FIDRES	0.114212 Hz
AQ	4.3778548 sec
RG	2048
DW	133.600 usec
DE	15.00 usec
TE	297.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

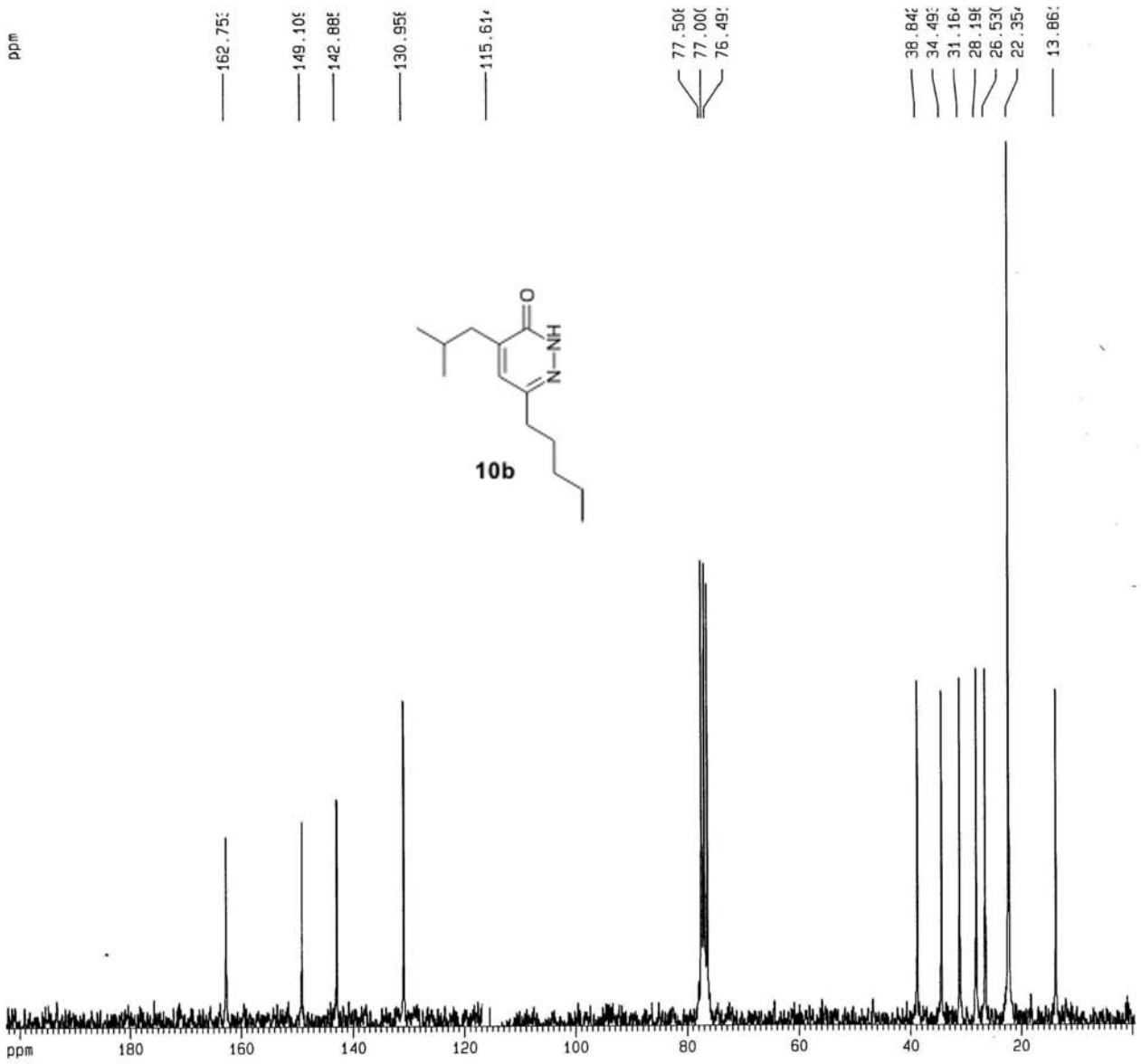
NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	250.1316258 MHz

F2 - Processing parameters

SI	32768
SF	250.1300083 MHz
WDW	EM
SSB	0
LB	0.05 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	21.50 cm
CY	12.50 cm
F1P	11.000 ppm
F1	2751.43 Hz
F2P	-0.500 ppm
F2	-125.06 Hz
PPMCM	0.53488 ppm/cm
HZCM	133.79047 Hz/cm



A.ALBRECHT

Current Data Parameters

NAME	AA-47-A1
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20050128
Time	11.48
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	185
DS	4
SWH	19960.080 Hz
FIDRES	0.609133 Hz
AQ	0.8208884 sec
RG	7298.2
DW	25.050 usec
DE	30.00 usec
TE	299.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	7.00 usec
PL1	-6.00 dB
SFO1	62.9025098 MHz

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

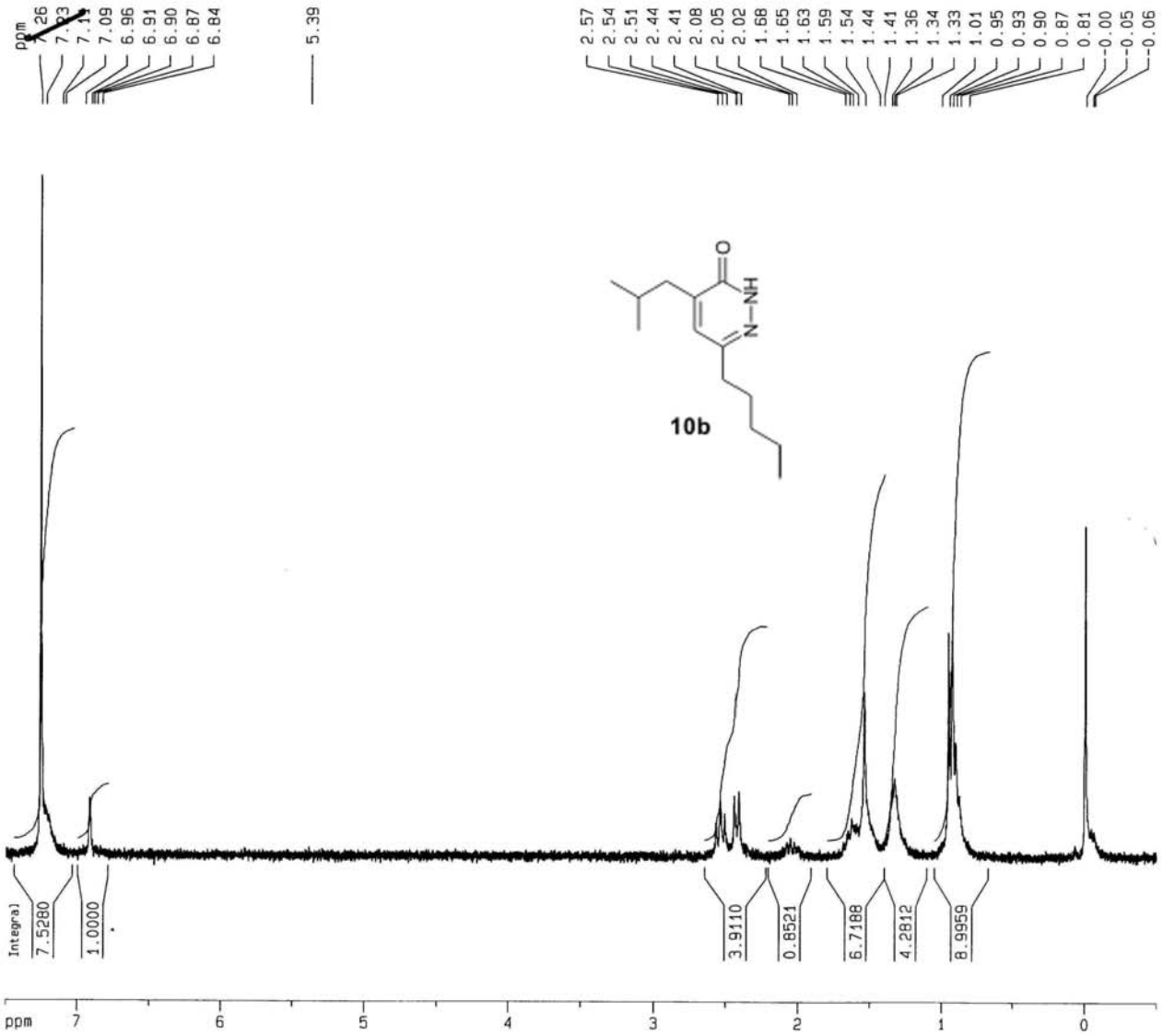
CPDPRG2	waltz16
NUC2	1H
PCPD2	120.00 usec
PL2	-6.00 dB
PL12	16.00 dB
PL13	16.00 dB
SFO2	250.1310005 MHz

F2 - Processing parameters

SI	65536
SF	62.8952432 MHz
WDW	EM
SSB	0
LB	4.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	21.50 cm
CY	16.50 cm
F1P	202.431 ppm
F1	12731.94 Hz
F2P	-0.449 ppm
F2	-28.26 Hz
PPMCM	9.43629 ppm/cm
HZCM	593.49744 Hz/cm



A. ALBRECHT

Current Data Parameters

NAME	AA-47-A1
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

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Time	14.47
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PROBHD	5 mm QNP 1H/1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	4
SWH	3742.515 Hz
FIDRES	0.114212 Hz
AQ	4.3778548 sec
RG	2896.3
DW	133.600 usec
DE	15.00 usec
TE	298.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

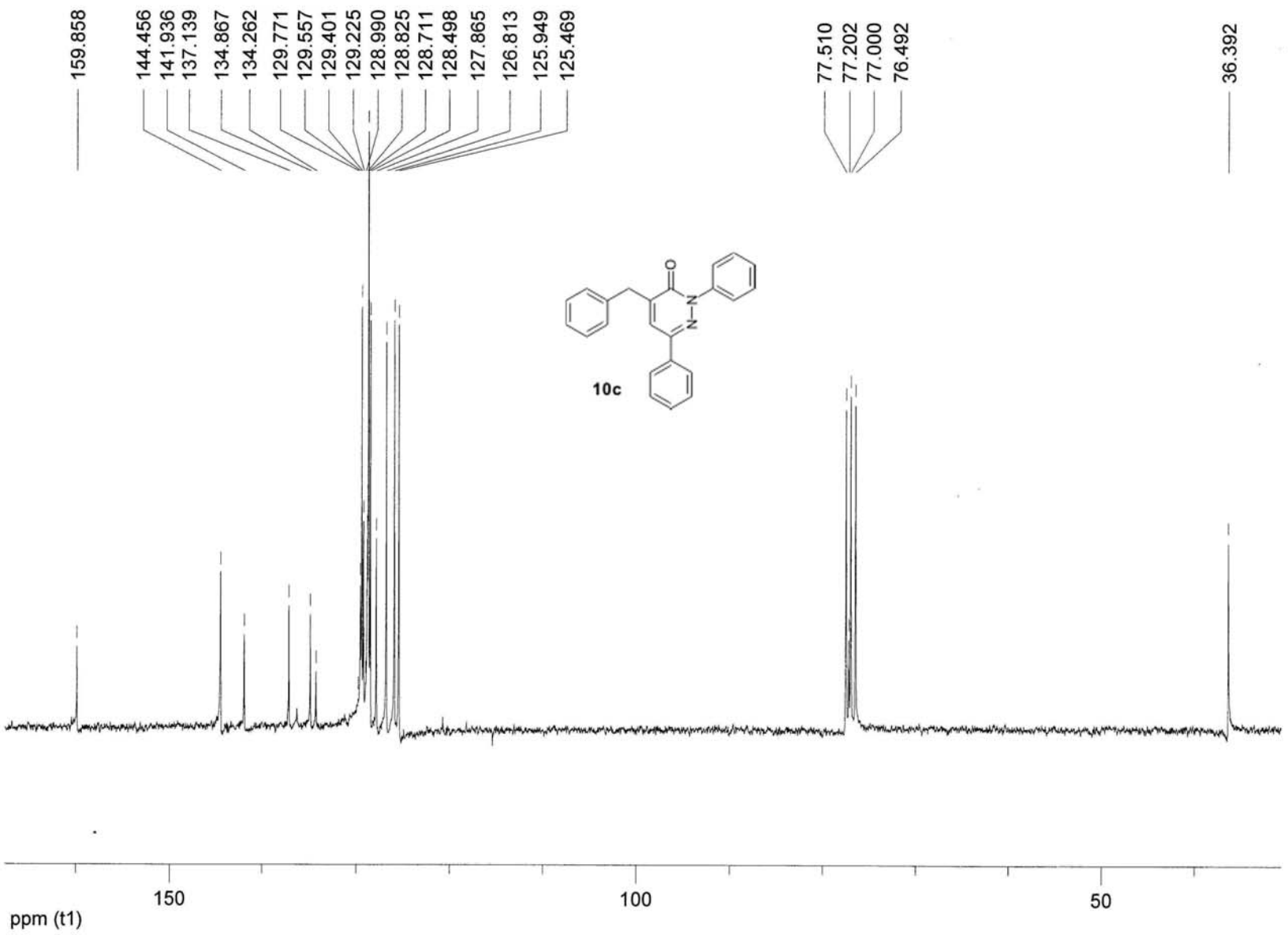
NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	250.1316258 MHz

F2 - Processing parameters

SI	32768
SF	250.1300084 MHz
WDW	EM
SSB	0
LB	0.05 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	21.50 cm
CY	12.50 cm
F1P	7.500 ppm
F1	1875.98 Hz
F2P	-0.500 ppm
F2	-125.07 Hz
PPMCM	0.37209 ppm/cm
HZCM	93.07163 Hz/cm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128.498
127.865
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10c
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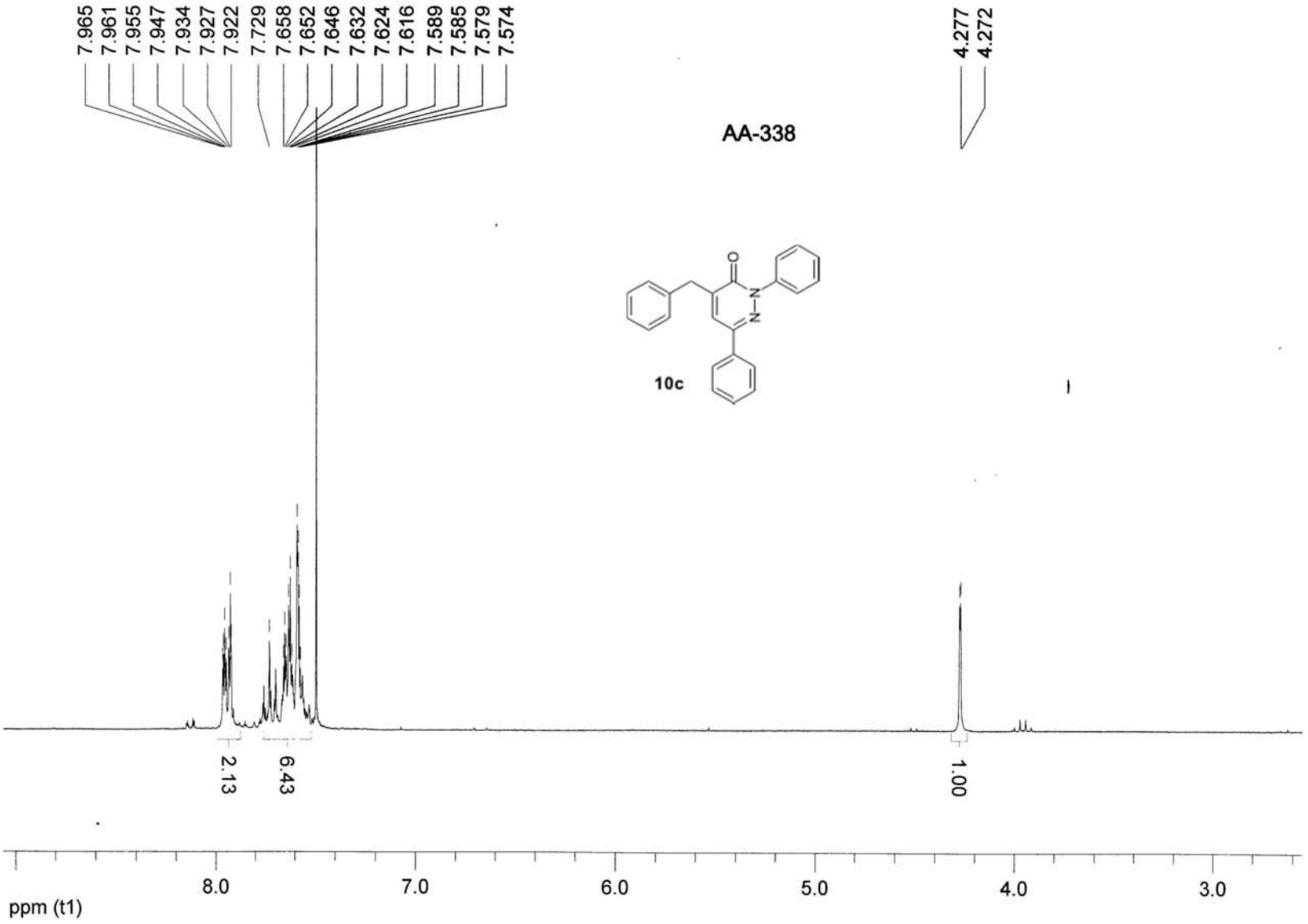
50
ppm (t1)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7.632
7.624
7.616
7.589
7.585
7.579
7.574
4.277
4.272
AA-338
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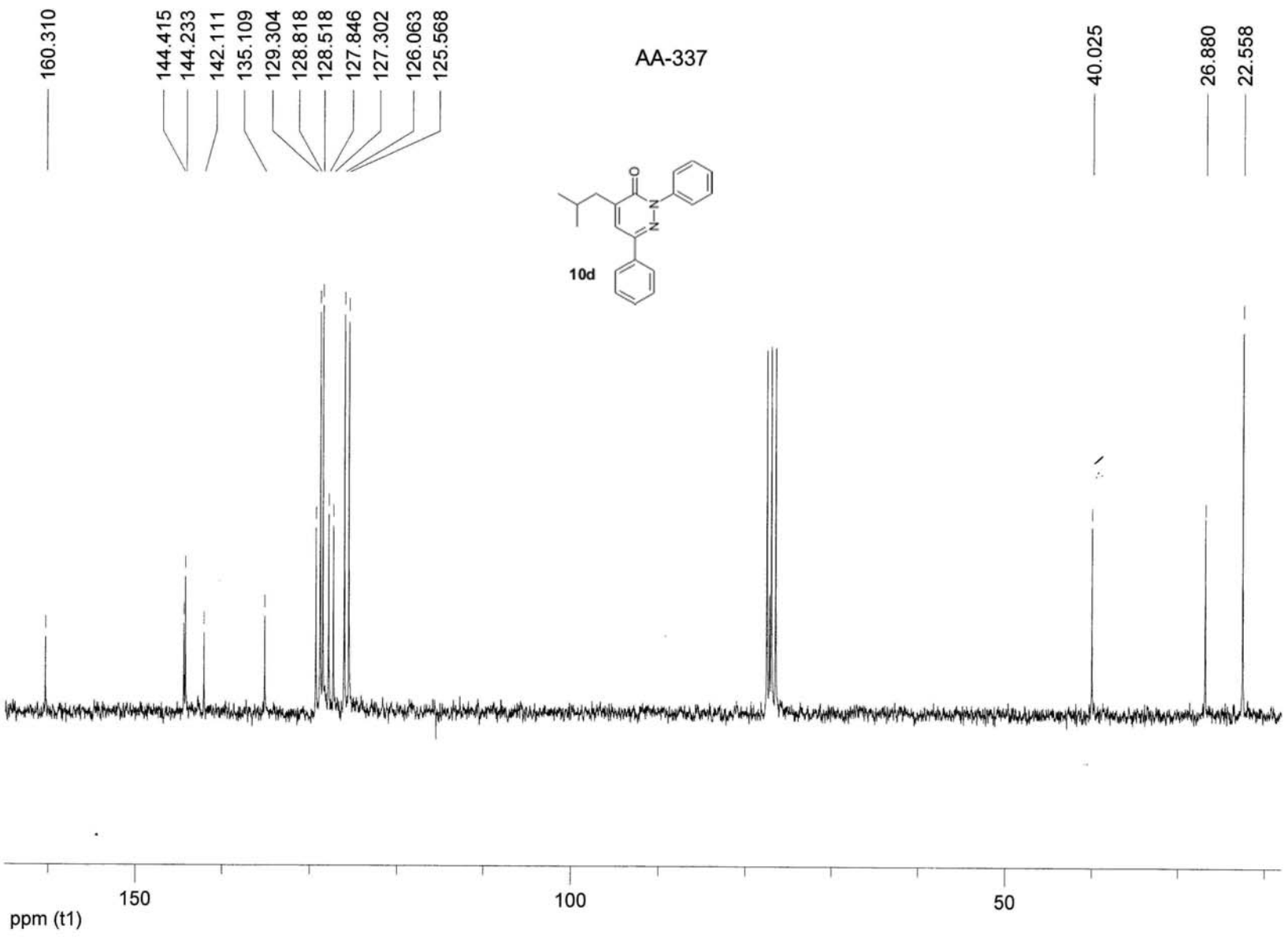
ppm (t1)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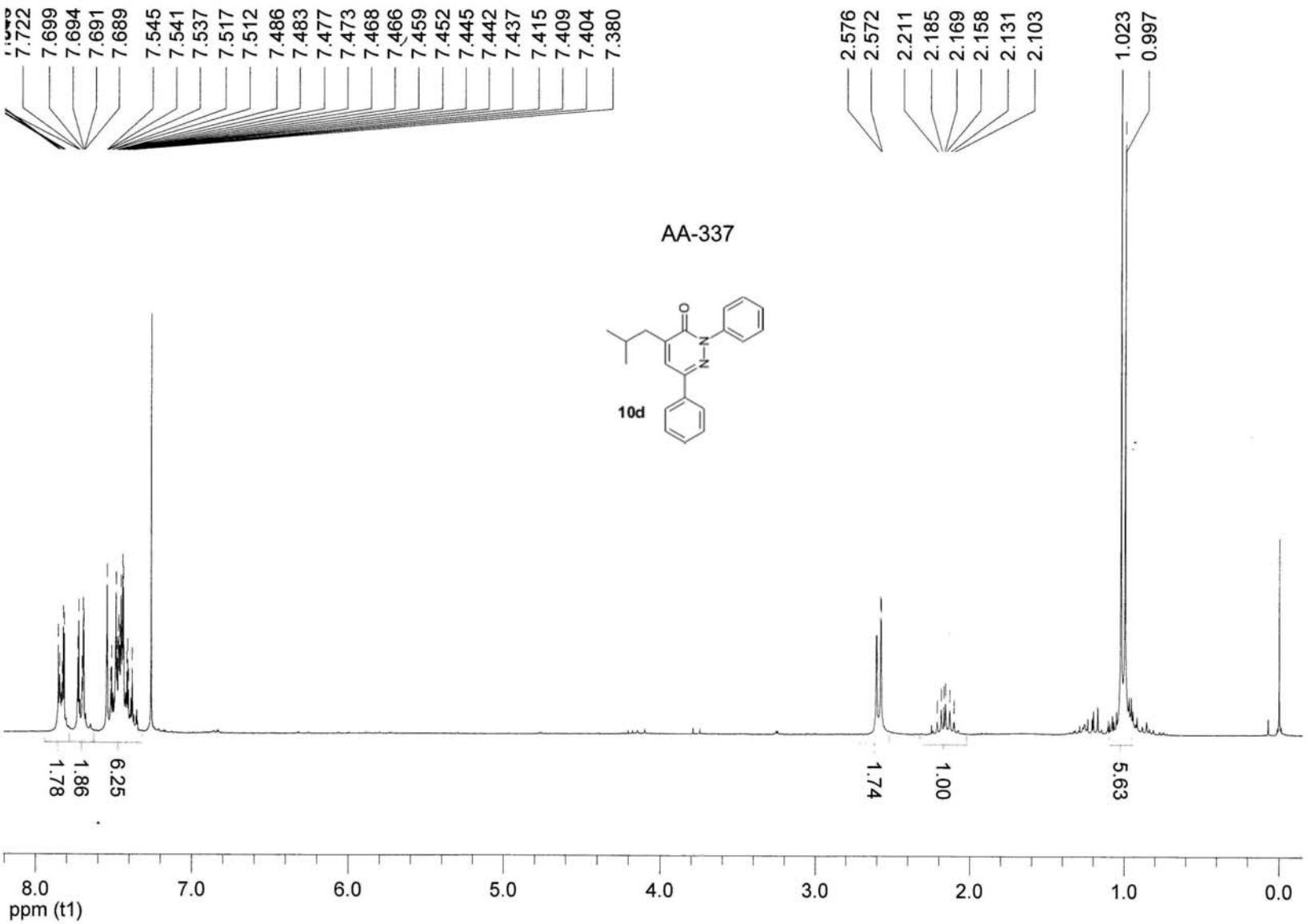
10d
150
100
50
ppm (t1)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7.483
7.477
7.473
7.468
7.466
7.459
7.452
7.445
7.442
7.437
7.415
7.409
7.404
7.380
2.576
2.572
2.211
2.185
2.169
2.158
2.131
2.103
1.023
0.997
AA-337
10d
1.78
1.86
6.25
1.74
1.00
5.63
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)