Supporting Information:

CH-01 is a hypoxia-activated prodrug that sensitizes cells to hypoxia/reoxygenation through inhibition of Chk1 and Aurora A

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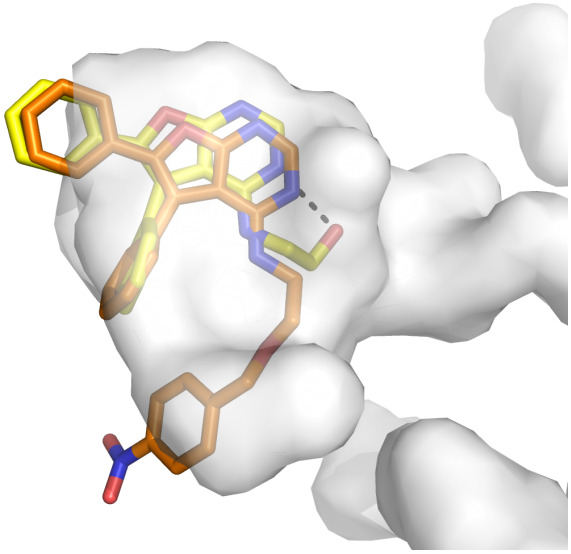


Figure S1. A representative image of compound **1** (carbon = orange) docked to the X-ray crystal structure of compound **6** (carbon = yellow) bound to Chk1 (PDB ID, 2BRB). The surface of the binding site is shown. Docking indicated that the binding of the 4-nitrobenzyl derivative **1** to Chk1 was less favorable than binding of **6**.

A **B**

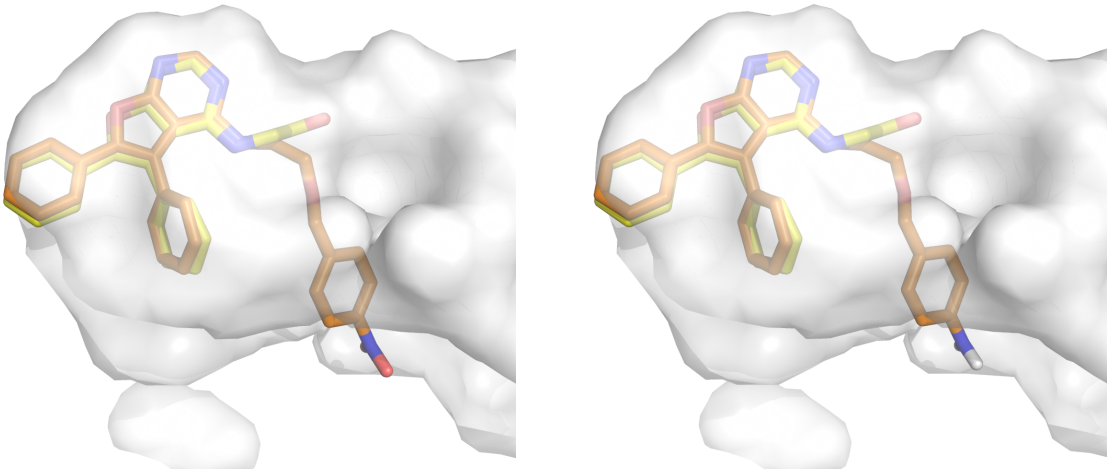
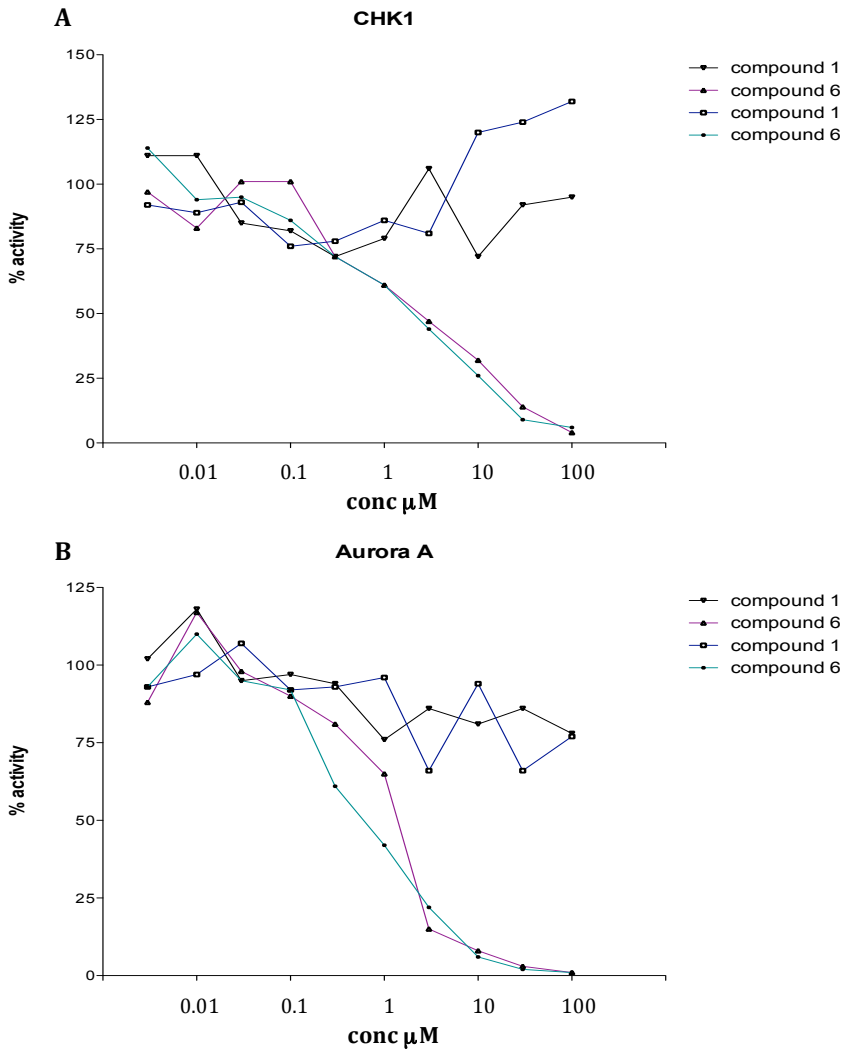


Figure S2. (A). A representative image of compound **1** (carbon = orange) docked to the X-ray crystal structure of compound **6** (carbon = yellow) bound to Aurora A (PDB ID, 3K5U). Docking indicated that the 4-nitrobenzyl group of **1** can potentially be accommodated in the ATP-binding site. (B). A representative image of amine **5** (carbon = orange) docked to the X-ray crystal structure of compound **6** (carbon = yellow) bound to Aurora A (PDB ID, 3K5U). Docking indicated that the 4-aminobenzyl group of **5** can potentially be accommodated in the ATP-binding site. The surface of the binding site is shown.



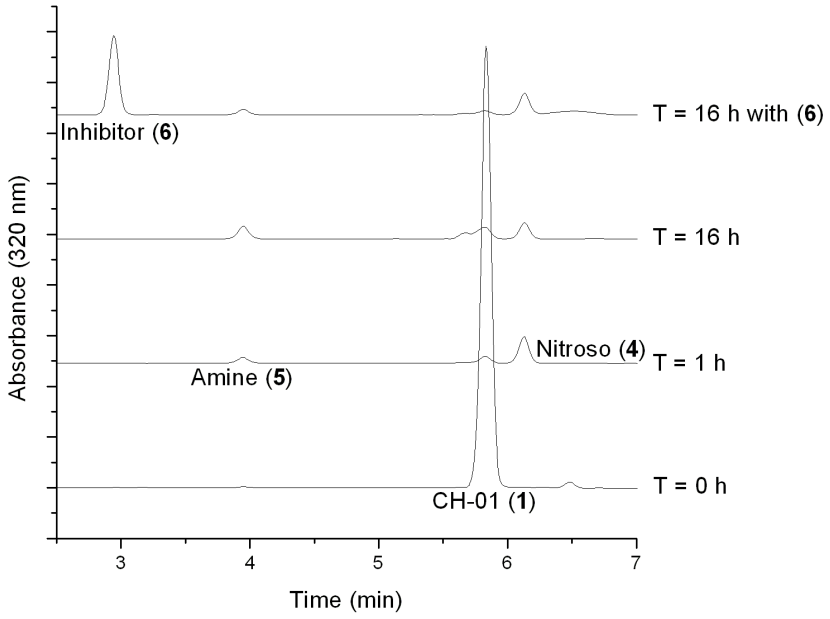
C

mean IC50 (uM)

	compound 1	compound 6
CHK1	no inhibition	1.75
Aurora A	no inhibition	0.81

Figure S3. The IC_{50} values of compounds **1** and **6** were obtained for Chk1 and Aurora kinase A using a radioactive (^{33}P-ATP) filter-binding assay. (A) Compound **1** shows no inhibition of Chk1 whereas compound **6** has an IC_{50} value of 1.75 μ M. (B) Compound **1** shows no inhibition of Aurora kinase A whereas compound **6** has an IC_{50} value of 0.81 μ M. This analysis was carried out by The International Centre for Kinase profiling, University of Dundee (http://www.kinase-screen.mrc.ac.uk/). (C) Mean IC_{50} values.

A



B

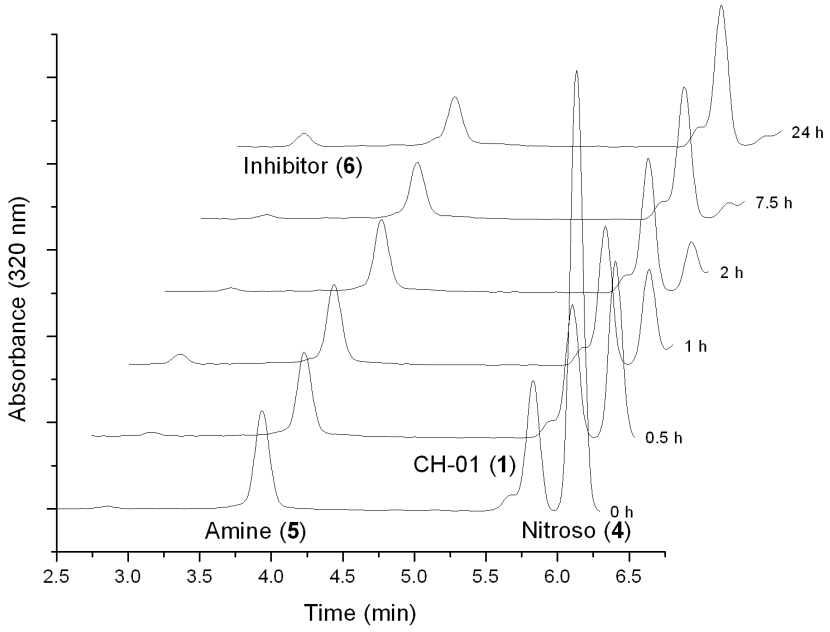


Figure S4. (A) Reduction of **1** using zinc powder and 10% ammonium chloride in DMF was monitored at 0, 1 and 16 h. The new peaks were identified as the corresponding amine and nitroso reduction products. An injection that contained the active inhibitor **6** as an internal control showed that none of the peaks correlated to **6**, confirming that release of **6** was not observed under these conditions. (B) The T = 1 h aliquot from the zinc reduction was injected into potassium phosphate buffer pH 7.4 and incubated at 37 °C. HPLC analysis of the formed precipitate reveals loss of the nitroso **4** and amine **5**.

Docking with AutoDock Vina (version 1.1.2):

Preparation of the receptors:

The receptors (PDB IDs: 2BRB and 3K5U) were initially prepared by adding polar hydrogens at pH 7.4 using Protonate3D in Molecular Operating Environment (MOE) 2011.10. Gasteiger charges were then assigned using AutoDock's graphical user interface AutoDockTools (ADT; version 1.5.4). Following the addition of Gasteiger charges, ADT was implemented to build a "united atom model" of the receptor by merging non-polar hydrogens and adding their partial charges to their parent carbon atoms.

Preparation of the ligands:

The ligands were prepared by adding polar hydrogens at pH 7.4 using Protonate3D in MOE. MOE then assigned Gasteiger charges, before performing an energy minimisation using an MMFF94x forcefield with a 0.05 gradient. AutoDock's graphical user interface AutoDockTools (ADT; version 1.5.4) was subsequently used to build a "united atom model" of the ligands, by merging non-polar hydrogens and adding their partial charges to their parent carbon atoms.

Individual docking with AutoDock Vina (version 1.1.2):

The search space for docking into the receptor 2BRB was defined as a cubic box with dimensions 18.75 Å × 18.75 Å × 18.75 Å and center x = 17.238, y = -2.877, z = 10.364. The exhaustiveness and number of modes were both set to 20 and all other parameters were kept at their default values.

The search space for docking into the receptor 3K5U was defined as a cubic box with dimensions 18.75 Å × 18.75 Å × 18.75 Å and center x = -5.496, y = -31.095, z = 6.03. The exhaustiveness and number of modes were both set to 20 and all other parameters were kept at their default values.

General Experimental

^{1}H NMR spectra were recorded on Bruker DPX400 or DQX400 (400 MHz) or Bruker AVII 500 (500 MHz) using deuterochloroform (unless indicated otherwise) as a reference for internal deuterium lock. The chemical shift data for each signal are given as δH in units of parts per million (ppm) relative to tetramethylsilane (TMS) where δH (TMS) = 0.00 ppm. The multiplicity of each signal is indicated by: s (singlet); br s (broad singlet); d (doublet); t (triplet); q (quartet); dd (doublet of doublets); combinations thereof; or m (multiplet). The number of protons (n) for a given resonance signal is indicated by nH. Coupling constants (*J*) are quoted in Hz and are recorded to the nearest 0.1 Hz. Identical proton coupling constants (*J*) are averaged in each spectrum and reported to the nearest 0.1 Hz. The coupling constants are determined by analysis using Bruker TopSpin software.

^{13}C NMR spectra were recorded on Bruker DQX400 (100 MHz) or Bruker AVII 500 (126 MHz) spectrometers with broadband proton decoupling and internal deuterium lock. The chemical shift data for each signal are given as δC in units of parts per million (ppm) relative to tetramethylsilane (TMS) where δC (TMS) = 0.00 ppm.

Mass spectra were acquired on a VG platform spectrometer. Electrospray ionization spectra were obtained on Micromass LCT Premier and Bruker MicroTOF spectrometers, operating in positive or negative mode, from solutions of methanol. *m/z* values are reported in Daltons and followed by their percentage abundance in parentheses.

Melting points were determined using a Kofler hot stage microscope and are uncorrected.

Microanalyses were obtained at the Elemental Analysis Service, London Metropolitan University, London.

Infrared Specta were obtained from neat samples, either as solids or liquids, using a diamond ATR module. The spectra were recorded on a Bruker Tensor 27 spectrometer. Absorption maxima are reported in wavenumbers (cm^{-1}).

Analytical thin layer chromatography (TLC) was carried out on Merck silica gel 60 F_{254} aluminum-supported thin layer chromatography sheets. Visualization was by absorption of UV light (λ_{max} 254 nm), or thermal development after dipping in one of: **a** ethanolic solution of phosphomolybdic acid (PMA), ninhydrin or 4-anisaldehyde; **b** aqueous solution of cerium-ammonium-molybdate and sulfuric acid or potassium permanganate, potassium carbonate and sodium hydroxide.

Flash Column chromatography was carried out on VWR Prolabo silica gel 60 (240-400 mesh), eluting with solvents as supplied, under a positive pressure of compressed air (unless otherwise stated).

Anhydrous solvents Anhydrous CH_2Cl_2, Et_2O, toluene, and THF were obtained using a Dalek drying column, where solvent was dried by passage

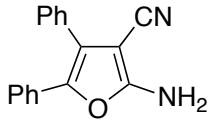
through filter columns and dispensed under an atmosphere of N_2 gas, before being stored over activated 3 Å molecular sieves under a N_2 atmosphere. Dry *N*,*N*-dimethylformamide was purchased from SigmaAldrich UK in SureSeal™ bottles and used without further purification as was dry 1,4-dioxane which was purchased from Fluka UK. All other solvents were used as supplied (analytical or HPLC grade) without purification.

Chemicals were purchased from Acros UK, Sigma Aldrich UK, Alfa Aesar UK, Fisher UK, Fluka UK, Fluorochem, Merck or TCI-Europe. All solvents and reagents were purified, when necessary, by standard techniques. Where appropriate and if not stated otherwise, all non-aqueous reactions were performed in a flame-dried flask under an inert atmosphere of nitrogen or argon.

In vacuo refers to the use of a rotary evaporator attached to a diaphragm pump. Brine refers to a saturated aqueous solution of sodium chloride. Petroleum ether refers to the fraction boiling between 30–40 °C unless otherwise stated.

Experimental Procedures

2-Amino-4,5-diphenylfuran-3-carbonitrile (**8**)

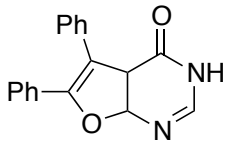


8

Benzoin (**7**, 5.00 g, 23.5 mmol, 1.0 eq), malononitrile (2.02 g, 30.6 mmol, 1.3 eq) and diethylamine (0.95 mL, 9.19 mmol, 0.4 eq) were added to dry dioxane (25 mL) stirring over 4 Å molecular sieves. The reaction vessel was covered with foil and heated under reflux overnight under an atmosphere of argon. The

reaction solution was filtered and the filtrate concentrated *in vacuo*. The resulting residue was crystallized from dioxane to yield (**8**) (4.60 g, 75%) as a beige solid: R_f 0.3 (1:4 ethyl acetate/petroleum ether); mp 204–207 °C (dioxane) (lit. 204–206 °C [dioxane]);[2] ν_{max} (neat) cm^{-1}: 3457, 2215; ^1H NMR (500 MHz; DMSO-D_6): δ 7.72 (s, 2H), 7.49–7.39 (m, 5H), 7.29–7.17 (m, 5H, Ar C*H*); ^{13}C NMR (126 MHz; DMSO-D_6): δ 163.5, 136.6, 131.2, 129.4, 129.0, 128.9, 128.6, 128.3, 126.9, 124.2, 121.8, 115.5, 69.2; (ESI$^+$) *m/z* 543.18 ([2M + Na]$^+$, 100%). These data are in good agreement with literature values.[1]

5,6-Diphenylfuro[2,3-d]pyrimidin-4(3H)-one (**10**)

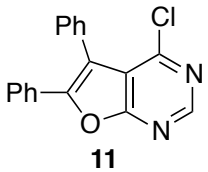


10

Formic acid (13.85 mL, 367.1 mmol) was added to acetic anhydride (13.85 mL, 146.8 mmol) stirring over 4 Å molecular sieves. The reaction solution was stirred at 60 °C for 2 h, generating acetic formic anhydride as a colorless liquid. Compound **8** (3.00 g, 11.5 mmol, 1.0 eq) was added to the acetic formic anhydride and the resulting solution heated to 85 °C for 6 h. The solution was filtered and adjusted to pH 6 using aqueous NaOH (2 M). The filtrate was extracted with CH_2Cl_2 (50 mL) and the organic layer washed with distilled water (3 × 50 mL). The organic layer was dried over $MgSO_4$, filtered and concentrated *in vacuo*. The resulting residue took the form of a brown solid (2.77 g), containing **9** {*m/z* (ES$^+$) 311 ([M+Na]$^+$, 100%)}, and was used without further purification.

The brown solid (3.79 g) containing **9** was heated to 220 °C for 30 min. The resulting solid was crystallized from methanol to yield **10** (1.70 g, 51% over two steps) as a brown solid: R_f 0.2 (3:7 ethyl acetate:petroleum ether); mp 258–260 °C (MeOH) (lit. > 240 °C [MeOH]);[2] ν_{max} (neat) cm^{-1}: 3443, 1675; ^1H NMR (500 MHz; DMSO-D_6): δ 12.65 (s, 1H), 8.17 (s, 1H), 7.45–7.33 (m, 10H); ^{13}C NMR (126 MHz; DMSO-D_6): δ 164.6, 159.0, 148.0, 146.8, 131.7, 131.0, 129.9, 129.62, 129.55, 129.2, 128.8, 127.2, 119.5, 108.9; (ESI^+) *m/z* 599.18 ([2M + Na]$^+$, 100%). These data are in good agreement with literature values.[2]

4-Chloro-5,6-diphenylfuro[2,3-d] pyrimidine (**11**)

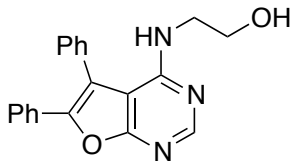


11

Phosphorus(V) oxychloride (9.93 mL, 106.53 mmol, 30.7 eq) was added to dry **10** (1.00 g, 3.47 mmol, 1.0 eq). The reaction solution was stirred at 55 °C under argon for 2 h, then quenched by pouring over crushed ice and adjusted to pH 7 using a saturated aqueous solution of Na_2CO_3. The product was extracted with CH_2Cl_2 (100 mL) and washed with distilled water (3 × 50 mL). The organic layer was dried over $MgSO_4$, filtered and concentrated *in vacuo*. The resulting residue was adsorbed onto silica gel and purified using silica gel column chromatography (elution: 1:9:90 triethylamine:ethyl acetate:petroleum ether) to give **11** (0.86 g, 81%) as a pale yellow solid: R_f 0.9 (1:4 ethyl acetate:petroleum ether); mp 103–105 °C (ethyl acetate/petroleum ether) (lit. 121–122 °C);[2] ^1H NMR (500 MHz;

DMSO-D_6): δ 8.86 (s, 1H), 7.53–7.40 (m, 10H); ^{13}C NMR (126 MHz; DMSO-D_6): δ 165.3, 153.0, 151.7, 150.9, 130.5, 130.1, 129.9, 129.0, 128.8, 128.0, 126.9, 118.4, 115.0; *m/z* (ES^+) 307 ($[M+H]^+$, 100%). These data are in good agreement with literature values.[2]

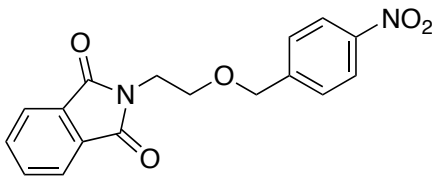
2-(5,6-Diphenylfuro[2,3-d]pyrimidin-4-ylamino)ethanol (**6**)



6

Chloride **11** (0.70 g, 2.29 mmol, 1.0 eq) and ethanolamine (0.30 mL, 5.03 mmol, 2.2 eq) were added to ethanol (7 mL). The reaction was heated under reflux for 6 h and then concentrated *in vacuo*. The resulting residue was adsorbed onto Celite® and purified by silica gel column chromatography, eluting with Et_3N, MeOH, ethyl acetate and petroleum ether (1:4:30:65) to afford **6** (0.72 g, 95%) as a beige solid: R_f 0.3 (1:4:30:65 Et_3N:MeOH:ethyl acetate:petroleum ether); mp 154–157 °C (ethyl acetate/petroleum ether) (lit. 163-165 °C);[2] ^{1}H NMR (500 MHz; $CDCl_3$): δ 8.32 (s, 1H, 3.56), 7.52–7.22 (m, 10H), 5.16 (t, *J* = 5.2 , 1H), 4.18 (br s, 1H), 3.72 (t, *J* = 4.2, 2H), 3.56 (dt, *J* = 5.2, 4.6, 2H); ^{13}C NMR (126 MHz; $CDCl_3$): δ 164.7, 157.9, 153.6, 147.0, 132.1, 129.72, 129.70, 129.3, 129.0, 128.5, 128.5, 126.4, 114.9, 103.3, 62.4, 44.2; *m/z* (ES^+) 333 (100%), 332 ($[M+H]^+$, 98%), 370 ($[M+K]^+$, 78%). These data are in good agreement with literature values.[2]

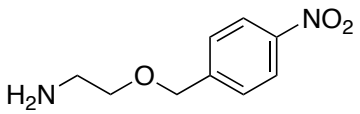
2-(2-([4-Nitrobenzyl]oxy)ethyl)isoindoline-1,3-dione



Sodium hydride (0.63 g 60% dispersion in mineral oil, 15.69 mmol, 1.5 eq) was added to a stirred solution of *N*-(2-hydroxyethyl)phthalimide (2.00 g, 10.46 mmol, 1.0 eq) in dry THF (20 mL). The reaction mixture was stirred for 15 min under argon at ambient temperature and then 4-nitrobenzyl bromide (3.39 g, 15.69 mmol, 1.5 eq) and TBAI (0.39 g, 1.05 mmol, 0.1 eq) were added. The reaction mixture was stirred at ambient temperature for a further 24 h, quenched by the addition of methanol (20 mL) and the solvents removed *in vacuo*. The residue was dissolved in CH_2Cl_2 (50 mL), washed with distilled water (3 × 50 mL) and the organic layer dried over $MgSO_4$, filtered and concentrated *in vacuo*. The resulting residue was purified by silica gel column chromatography, eluting with ethyl acetate and petroleum ether (20:80) to afford *2-(2-([4-nitrobenzyl]oxy)ethyl)isoindoline-1,3-dione* (0.78 g, 23%) as a yellow solid: R_f 0.2 (1:4 ethyl acetate:petroleum ether); mp 142–143 °C (ethyl acetate/petroleum ether); ν_{max} (neat) cm^{-1}: 1739, 1515, 1366; ^1H NMR (500 MHz; $CDCl_3$): δ 8.12 (d, *J* = 8.7, 2H), 7.87–7.85 (m, 2H), 7.74–7.73 (m, 2H), 7.43 (d, *J* = 8.7, 2H), 4.63 (s, 2H), 3.98 (t, *J* = 5.6, 2H), 3.80 (t, *J* = 5.6); ^{13}C NMR (126 MHz; $CDCl_3$): δ 168.2, 147.3, 145.5, 134.1, 132.0, 127.6, 123.6, 123.3, 71.4, 67.7, 37.4; HRMS *m/z* (ESI^+) found $[M+Na]^+$ 349.0791, $C_{17}H_{14}N_2O_5Na$ requires $[M+Na]^+$ 349.0795; *m/z*

(ES$^+$) 349 ([M+Na]$^+$, 100%), 675 ([2M+Na]$^+$, 42%). Anal. Calcd for $C_{17}H_{14}N_2O_5$: C, 62.6; H, 4.3; N, 8.6. Found C, 62.5; H, 4.4; N, 8.5.

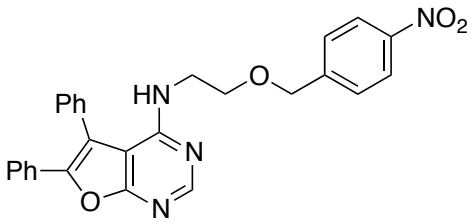
2-([4-Nitrobenzyl]oxy)ethanamine (**12**)



12

Hydrazine monohydrate (1.98 g, 1.92 mL, 39.6 mmol, 43.1 eq) was added to a solution of 2-(2-([4-nitrobenzyl]oxy)ethyl)isoindoline-1,3-dione (0.30 g, 0.92 mmol, 1.0 eq.) in ethanol (20 mL). The reaction mixture was stirred at ambient temperature for three days under argon then filtered, washed with ethanol and the filtrate concentrated *in vacuo*. The resulting residue was dissolved in CH_2Cl_2 (20 mL) and washed with aqueous HCl (2 M, 2 × 20 mL). The aqueous phases were combined, washed with diethyl ether (2 × 20 mL) and then adjusted to pH > 11 using NaOH pellets. The organic material was extracted from this mixture with CH_2Cl_2 (20 mL), the combined CH_2Cl_2 layers dried over $MgSO_4$, filtered and the solvent was removed *in vacuo* to yield *2-([4-nitrobenzyl]oxy)ethanamine* (**12**) (0.14 g, 80%) as an orange liquid: R_f 0.2 (2:3, ethyl acetate:petroleum ether); ν_{max} ($CHCl_3$) cm^{-1}: 1518, 1345; ^{1}H NMR (400 MHz; $CDCl_3$): δ 8.11 (d, *J* = 8.6, 2H), 7.44 (d, *J* = 8.6, 2H), 4.57 (s, 2H), 3.50 (t, *J* = 5.2, 2H), 2.86 (t, *J* = 5.2, 2H); ^{13}C NMR (100 MHz; $CDCl_3$): δ 147.2, 146.1, 127.6, 123.5, 73.1, 71.7, 41.8; HRMS *m/z* (ESI$^+$) found [M+H]$^+$ 197.0929, $C_9H_{13}N_2O_3$ requires [M+H]$^+$ 197.0921; *m/z* (ES$^+$) 197 ([M+H]$^+$, 100%).

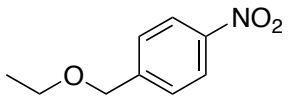
N-(2-([4-Nitrobenzyl]oxy)ethyl)-5,6-diphenylfuro[2,3-d]pyrimidin-4-amine (**1**)



1

A solution of **11** (0.05 g, 0.17 mmol, 1.0 eq), amine **12** (0.07 g, 0.38 mmol, 2.2 eq) and Et_3N (0.05 mL, 0.38 mmol, 2.2 eq) in DMF (3 mL) was stirred at 80 °C under nitrogen for 6 h and then concentrated *in vacuo*. The resulting residue was dissolved in CH_2Cl_2 (20 mL) and washed with distilled water (3 × 20 mL). The organic layer was dried over $MgSO_4$, filtered and concentrated *in vacuo* and the resulting residue purified by silica gel chromatography, eluting with Et_3N, MeOH, ethyl acetate and petroleum ether (1:4:20:75) to afford *N-(2-([4-nitrobenzyl]oxy)ethyl)-5,6-diphenylfuro[2,3-d]pyrimidin-4-amine* (**1**) (0.1 g, 93%) as a yellow solid: R_f 0.2 (1:1, ethyl acetate:petroleum ether); mp 127–129 °C (ethyl acetate); ν_{max} (neat) cm^{-1}: 3426, 1520, 1340; ^1H NMR (400 MHz; $CDCl_3$): δ 8.42 (s, 1H), 8.22 (d, *J* = 8.7, 2H), 7.52–7.27 (m, 10H), 7.35 (d, *J* = 8.7, 2H), 5.12 (t, *J* = 5.2, 1H), 4.51 (s, 2H), 3.74 (dt, *J* = 5.2, 5.2, 2H), 3.61 (t, *J* = 5.2, 2H); ^{13}C NMR (126 MHz; $CDCl_3$): δ 165.0, 157.4, 154.0, 147.4, 146.9, 145.4, 132.4, 129.7, 129.5, 129.4, 128.7, 128.5, 127.5, 126.4, 123.6, 114.8, 103.3, 71.7, 69.3, 40.4; HRMS *m/z* (ESI^-) [Found: $[M-H]^-$ 465.1575, $C_{27}H_{21}N_4O_4$ requires $[M-H]^-$ 465.1568]; *m/z* (ES^-) 465 ($[M-H]^-$, 100%); Anal. Calcd for $C_{27}H_{22}N_4O_4$: C, 69.5; H, 4.8; N, 12.0. Found C, 69.4; H, 4.6; N, 11.9.

1-(Ethoxymethyl)-4-nitrobenzene (**13**)



13

Anhydrous ethanol (6 mL) was added to dry THF (30 mL) and the solution cooled with an ice-water bath. Sodium hydride was then added in portions and the resulting mixture left to stir at the ambient temperature for 10 min. This mixture was syringed drop wise into an ice-cooled solution of 4-nitrobenzylbromide (1.0 g, 4.62 mmol) in dry THF (20 mL) and the reaction left stirring at the ambient temperature for an additional 2 h. A saturated aqueous solutions of NH_4Cl was added, the mixture concentrated *in vacuo* and then re-dissolved in EtOAc. This solution washed with brine, dried over anhydrous $MgSO_4$, filtered and the solvent removed *in vacuo*. Purification by column chromatography eluting with petroleum ether and ethyl acetate (gradient: 10:0 to 9:1) gave 1-(ethoxymethyl)-4-nitrobenzene (**13**) as a yellow oil (161 mg, 19%): R_f 0.4 (1:10 ethyl acetate:petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.1, 2H), 7.51 (d, *J* = 8.1, 2H), 4.61 (s, 2H), 3.60 (q, *J* = 7.0), (t, *J* = 7.0); *m/z* (FI^+) 181.07 ($[M]^+$, 100%). These data are in good agreement with literature values.[3]

References

1. Johannsen, F.; Jorgensen, A.; Pedersen, E. B., Reactions of Heterocyclic Ortho-Aminonitriles with Acetic Formic Anhydride. *Chem. Scripta* **1986,** *26*, 347-351.

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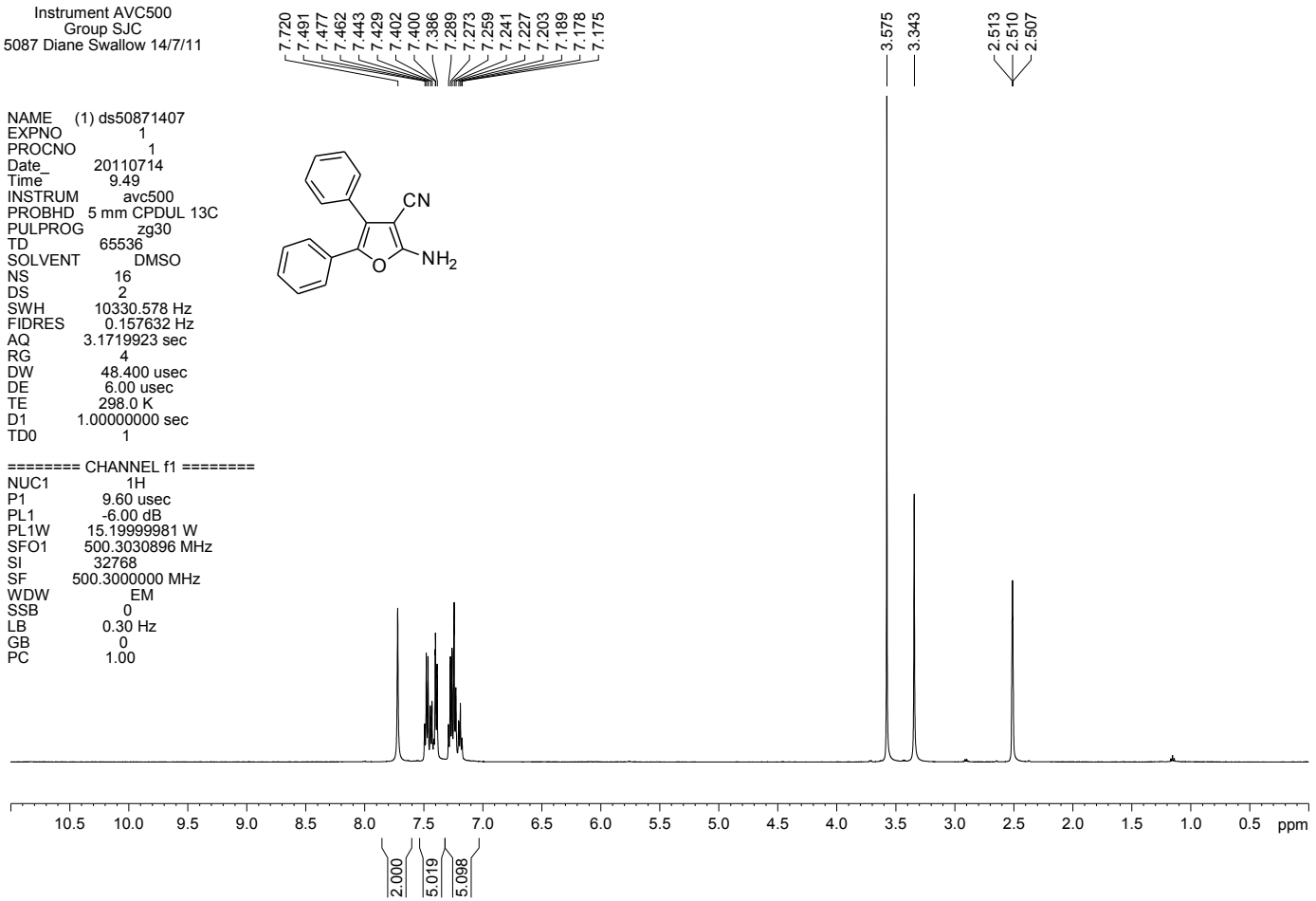
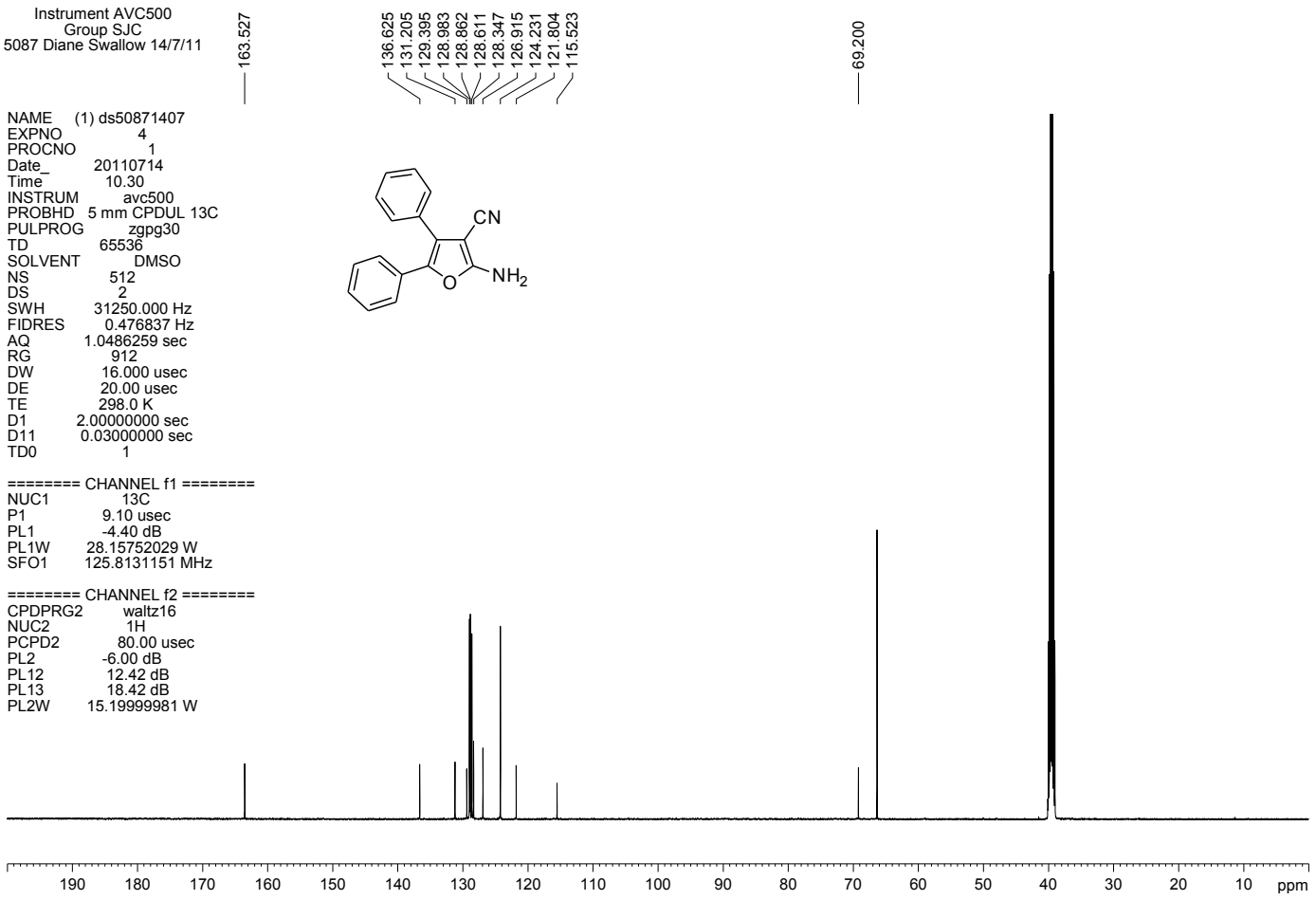
3. Joshi, G.; Adimurthy, S., New Method for the Synthesis of Benzyl Alkyl Ethers Mediated by $FeSO_4$. *Synth. Commun.* **2011,** *41*, 720-728.

^{1}H and ^{13}C NMR Spectra

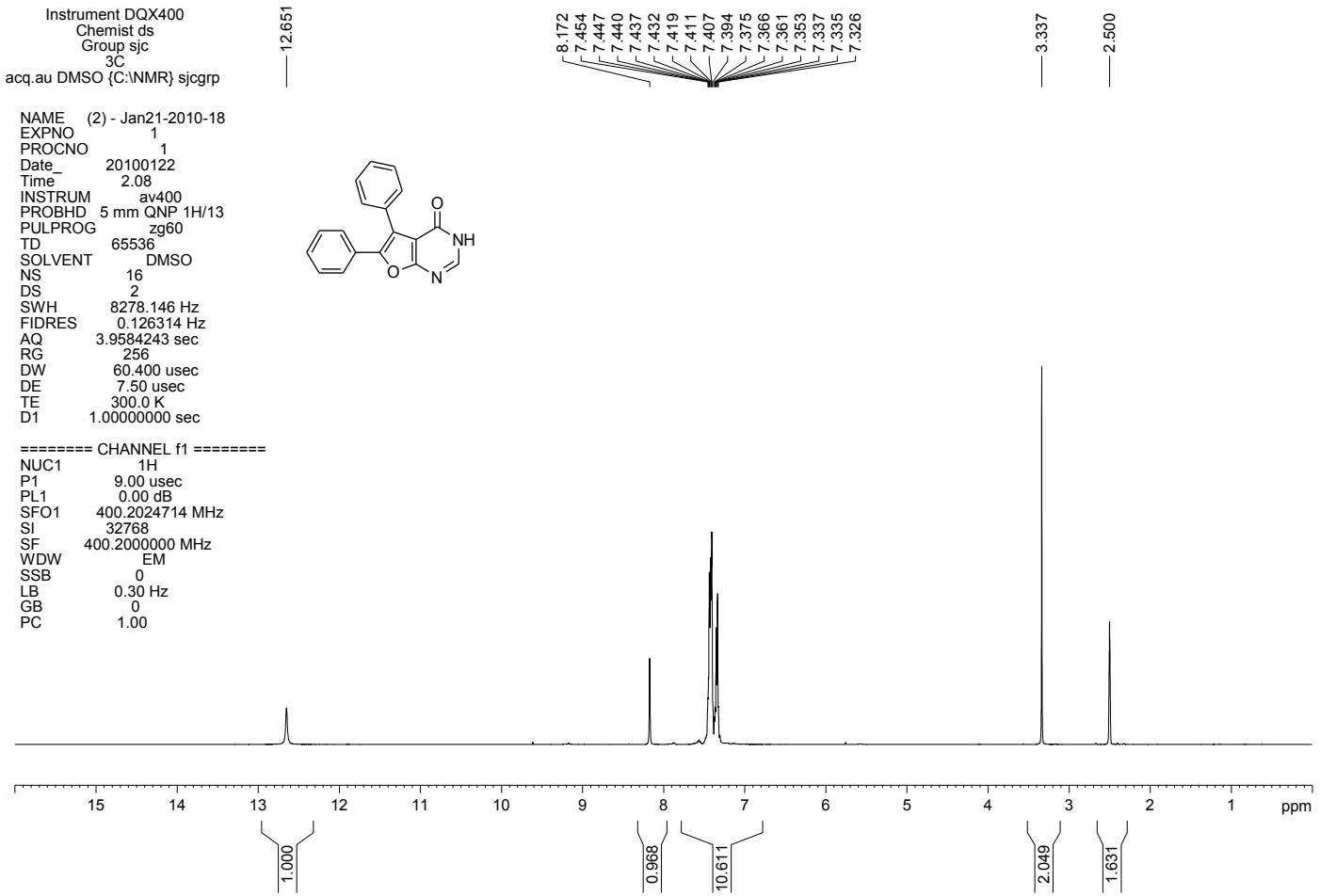
2-Amino-4,5-diphenylfuran-3-carbonitrile (**8**) – ^{1}H NMR spectrum



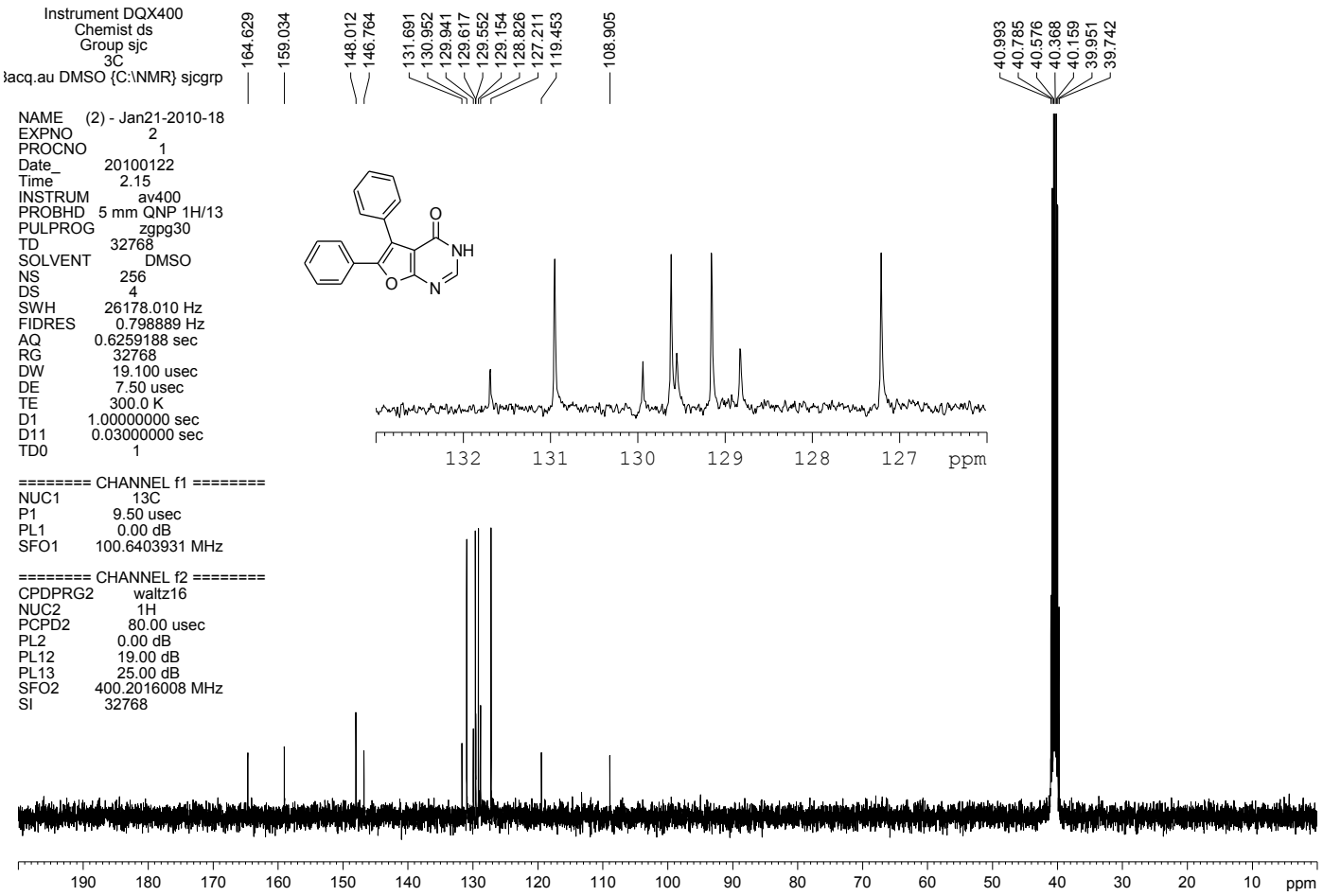
2-Amino-4,5-diphenylfuran-3-carbonitrile (**8**) – ^{13}C NMR spectrum



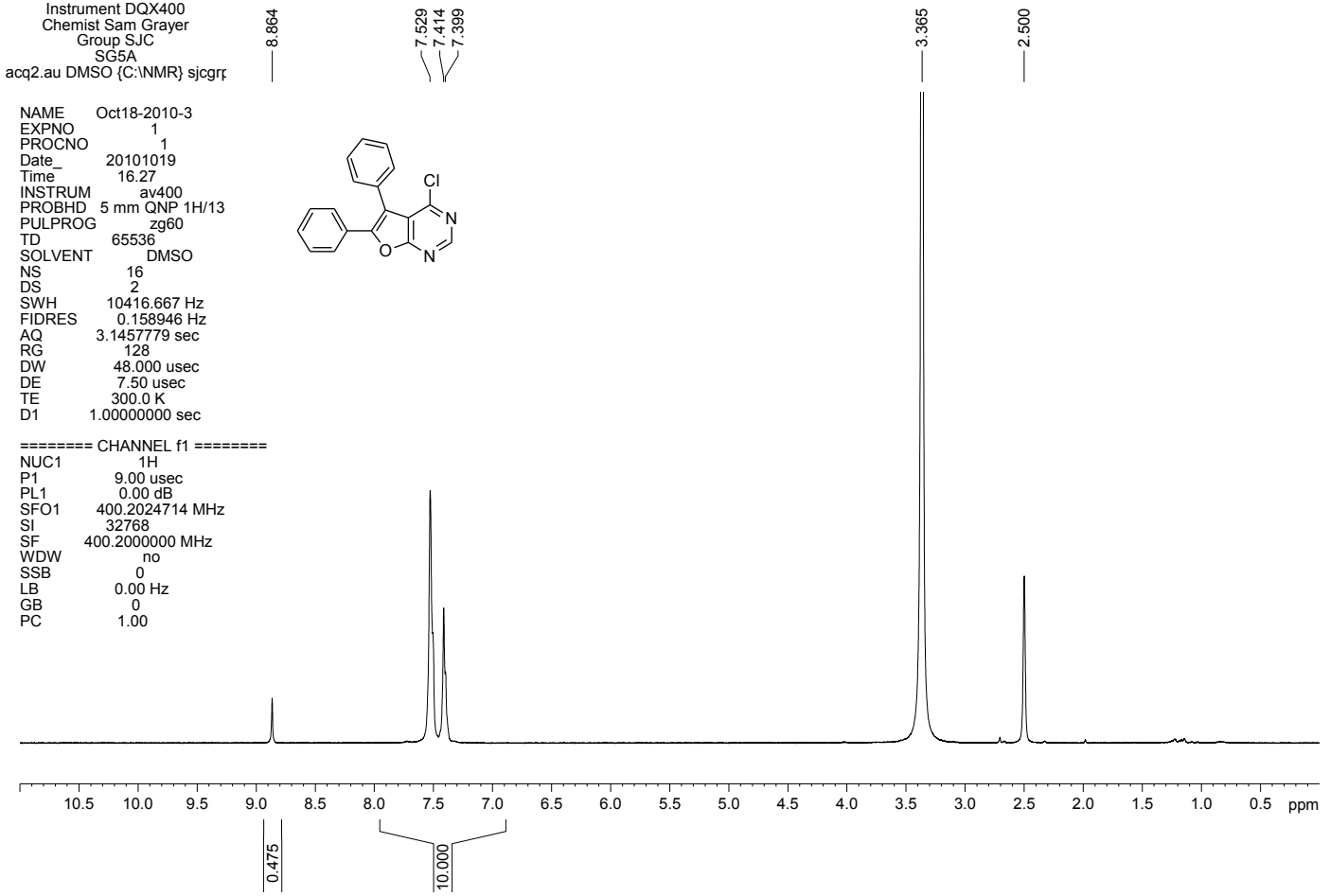
5,6-Diphenylfuro[2,3-d]pyrimidin-4(3H)-one (**10**) – ^{1}H NMR spectrum



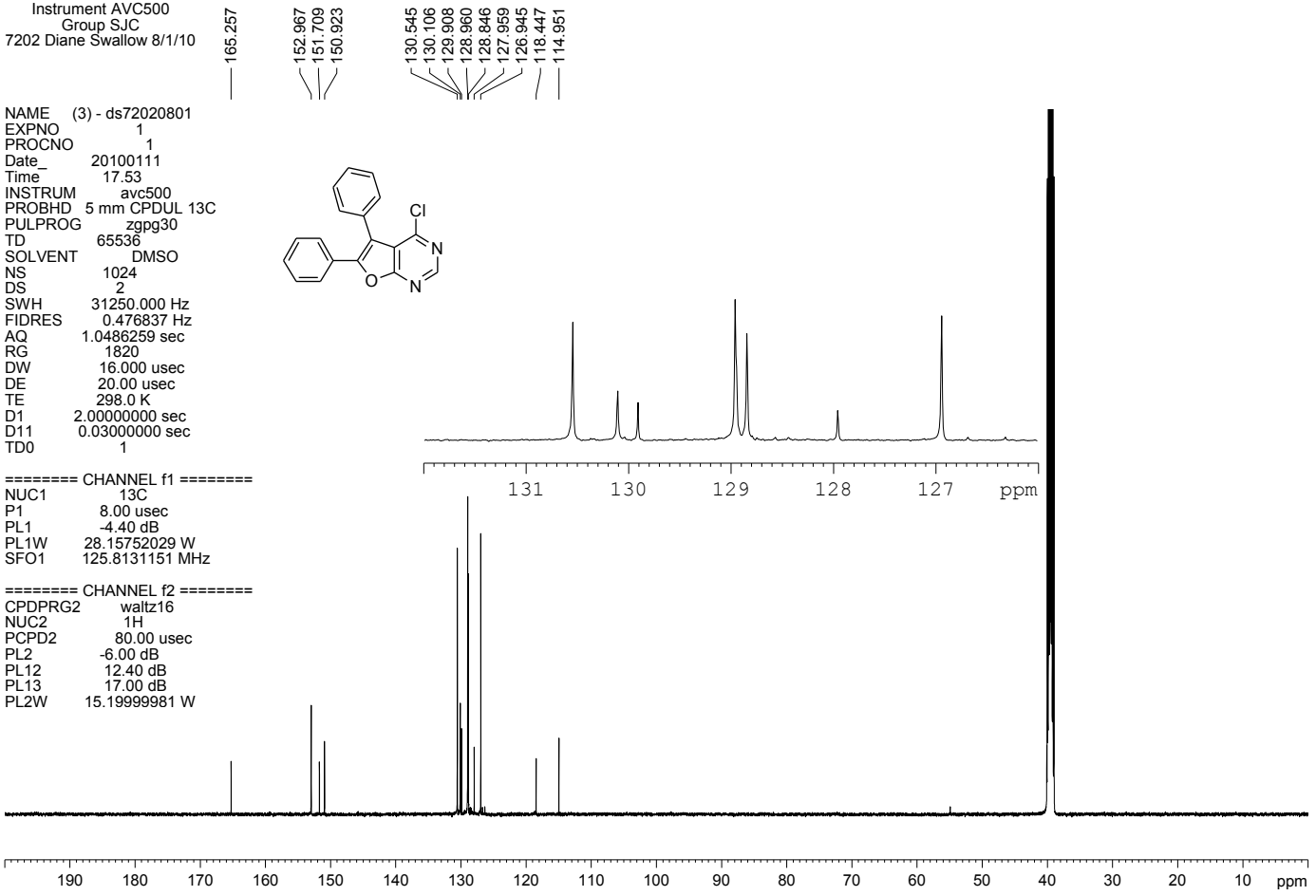
5,6-Diphenylfuro[2,3-d]pyrimidin-4(3H)-one (**10**) – ^{13}C NMR spectrum



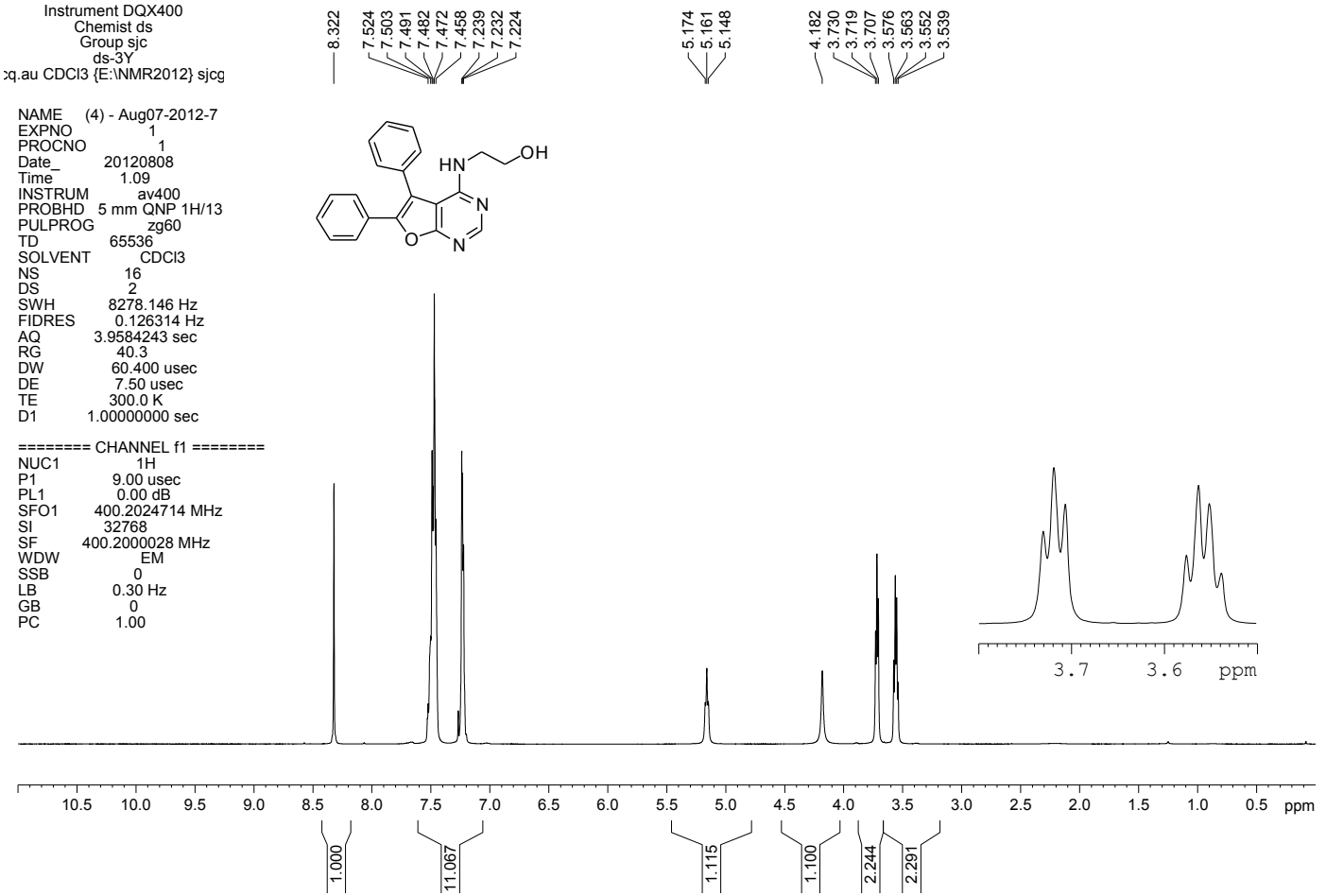
4-Chloro-5,6-diphenylfuro[2,3-d] pyrimidine (**11**) – ^{1}H NMR spectrum



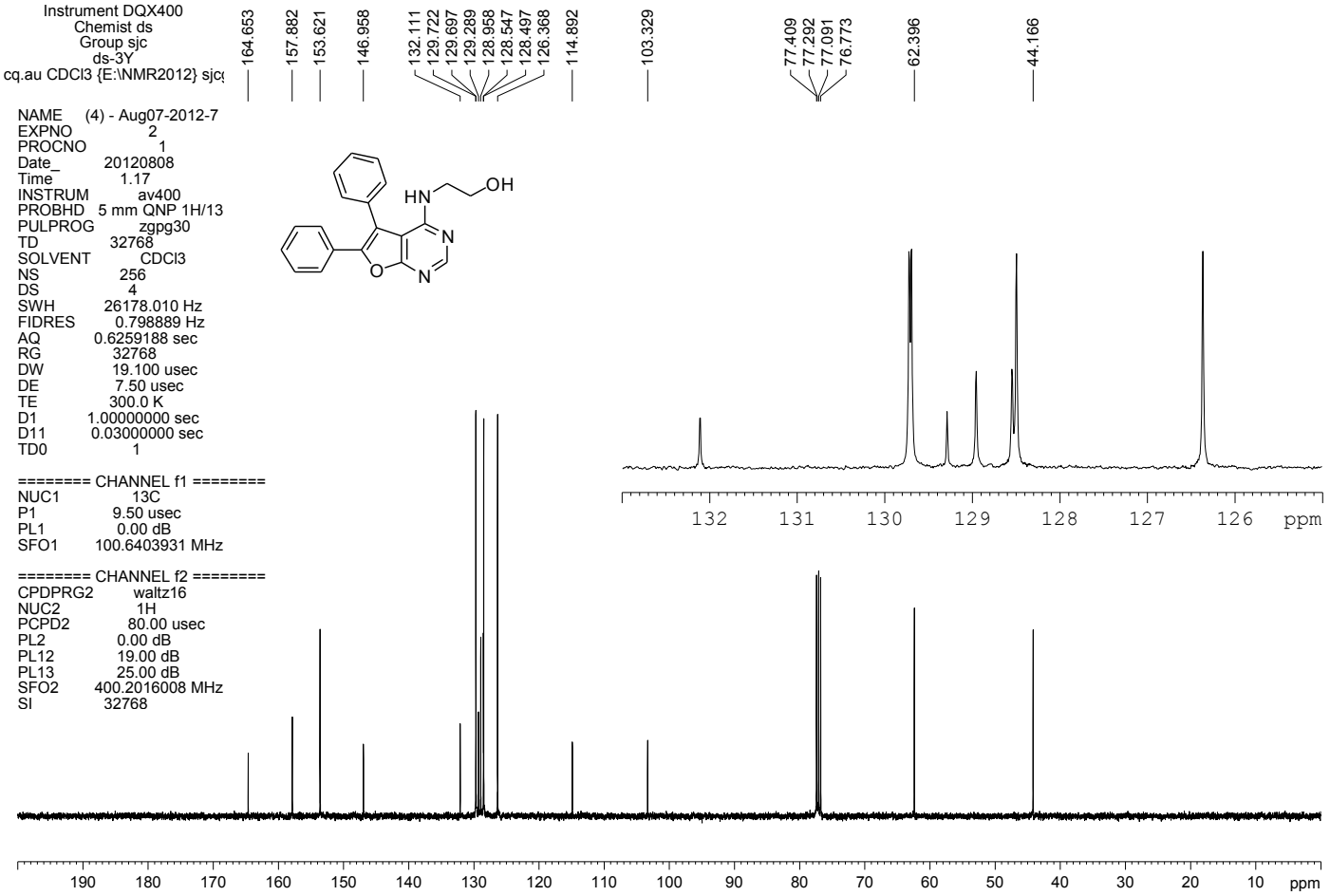
4-Chloro-5,6-diphenylfuro[2,3-d] pyrimidine (**11**) – ^{13}C NMR spectrum



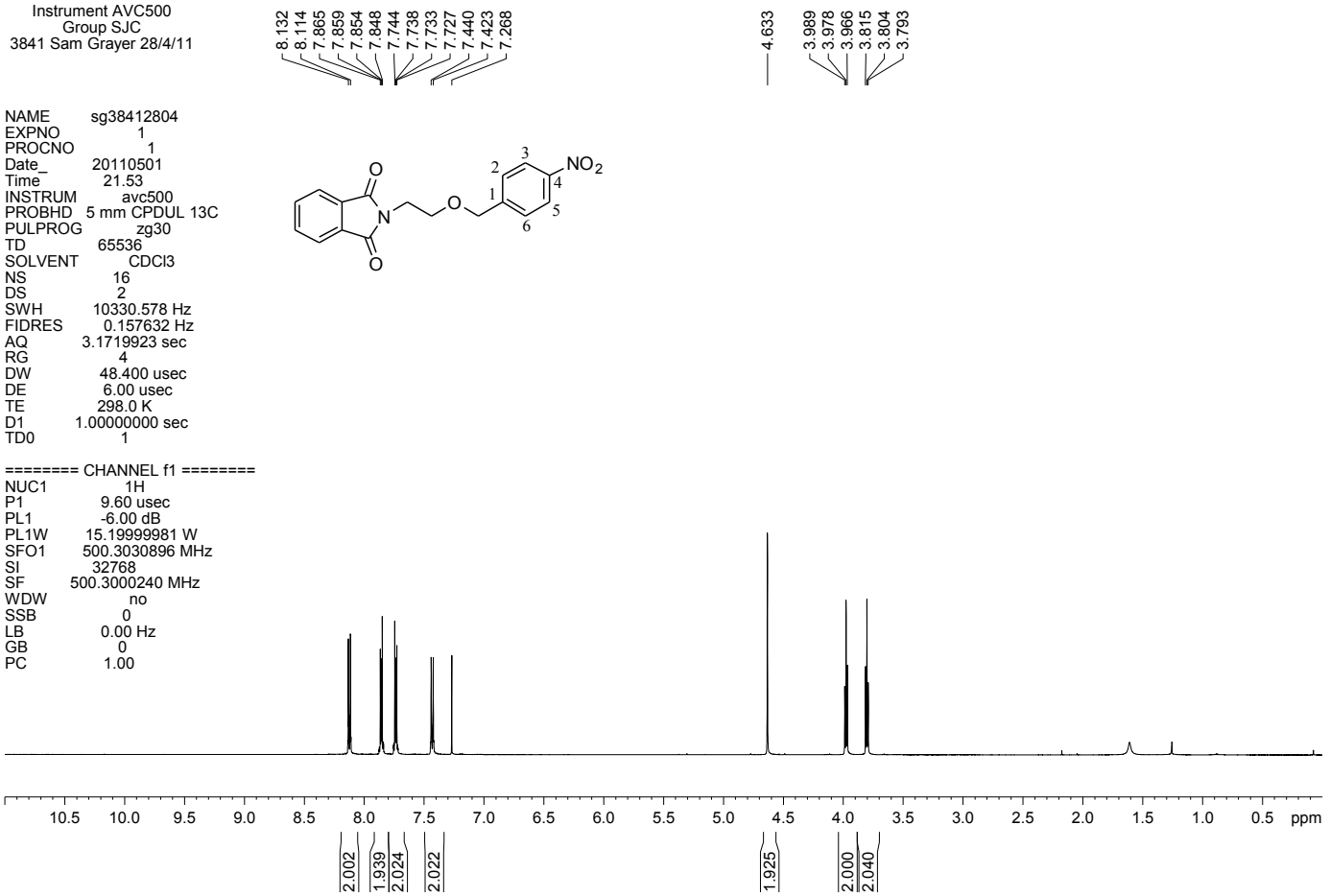
2-(5,6-Diphenylfuro[2,3-d]pyrimidin-4-ylamino)ethanol (**6**) – ^{1}H NMR spectrum



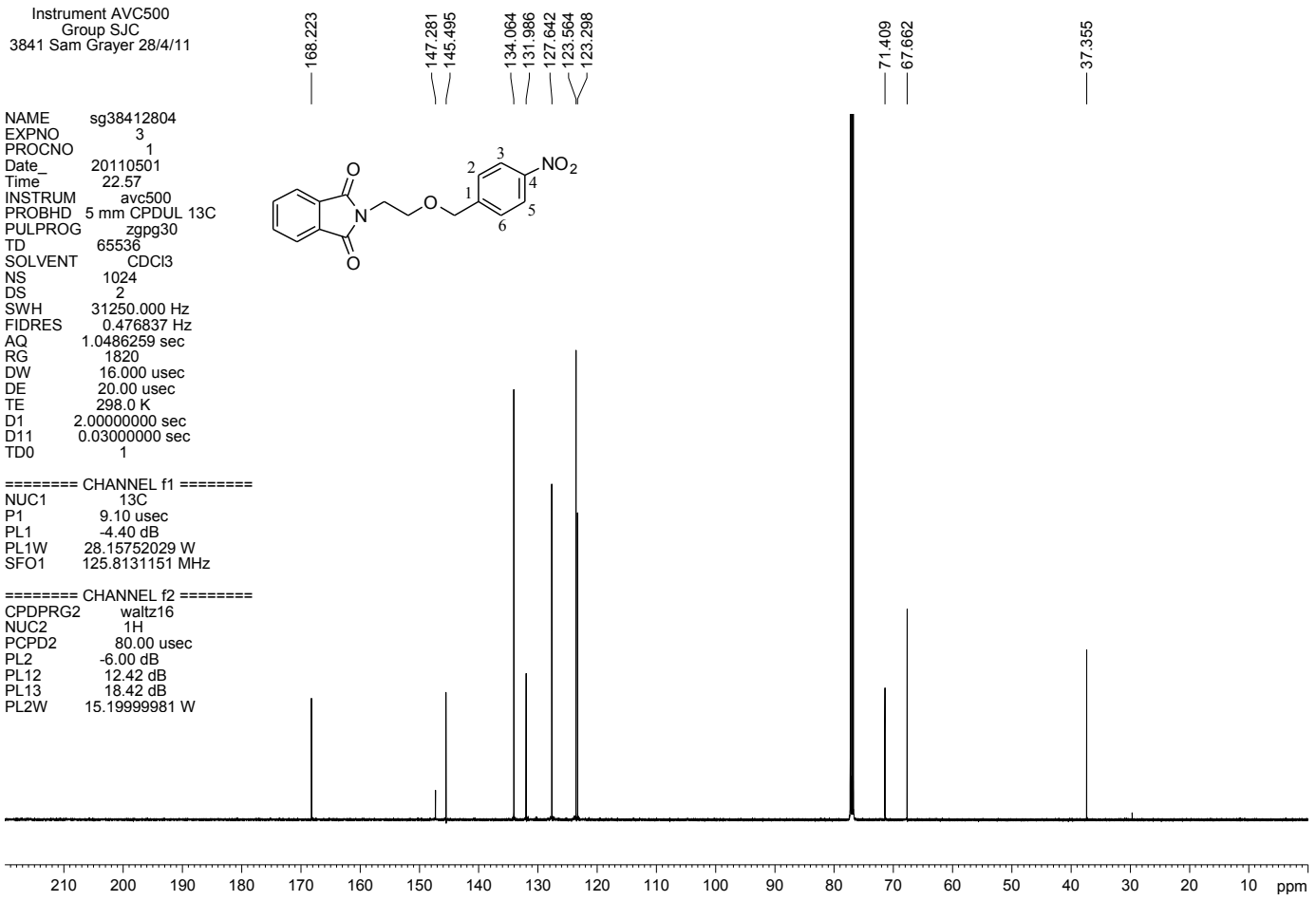
2-(5,6-Diphenylfuro[2,3-d]pyrimidin-4-ylamino)ethanol (**6**) – ^{13}C NMR spectrum



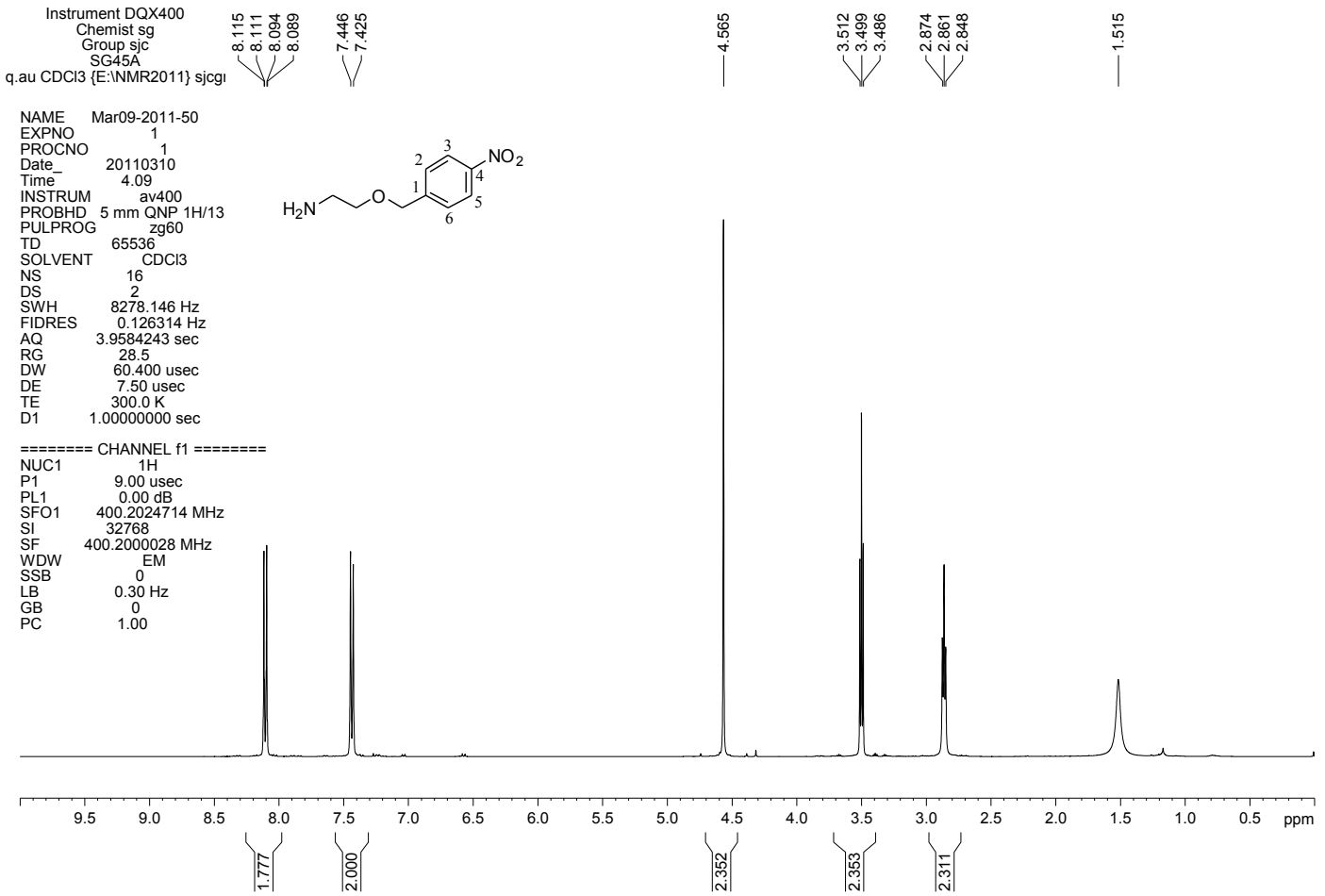
2-(2-([4-Nitrobenzyl]oxy)ethyl)isoindoline-1,3-dione – ^{1}H NMR spectrum



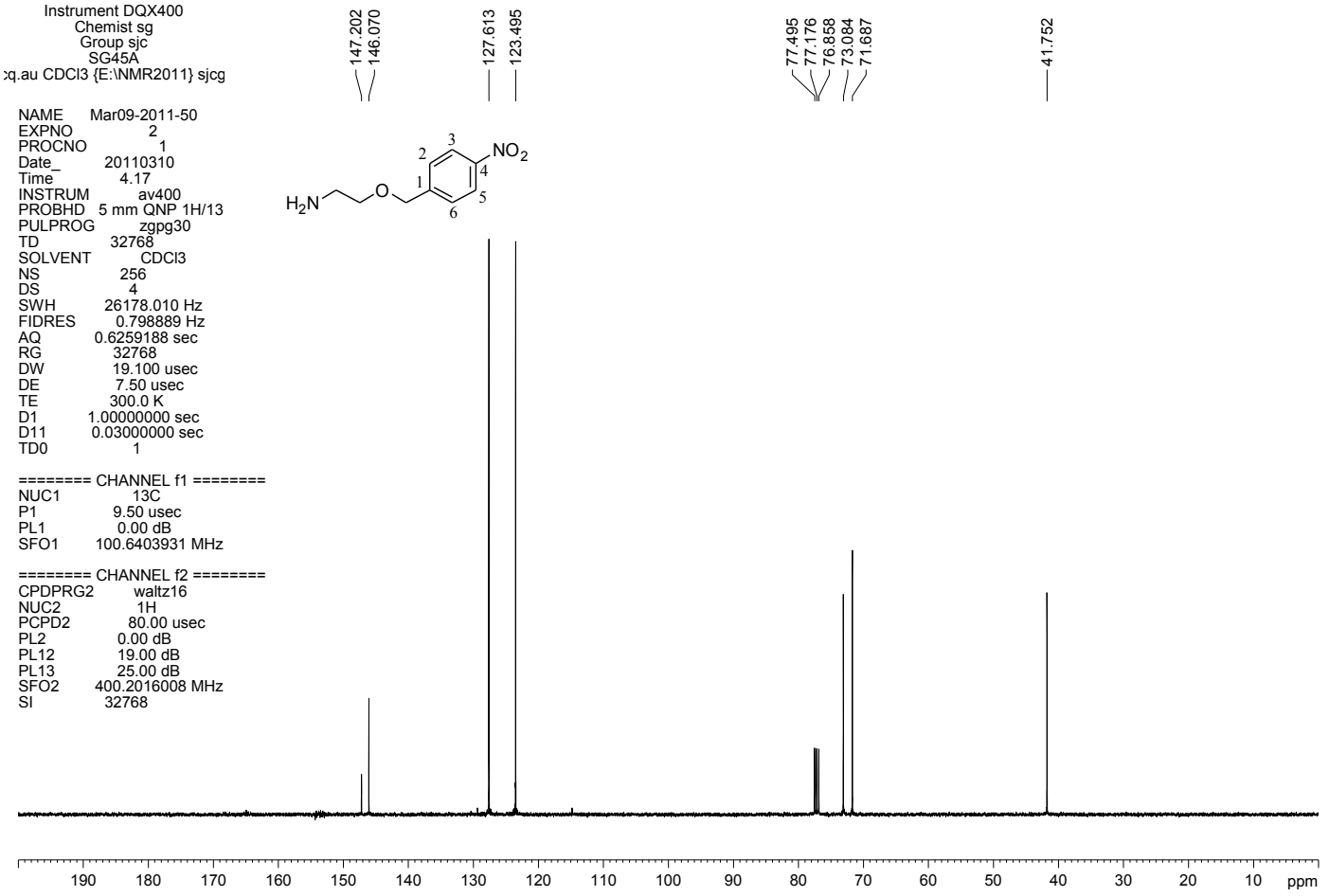
2-(2-([4-Nitrobenzyl]oxy)ethyl)isoindoline-1,3-dione – ^{13}C NMR spectrum



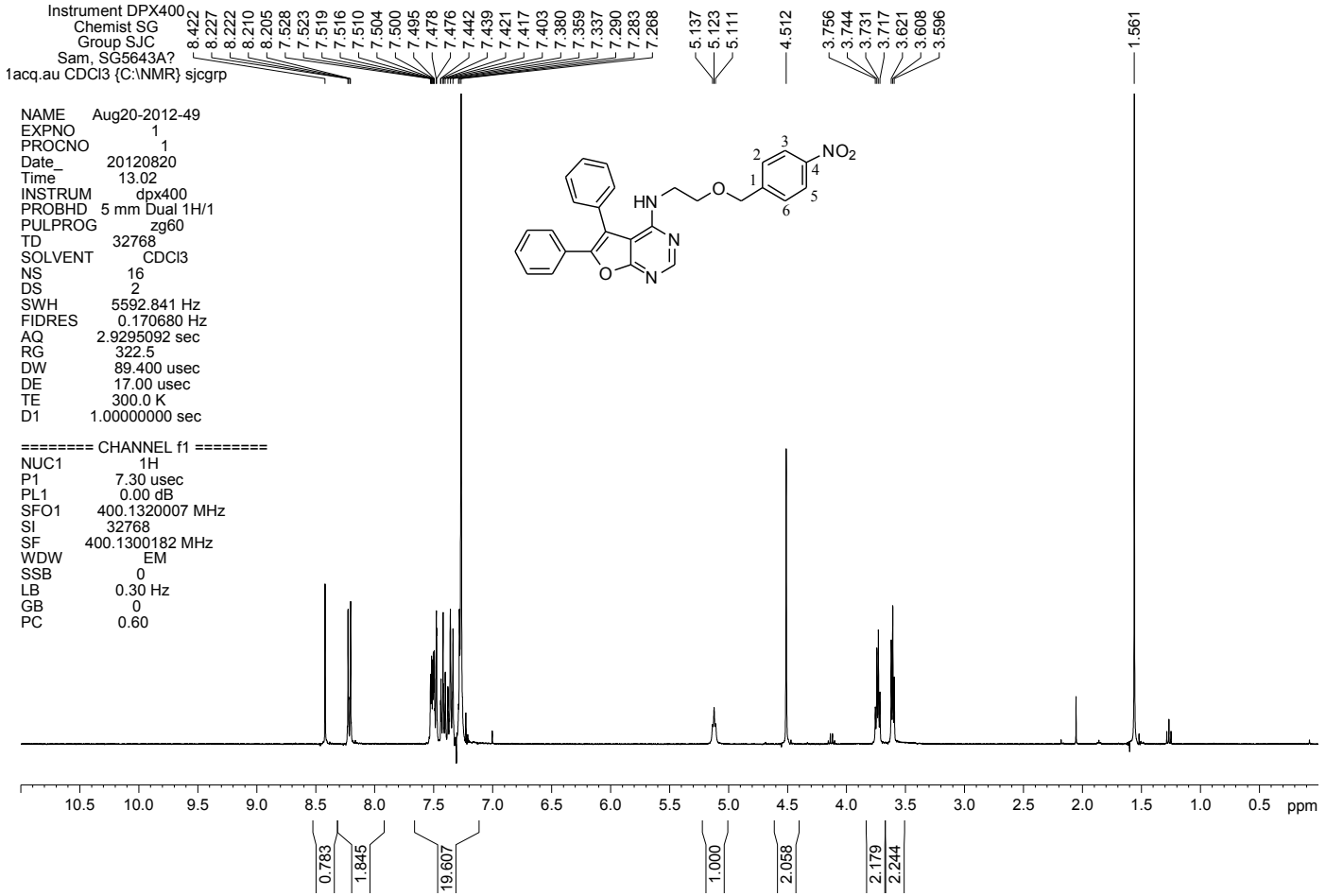
2-([4-Nitrobenzyl]oxy)ethanamine (**12**) – ^{1}H NMR spectrum



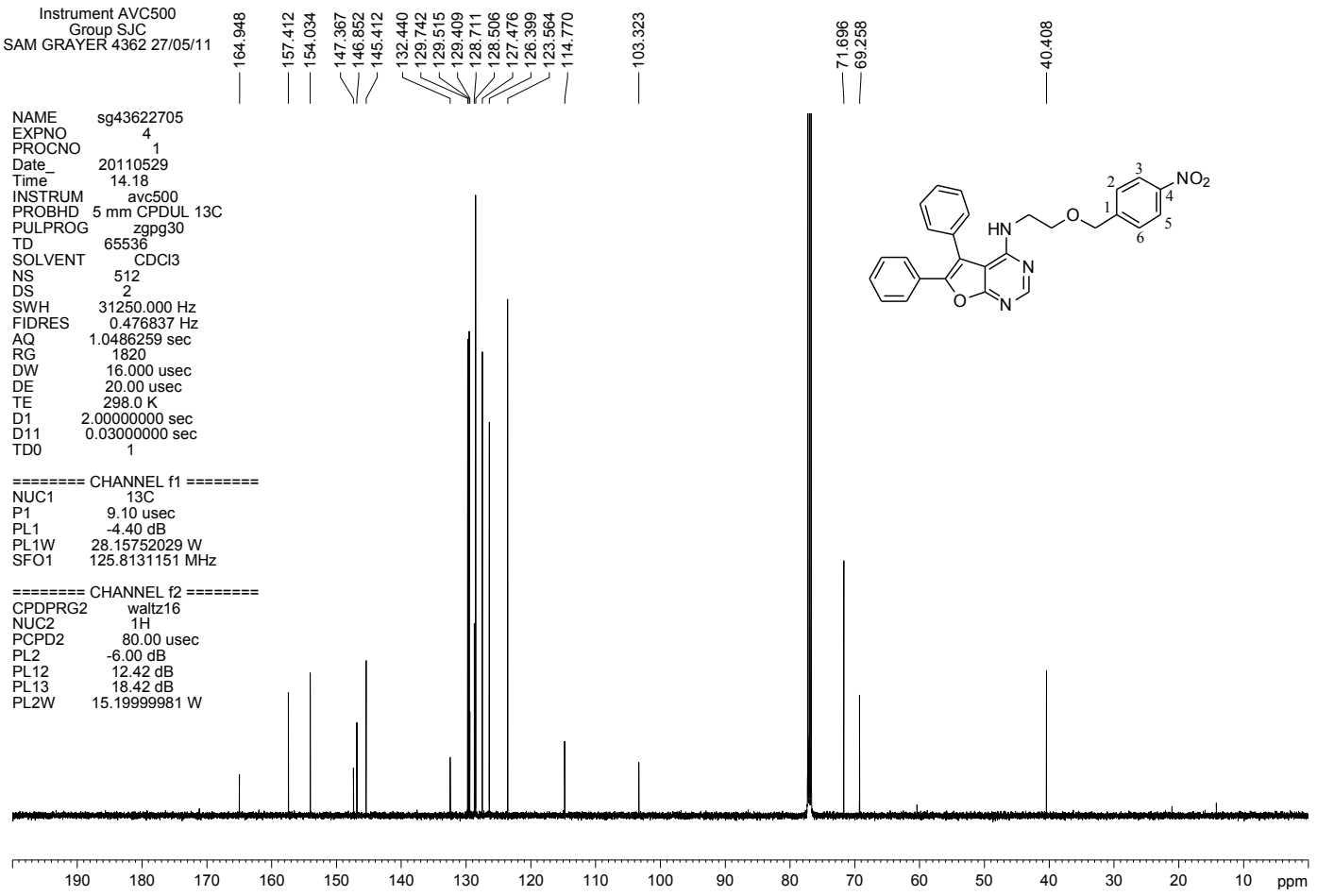
2-([4-Nitrobenzyl]oxy)ethanamine (**12**) – ^{13}C NMR spectrum



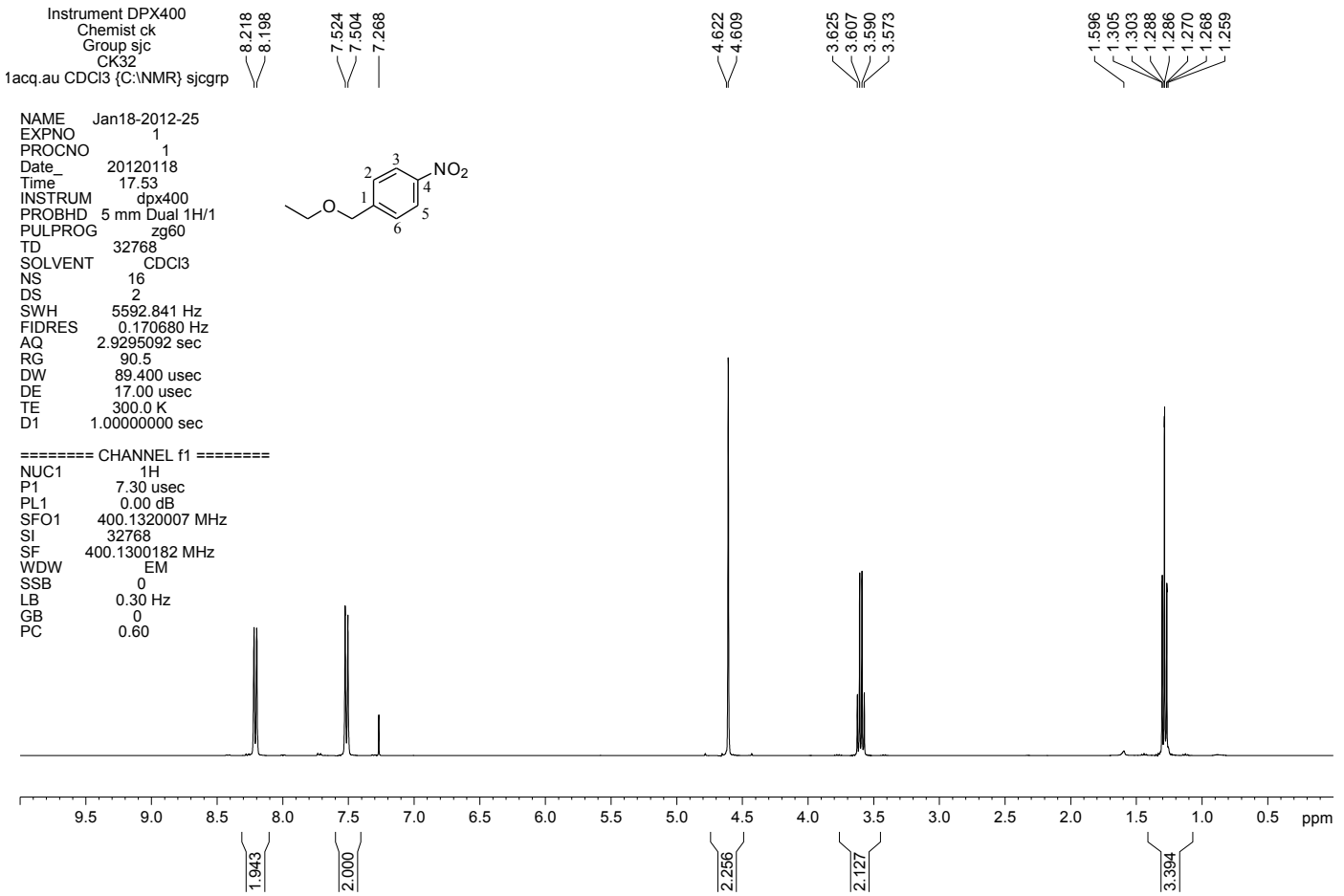
N-(2-([4-Nitrobenzyl]oxy)ethyl)-5,6-diphenylfuro[2,3-d]pyrimidin-4-amine (**1**) – ^{1}H NMR spectrum



N-(2-([4-Nitrobenzyl]oxy)ethyl)-5,6-diphenylfuro[2,3-d]pyrimidin-4-amine (**1**) – ^{13}C NMR spectrum



1-(Ethoxymethyl)-4-nitrobenzene (**13**) – ^{1}H NMR spectrum



1-(Ethoxymethyl)-4-nitrobenzene (**13**) – ^{13}C NMR spectrum