Supporting Information

For

Palladium(II)-catalysed regioselective synthesis of 3,4-disubstituted quinolines and 2,3,5-trisubstituted pyrroles from alkenes via *anti*-Markovnikov selectivity

Gopal Chandru Senadi,[a] Wan-Ping Hu,[b] Amol Milind Garkhedkar,[a] Siva Senthil Kumar Boominathan,[a] and Jeh-Jeng Wang[,a]*

[a]Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, No. 100, Shih-Chuan 1st Rd, Sanmin district, Kaohsiung City, 807 (Taiwan).

[b]Department of Biotechnology, Kaohsiung Medical University, No. 100, Shih-Chuan 1st Rd, Sanmin district, Kaohsiung City, 807 (Taiwan).

E-mail: jjwang@kmu.edu.tw.

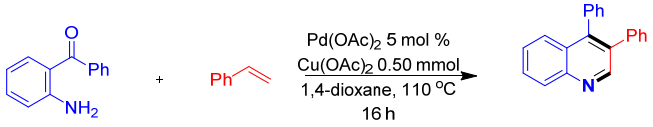
Table of Contents

1. General Information

^{1}H, ^{13}C and DEPT NMR spectra were recorded on a 400 MHz Varian Unity Plus or Varian Mercury plus spectrometer. The chemical shift (δ) values are reported in parts per million (ppm), and the coupling constants (*J*) are given in Hz. The spectra were recorded using $CDCl_3$ as a solvent. ^{1}H NMR chemical shifts are referenced to tetramethylsilane (TMS) (0 ppm). ^{13}C NMR was referenced to $CDCl_3$ (77.0 ppm). The abbreviations used are as follows: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublet; ddd, doublet of doublet of doublet; dt, doublet of triplets; td, triplet of doublet; m, multiplet. Mass spectra and high-resolution mass spectra (HRMS) was measured using the ESI (FT-MS solariX) at NSYSU, Kaohsiung, Taiwan. Melting points were determined on an EZ-Melt (Automated melting point apparatus). All products reported showed ^{1}H NMR spectra in agreement with the assigned structures. Reaction progress and product mixtures were routinely monitored by TLC using Merck TLC aluminum sheets (silica gel 60 F254). Column chromatography was carried out with 230–400 mesh silica gel 60 (Merck) and a mixture of hexane/ethyl acetate as an eluent.

2. Optimization of reaction conditions for quinolines and pyrroles

2.1 Table S1. Optimization of the additive



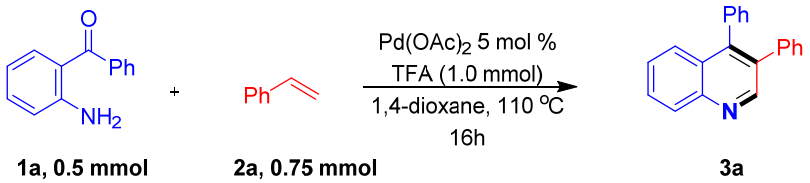
1a, 0.5 mmol **2a, 0.75 mmol** **3a**

Entry	Additive (mmol)	Yield (%)[a]
1	---	NR
2	TFA (1.0)	33
3	AcOH (1.0)	<20
4	PivOH (1.0)	NR
5	TfOH (1.0)	NR
6	TFA (0.5)	16
7	TFA (1.5)	25

[a] Isolated yield. NR = No reaction

Our initial investigation began by using commercially available 2-aminobenzophenone **1a** and styrene **2a** as substrate with 5 mol % $Pd(OAc)_2$, 1.0 equiv of $Cu(OAc)_2$ in 1,4-dioxane at 90 °C for 16h (Table S1, entry 1). But, the reaction did not proceeded to generate compound **3a**. Then the feasibility of the reaction was tested with various other Bronsted acids such as TFA, AcOH, PivOH and TfOH (entries 2-5). To our surprise, the desired compound was obtained in 33% yield with TFA (entry 2) and very low yield with AcOH (entry 3). Whereas, no progress of reaction with PivOH and TfOH (entries 4-5). Finally, the equivalents of TFA was evaluated and the results shown that 2.0 equivalents as the best choice. (entries 6 and 7).

2.2 Table S2. Optimization of the oxidant



1a, 0.5 mmol **2a, 0.75 mmol** **3a**

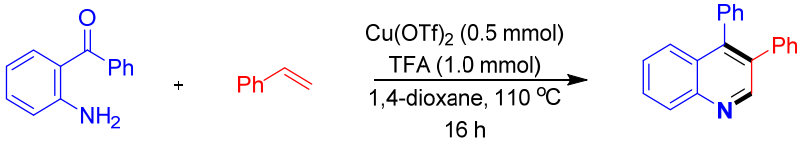
Entry	Oxidant (mmol)	Yield (%)[a]
1	$Cu(OTf)_2$ (0.5)	55
2	$CuCl_2$ (0.5)	---
3	$Cu(OAc)_2.H_2O$ (0.5)	28
4	AgOAc (0.5)	---
5	CuCl (0.5)	---
6	Cu_2O (0.5)	---
7	PIDA (0.5)	---[b]
8	$Cu(OTf)_2$ (1)	51
9	----	---[c]

[a] Isolated yield. [b] 3-phenylbenzo[*c*]isoxazole was observed instead of **3a**. [c] (5*Z*,11*Z*)-6,12-diphenyldibenzo[*b*,*f*][1,5]diazocine was formed.

With the optimized condition for additives, we next focused on the screening of various oxidant as shown in Table S2. The desired compound **3a** was obtained in 55% using $Cu(TFA)_2$ (entry 1). While other oxidants such as $CuCl_2$, $Cu(OAc)_2.H_2O$, AgOAc, CuCl, Cu_2O did not create the desired compound **3a** except with $Cu(OAc)_2.H_2O$ (entries 2-6). Interestingly, Then the reaction was carried with iodobenzene diacetate (PIDA) as

an oxidant, 3-phenylbenzo[*c*]isoxazole was isolated (entry 7). Next, the equivalents of $Cu(TFA)_2$ was increased to 2.0 and found that the yield of desired compound was reduced. Finally, in the absence of copper triflate, the starting material **1a** was consumed to generate (5*Z*,11*Z*)-6,12-diphenyldibenzo[*b*,*f*][1,5]diazocine.

2.3 Table S3. **Optimization of the metal catalyst**



1a, 0.5 mmol **2a, 0.75 mmol** **3a**

Entry	Metal (mol %)	Yield (%)[a]
1	$PdCl_2$ (5)	trace
2	PdI_2 (5)	<10
3	$PdCl_2(PPh_3)_2$ (5)	<10
4	$Pd(TFA)_2$ (5)	65
5	$NiCl_2$ (5)	<10
6	$NiCl_2$(dppp)[b] (5)	trace
7	---	---

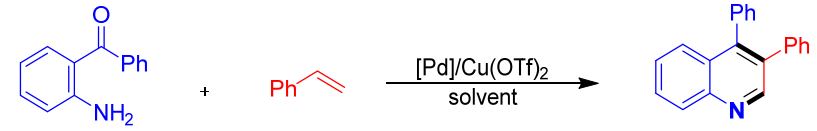
[a] Isolated yield. [b] [1,3-Bis(diphenylphosphino)propane]dichloronickel(II)

With the optimized condition of additive and oxidant we next performed the screening of various metal(II) salts as shown in Table S3. The reaction of 2-aminobenzophenone **1a** and styrene **2a** with various metals such as $PdCl_2$, PdI_2, $PdCl_2(PPh_3)_2$, $Pd(TFA)_2$, $NiCl_2$ and $NiCl_2$(dppp) entries (1-6). The desired compound **3a** was generated in 65% yield with $Pd(TFA)_2$ (entry 4). In the absence of metal, there is no progress in the reaction (entry 7).

After the evaluation of additive, oxidant and metal we have screened the choice of solvent as shown in Table S4 and the best result was obtained using chlorobenzene (entry 1-8). Interestingly, the target compound **3a** was generated in 87% yield by reducing the amount of $Cu(OTf)_2$ to a catalytic quantity (20 mol %) in the presence of O_2 as a terminal oxidant (entry 9). The reaction did not generate the desired compound **3a** in the absence of $Cu(OTf)_2$ (entry 10) as well as with $Cu(OTf)_2/O_2$ (entry 11). The reaction was

unsuccessful in the absence of TFA (entry 12) and also in the basic condition using acetate salt (entry 13). By replacing the $Pd(TFA)_2$/Chlorobenzene with $Pd(OAc)_2$/1,4-dioxane also failed to create compound **3a** (entry 14). Then, the equivalent studies of $Pd(TFA)_2$ and $Cu(OTf)_2$ (entries 15-18) revealed that 5 mol% of $Pd(TFA)_2$ and 20 mol % of $Cu(OTf)_2$ as the best combination (entry 9).

2.4 Table S4. Optimization of the solvent and other parameters

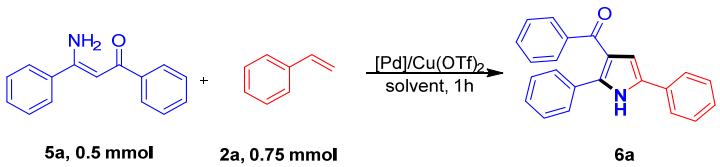


1a (0.507 mmol) **2a (0.761 mmol)** **3a**

Entry	Catalyst (x mol %)	Oxidant (y mmol)	Solvent	Additives (mmol)	Time, h	Temp, °C	Yield (%)[a]
1	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	1,4-dioxane	TFA (1)	16	110	65
2	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	DMSO	TFA (1)	16	110	12
3	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	DMF	TFA (1)	16	110	27
4	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	CH_3CN	TFA (1)	16	80	14
5	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	1,2-DCE	TFA (1)	16	80	39
6	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	THF	TFA (1)	16	65	68
7	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	Toluene	TFA (1)	4	110	82
8	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.5)	Chlorobenzene	TFA (1)	4	110	89
9[b]	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.1)	Chlorobenzene	TFA (1)	4	110	87
10[b]	$Pd(TFA)_2$ (5)	---	Chlorobenzene	TFA (1)	4	110	ND
11	$Pd(TFA)_2$ (5)	---	Chlorobenzene	TFA (1)	4	110	NR
12[b]	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.1)	Chlorobenzene	---	16	110	ND
13[b]	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.1)	Chlorobenzene	NaOAc (1)	16	110	ND
14[b]	$Pd(OAc)_2$ (10)	$Cu(OTf)_2$ (0.1)	1,4-dioxane	TFA (1)	16	110	Trace
15[b]	$Pd(TFA)_2$(2.5)	$Cu(OTf)_2$ (0.1)	Chlorobenzene	TFA (1)	12	110	75
16[b]	$Pd(TFA)_2$(10)	$Cu(OTf)_2$ (0.1)	Chlorobenzene	TFA (1)	4	110	85
17[b]	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.05)	Chlorobenzene	TFA (1)	12	110	85
18[b]	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.15)	Chlorobenzene	TFA (1)	4	110	70

[a] Isolated yield. [b] O_2 balloon was used. NR = No reaction. ND = Not detected

2.5 Table S5. Optimization of the reaction condition for pyrrole derivative 6a



5a, 0.5 mmol 2a, 0.75 mmol 6a

Entry	Metal (mol %)	Oxidant (mmol)	Solvent	Temp, °C	Yield (%)[a]
1	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.1)	PhCl	110	< 10
2	$Pd(TFA)_2$ (5)	$Cu(OTf)_2$ (0.1)	1,4-dioxane	90	< 20
3	$Pd(OAc)_2$ (5)	$Cu(OTf)_2$ (0.1)	PhCl	110	30
4	$Pd(OAc)_2$ (5)	$Cu(OTf)_2$ (0.1)	1,4-dioxane	90	48
5	$Pd(OAc)_2$ (10)	$Cu(OTf)_2$ (0.1)	1,4-dioxane	90	75

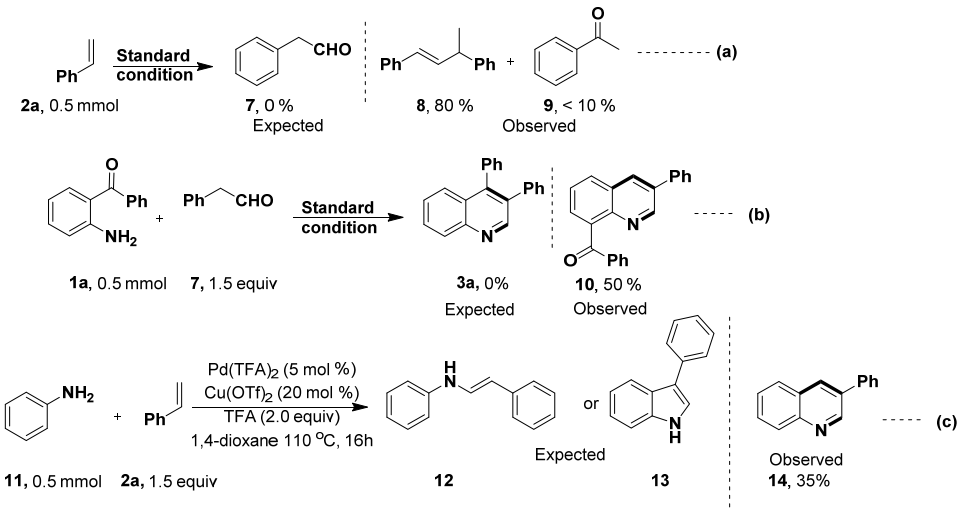
[a] Isolated yield.

The reaction didn't proceed well to generate the pyrrole derivative **6a** under the optimized condition of quinolines. Hence, the feasibility of the reaction was screened with $Pd(OAc)_2$ and 1,4-dioxane as shown in Table S5. The best yield of compound **6a** was obtained using 10 mol % of $Pd(OAc)_2$, 20 mol % of $Cu(OTf)_2$ in 1,4-dioxane at 90 °C for 1h (entry 5).

3. Control Studies

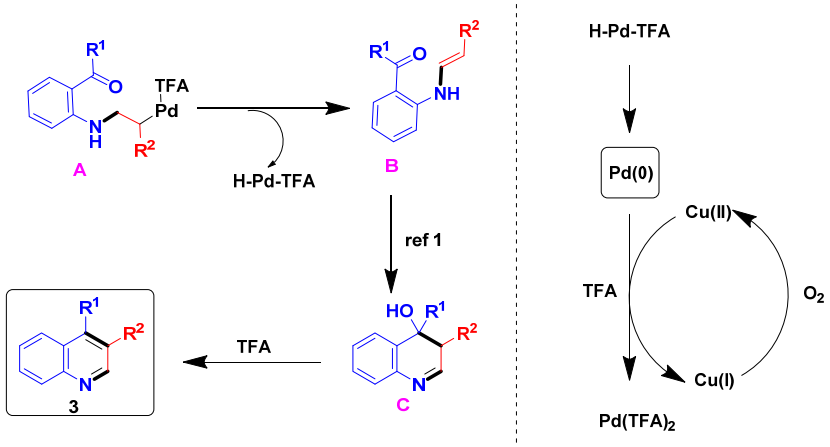
To gain some preliminary understanding on the mechanism, control experiments were carried out under standard conditions (Scheme S1a). The reaction of compound **2a** under optimized condition gave the dimerized product **8** in 80% and trace amount of Wacker oxidation product **9**, but not the expected aldehyde selective Wacker oxidation product **7**[1].This result eliminated the formation of phenyl acetaldehyde intermediate **7**. Next, 2-aminobenzophenone **1a** and phenyl acetaldehyde **7** were treated under standard protocol, but the desired compound **3a** was not formed, instead phenyl(3-phenylquinolin-8-yl)methanone **10** was isolated in 50 % yield (Scheme S1b). A similar observation was reported by Huang et al. using aniline and phenyl acetaldehyde **7** in the presence of CuBr/TfOH and they proposed that the reaction proceeds *via* enamine intermediate.[2] These results indicated that our present protocol might involve trapping of *in situ* generated 2-

amino alkyl palladium with ketone and ruled out the formation of enamine intermediate via *β*-hydride elimination. Our point of reaction in Scheme S1c was to know that the formed 2-amino alkyl intermediate from styrene **2a** and aniline **11 (**instead of ***ortho***-acyl aniline,**1a**) under standard condition would undergo β-hydride elimination to afford enamine or *ortho*-C-H functionalization followed by oxidation to for 3-aryl indoles. But to our surprise, the observed product was found to be 3-phenyl quinolines and their structure was confirmed by NMR analysis (NMR is slightly impure). Further mechanistic studies are under investigation.



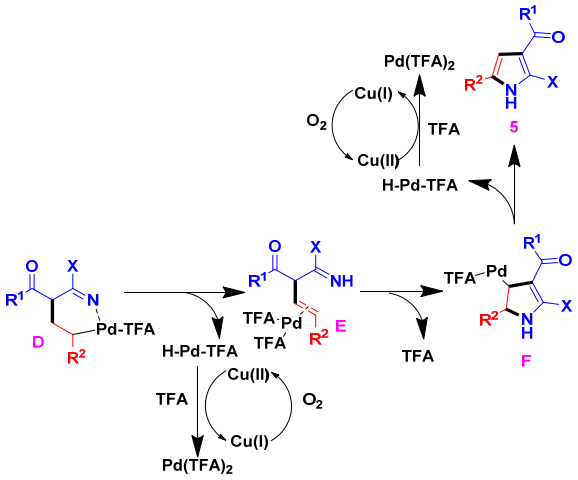
Scheme S1. Control Studies

4. proposed reaction mechanism pathway



Scheme S2. Alternative pathway for quinolines

We have also proposed an alternative route for quinoline derivatives as shown in Scheme S2. The *β*-elimination of intermediate **A** would provide enamine intermediate **B**, which can undergo an intramolecular annulation to form the intermediate **C**[3] followed by dehydration to beget the quinolines **3**.



Scheme S3. Alternative pathway for pyrroles

On the other hand, we have also proposed an alternative route for pyrrole derivatives as shown in Scheme S3. The *β*-hydride elimination of **D** would generate alkene intermediate **E** and active Pd(II) will be regenerated in the presence of oxidant. Then, the intramolecular aminopalladation via a 5-*endo–trig* annulation of **E** gave the annulated compound **F**[4] followed by *β*-hydride elimination also produce the target pyrrole **6**.

5. General experimental procedure

5.1 General procedure for synthesis of 3,4-disubstituted quinolines 3a-s

A 2 dram vial was charged with respective *o*-acyl aniline **1a-e** (0.5 mmol) and alkenes **2a-k** (0.75 mmol) in chlorobenzene (2.0 mL) followed by the addition of $Pd(TFA)_2$ (5 mol %), $Cu(OTf)_2$ (20 mol %) and TFA (1.0 mmol). The resultant reaction mixture was stirred under O_2 balloon at 110 $^{\circ}$C until the completion of reaction by TLC (2-6 h). The reaction mass was cooled to room temperature (25 ^{o}C) and successively diluted with H_2O. The aqueous layer was extracted with ethyl acetate (3X10ml), and combined organic layer was washed with 10 % $NaHCO_3$ (1X10 mL) followed by water (3X10ml) and brine

solution. The final solution was dried over Na_2SO_4 and concentrated under reduced pressure and then purified by column chromatography using hexane to 5% EA/hexane to obtain the pure compound **3a-s**.

5.2 General procedure for synthesis of 3,4-disubstituted quinolines 4a-i

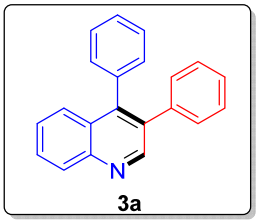
A 2 dram vial was charged with respective *o*-acyl aniline **1a-b** (0.5 mmol) and alkenes **2l-q** (0.75 mmol) in chlorobenzene (2.0 mL) followed by the addition of $Pd(TFA)_2$ (5 mol %), $Cu(OTf)_2$ (20 mol % or 0.5 mmol) and TFA (1.0 mmol). The resultant reaction mixture was stirred with or without O_2 balloon at mentioned time and temperature in Scheme 4. The reaction mass was cooled to room temperature (25 ^oC) and successively diluted with H_2O. The aqueous layer was extracted with ethyl acetate (3X10ml), and combined organic layer was washed with 10 % $NaHCO_3$ (1X10 mL) followed by water (3X10ml) and brine solution. The final solution was dried over Na_2SO_4 and concentrated under reduced pressure and then purified by column chromatography using hexane to 5% EA/hexane to obtain the pure compound **4a-i**.

5.3 General procedure for synthesis of 2,3,5-trisubstituted pyrroles 6a-k

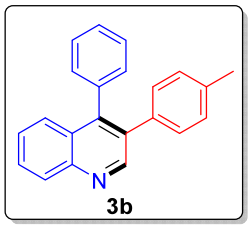
The starting material 5a-5d were prepared according to the previously reported literature methods.[5] A 2 dram vial was charged with respective enaminoketones **5a-c/enaminoesters 5d** (0.5 mmol) and **2a-c**, **f-i** (0.75 mmol) in 1,4-dioxane (2.0 mL) followed by the addition of $Pd(OAc)_2$ (10 mol %), $Cu(OTf)_2$ (20 mol %) and TFA (1.0 mmol). The resultant reaction mixture was stirred under O_2 balloon at 90 $^\circ C$ until the completion of reaction by TLC (1-6 h). The reaction mass was cooled to room temperature (25 ^oC) and successively diluted with H_2O. The aqueous layer was extracted with ethyl acetate (3X10ml), and combined organic layer was washed with 10 % $NaHCO_3$ (1X10 mL) followed by water (3X10ml) and brine solution. The final solution was dried over Na_2SO_4 and concentrated under reduced pressure and then purified by column chromatography using hexane to 5% EA/hexane to obtain the pure compound **6a-j**.

6. Experimental characterization of compounds 3, 4 and 6

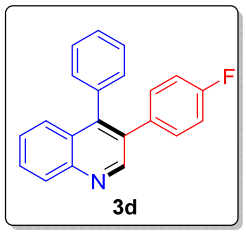
3,4-diphenylquinoline (3a) Yellow solid; Mp: 141-142 °C; Yield: 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (s, 1H), 8.21 (d, J = 8.4 Hz, 1H), 7.75-7.69 (m, 2H), 7.48 (t, J = 8.0 Hz, 1H), 7.36-7.34 (m, 3H), 7.25-7.16 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 147.3, 145.6, 138.0, 136.1, 133.1, 130.4, 130.1, 129.3, 129.1, 128.1, 128.0, 127.7, 127.2, 127.0, 126.9, 126.5; HRMS (ESI) calcd for $C_{21}H_{16}N$ $[M + H]^+$: 282.1275; found: 282.1277.



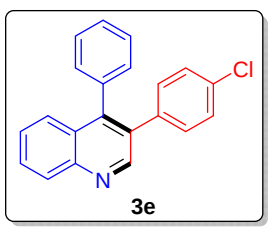
4-phenyl-3-(*p*-tolyl)quinoline (3b) White solid; Mp: 154-155 °C; Yield: 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 8.21 (d, J = 8.4 Hz, 1H), 7.72 (ddd, J = 15.2, 8.4, 1.6 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.48 (t, J = 8.0, 1H), 7.37-7.34 (m, 3H), 7.22-7.19 (m, 2H), 7.07-7.05 (m, 4H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 146.9, 145.7, 136.8, 136.3, 134.9, 133.1, 130.4, 129.9, 129.17, 129.10, 128.8, 128.1, 127.7, 127.3, 126.9, 126.5, 21.1; HRMS (ESI) calcd for $C_{22}H_{18}N$ $[M + H]^+$: 296.1433; found: 293.1433.



3-(4-fluorophenyl)-4-phenylquinoline (3d) Pale yellow Solid; Mp:119-120 °C; Yield: 79%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.26 (d, J = 8.4 Hz, 1H), 7.76 (ddd, J = 14.8, 8.0, 1.6, 1H), 7.70 (d, J = 8.8 Hz, 1H), 7.52 (ddd, J = 15.6, 8.0, 1.2 Hz, 1H), 7.38-7.36 (m, 3H), 7.20-7.11 (m, 4H), 6.94 (t, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.9, 163.2, 160.7, 150.7, 146.5, 135.8, 132.2, 131.7 (d, J_F = 9 Hz), 130.4, 129.6, 128.8, 128.3, 128.0, 127.2, 126.4, 115.2 (d, J_F = 21 Hz), 114.3; HRMS (ESI) calcd for $C_{21}H_{15}FN$ $[M + H]^+$: 300.3484; found: 300.3487.

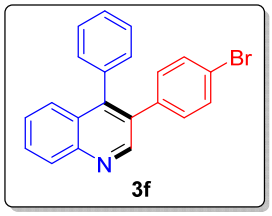


3-(4-chlorophenyl)-4-phenylquinoline (3e) Off-white solid; Mp: 150-151 °C; Yield: 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.25 (d, J = 8.4 Hz, 1H), 7.76 (ddd, J = 15.6, 8.4, 1.2 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.51 (ddd, J = 15.6, 8.0, 1.6 Hz, 1H), 7.39-7.36 (m, 3H), 7.24-7.17 (m, 4H), 7.09 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100



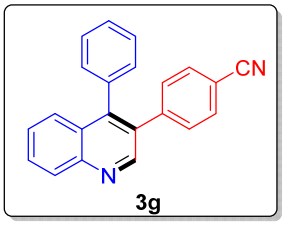
MHz, $CDCl_3$) δ 150.7, 146.8, 146.4, 136.2, 135.7, 133.4, 132.0, 131.3, 130.3, 129.7, 129.0, 128.9, 128.4, 128.3, 128.0, 127.2, 126.6; HRMS (ESI) calcd for $C_{21}H_{15}ClN$ $[M + H]^+$: 316.0815; found: 316.0817.

3-(4-bromophenyl)-4-phenylquinoline (3f) Yellow solid; Mp: 155-156 °C; Yield: 83%;



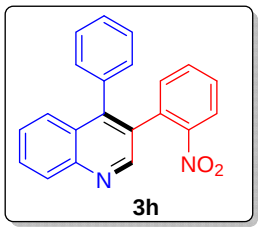
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.28 (d, J = 8.4 Hz, 1H), 7.77 (ddd, J = 14.0 ,8.4,1.2 Hz, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.52 (ddd, J = 15.6, 8.4, 1.2 Hz, 1H), 7.40-7.36 (m, 5H), 7.21-7.17 (m, 2H), 7.03 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.6, 149.9, 135.7, 133.3, 132.9, 132.3, 131.6, 131.3, 130.3, 130.1, 129.8, 129.6, 128.9, 128.3, 128.0, 127.8, 127.2; HRMS (ESI) calcd for $C_{21}H_{15}BrN$ $[M + H]^+$: 360.0381; found: 360.0379.

4-(4-phenylquinolin-3-yl)benzonitrile (3g) White solid; Mp: 180-181 °C; Yield: 72%;



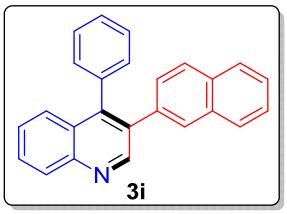
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.17 (d, J = 8.4 Hz, 1H), 7.73 (ddd, J = 15.2, 6.8, 1.2 Hz, 1H), 7.67 (dd, J = 8.4, 1.2 Hz, 1H), 7.51-7.46 (m, 3H), 7.36-7.33 (m, 3H), 7.24 (d, J = 8.4 Hz, 2H), 7.15-7.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 147.8, 146.0, 143.0, 135.3, 131.7, 131.2, 130.7, 130.2, 130.1, 129.7, 129.4, 128.3, 127.2, 126.5, 118.5, 110.8; HRMS (ESI) calcd for $C_{22}H_{15}N_2$ $[M + H]^+$: 307.1231; found: 307.1229.

3-(2-nitrophenyl)-4-phenylquinoline (3h) Yellow solid; Mp: 111-112 °C; Yield: 64%;

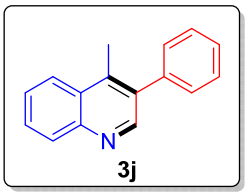


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.26 (d, J = 8.8 Hz, 1H), 7.92 (dd, J = 8.0, 1.6 Hz, 1H), 7.78 (ddd, J = 15.2, 8.4, 1.6, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.52 (t, J = 7.6 Hz, 2H), 7.42 (t, J = 8.4 Hz, 1H), 7.32-7.27 (m, 4H), 7.21-7.18 (m, 1H), 7.10 (dd, J = 7.6, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 148.8, 147.2, 146.3, 135.1, 133.3, 132.6, 129.9, 129.8, 129.1, 128.8, 128.5, 128.1, 127.8, 127.3, 126.5, 124.5; HRMS (ESI) $[M + H]^+$ calcd for $C_{21}H_{15}N_2O_2$: 327.1127; found: 327.1130.

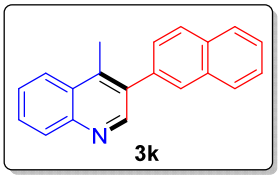
3-(naphthalen-2-yl)-4-phenylquinoline (3i) Bright yellow solid; Mp: 138-139 °C; Yield: 79%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.23 (d, J = 8.8 Hz, 1H), 7.78-7.72 (m, 5H), 7.64 (d, J = 8.4 Hz, 1H), 7.51 (ddd, J = 14.4, 8.4, 1.2 Hz, 1H), 7.47-7.45 (m, 2H), 7.34-7.31 (m, 3H), 7.25-7.23 (m, 2H), 7.18 (dd, J = 8.4, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.5, 136.1, 135.6, 133.1, 132.9, 132.0, 130.5, 129.4, 129.1, 129.0, 128.8, 128.2, 128.0, 127.8, 127.7, 127.5, 127.4, 127.2, 126.9, 126.5, 126.1, 125.0, 123.1; HRMS (ESI) calcd for $C_{25}H_{18}N$ $[M + H]^+$: 332.1436; found: 332.1433.



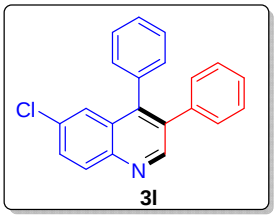
4-methyl-3-phenylquinoline (3j) Yellow solid; Mp: 58-61 °C; Yield: 58% (63.6 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.14 (dd, J = 8.4, 0.8 Hz, 1H), 8.09 (dd, J = 8.4, 1.2 Hz, 1H), 7.73 (ddd, J = 15.2, 6.8, 1.6 Hz, 1H), 7.61 (ddd, J = 15.2, 8.4, 1.2 Hz, 1H), 7.52-7.38 (m, 5H), 2.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 146.9, 140.6, 138.6, 134.4, 129.94, 129.93, 128.8, 128.4, 127.9, 127.5, 126.7, 124.1, 15.6; HRMS (ESI) calcd for $C_{16}H_{14}N$ $[M + H]^+$: 220.1048; found: 220.1045.



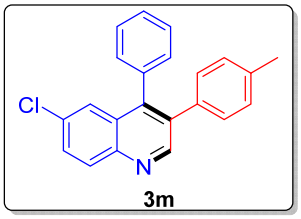
4-methyl-3-(naphthalen-2-yl)quinoline (3k) Dark brown solid; Yield: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (s, 1H), 8.46 (d, J = 8.4 Hz, 1H), 8.21 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 8.4 Hz, 2H), 7.96-7.86 (m, 3H), 7.76 (t, J = 7.6 Hz, 1H), 7.61-7.56 (m, 2H), 7.50 (dd, J = 8.4, 1.6 Hz, 1H), 2.79 (s, 3H); HRMS (ESI) calcd for $C_{20}H_{16}N$ $[M + H]^+$: 270.1277; found: 270.1276.



6-chloro-3,4-diphenylquinoline (3l) Yellow solid; Mp:177-178 °C; Yield: 69%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.15 (d, J = 9.6 Hz, 1H), 7.67-7.64 (m, 2H), 7.38-7.34 (m, 3H), 7.27-7.22 (m, 3H), 7.20-7.13 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 145.6, 144.9, 137.5, 135.4, 133.9, 132.9, 130.9, 130.3, 130.1, 130.0, 128.3, 128.1, 128.0, 127.6, 127.3, 125.3; HRMS (ESI) calcd for $C_{21}H_{15}ClN$ $[M + H]^+$: 316.0815; found: 316.0817.

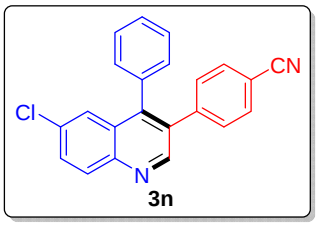


6-chloro-4-phenyl-3-(*p*-tolyl)quinoline (3m) White solid; Mp: 181-182 °C; Yield: 68%;

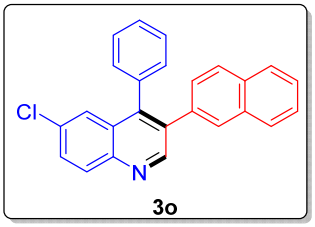


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.16 (d, J = 8.8 Hz, 1H), 7.67-7.65 (m, 2H), 7.40-7.37 (m, 3H), 7.20-7.16 (m, 2H), 7.07-7.02 (m, 4H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 137.1, 135.6, 134.5, 134.1, 132.9, 130.8, 130.3, 130.0, 129.8, 129.4, 128.9, 128.4, 128.1, 127.7, 125.3, 120.0, 21.4; HRMS (ESI) calcd for $C_{22}H_{17}ClN$ $[M + H]^+$: 330.1046; found: 330.1044.

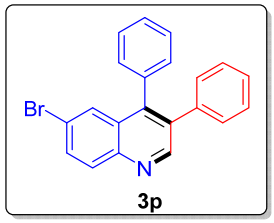
-(6-chloro-4-phenylquinolin-3-yl)benzonitrile (3n) White solid; Mp: 198-199 °C; Yield: 64%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.13 (d, J = 8.8 Hz, 1H), 7.70-7.65 (m, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.42-7.36 (m, 3H), 7.26 (d, J = 8.4 Hz, 2H), 7.17-7.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.8, 146.3, 145.2, 142.5, 134.7, 133.3, 132.0, 131.8, 131.2, 130.7, 130.6, 128.6, 128.5, 127.7, 125.3, 118.4, 111.1; HRMS (ESI) calcd for $C_{22}H_{14}ClN_2$ $[M + H]^+$: 341.0839; found: 341.0840.



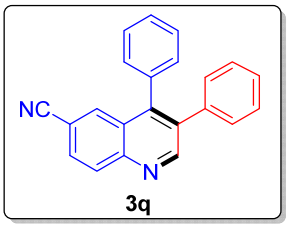
6-chloro-3-(naphthalen-2-yl)-4-phenylquinoline (3o) Light yellow solid; Mp: 204-205 °C; Yield: 67%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (s, 1H), 8.20 (d, J = 9.2 Hz, 1H), 7.79-7.63 (m, 6H), 7.49-7.45 (m, 2H), 7.36-7.33 (m, 3H), 7.24-7.21 (m, 2H), 7.15 (dd, J = 8.4, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 145.5, 135.4, 135.0, 133.1, 132.5, 132.1, 130.8, 130.4, 130.2, 129.4, 129.2, 128.8, 128.4, 128.3, 128.2, 128.0, 127.7, 127.5, 127.0, 126.4, 125.3, 120.4; HRMS (ESI) calcd for $C_{25}H_{17}ClN$ $[M + H]^+$: 366.1044; found: 366.1044.



6-bromo-3,4-diphenylquinoline (3p) Pale yellow solid; Mp: 220-221 °C; Yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (s, 1H), 8.10 (d, J = 8.8 Hz, 1H), 7.81 (ddd, J = 20.0, 11.2, 2.0 Hz, 2H), 7.39-7.35(m, 3H), 7.26-7.22 (m, 3H), 7.20-7.13 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 145.5, 145.1, 137.4, 135.3, 132.8, 130.8, 130.3, 130.0, 128.6, 128.4, 128.1, 127.3, 121.3; HRMS (ESI) calcd for $C_{21}H_{15}BrN$ $[M + H]^+$: 360.0394; found: 360.0396.

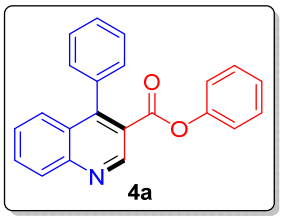


7,8-diphenyl-2-naphthonitrile (3q) Grey solid; Mp: 203-204°C; Yield: 48% (73.5 mg);



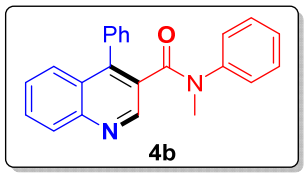
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.27 (d, J = 8.8 Hz, 1H), 8.09 (s, 1H), 7.85 (dd, J = 8.8, 1.6 Hz, 1H), 7.42-7.38 (m, 3H), 7.28-7.26 (m, 3H), 7.19-7.14 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 148.3, 145.9, 137.0, 134.7, 133.2, 131.0, 130.2, 129.9, 129.6, 128.5, 128.4, 128.2, 127.6, 118.7, 110.5; HRMS (ESI) calcd for $C_{22}H_{15}N_2$ $[M + H]^+$: 307.1229; found: 307.1228.

Phenyl 4-phenylquinoline-3-carboxylate (4a) Off-white solid; Mp: 142-143 °C; Yield:



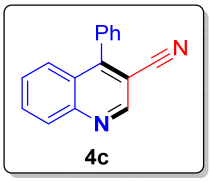
55% (89.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.48 (s, 1H), 8.23 (d, J = 8.0 Hz, 1H), 7.90 (ddd, J = 15.2, 6.8, 1.2 Hz, 1H), 7.65 (dd, J = 8.4, 0.8 Hz, 1H), 7.56-7.51 (m, 4H), 7.41-7.38 (m, 2H), 7.31 (t, J = 8.4 Hz, 2H), 7.19 (ddd, J = 14.8, 7.6, 1.2 Hz, 1H), 6.84 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 150.39, 150.33, 149.9, 149.3, 136.2, 131.3, 129.6, 129.3, 128.9, 128.4, 128.2, 127.6, 127.4, 126.9, 125.9, 122.6, 121.2; HRMS (ESI) calcd for $C_{22}H_{16}NO_2$ $[M + H]^+$: 326.1174; found: 326.1175.

***N*-methyl-*N*,4-diphenylquinoline-3-carboxamide (4b)** Yellow solid; Mp: 125-126 °C;



Yield: 61%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (s, 1H), 8.08 (d, J = 8.4 Hz, 1H), 7.67 (ddd, J = 15.2, 8.0, 1.2 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.51-7.37 (m, 4H), 7.08 (s, 2H), 6.97-6.95 (m, 3H), 6.45-6.43 (m, 2H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 149.2, 148.0, 143.7, 142.1, 134.5, 130.3, 129.7, 129.5, 129.2, 128.6, 128.5, 128.0, 127.0, 126.5, 126.4, 126.2, 125.8, 37.0; HRMS (ESI) calcd for $C_{23}H_{19}N_2O$ $[M + H]^+$: 339.1490; found: 339.1491.

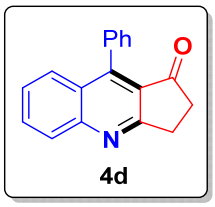
4-phenylquinoline-3-carbonitrile (4c) White solid; Mp: 182-183 °C; Yield: 58%; ^{1}H



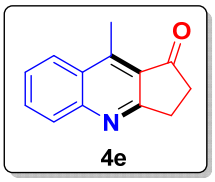
NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.22 (d, J = 8.4 Hz, 1H), 7.87 (ddd, J = 15.2, 8.4, 1.2 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.62-7.58 (m, 4H), 7.50-7.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 150.0, 149.0, 133.8, 132.2, 130.0, 129.8, 129.4, 128.8, 128.3,

127.0, 125.8, 122.3, 116.9; HRMS (ESI) calcd for $C_{16}H_{11}N_2$ $[M + H]^+$: 231.0918; found: 231.0916.

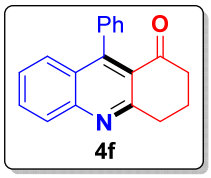
9-phenyl-2,3-dihydro-1*H*-cyclopenta[*b*]quinolin-1-one (4d) Grey solid; Mp: 185-186 °C; Yield: 65%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.4 Hz, 1H), 7.83 (ddd, J = 14.8, 8.0, 1.2 Hz, 1H), 7.76 (dd, J = 8.8, 1.2 Hz, 1H), 7.54 (d, J = 3.2 Hz, 3H), 7.49 (ddd, J = 15.2, 8.4, 1.2, 1H), 7.37-7.33 (m, 2H), 3.45 (t, J = 6.8, 2H), 2.84 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.7, 171.0, 151.2, 149.0, 133.1, 132.1, 129.3, 128.9, 128.8, 128.3, 128.0, 126.6, 123.8, 36.5, 28.4; HRMS (ESI) calcd for $C_{18}H_{14}NO$ $[M + H]^+$: 260.1072; found: 260.1069.



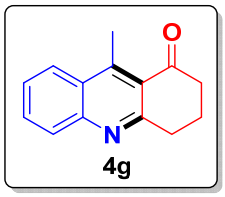
9-methyl-2,3-dihydro-1*H*-cyclopenta[*b*]quinolin-1-one (4e) Brown solid; Mp: 134-135 °C; Yield: 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.4 Hz, 1H), 8.06 (d, J = 8.4 Hz, 1H), 7.80 (ddd, J = 15.2, 8.4, 1.2 Hz, 1H), 7.58 (t, J = 7.2 Hz, 1H), 3.32 (t, J = 7.2 Hz, 2H), 3.04 (s, 3H), 2.83 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.2, 170.7, 150.1, 148.1, 131.9, 129.2, 127.0, 126.3, 125.4, 124.8, 36.5, 28.0, 12.5; HRMS (ESI) calcd for $C_{13}H_{12}NO$ $[M + H]^+$: 198.0910; found: 198.0913.



9-phenyl-3,4-dihydroacridin-1(2*H*)-one (4f) Off-white solid; Mp: 170-171 °C; Yield: 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.4 Hz, 1H), 7.76 (t, J = 7.2 Hz, 1H), 7.50-7.45 (m, 4H), 7.40 (t, J = 8.0 Hz, 1H), 7.18 (d, J = 7.6 Hz, 2H), 3.38 (t, J = 6.4 Hz, 2H), 2.70 (t, J = 6.4 Hz, 2H), 2.25 (quin, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 162.2, 151.4, 148.6, 137.6, 131.7, 128.4, 128.2, 128.09, 128.00, 127.5, 127.4, 126.4, 123.8, 40.6, 34.5, 21.3; HRMS (ESI) calcd for $C_{19}H_{20}NO$ $[M + H]^+$: 274.1128; found: 274.1131.

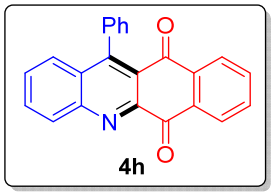


9-methyl-3,4-dihydroacridin-1(2*H*)-one (4g) The spectral data are in accordance with the previously reported literature.[6] Pale yellow solid; Mp: 131-132 °C; Yield: 61%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (dd, J = 8.8, 0.8, Hz, 1H), 8.06 (d, J = 8.4 Hz, 1H), 7.79 (ddd, J = 15.2, 8.4, 1.6, 1H),



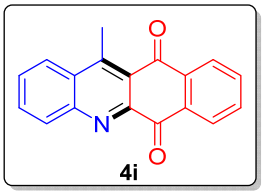
7.58 (ddd, J = 15.6, 8.4, 1.6, 1H), 3.31 (t, J = 6.4 Hz, 2H), 3.06 (s, 3H), 2.81 (t, J = 6.4 Hz, 2H), 2.21 (quin, J = 6.4 Hz, 2H); HRMS (ESI) calcd for $C_{14}H_{14}NO$ $[M + H]^+$: 212.0997; found: 212.1002.

12-phenylbenzo[*b*]acridine-6,11-dione (4h) Yellow solid; Mp: 219-220 °C; Yield: 67%;

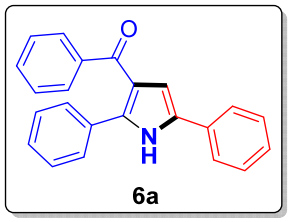


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, J = 8.4 Hz, 1H), 8.45 (d, J = 8.0 Hz, 1H), 8.17 (dd, J = 7.6, 1.6 Hz, 1H), 7.91 (t, J = 6.0 Hz, 1H), 7.84-7.76 (m, 2H), 7.63-7.59 (m, 5H), 7.29-7.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.6, 182.0, 152.9, 149.3, 148.3, 137.1, 134.7, 134.2, 133.5, 132.7, 131.5, 129.8, 129.6, 128.4, 128.1, 128.0, 127.8, 127.6, 124.0; HRMS (ESI) calcd for $C_{23}H_{14}NO_2$ $[M + H]^+$: 336.1019; found: 336.1019.

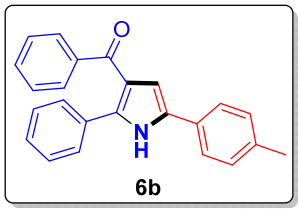
12-methylbenzo[*b*]acridine-6,11-dione (4i) Dark brown solid; Mp: 182-183 °C; Yield: 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, J = 8.4 Hz, 1H), 8.39 (d, J = 8.0 Hz, 1H), 8.35 (d, J = 8.0 Hz, 1H), 8.31 (d, J = 7.6 Hz, 1H), 7.90 (t, J = 8.0 Hz, 1H), 7.83 (t, J = 8.0 Hz, 2H), 7.75 (t, J = 8.4 Hz, 1H), 3.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.0, 182.0, 152.1, 148.3, 148.1, 135.3, 134.7, 134.0, 133.2, 132.5, 132.1, 129.8, 129.5, 127.54, 127.52, 125.3, 16.6; HRMS (ESI) calcd for $C_{18}H_{12}NO_2$ $[M + H]^+$: 274.0860; found: 274.0862.



(2,5-diphenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (6a) Pale yellow solid; Mp: 161-162 °C; Yield: 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (s, 1H), 7.80 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 7.6 Hz, 2H), 7.46-7.43 (m, 3H), 7.39 (t, J = 8.0 Hz, 2H), 7.32 (t, J = 8.0 Hz, 2H), 7.29-7.23 (m, 4H), 6.85 (d, J = 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 139.3, 137.8, 131.8, 131.7, 131.3, 129.6, 129.0, 128.4, 128.3, 128.1, 127.8, 127.1, 124.1, 121.9, 110.4; HRMS (ESI) calcd for $C_{23}H_{18}NO$ $[M + H]^+$: 324.1383; found: 324.1382.

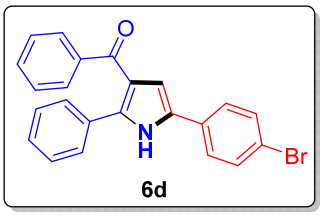


Phenyl(2-phenyl-5-(*p*-tolyl)-1*H*-pyrrol-3-yl)methanone (6b) Yellow solid; Mp: 154-155 °C; Yield: 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 7.79 (d, J = 8.4 Hz, 2H), 7.45-7.40 (m, 5H), 7.31 (t, J = 8.0 Hz, 2H), 7.28-7.24 (m, 3H), 7.20 (d, J = 7.6 Hz, 2H), 6.80 (d, J = 2.8 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 139.4, 137.5, 137.0, 132.0, 131.8, 131.6, 129.9, 129.7, 128.7, 128.4, 128.0, 127.1, 126.1, 124.0, 121.8, 109.9, 21.1; HRMS (ESI) calcd for $C_{24}H_{20}NO$ $[M + H]^+$: 338.1540; found: 338.1539.



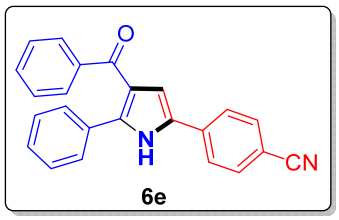
6b

(5-(4-bromophenyl)-2-phenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (6d) Off-white solid; Mp: 188-189 °C; Yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 7.75 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.45-7.35 (m, 5H), 7.30 (t, J = 8.0 Hz, 2H), 7.20-7.17 (m, 3H), 6.78 (d, J = 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 139.1, 138.3, 132.0, 131.8, 131.4, 130.8, 130.3, 129.6, 128.4, 128.3, 128.1, 127.9, 125.6, 121.9, 120.6, 110.8; HRMS (ESI) calcd for $C_{23}H_{17}BrNO$: 402.0485; found: 402.0487.



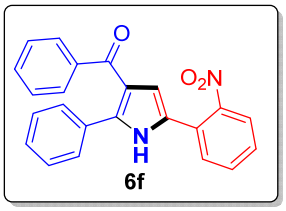
6d

4-(4-benzoyl-5-phenyl-1*H*-pyrrol-2-yl)benzonitrile (6e) White solid; Mp: 205-206 °C; Yield: 70%; 1H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 7.79 (d, J = 8.0 Hz, 2H), 7.65-7.59 (m, 4H), 7.46 (ddd, J = 14.8, 7.6, 1.2 Hz, 1H), 7.43-7.40 (m, 2H), 7.33 (t, J = 8.0 Hz, 2H), 7.24-7.22 (m, 3H), 6.95 (d, J = 2.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.2, 139.4, 138.9, 135.4, 132.8, 132.0, 131.1, 129.8, 129.6, 128.5, 128.4, 128.0, 124.1, 122.4, 118.8, 112.8, 109.8; HRMS (ESI) calcd for $C_{24}H_{17}N_2O$ $[M + H]^+$: 349.1335; found: 349.1335.



6e

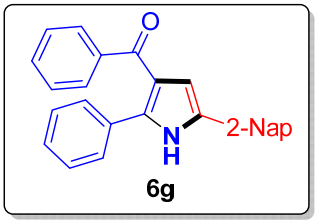
(5-(2-nitrophenyl)-2-phenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (6f) Green solid; Mp: 87-88 °C; Yield: 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (s, 1H), 7.85 (dd, J = 8.0, 1.2 Hz, 1H), 7.80 (d, J = 8.0 Hz, 2H), 7.68 (dd, J = 8.0, 1.6 Hz, 1H), 7.62 (dt, J = 8.0, 1.6 Hz, 1H), 7.50-7.42 (m, 4H), 7.35-7.28 (m, 5H), 6.83 (d, J = 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 139.1, 132.1, 131.8, 131.4, 131.2, 129.6, 128.5,



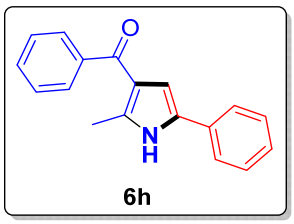
6f

128.47, 128.43, 128.1, 127.9, 126.3, 126.0, 124.9, 121.6, 115.8; HRMS (ESI) calcd for $C_{23}H_{17}N_2O_3$: 369.1232; found: 369.1235.

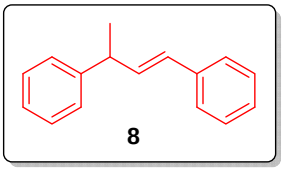
(5-(naphthalen-2-yl)-2-phenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (6g) Pale yellow solid; Mp: 102-103 °C; Yield: 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (s, 1H), 7.92 (s, 1H), 7.85-7.77 (m, 5H), 7.66 (dd, J = 8.8, 1.6 Hz, 1H), 7.48-7.42 (m, 5H), 7.33 (t, J = 7.6 Hz, 2H), 7.27-7.22 (m, 3H), 6.95 (d, J = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 139.3, 138.2, 133.5, 132.4, 131.8, 131.7, 129.7, 128.7, 128.4, 128.3, 128.1, 127.7, 126.6, 125.8, 122.9, 122.0, 121.7, 111.0; HRMS (ESI) calcd for $C_{27}H_{20}NO$ $[M + H]^+$: 374.1539; found: 374.1541.



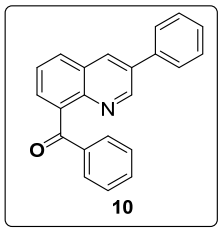
(2-methyl-5-phenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (6h) White solid; Mp: 185-186 °C ; Yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (s, 1H), 7.84 (d, J = 8.4 Hz, 2H), 7.53 (tt, J = 7.2, 1.2 Hz, 1H), 7.48-7.44 (m, 4H), 7.36 (t, J = 8.0 Hz, 2H), 7.23 (tt, J = 7.2, 1.2 Hz, 2H), 6.67 (d, J = 2.8 Hz, 1H), 2.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 140.4, 137.4, 131.6, 131.2, 129.6, 129.0, 128.9, 128.0, 126.7, 123.7, 121.2, 109.1, 13.9; HRMS (ESI) calcd for $C_{18}H_{16}NO$ $[M + H]^+$: 262.1226; found: 262.1223.



(*E*)-but-1-ene-1,3-diyldibenzene (8) Colourless liquid; Yield: 80 % (83.3 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.25 (m, 10 H), 6.51-6.42 (m, 2H), 3.74-3.67 (m, 1H), 1.53 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 137.5, 135.1, 128.48, 128.45, 127.2, 127.0, 126.18, 126.11, 42.5, 21.1; HRMS (ESI) calcd for C16H17 $[M + H]^+$: 209.3040; found: 209.3037.

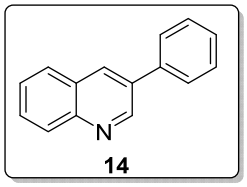


Phenyl(3-phenylquinolin-8-yl)methanone (10) Yellow solid; Mp: 121-122 °C; Yield: 50% (77.3 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (s, 1H), 8.37 (s, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.87 (d, J = 7.2 Hz, 2H), 7.75 (d, J = 6.8 Hz, 1H), 7.68 (t, J = 7.2 Hz, 3H), 7.59-7.41 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 153.3, 150.2, 144.3, 138.4, 137.6, 137.1, 134.4,



133.7, 133.3, 130.3, 130.1, 129.2, 128.7, 128.4, 128.1, 127.4, 126.5; HRMS (ESI) calcd for $C_{25}H_{16}NO$ 310.1154; found: 310.1151.

3-phenylquinoline (14) Yellow oil; Yield: 35% (35.9 mg); ^{1}H NMR (400 MHz, $CDCl_3$)



14

δ 9.18 (d, J = 2.0 Hz, 1H), 8.30 (d, J = 2.0 Hz, 1H), 8.15 (d, J = 8.4 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.74-7.70 (m, 3H), 7.60-7.51 (m, 3H), 7.46-7.42 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 147.2, 137.8, 133.5, 133.2, 129.3, 129.1, 128.3, 128.0, 127.4, 127.0; HRMS (ESI) calcd for $C_{15}H_{12}N$ $[M + H]^+$: 206.0891; found: 206.0894.

7. References

1. P. Teo, Z. K. Wickens, G. Dong, R. H. Grubbs, *Org. Lett*., 2012, **14**, 3237.

2. R. Yan, X. Liu, C. Pan, X. Zhou, X. Li, X. Kang and G. Huang, *Org. Lett.*, 2013, **15**, 4876.

3. L. Kong, Y. Zhou, H. Huang, Y. Yang, Y. Liu, Y. Li. *J. Org. Chem*. 2015, **80**, 1275.

4. W. Yang, L. Huang, H. Liu, W. Wang, H. Li. *Chem. Commun*. 2013, **49**, 4667.

5. (*a*) X. Sun, Y. Lyu, D. Zhang-Negrerie, Y. Du, K. Zhao, *Org. Lett*., 2013, **15**, 6222; (*b*) M. Sugiura, M. Kumahara, M. Nakajima, *Chem. Commun*., 2009, 3585; (*c*) A. Fuerstner, H. Weintritt, A. Hupperts, *J. Org. Chem*., 1995, **60**, 6637; (*d*) T. Sasada, F. Kobayashi, N. Sakai, T. Konakahara, *Org. Lett*., 2009, **11**, 2161.

6. J. Yang, J. -N. Tana, Y. Gu, *Green Chem*., 2012,**14**, 3304.

8. X-ray analysis

Compound 3g

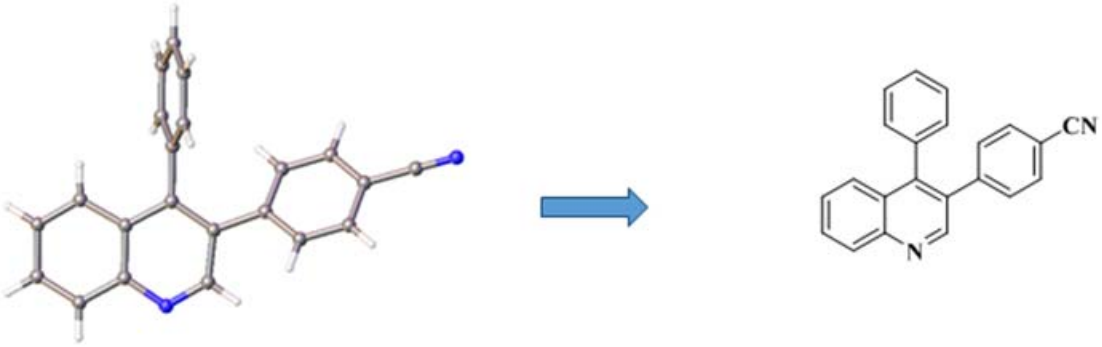


Table 1. Crystal data and structure refinement for compound **3g**.

Identification code	**3g**	
Empirical formula	$C_{22}H_{14}N_2$	
Formula weight	306.35	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 5.8666(5) Å	a= 83.981(8)°.
	b = 11.4535(10) Å	b= 81.526(8)°.
	c = 12.2113(12) Å	g = 76.578(8)°.
Volume	787.26(12) $Å^3$	
Z	2	
Density (calculated)	1.292 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	320	
Crystal size	0.40 x 0.36 x 0.32 mm^3	
Theta range for data collection	3.38 to 29.16°.	
Index ranges	-5<=h<=7, -15<=k<=12, -16<=l<=15	
Reflections collected	6123	
Independent reflections	3630 [R(int) = 0.0297]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	1.00000 and 0.99412
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3630 / 0 / 217
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0539, wR2 = 0.1098
R indices (all data)	R1 = 0.0837, wR2 = 0.1347
Largest diff. peak and hole	0.208 and -0.232 e.Å^{-3}

Compound 4a

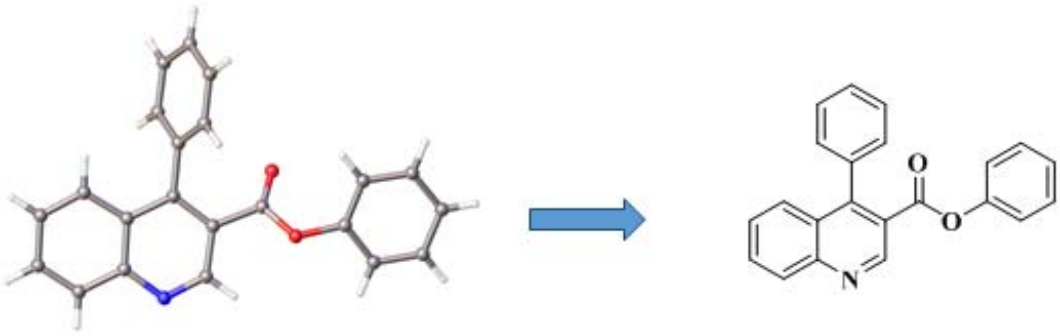


Table 1. Crystal data and structure refinement for compound **4a**.

Identification code	**4a**	
Empirical formula	C_{22} H_{15} N O_2	
Formula weight	325.35	
Temperature	152(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 10.0557(10) Å	= 90°.
	b = 10.3647(11) Å	= 97.658(4)°.
	c = 15.6302(17) Å	= 90°.
Volume	1614.5(3) Å^3	
Z	4	
Density (calculated)	1.338 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	680	
Crystal size	0.40 x 0.20 x 0.11 mm^3	

Theta range for data collection	3.01 to 26.38°.
Index ranges	-12<=h<=12, -12<=k<=12, -19<=l<=19
Reflections collected	41068
Independent reflections	3299 [R(int) = 0.0655]
Completeness to theta = 26.38°	99.8 %
Absorption correction	Semi-empirical from euivalents
Max. and min. transmission	0.9906 and 0.9664
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3299 / 0 / 226
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.0943
R indices (all data)	R1 = 0.0521, wR2 = 0.1097
Largest diff. peak and hole	0.241 and -0.203 e.$Å^{-3}$

Compound 4c

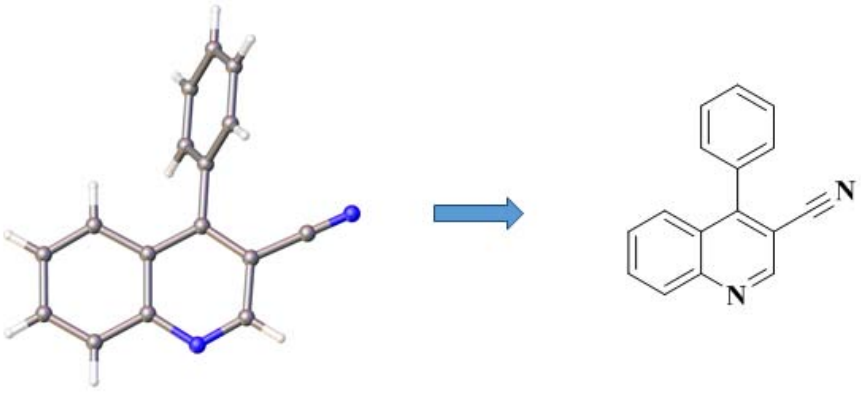


Table 1. Crystal data and structure refinement for compound **4c**.

Identification code	**4c**	
Empirical formula	$C_{16}H_{10}N_2$	
Formula weight	230.26	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.4760(11) Å	a= 90°.
	b = 6.7685(5) Å	b= 106.572(10)°.

	c = 15.8831(16) Å g = 90°.
Volume	1182.48(19) $Å^3$
Z	4
Density (calculated)	1.293 Mg/m^3
Absorption coefficient	0.078 mm^{-1}
F(000)	480
Crystal size	0.60 x 0.40 x 0.08 mm^3
Theta range for data collection	3.29 to 29.22°.
Index ranges	-11<=h<=15, -8<=k<=7, -19<=l<=21
Reflections collected	5267
Independent reflections	2774 [R(int) = 0.0263]
Completeness to theta = 26.00°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.98218
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2774 / 0 / 163
Goodness-of-fit on F^2	0.999
Final R indices [I>2sigma(I)]	R1 = 0.0550, wR2 = 0.1158
R indices (all data)	R1 = 0.1032, wR2 = 0.1447
Largest diff. peak and hole	0.175 and -0.205 $e.Å^{-3}$

Compound 6e

Table 1. Crystal data and structure refinement for compound **6e**.

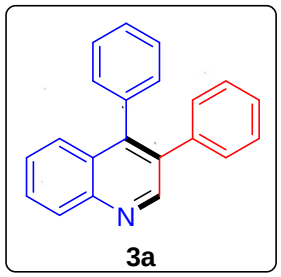
Identification code	**6e**
Empirical formula	$C_{24}H_{16}N_2O$
Formula weight	348.39
Temperature	297(2) K
Wavelength	0.71073 Å

Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 13.1944(9) Å = 90°.
	b = 9.7945(10) Å = 100.206(7)°.
	c = 14.6162(10) Å = 90°.
Volume	1859.0(3) $Å^3$
Z	4
Density (calculated)	1.245 Mg/m^3
Absorption coefficient	0.077 mm^{-1}
F(000)	728
Crystal size	0.43 x 0.41 x 0.38 mm^3
Theta range for data collection	2.83 to 29.26°.
Index ranges	-16<=h<=18, -13<=k<=7, -19<=l<=19
Reflections collected	8872
Independent reflections	4363 [R(int) = 0.0359]
Completeness to theta = 26.00°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.95339
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4363 / 0 / 248
Goodness-of-fit on F^2	0.979
Final R indices [I>2sigma(I)]	R1 = 0.0623, wR2 = 0.1157
R indices (all data)	R1 = 0.1403, wR2 = 0.1476
Largest diff. peak and hole	0.128 and -0.244 $e.Å^{-3}$

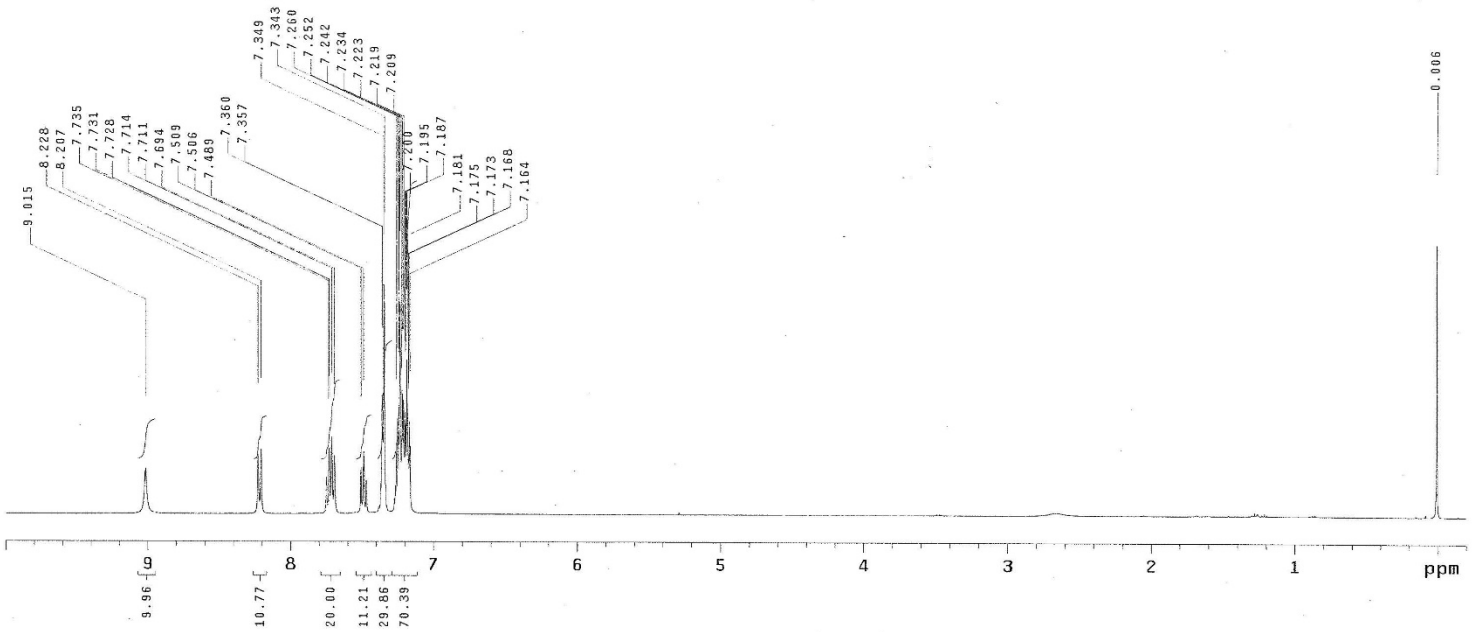
SGC/RP5/Q-11

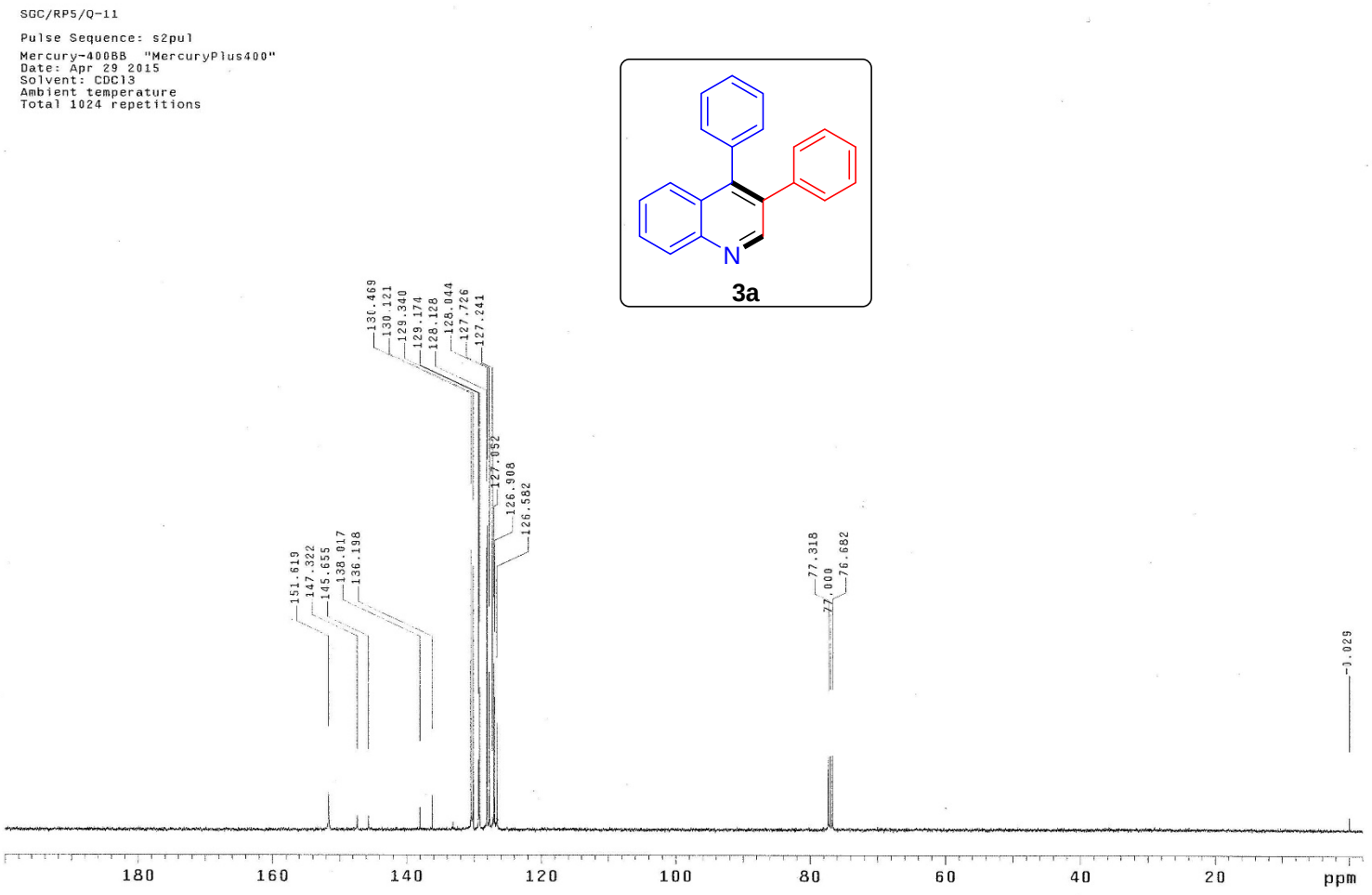
Pulse Sequence: s2pul

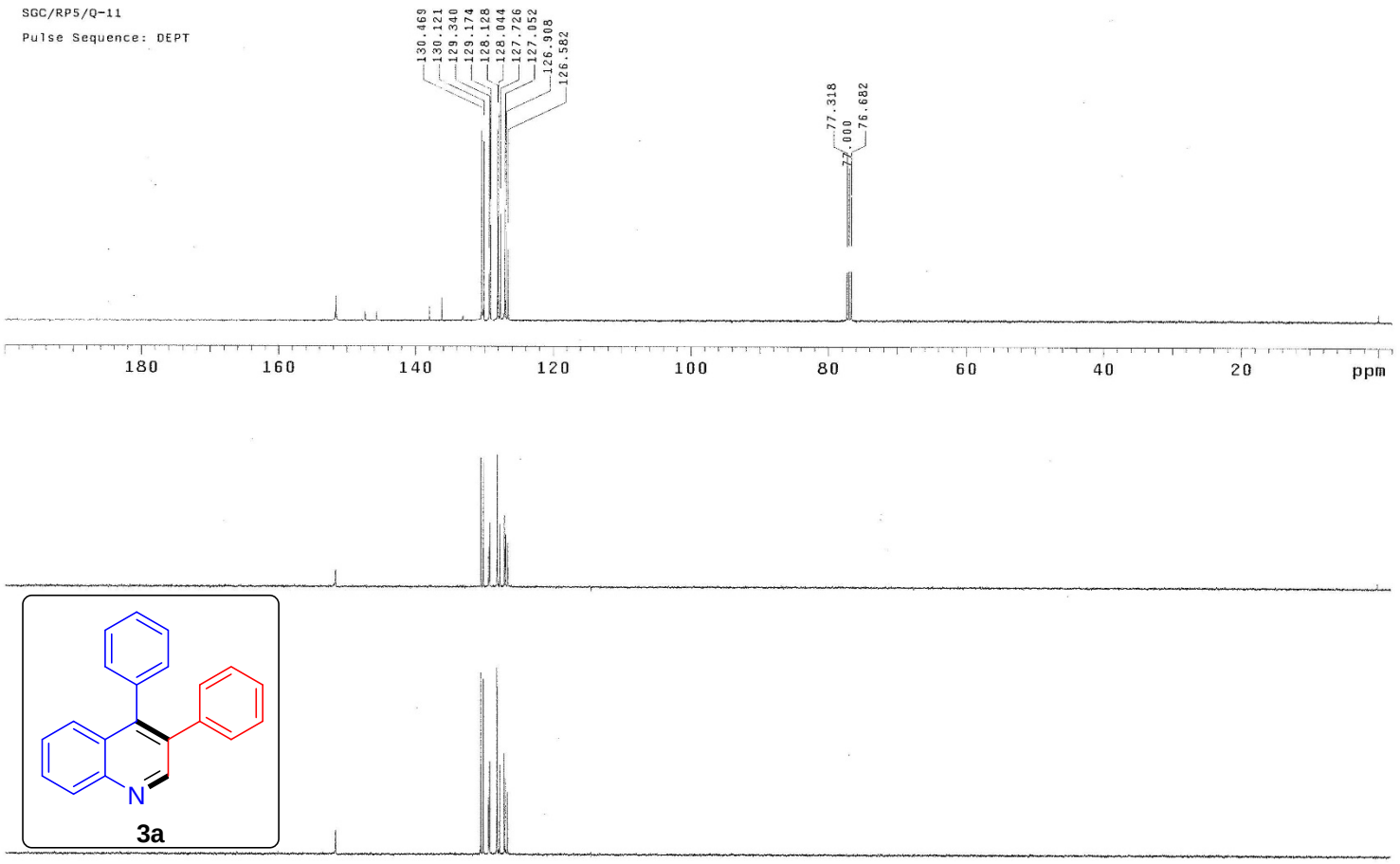
Mercury-400BB "MercuryPlus400"
Date: Apr 29 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



3a



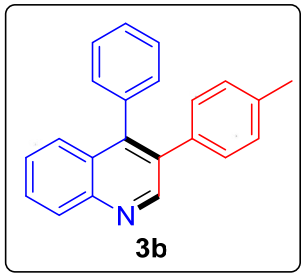

SGC/RP5/Q-11
Pulse Sequence: s2pul
Mercury-400BB "MercuryPlus400"
Date: Apr 29 2015
Solvent: CDCl3
Ambient temperature
Total 1024 repetitions
N
3a
130.469
130.121
129.340
129.174
128.128
128.044
127.726
127.241
127.052
126.908
126.582
151.619
147.322
145.655
138.017
136.198
77.318
77.000
76.682
-1.029
180
160
140
120
100
80
60
40
20
ppm


SGC/RP5/Q-11
Pulse Sequence: DEPT
130.469
130.121
129.340
129.174
128.128
128.044
127.726
127.052
126.908
126.582
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
N
3a

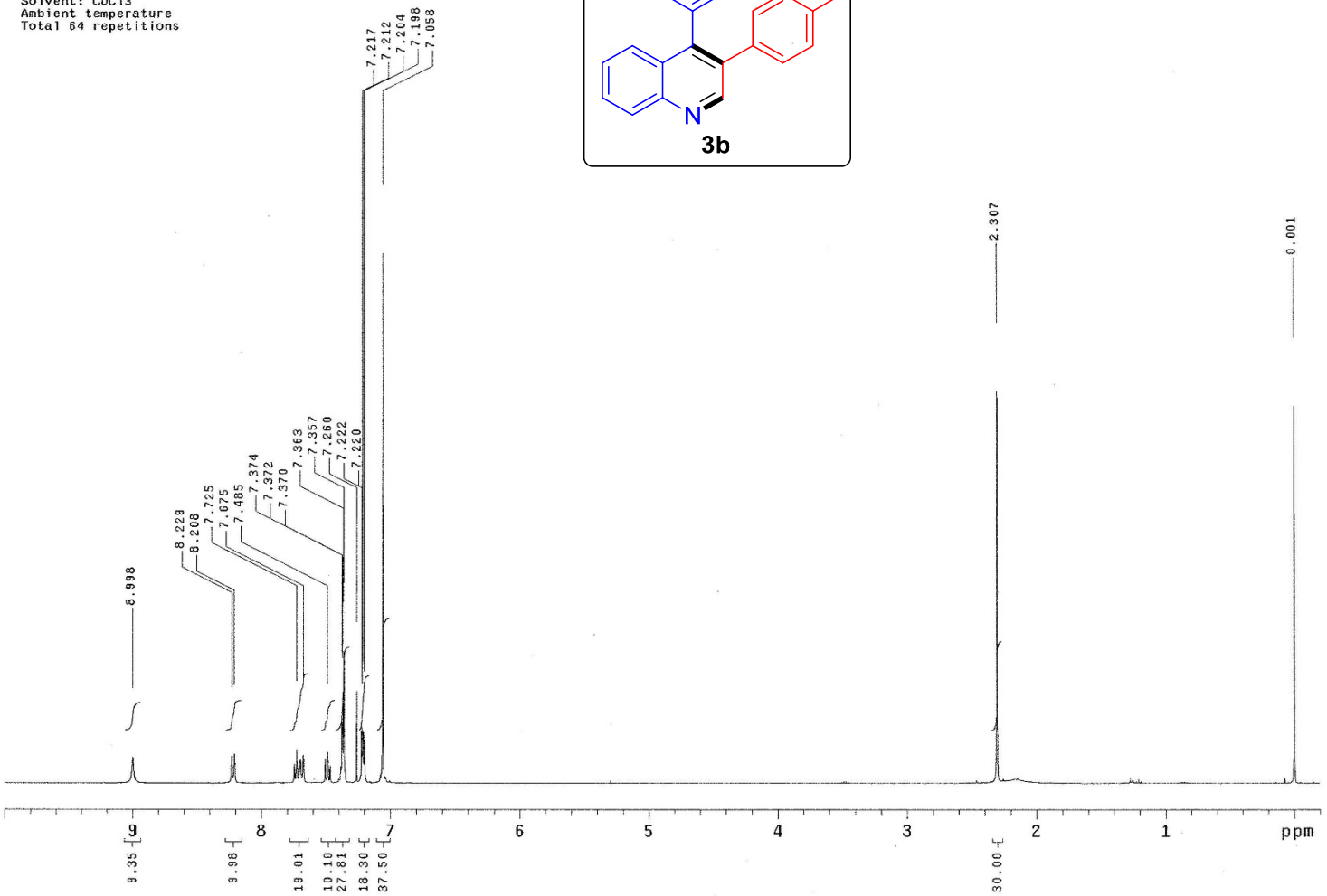
SGC/RP5/Q-13

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 29 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



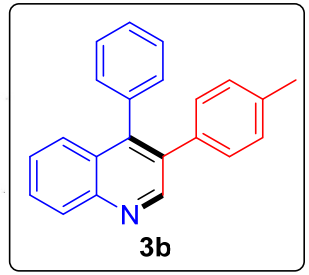
3b



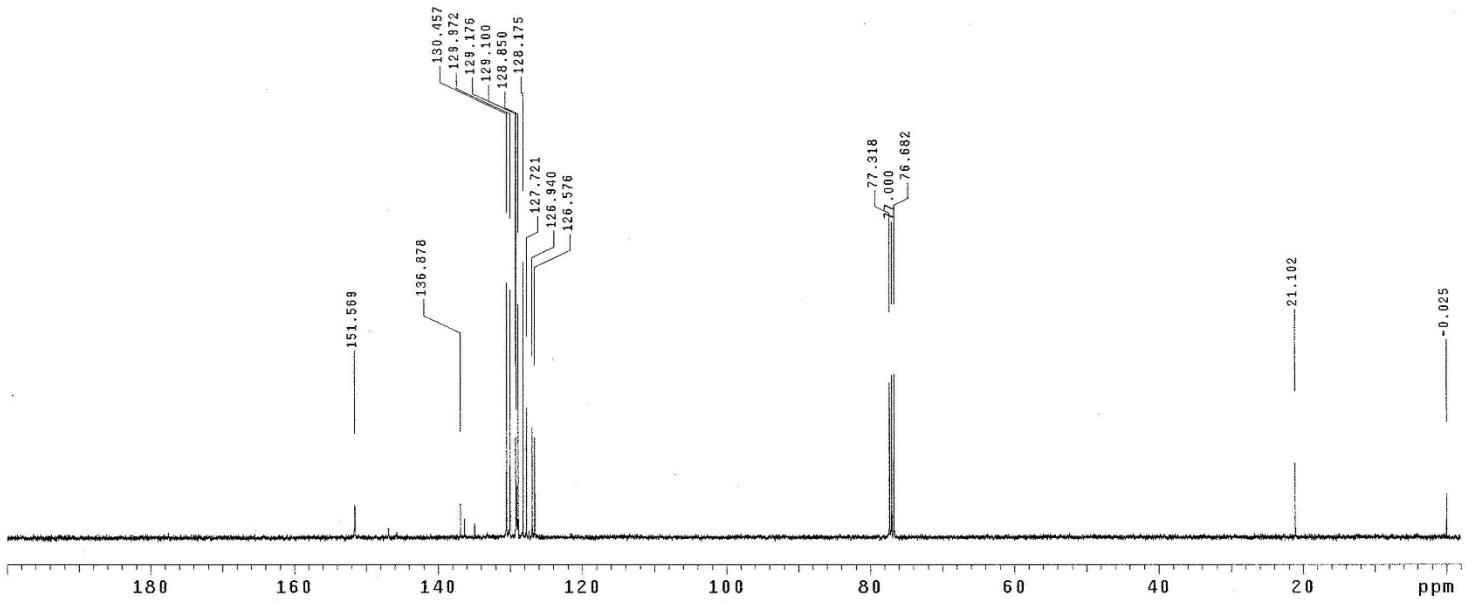
SGC/RP5/Q-13

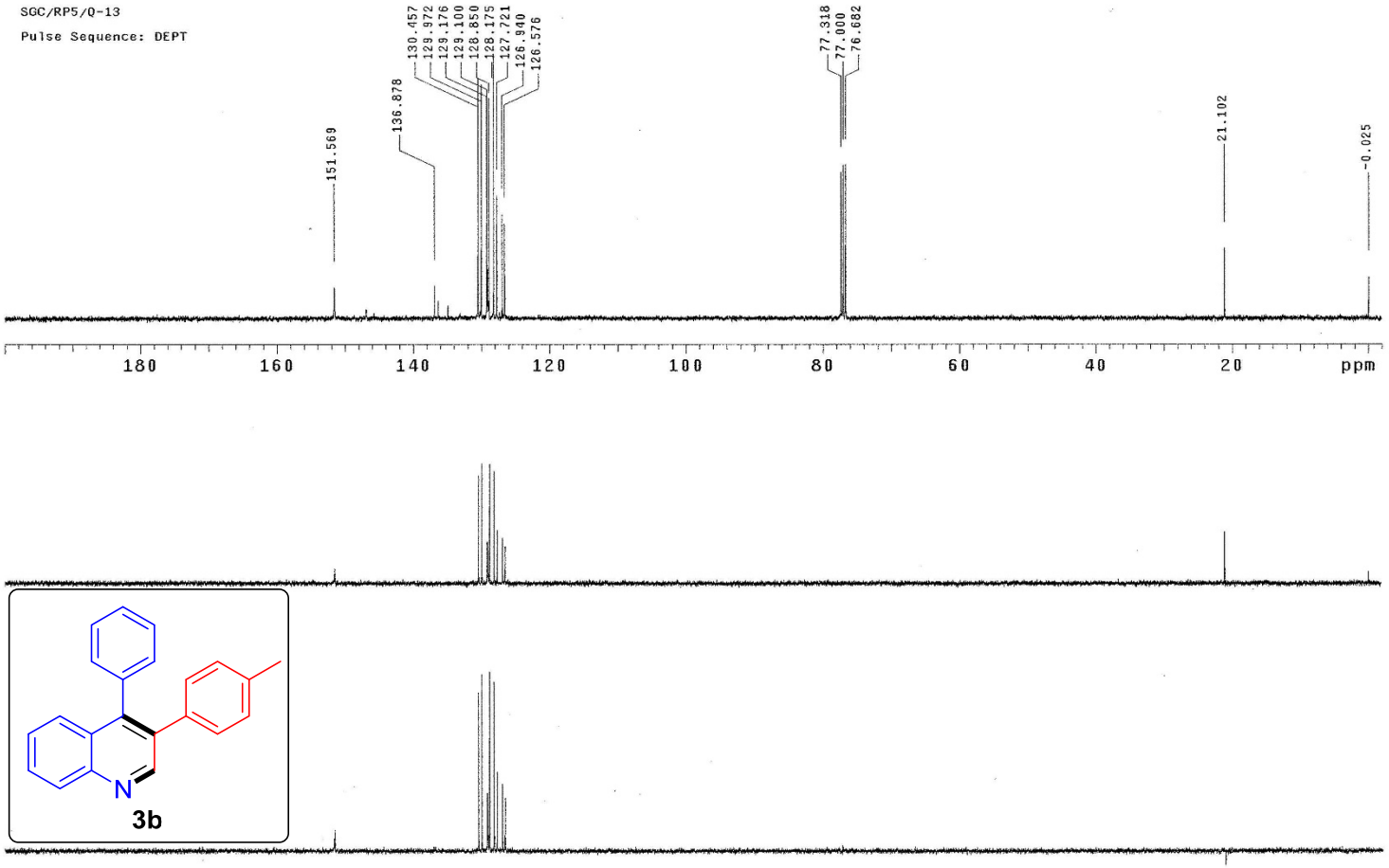
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 29 2015
Solvent: CDCl3
Ambient temperature
Total 8672 repetitions



3b

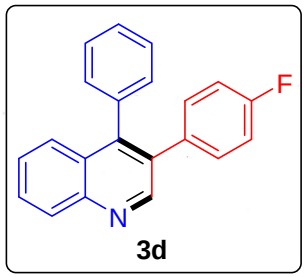



SGC/RP5/Q-13
Pulse Sequence: DEPT
151.569
136.878
130.457
129.972
129.176
129.100
128.850
128.175
127.721
126.940
126.576
77.318
77.000
76.682
21.102
-0.025
180
160
140
120
100
80
60
40
20
ppm
N
3b

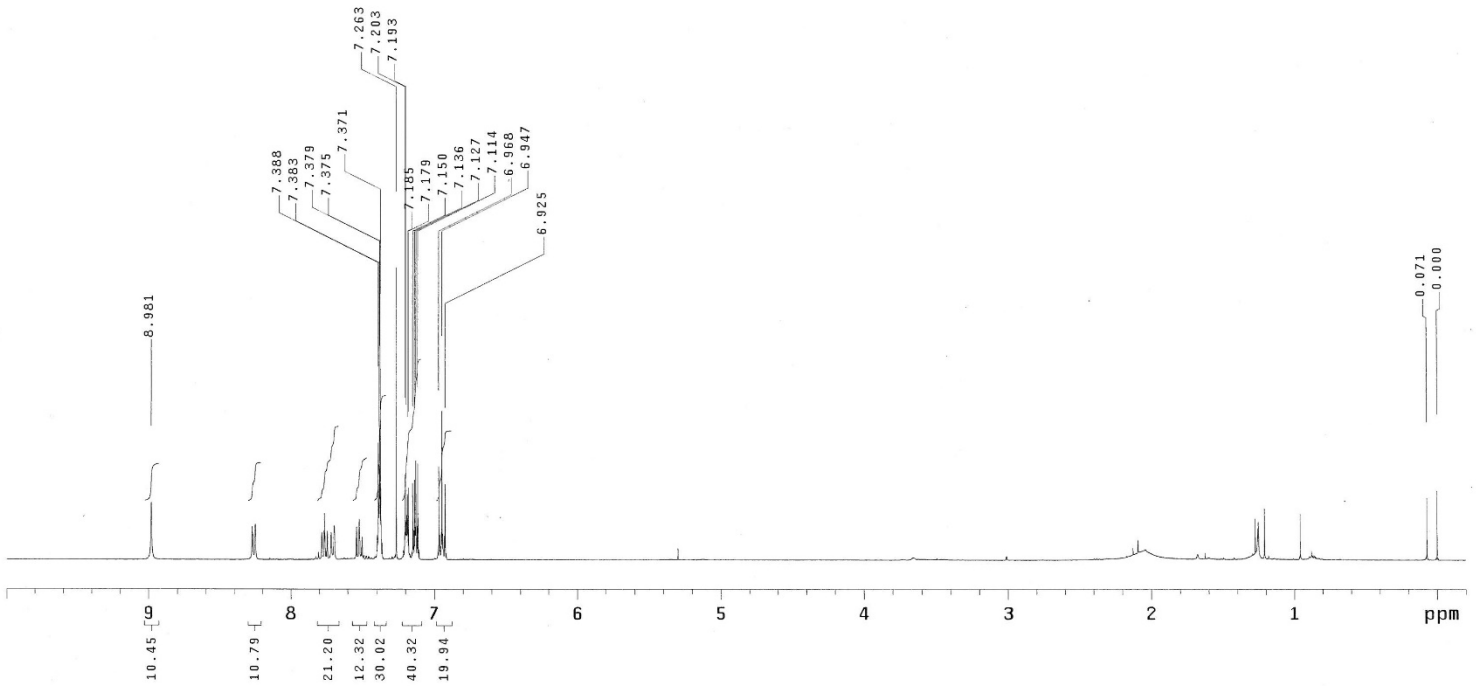
SGC/P-5/F

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 40 repetitions



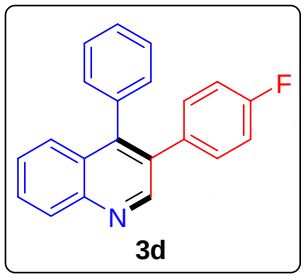
3d



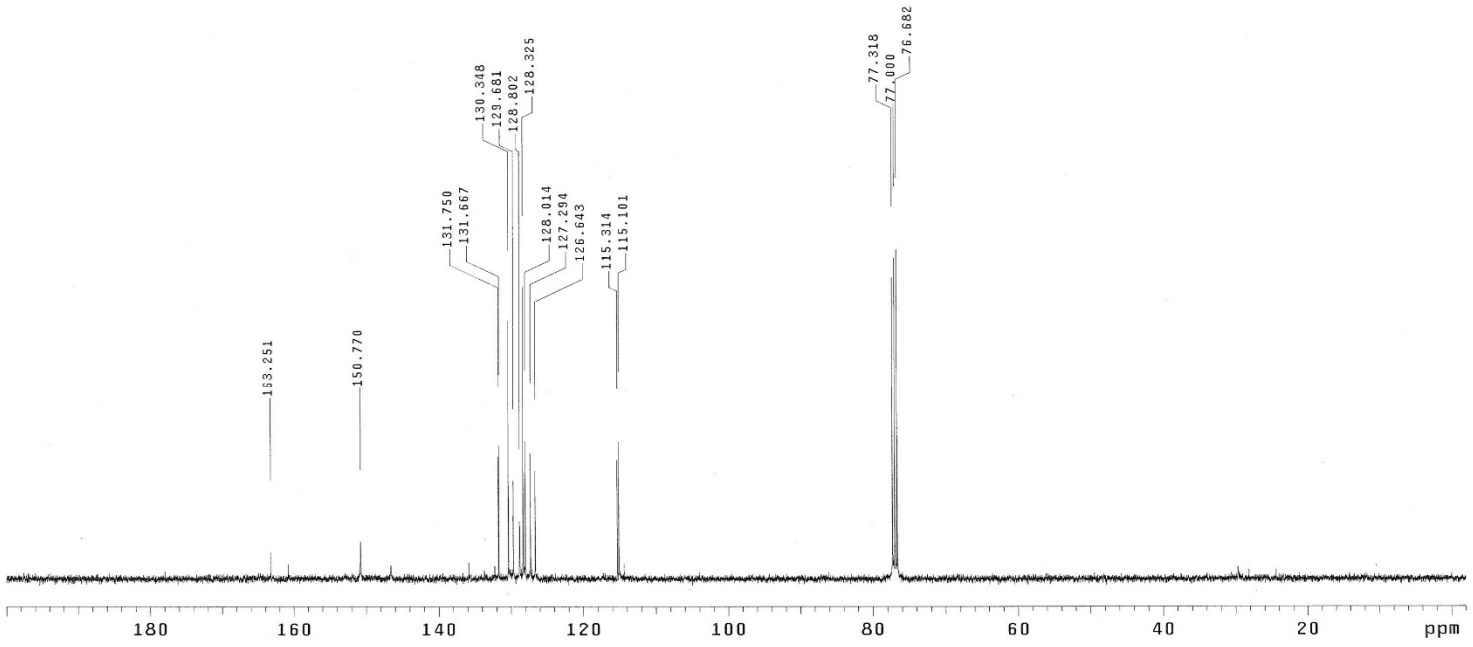
SGC/P-5/F

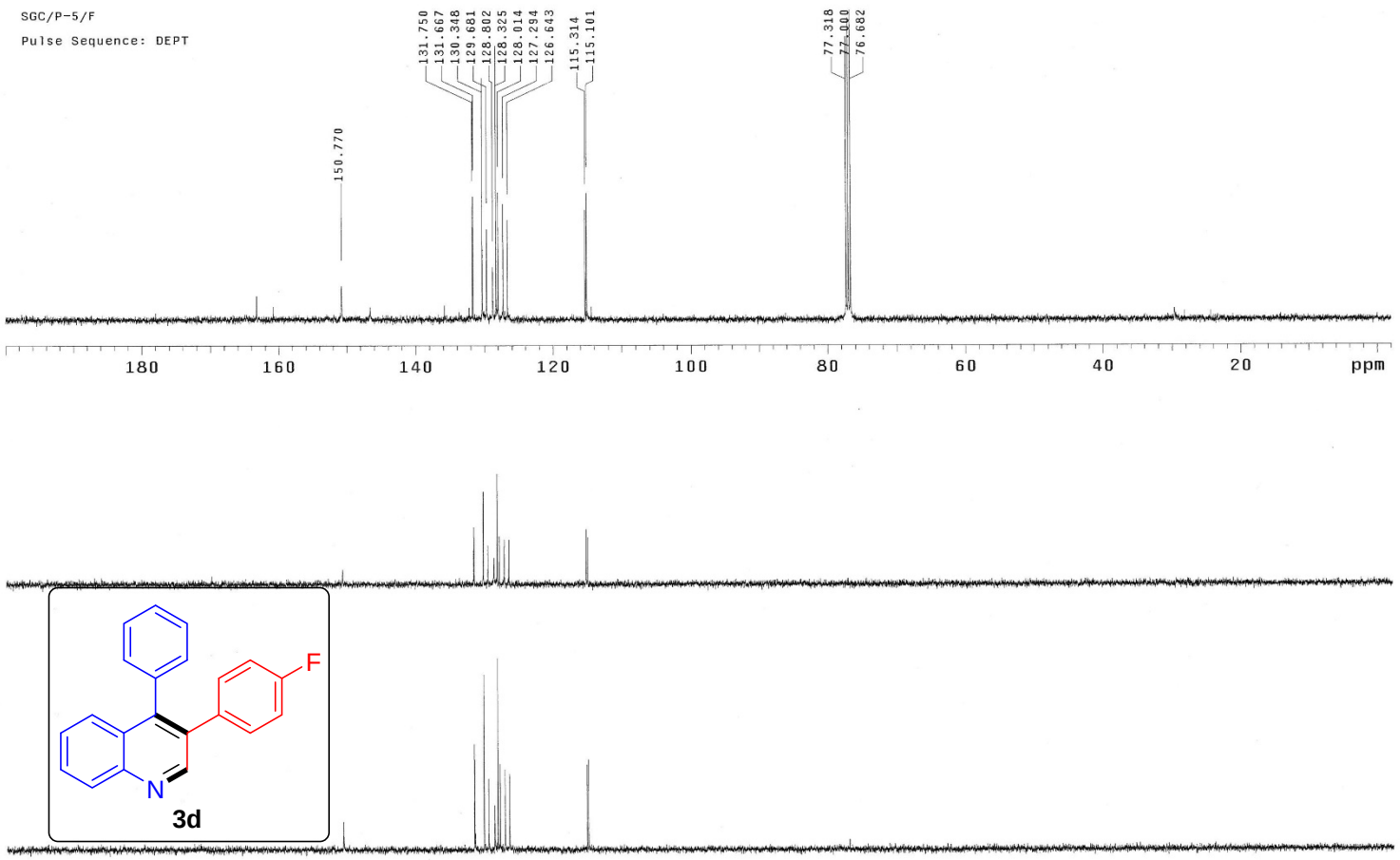
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 10848 repetitions



3d

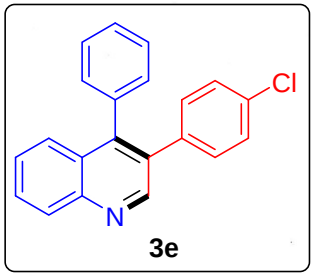



SGC/P-5/F
Pulse Sequence: DEPT
150.770
131.750
131.667
130.348
129.681
128.802
128.325
128.014
127.294
126.643
115.314
115.101
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
F
N
3d

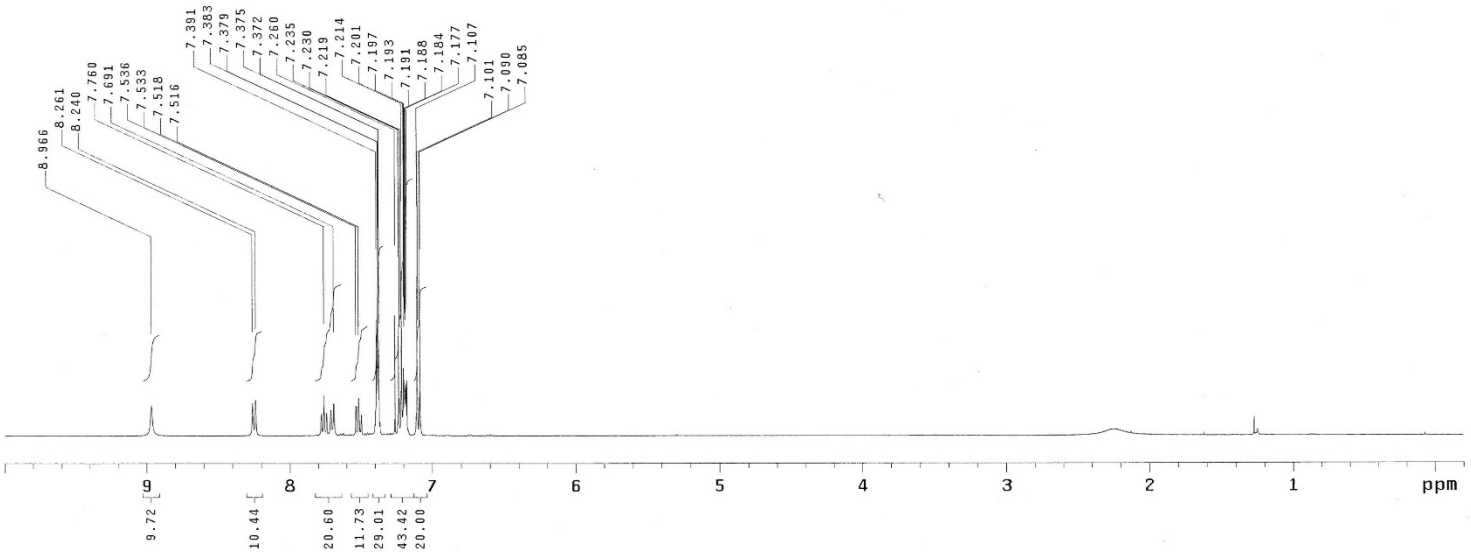
SGC/P-5/Cl

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 48 repetitions



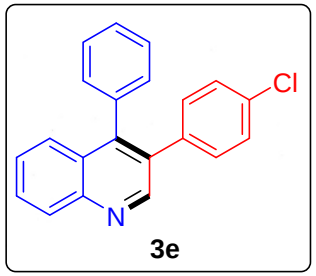
3e



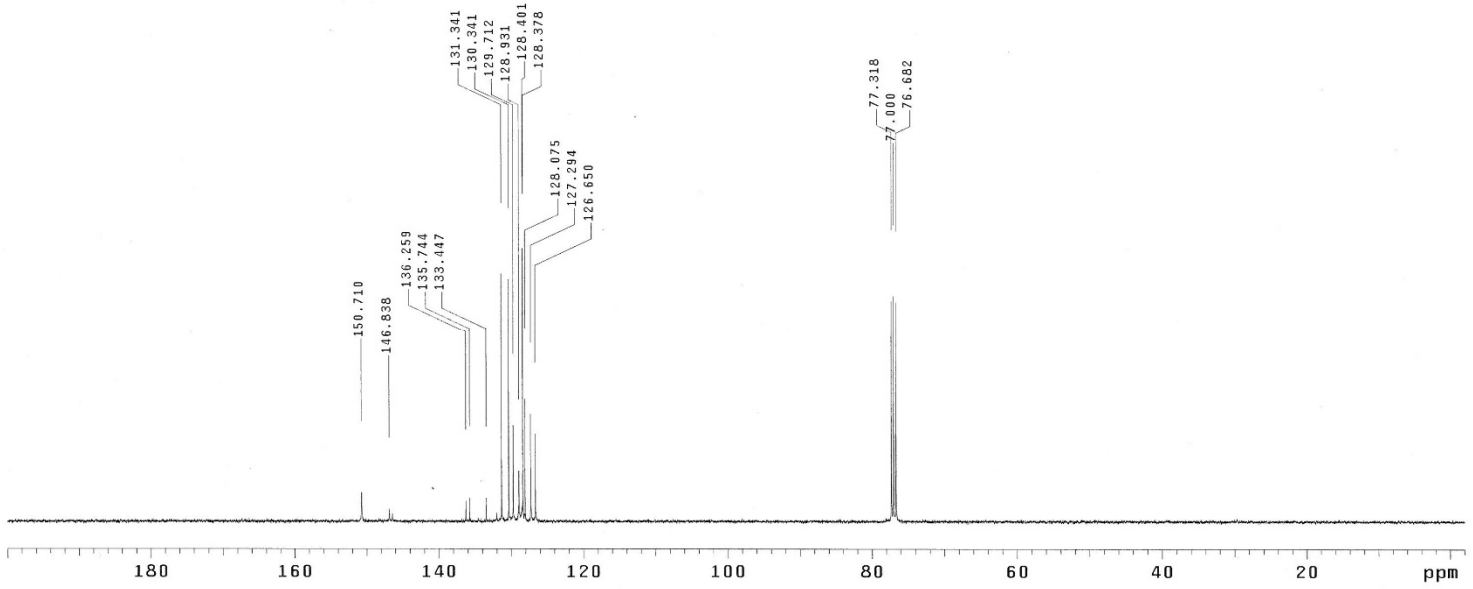
SGC/P-5/Cl

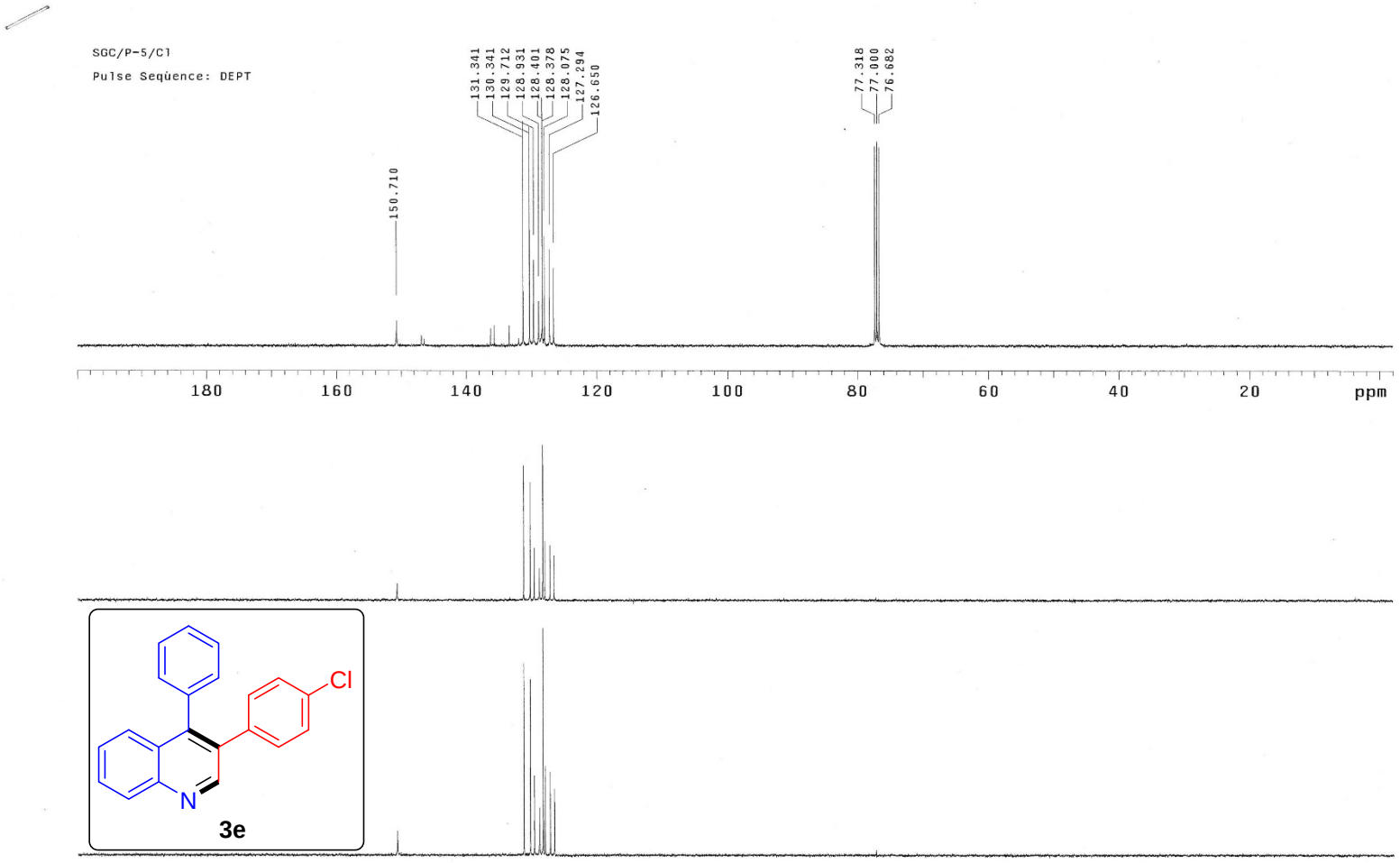
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 20480 repetitions



3e

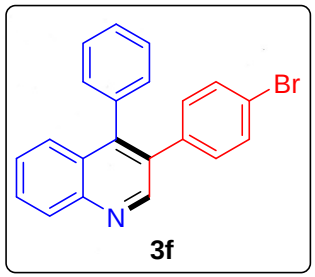



SGC/P-5/Cl
Pulse Sequence: DEPT
131.341
130.341
129.712
128.931
128.401
128.378
128.075
127.294
126.650
150.710
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Cl
N
3e

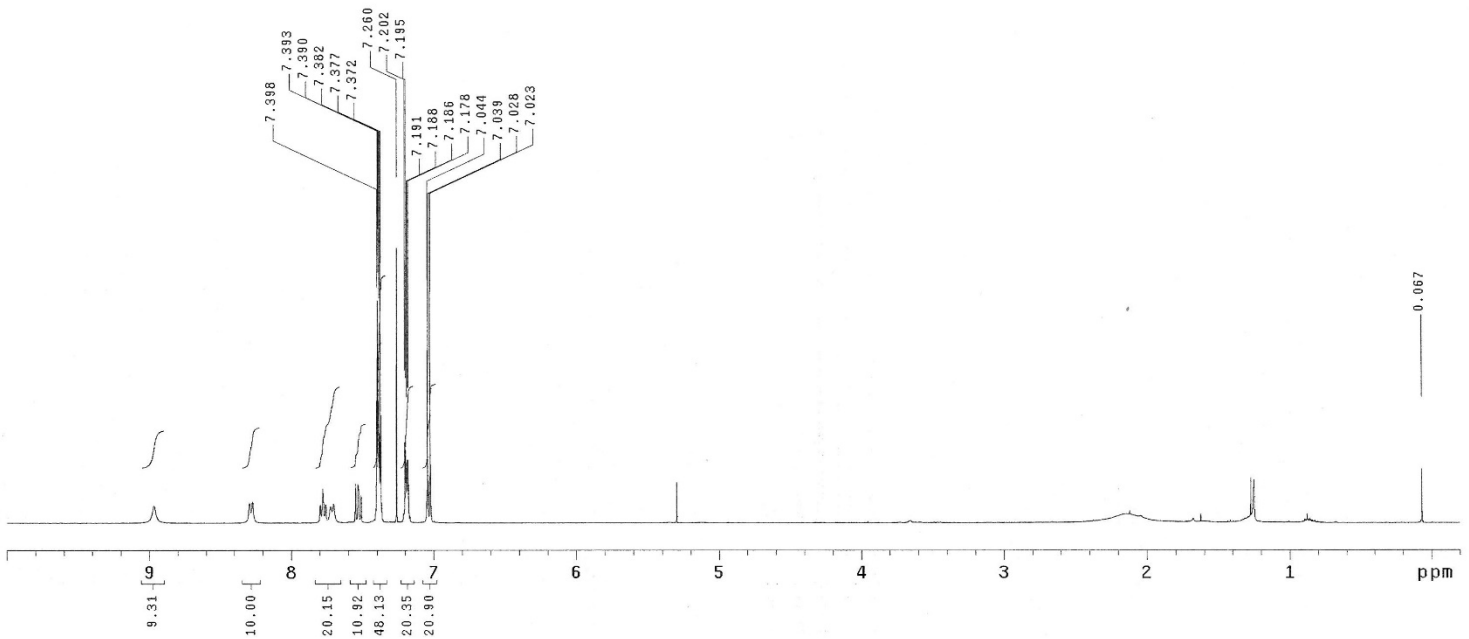
SGC/P-5/P-Br

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 80 repetitions



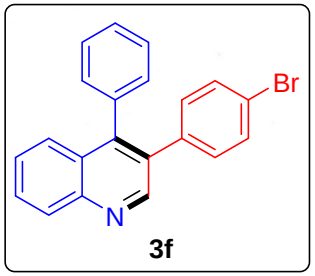
3f



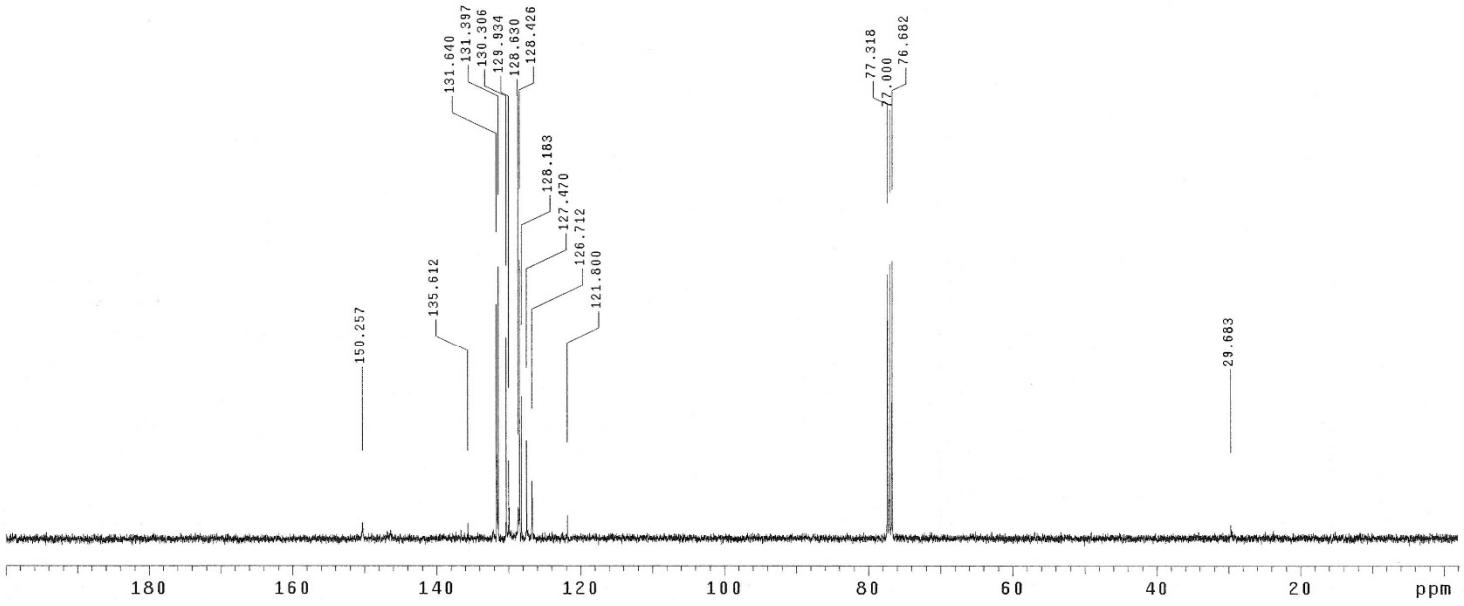
SGC/P-5/P-Br

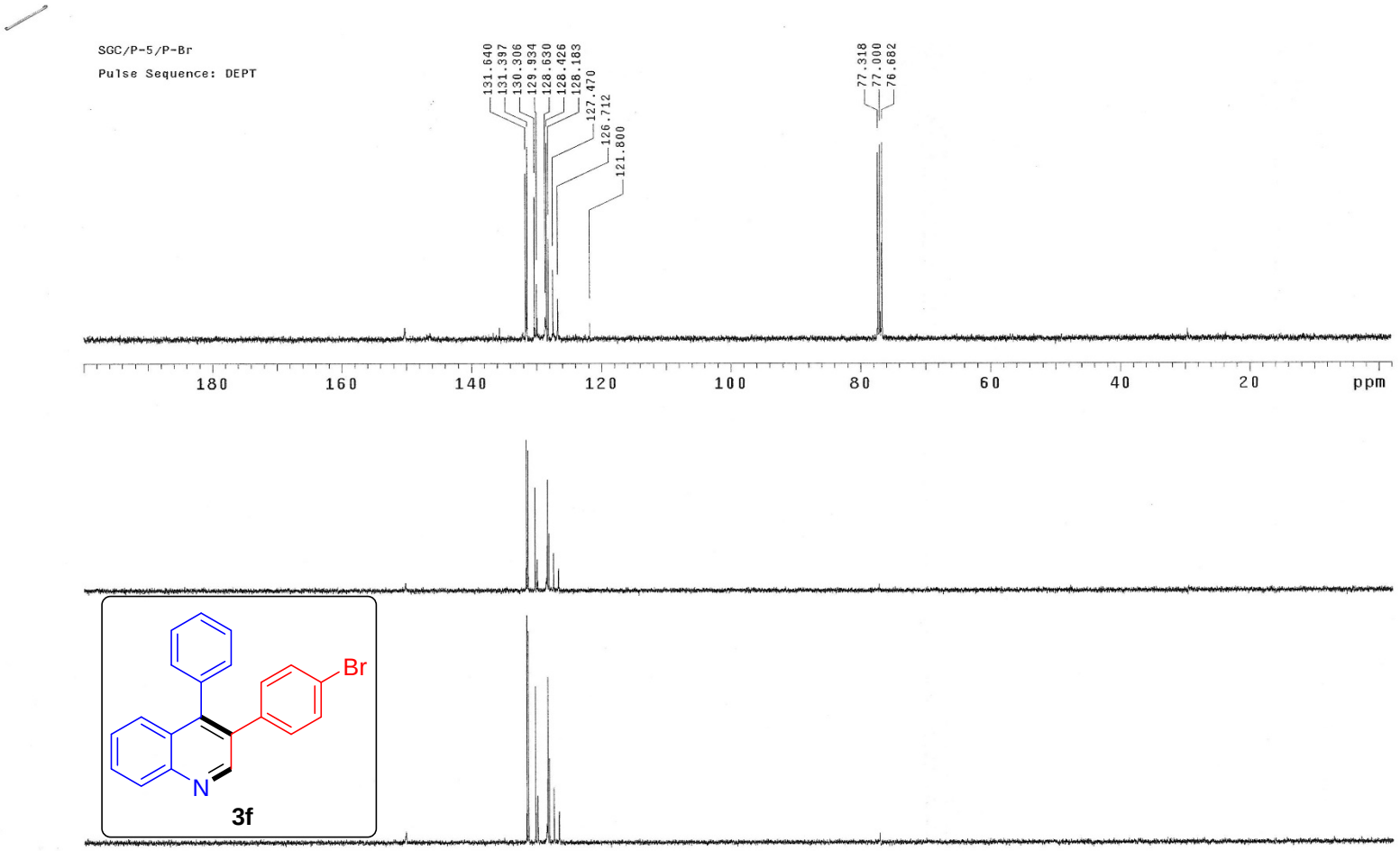
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 18368 repetitions



3f

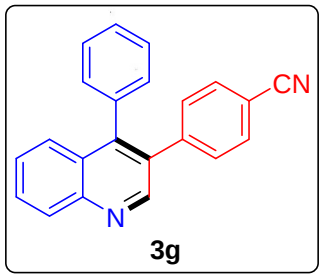



SGC/P-5/P-Br
Pulse Sequence: DEPT
131.640
131.397
130.306
129.934
128.630
128.426
128.183
127.470
126.712
121.800
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Br
N
3f

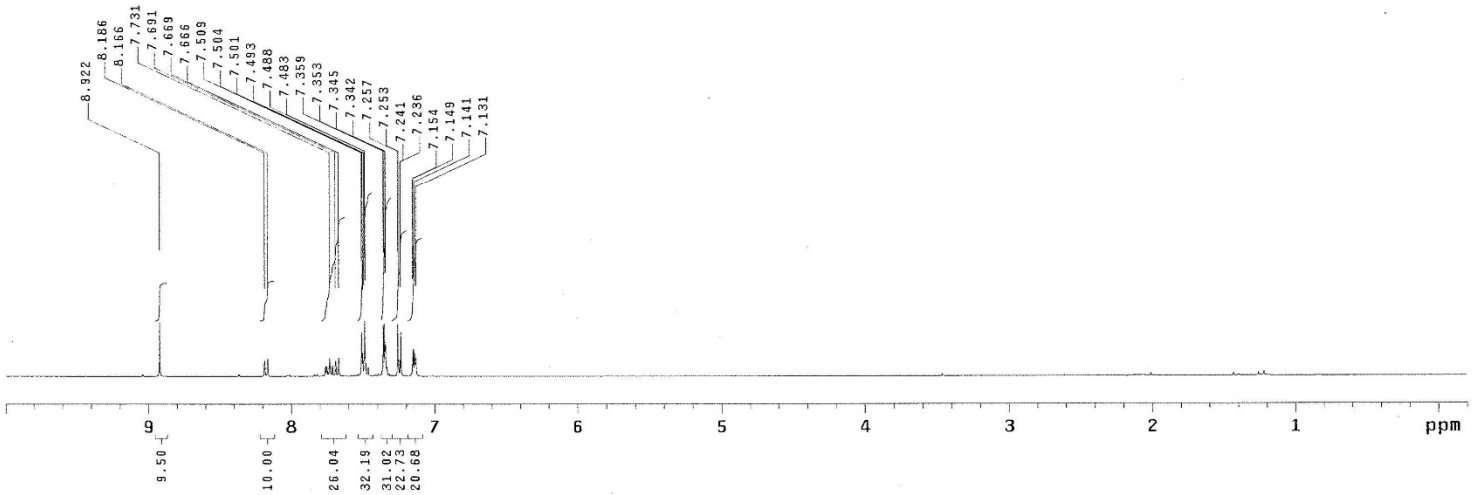
SGC/RP5/4

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 5 2015
Solvent: CDCl3
Ambient temperature
File: M0002-10
Total 64 repetitions



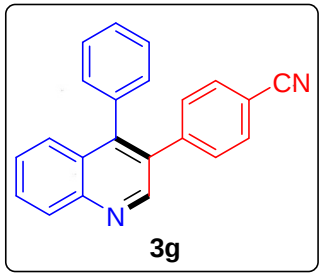
3g



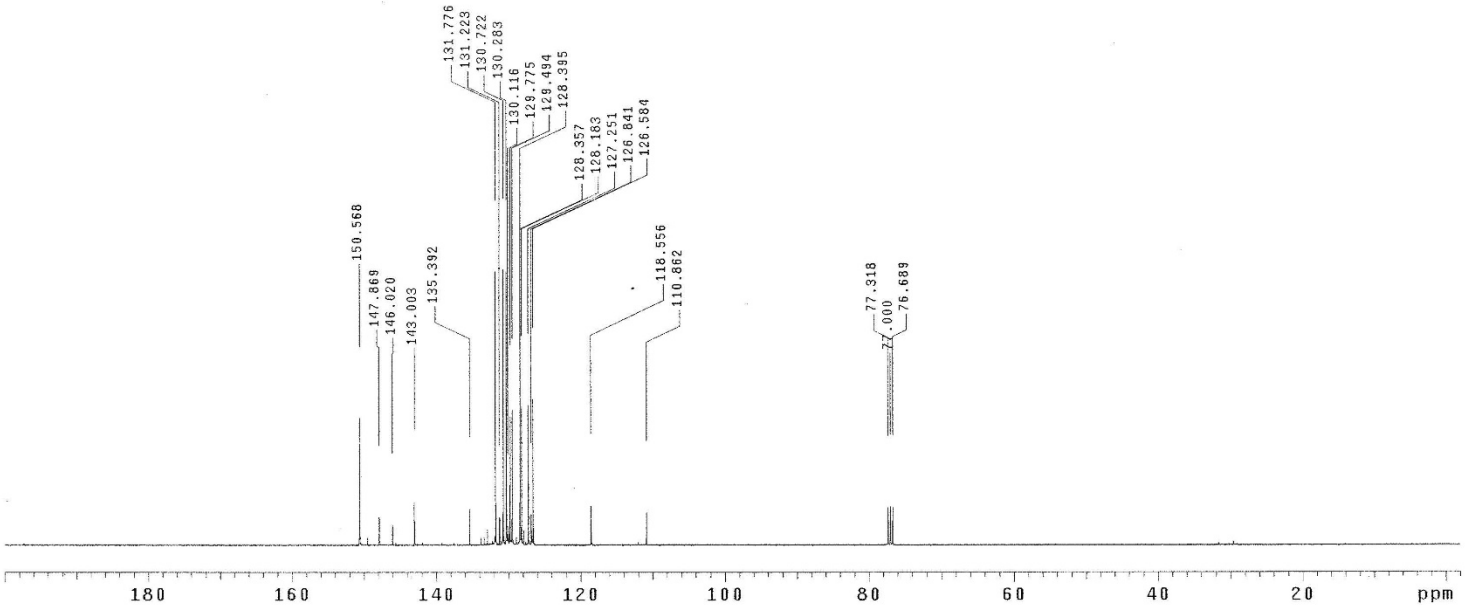
SGC/RP5/4

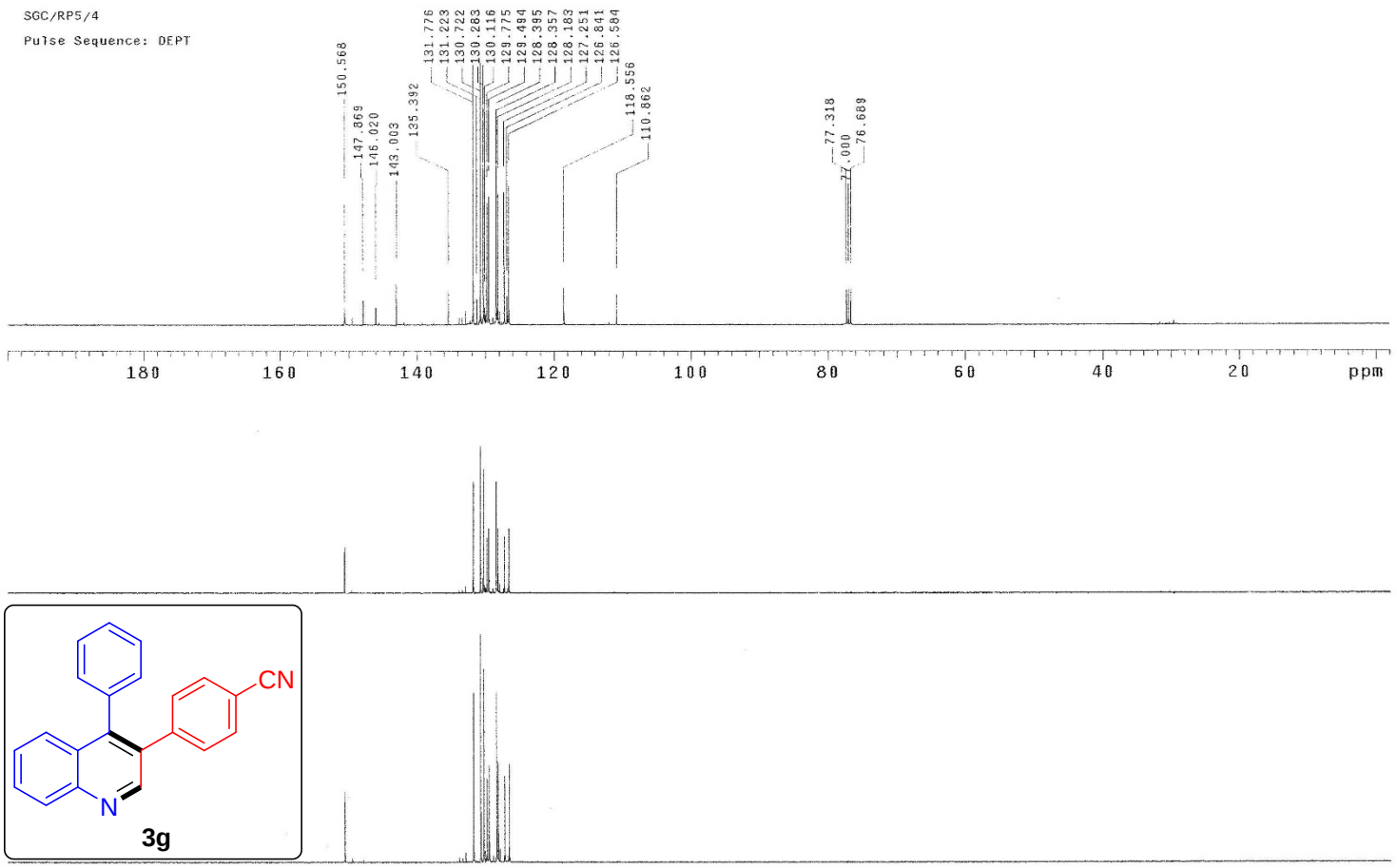
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 5 2015
Solvent: CDCl3
Ambient temperature
Total 6400 repetitions



3g

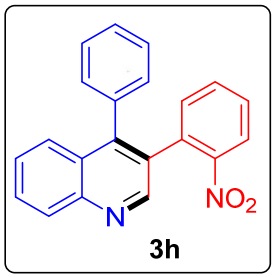



SGC/RP5/4
Pulse Sequence: DEPT
150.568
147.869
146.020
143.003
135.392
131.776
131.223
130.722
130.283
130.116
129.775
129.494
128.395
128.357
128.183
127.251
126.841
126.584
118.556
110.862
77.318
77.000
76.689
180
160
140
120
100
80
60
40
20
ppm
CN
N
3g

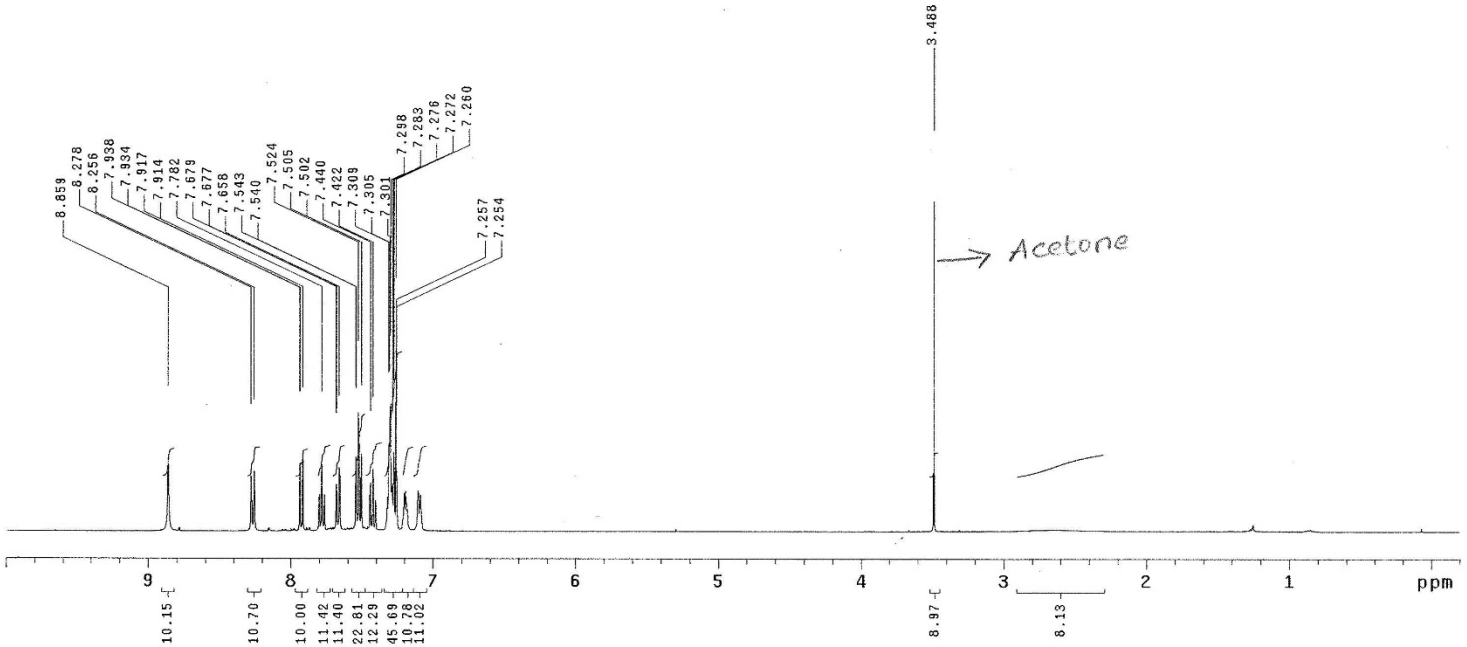
SGC/P-5/Q-8

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 28 2015
Solvent: CDCl3
Ambient temperature
Total 80 repetitions



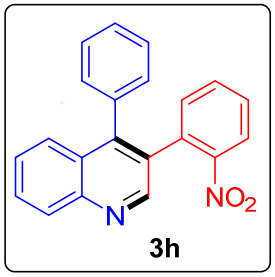
3h



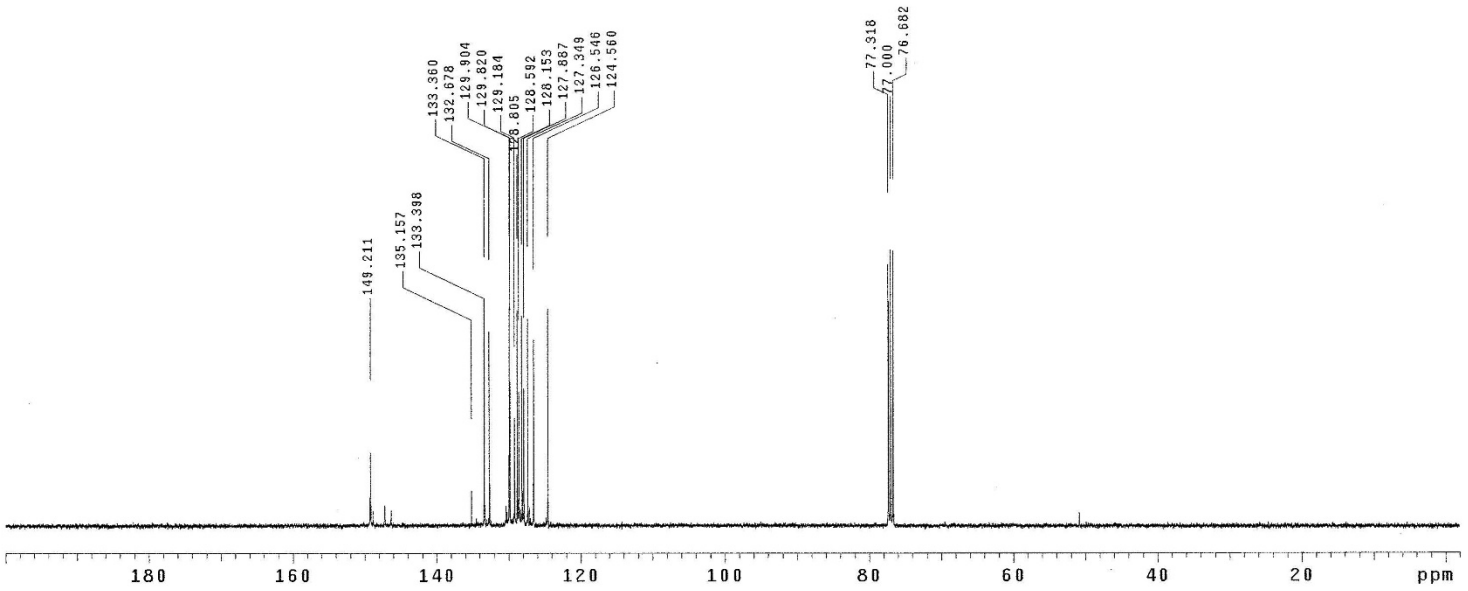
SGC/P-5/Q-8

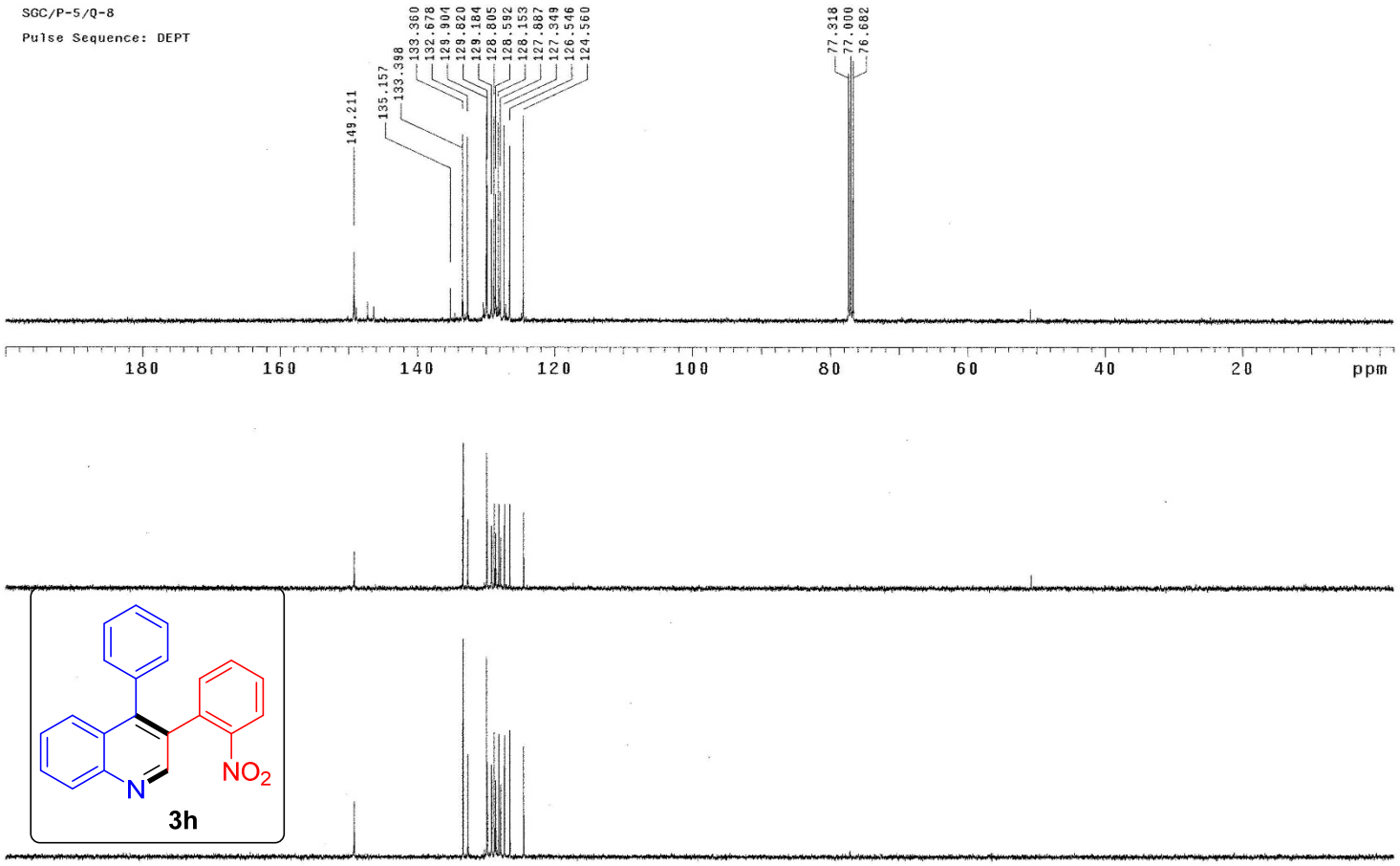
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 28 2015
Solvent: CDCl3
Ambient temperature
Total 16000 repetitions



3h

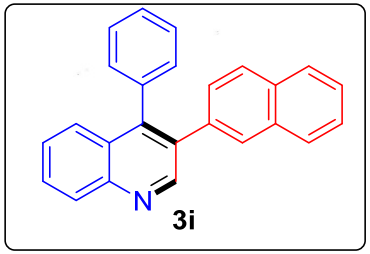


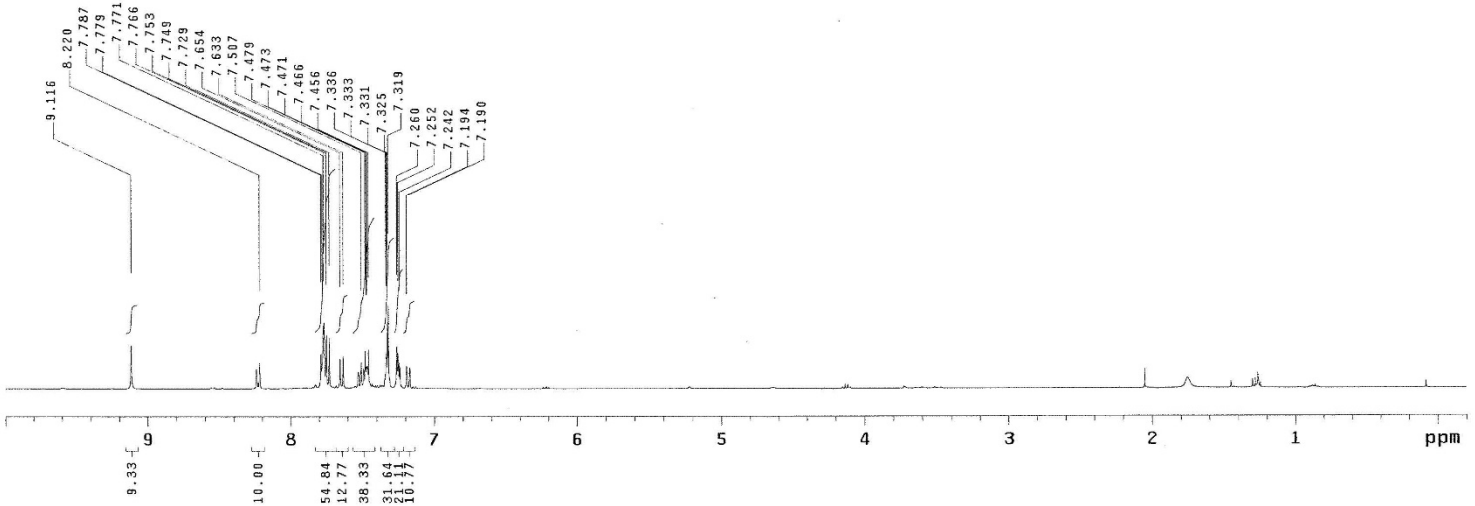

SGC/P-5/Q-8
Pulse Sequence: DEPT
149.211
135.157
133.398
133.360
132.678
129.904
129.820
129.184
128.805
128.592
128.153
127.887
127.349
126.546
124.560
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
N
NO2
3h

SGC/RP5/2

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 7 2015
Solvent: CDCl3
Ambient temperature
File: M0002-4
Total 64 repetitions

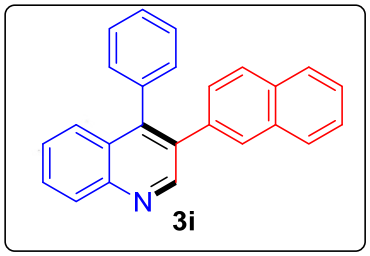


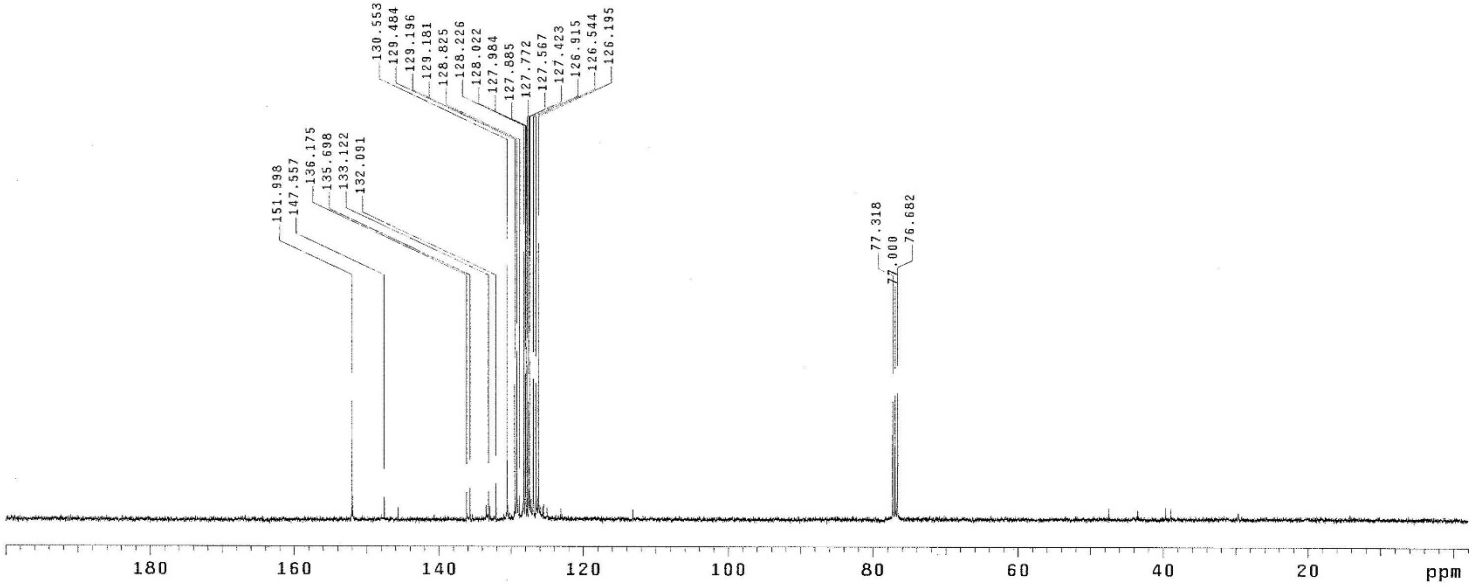


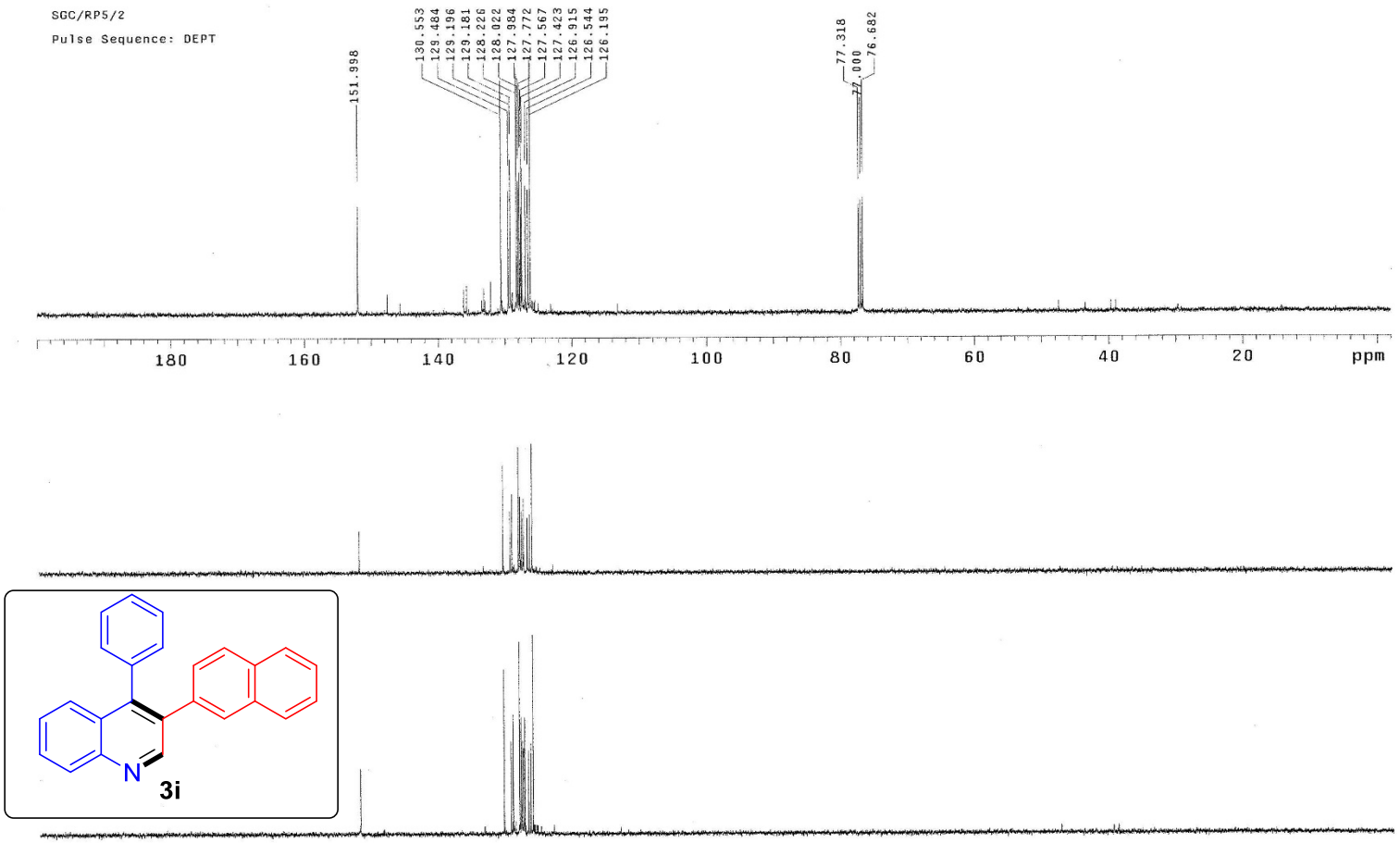
SGC/RP5/2

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 7 2015
Solvent: CDCl3
Ambient temperature
Total 64000 repetitions



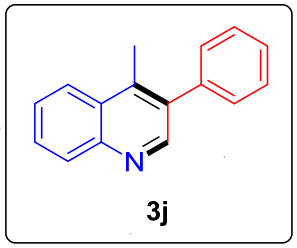



SGC/RP5/2
Pulse Sequence: DEPT
151.998
130.553
129.484
129.196
129.181
128.226
128.022
127.984
127.772
127.567
127.423
126.915
126.544
126.195
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
N
3i

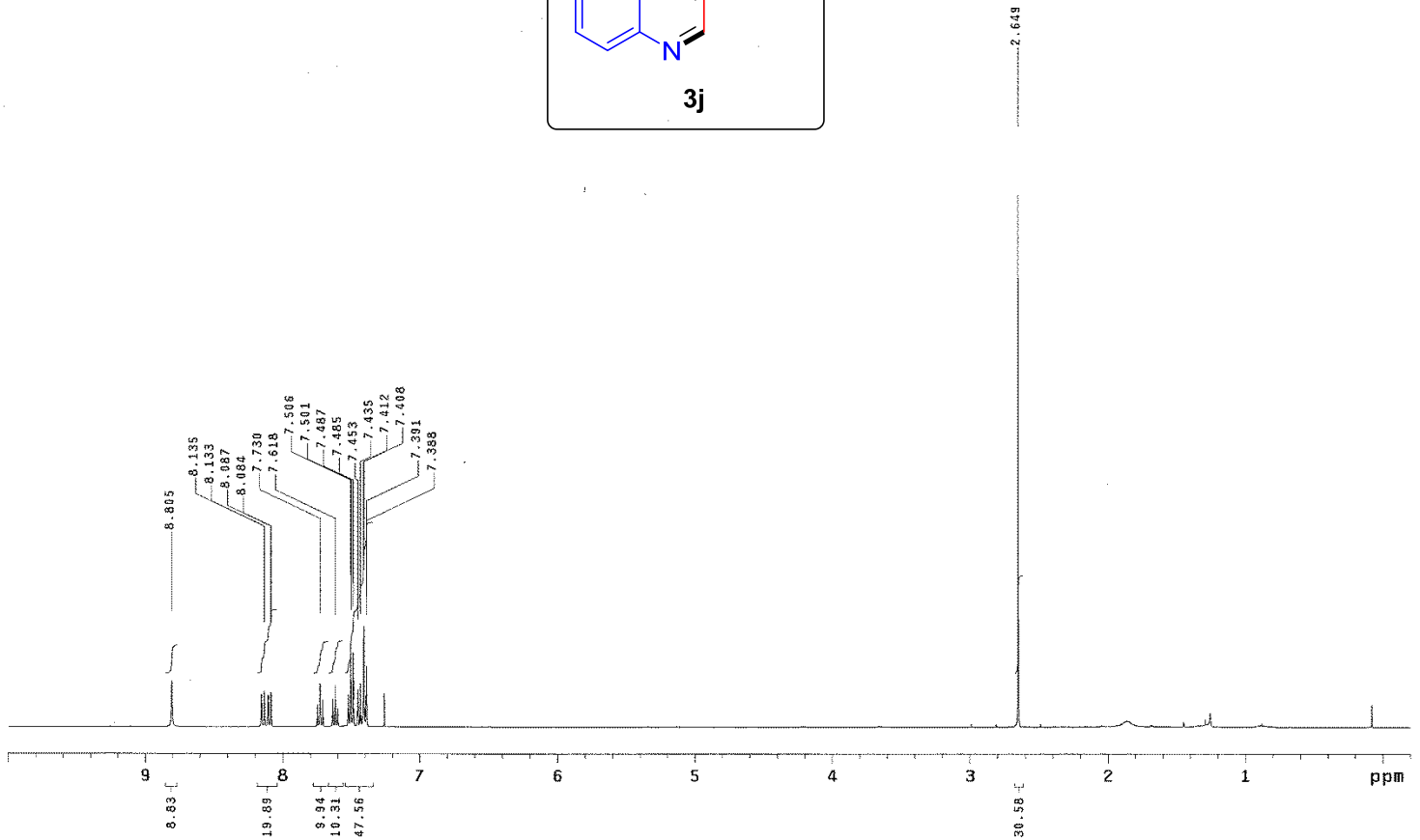
SGC/P-5/Q-Ph

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



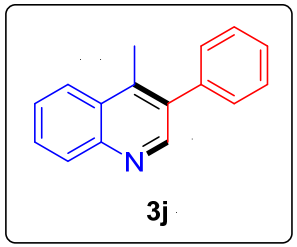
3j



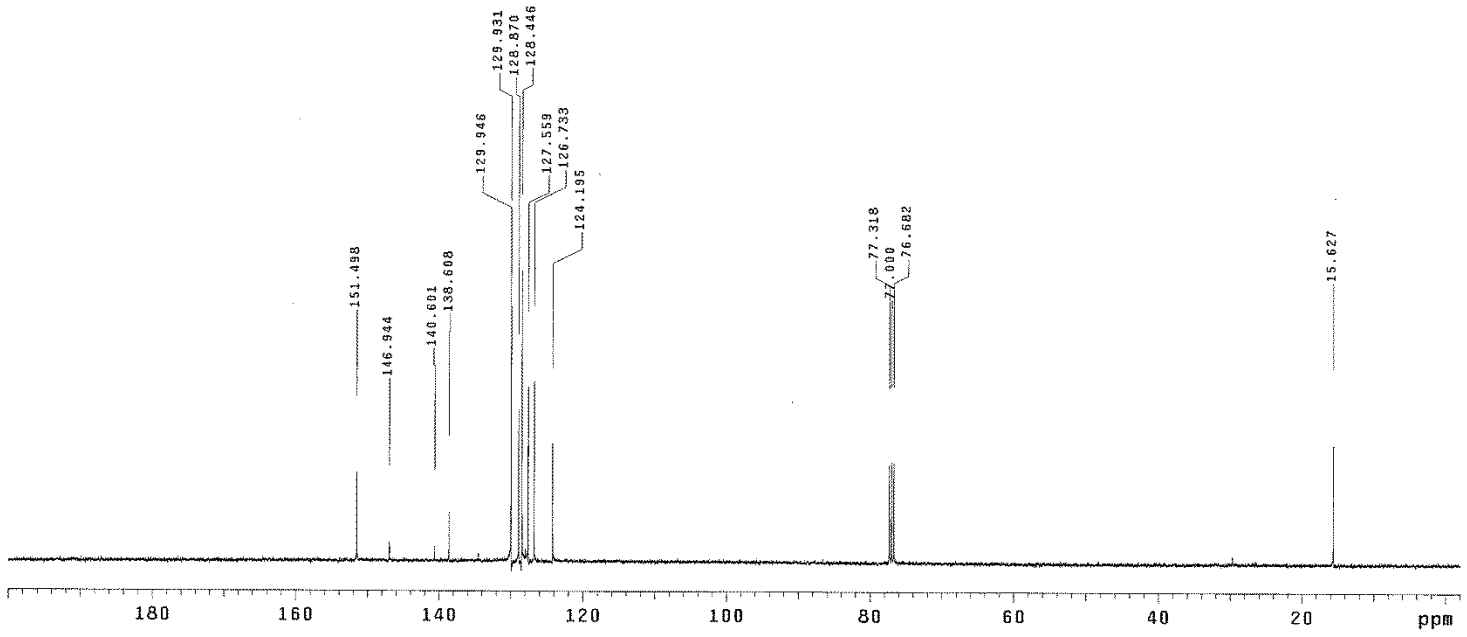
SGC/P-5/Q-Ph

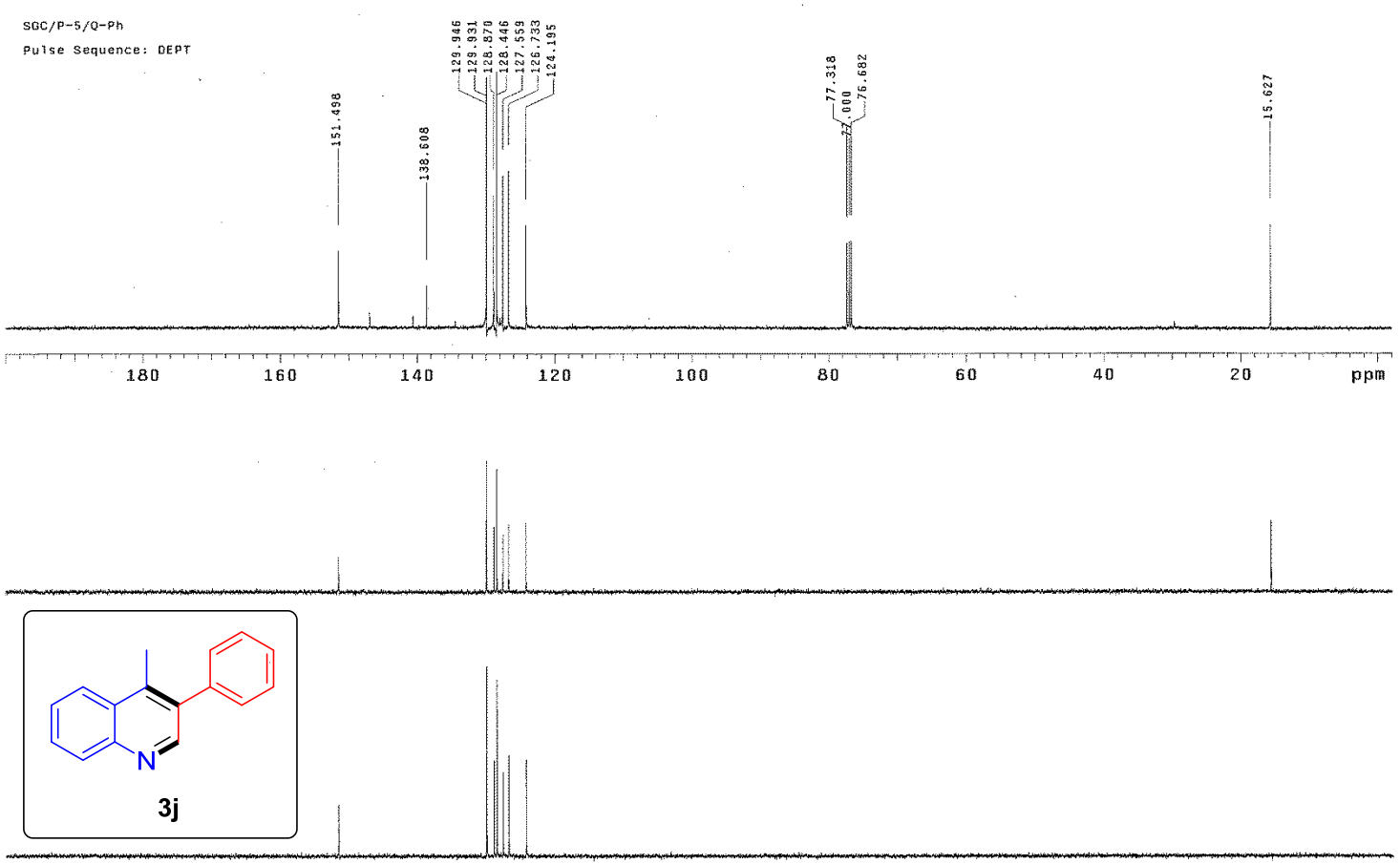
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 3040 repetitions



3j

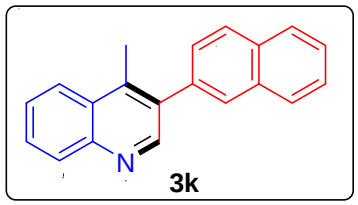



SGC/P-5/Q-Ph
Pulse Sequence: DEPT
151.498
138.608
129.946
129.931
128.870
128.446
127.559
126.733
124.195
77.318
77.000
76.682
15.627
180
160
140
120
100
80
60
40
20
ppm
N
3j

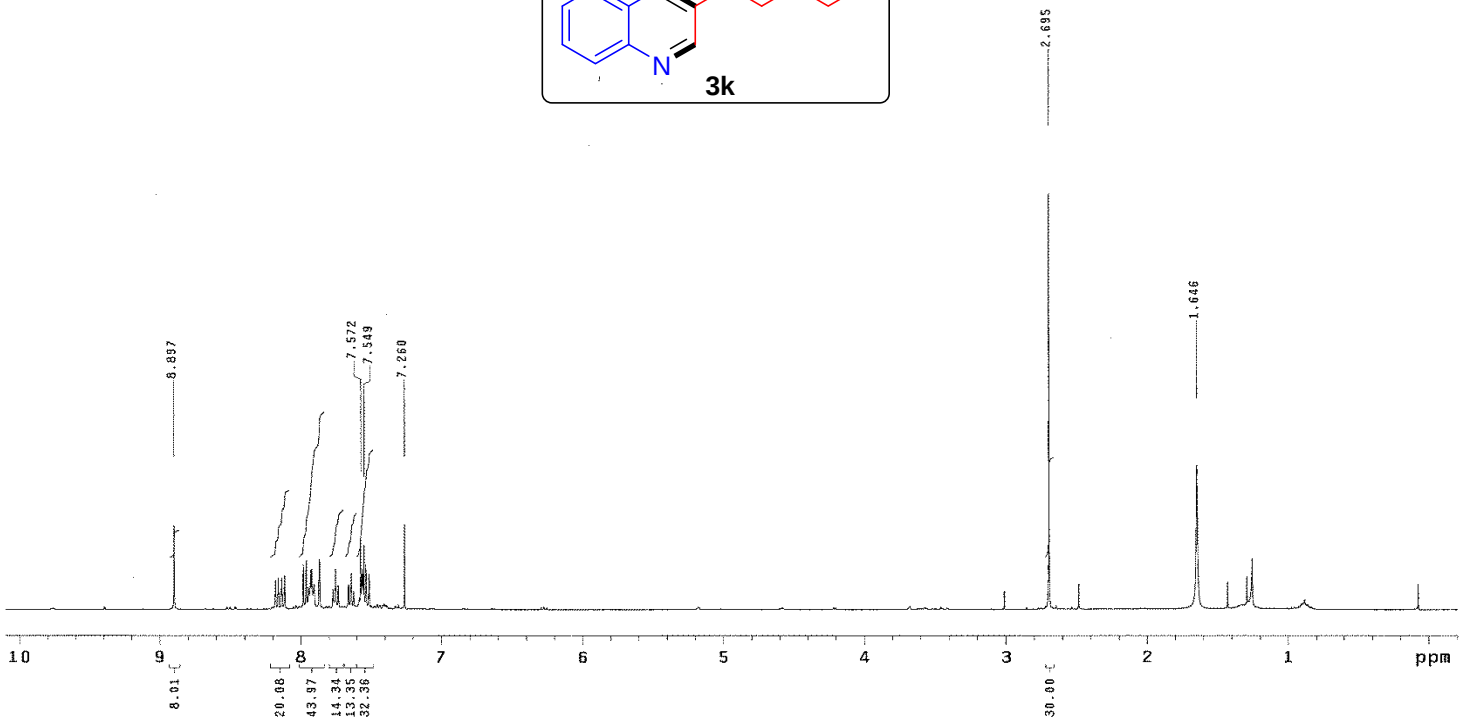
SGC/P-S/Q-Naph

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 56 repetitions



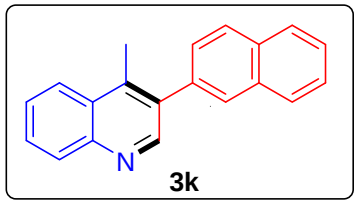
3k



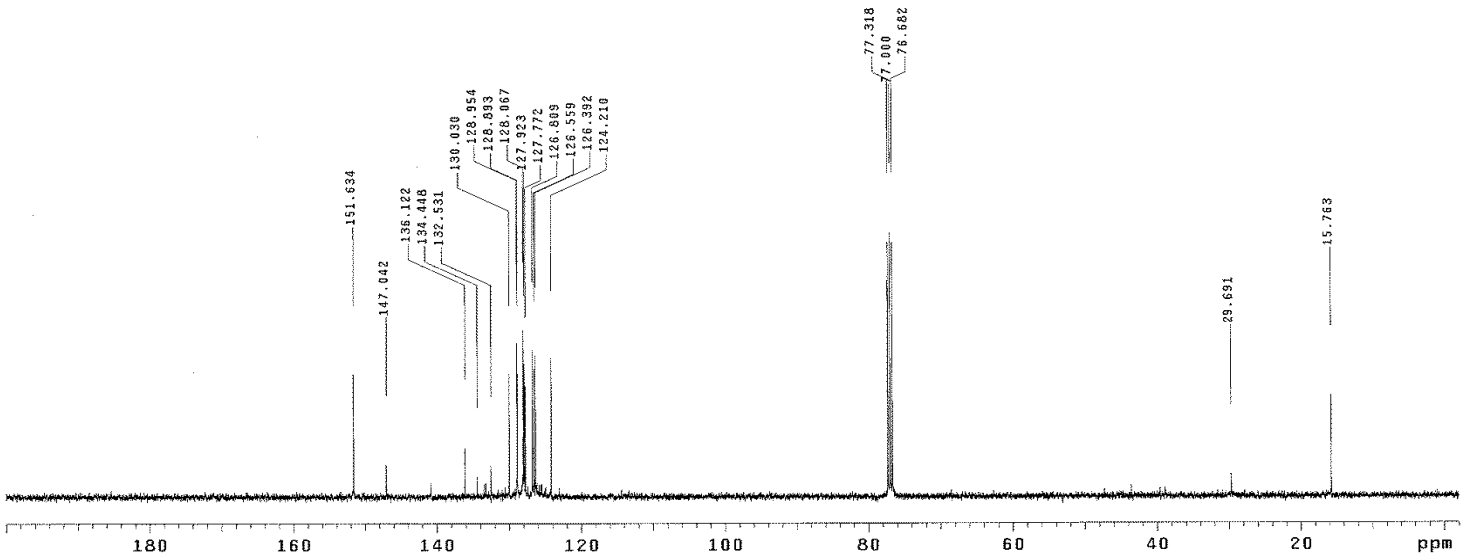
SGC/P-5/Q-Naph

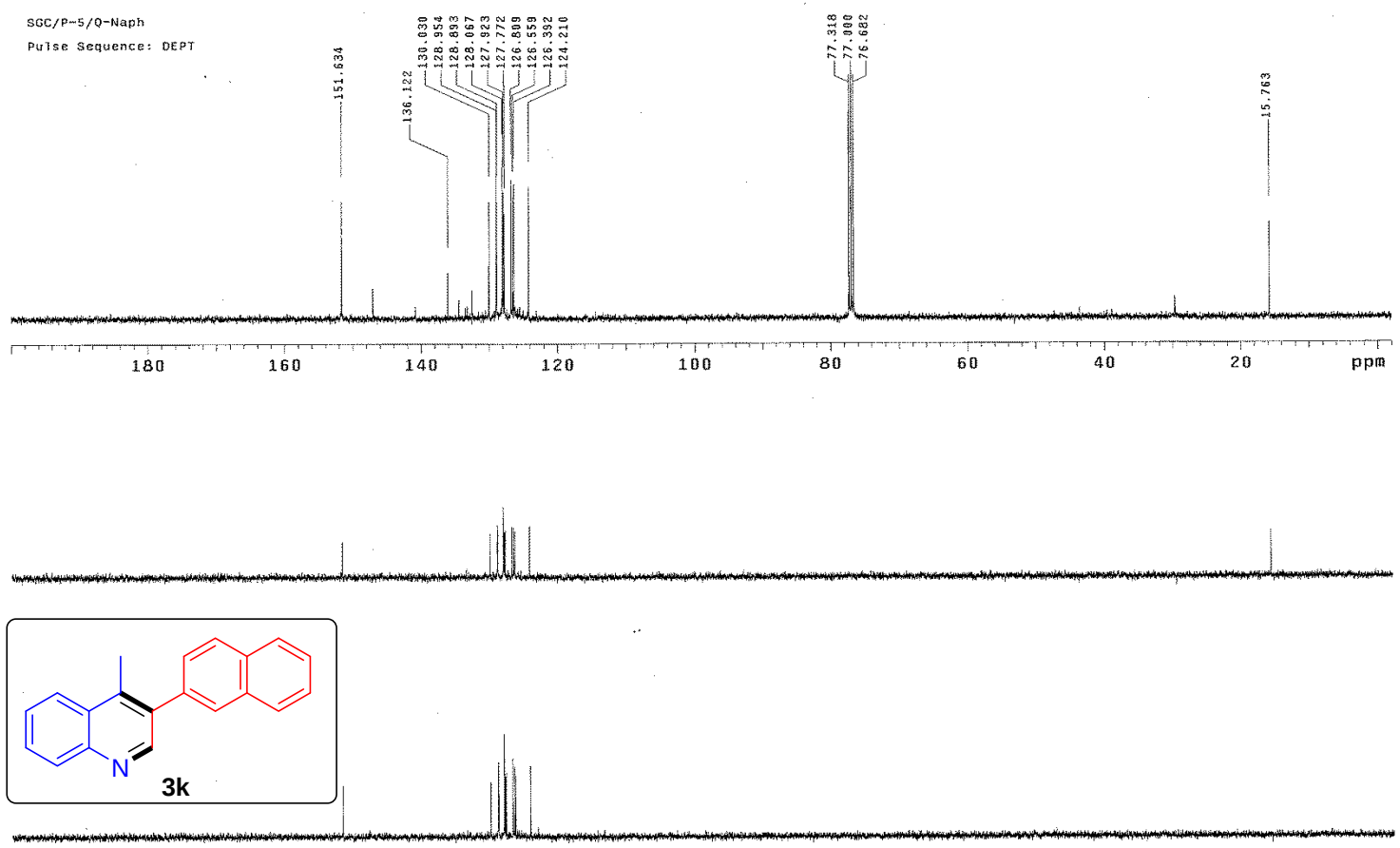
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 8400 repetitions



3k

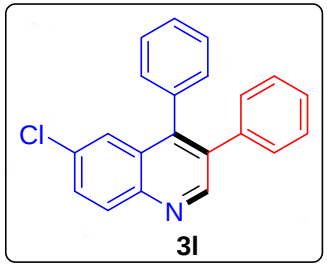



SGC/P-5/Q-Naph
Pulse Sequence: DEPT
151.634
136.122
130.030
128.954
128.893
128.067
127.923
127.772
126.809
126.559
126.392
124.210
77.318
77.000
76.682
15.763
180
160
140
120
100
80
60
40
20
ppm
N
3k

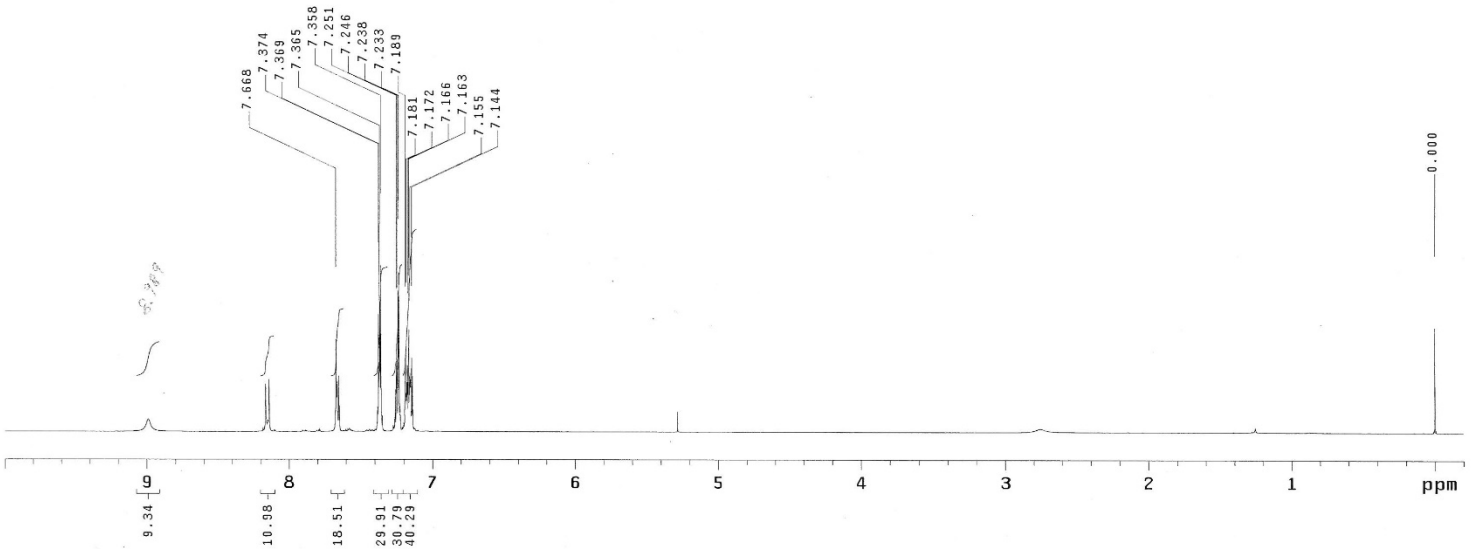
SGC/RP5/Cl-f

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jun 3 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



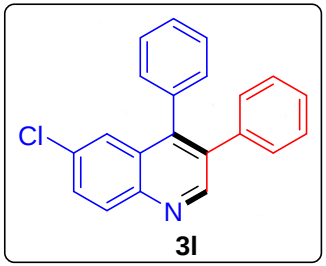
3l



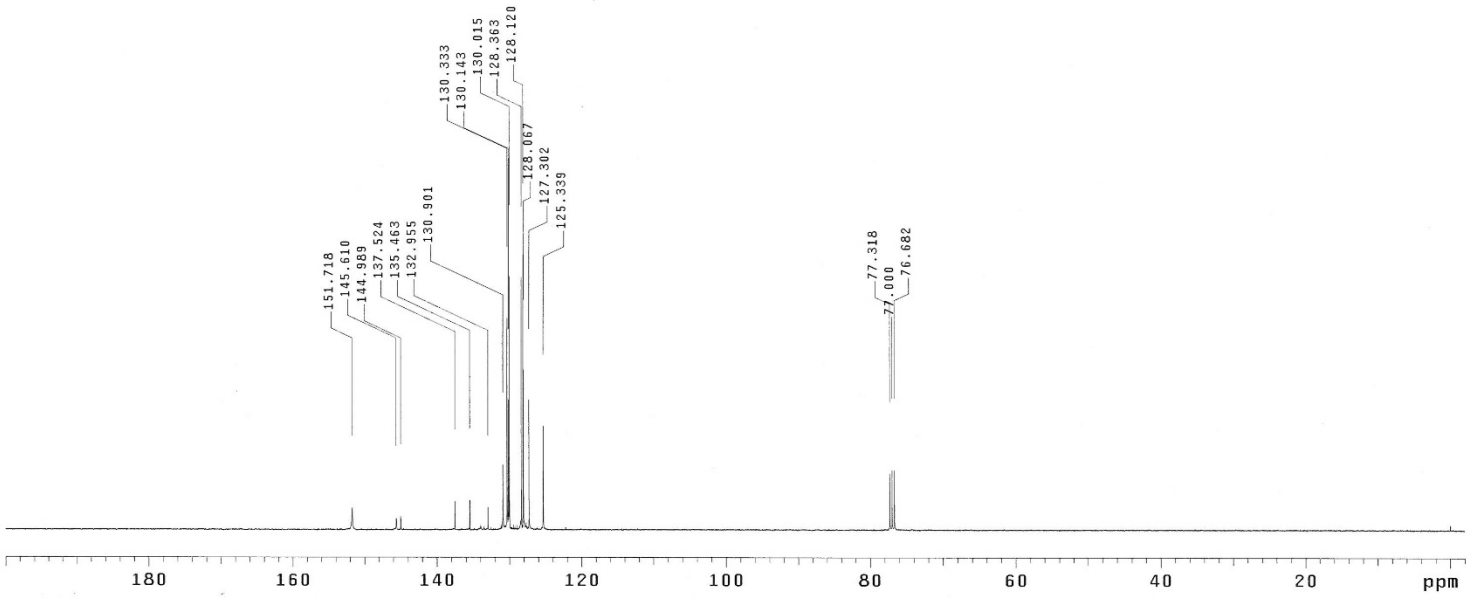
SGC/RP5/Cl-f

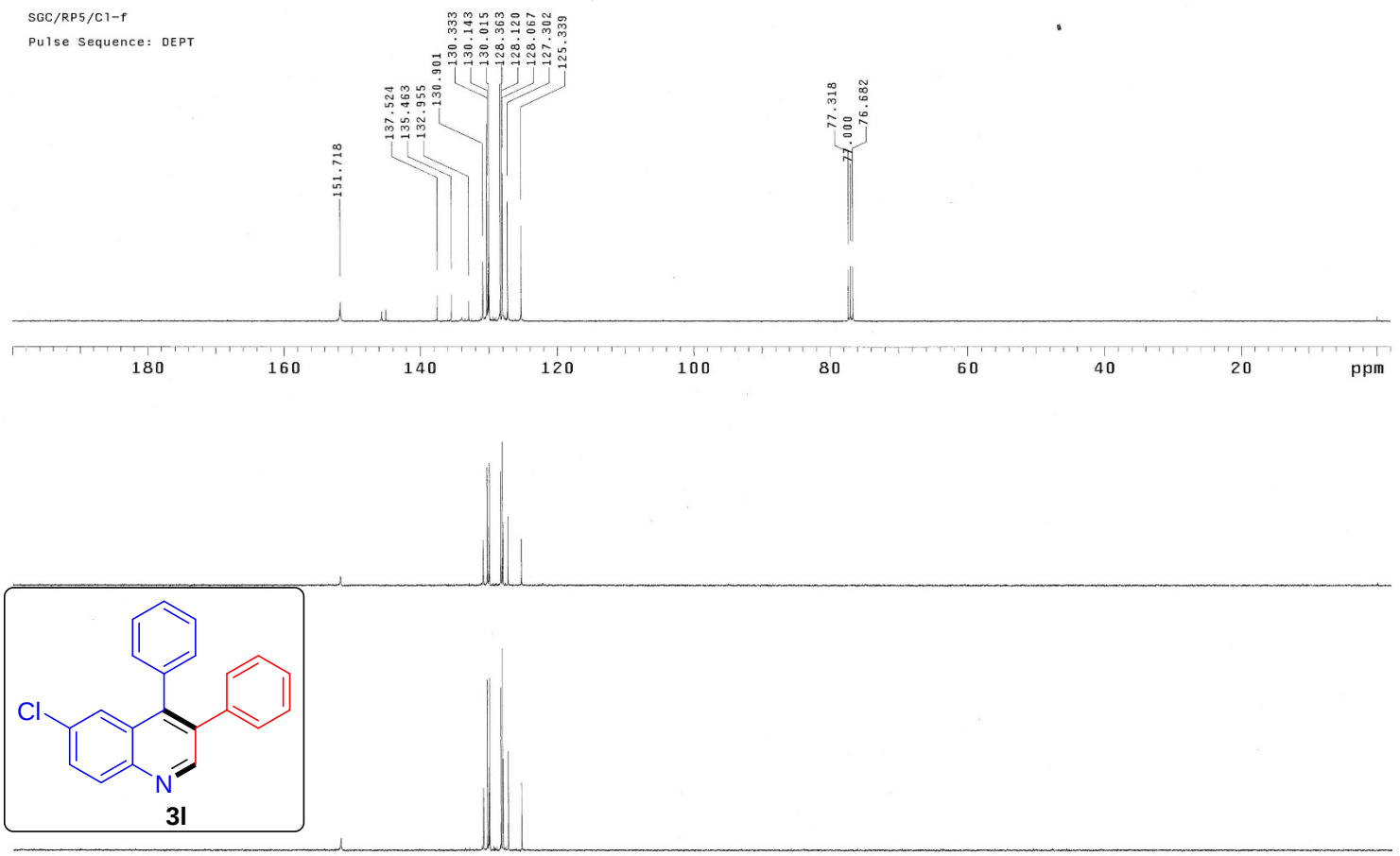
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jun 3 2015
Solvent: CDCl3
Ambient temperature
Total 3008 repetitions



3l

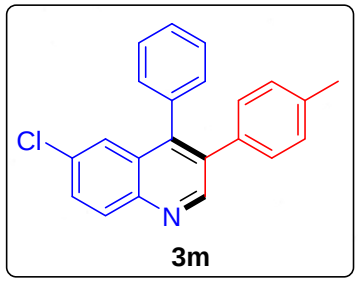



SGC/RP5/Cl-f
Pulse Sequence: DEPT
151.718
137.524
135.463
132.955
130.901
130.333
130.143
130.015
128.363
128.120
128.067
127.302
125.339
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Cl
N
3l

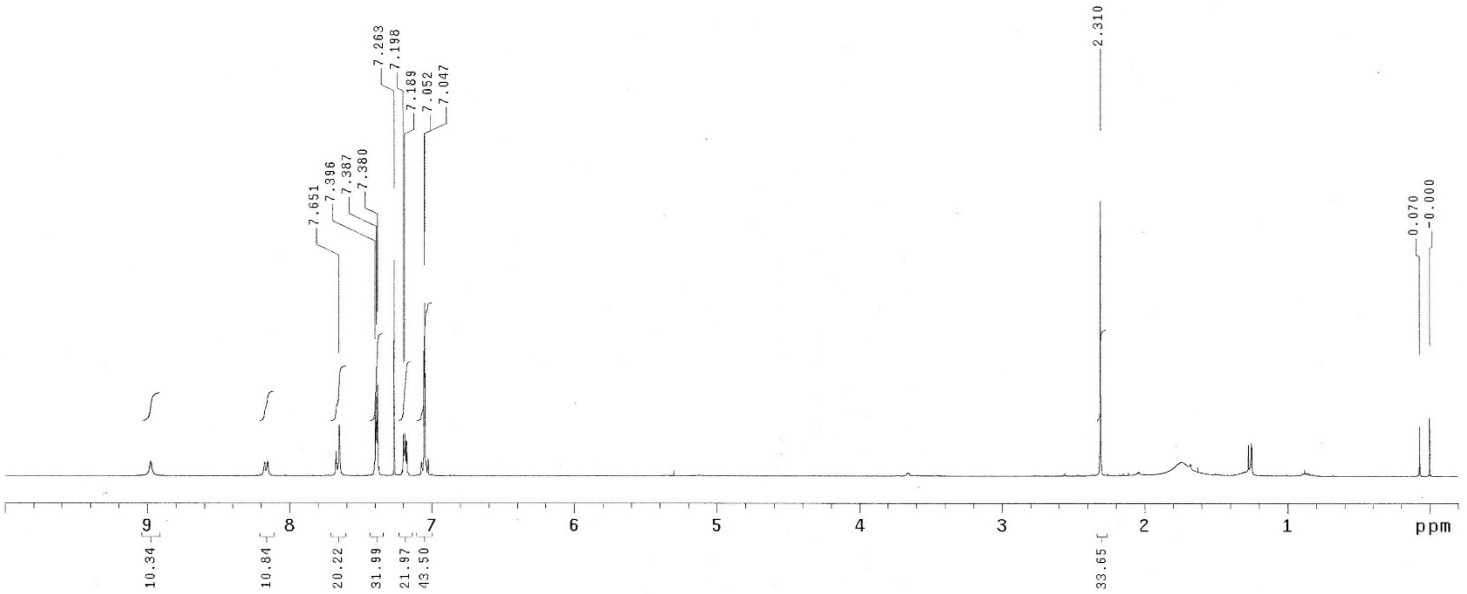
SGC/P-Cl/Me

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 132 repetitions



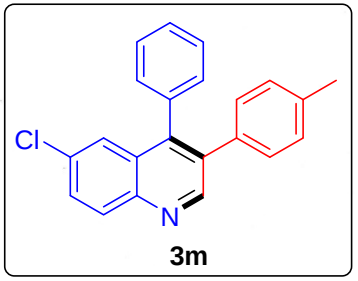
3m



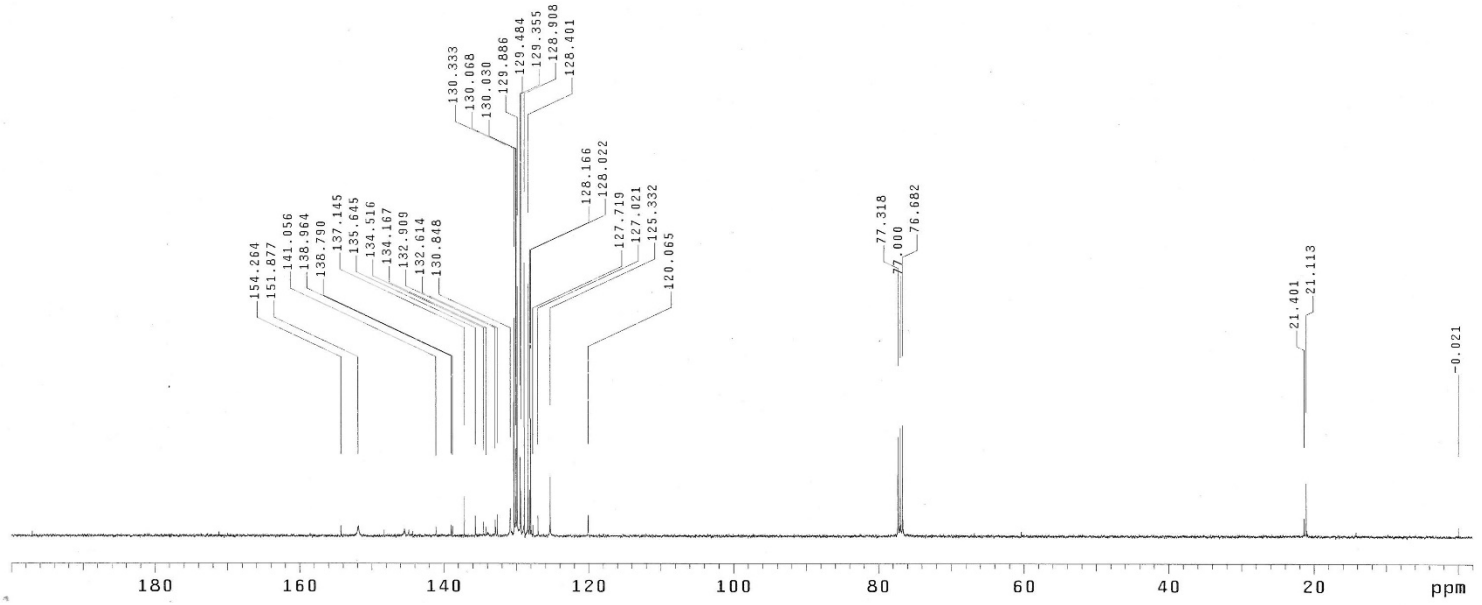
SGC/RP5/Q-12

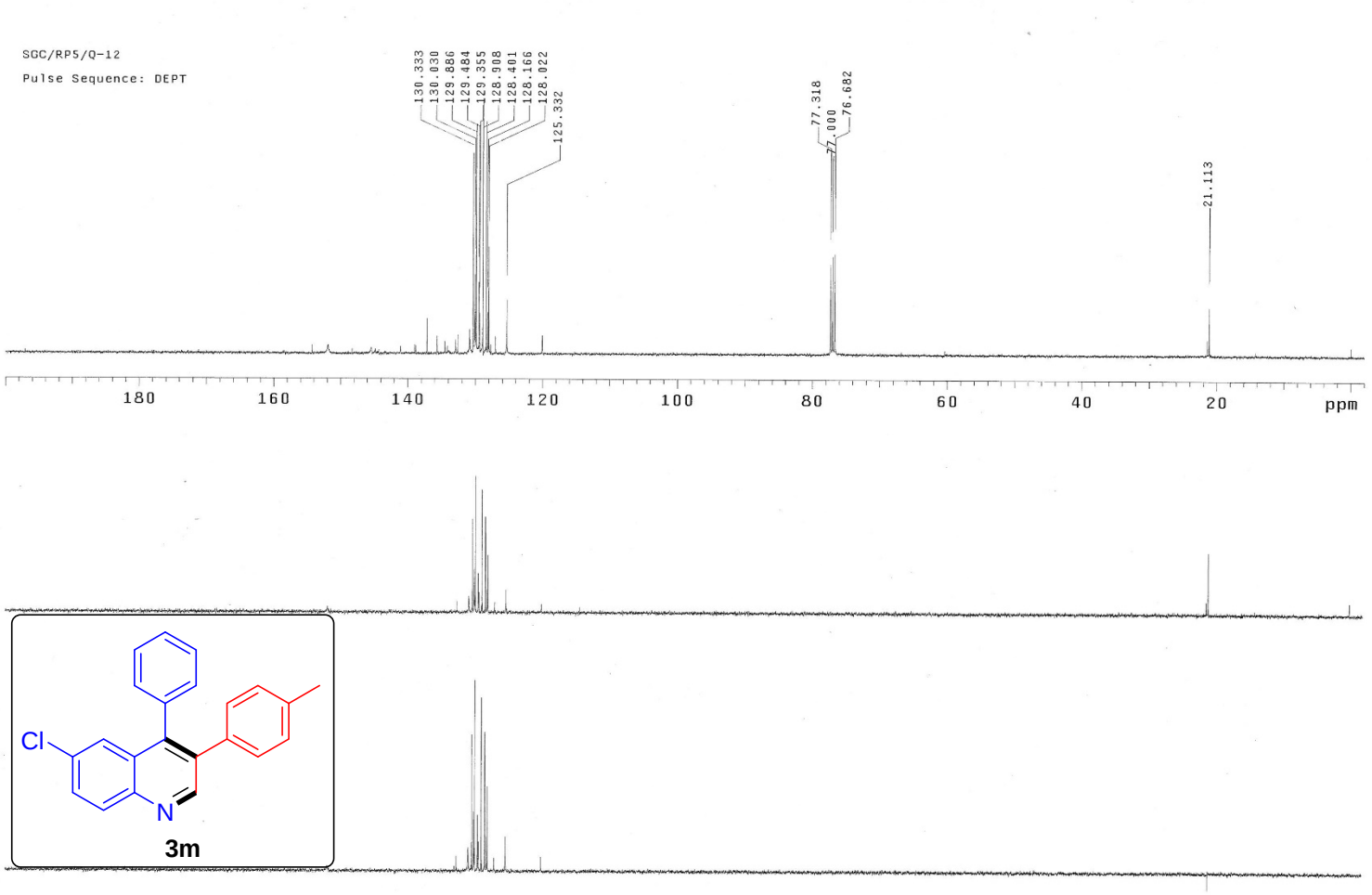
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 29 2015
Solvent: CDCl3
Ambient temperature
Total 7024 repetitions



3m

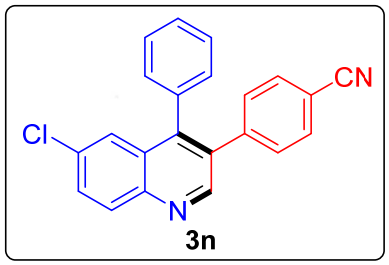



SGC/RP5/Q-12
Pulse Sequence: DEPT
130.333
130.030
129.886
129.484
129.355
128.908
128.401
128.166
128.022
125.332
77.318
77.000
76.682
21.113
180
160
140
120
100
80
60
40
20
ppm
Cl
N
3m

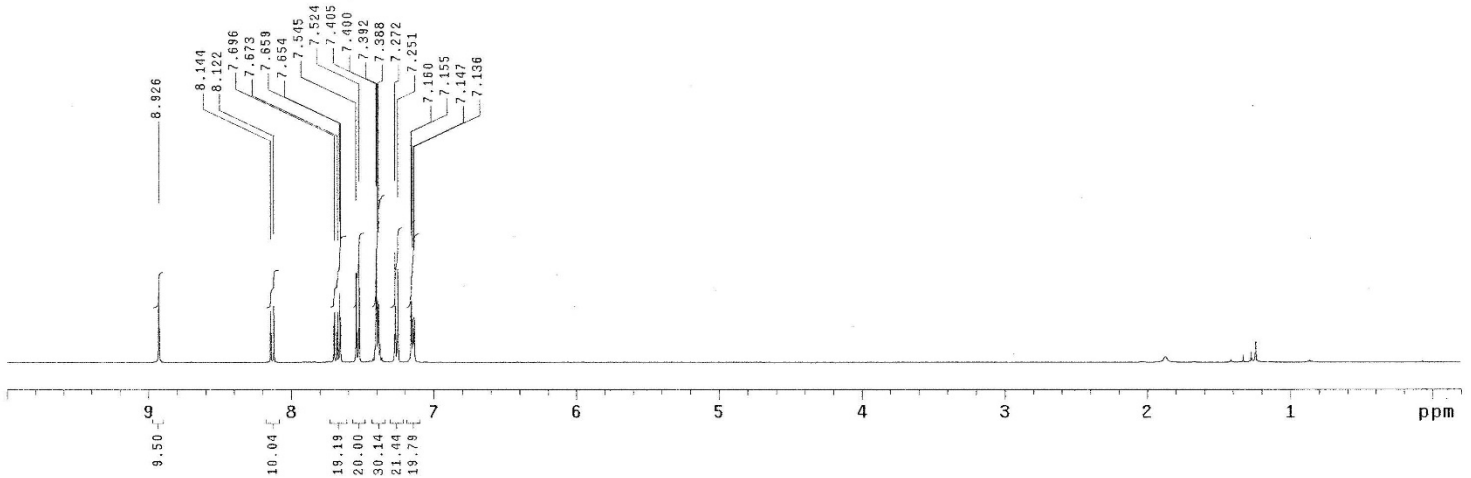
SGC/RP5/5

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 5 2015
Solvent: CDCl3
Ambient temperature
Total 16 repetitions



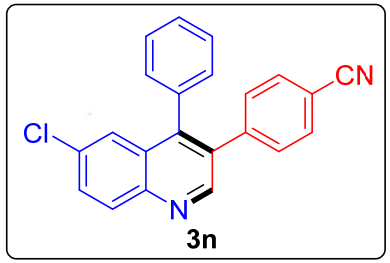
3n



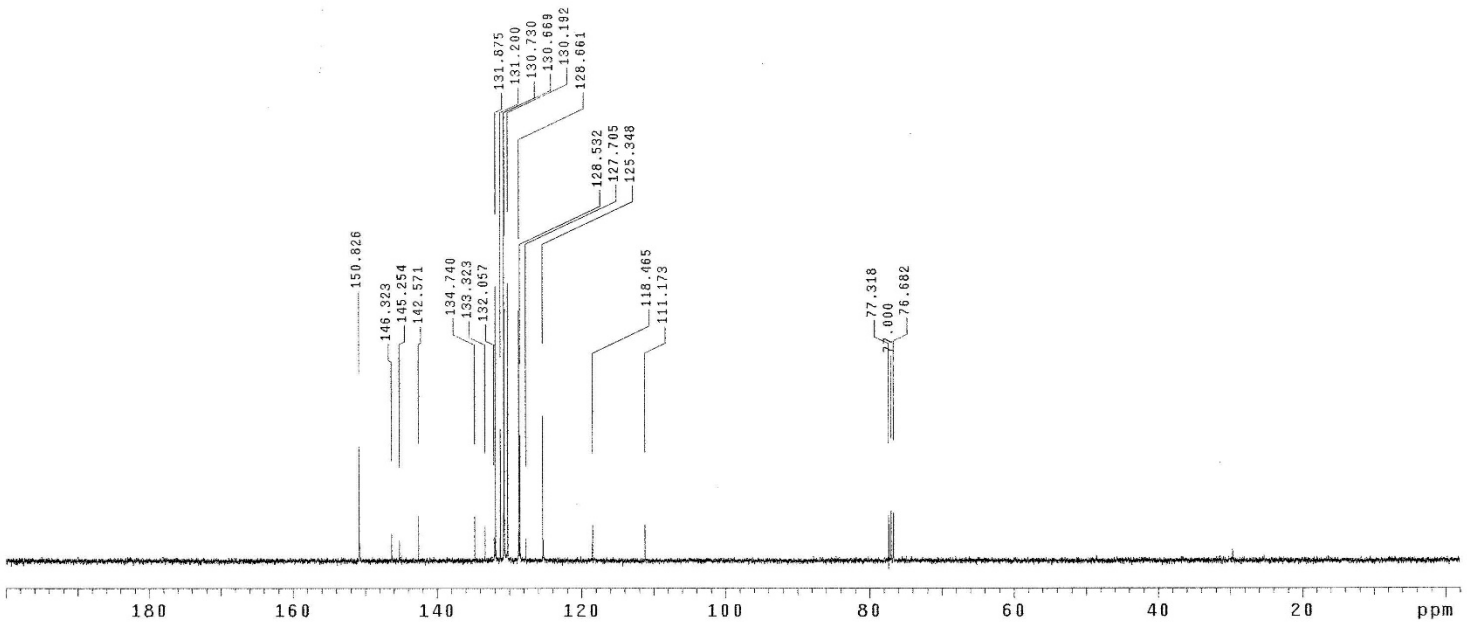
SGC/RP5/5

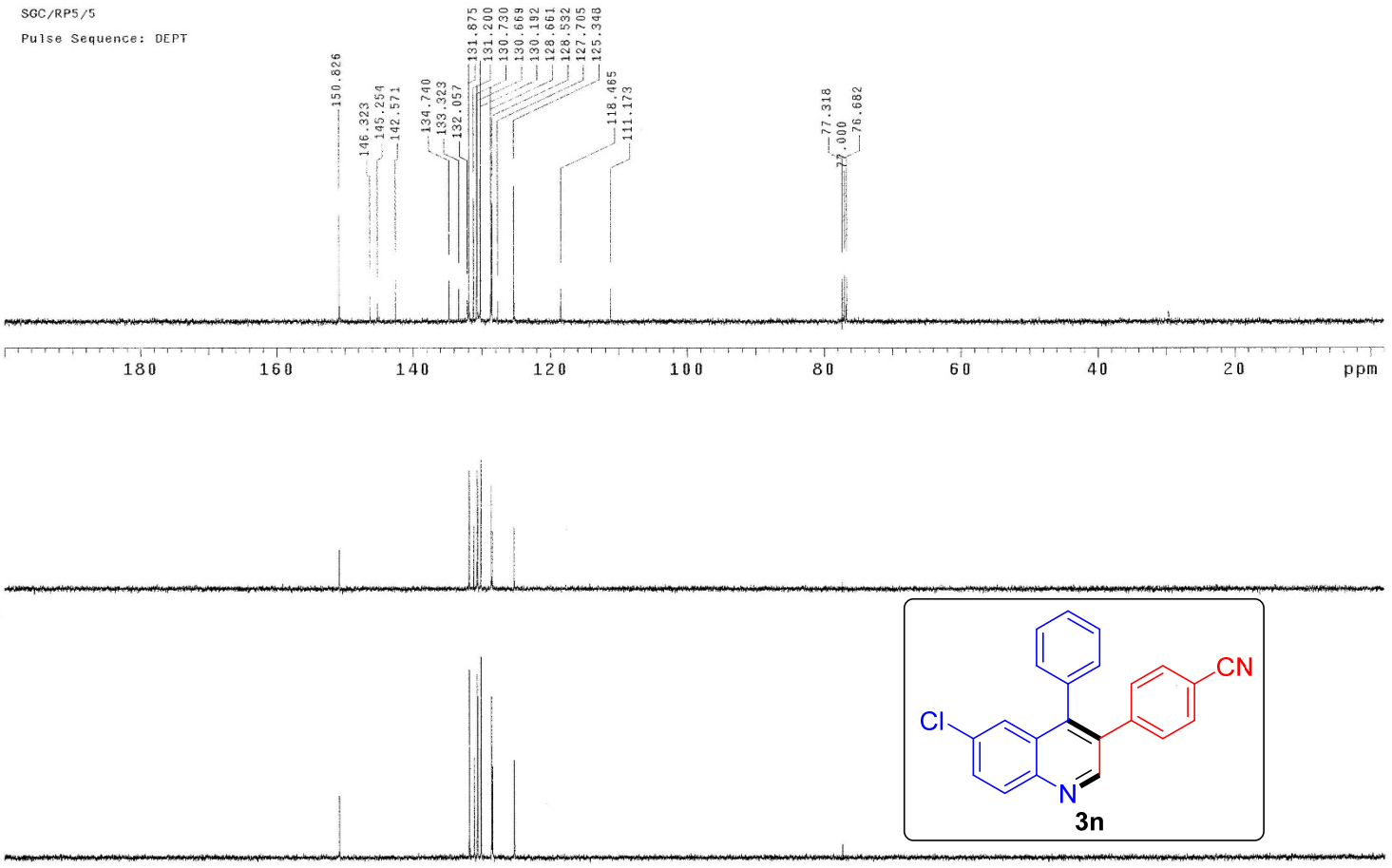
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 5 2015
Solvent: CDCl3
Ambient temperature
Total 432 repetitions



3n

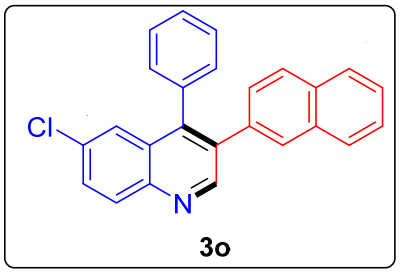



SGC/RP5/5
Pulse Sequence: DEPT
150.826
146.323
145.254
142.571
134.740
133.323
132.057
131.875
131.200
130.730
130.669
130.192
128.661
128.532
127.705
125.340
118.465
111.173
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Cl
CN
N
3n

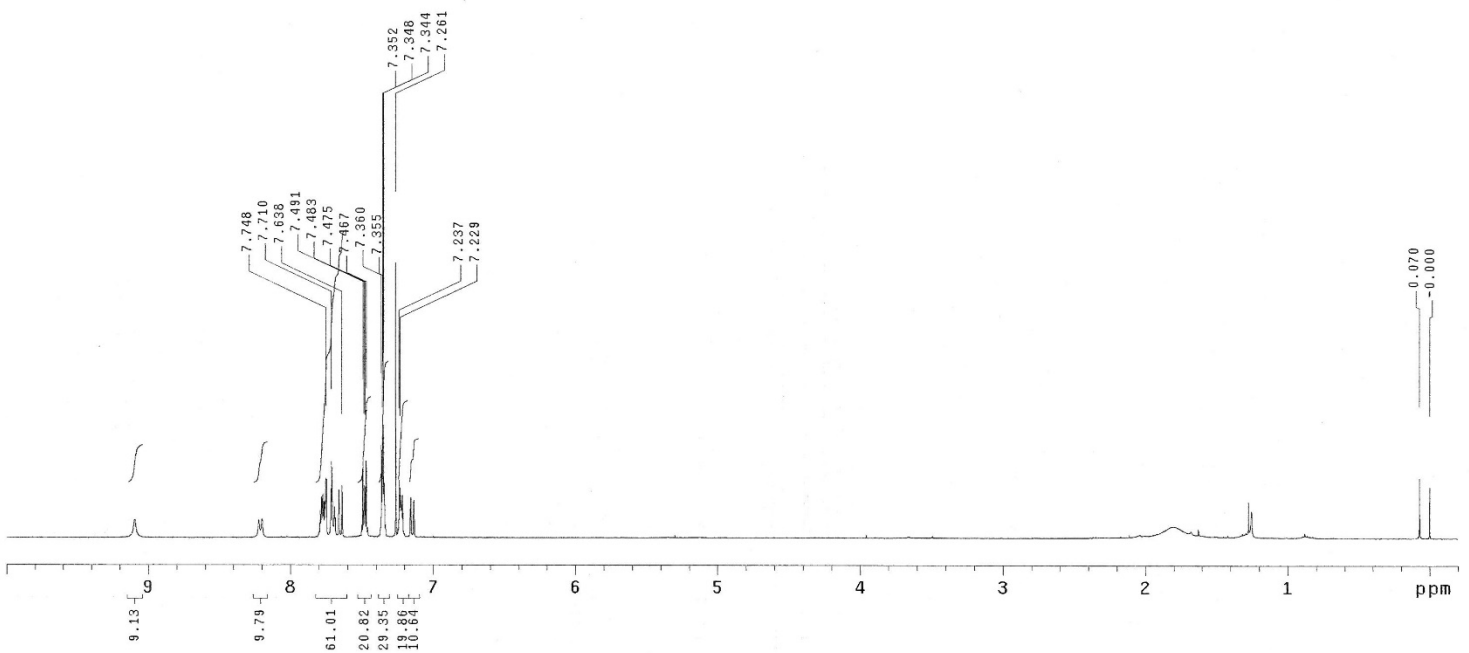
SGC/P-Cl/Nap

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



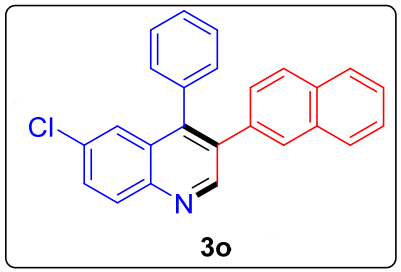
3o



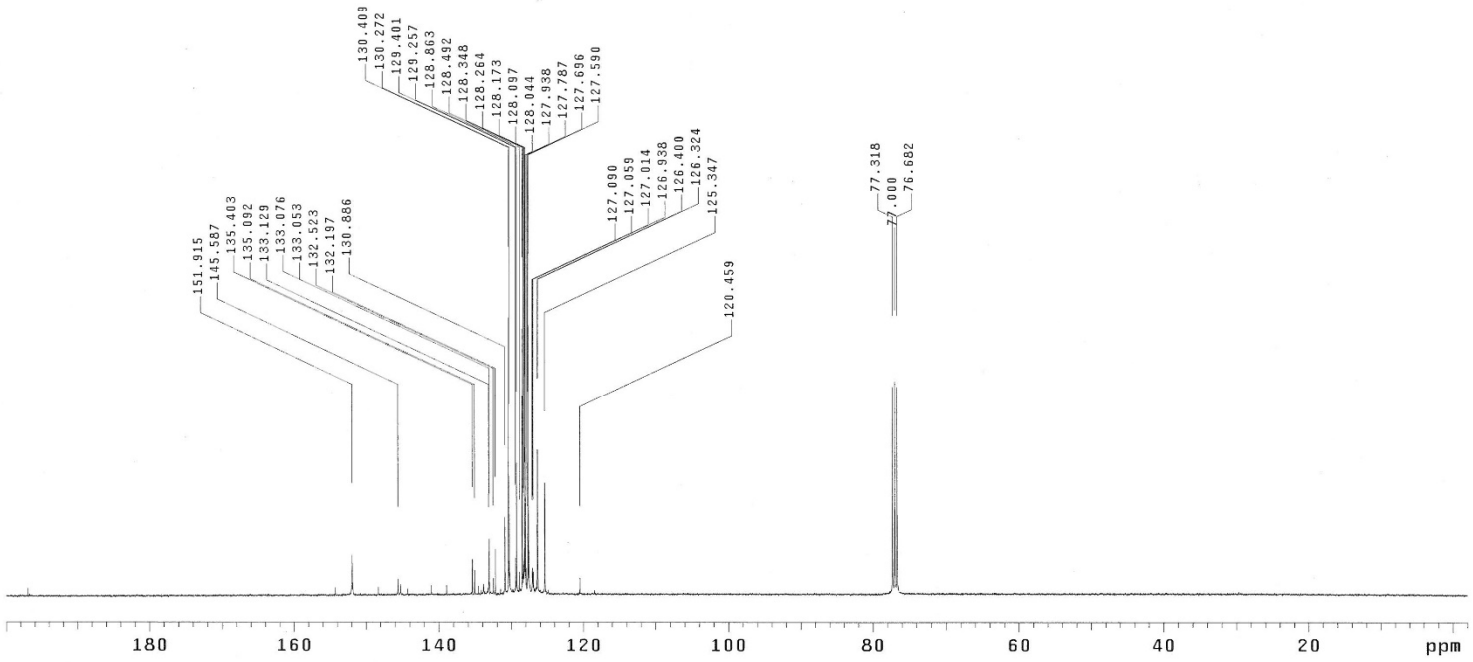
SGC/RP5/1

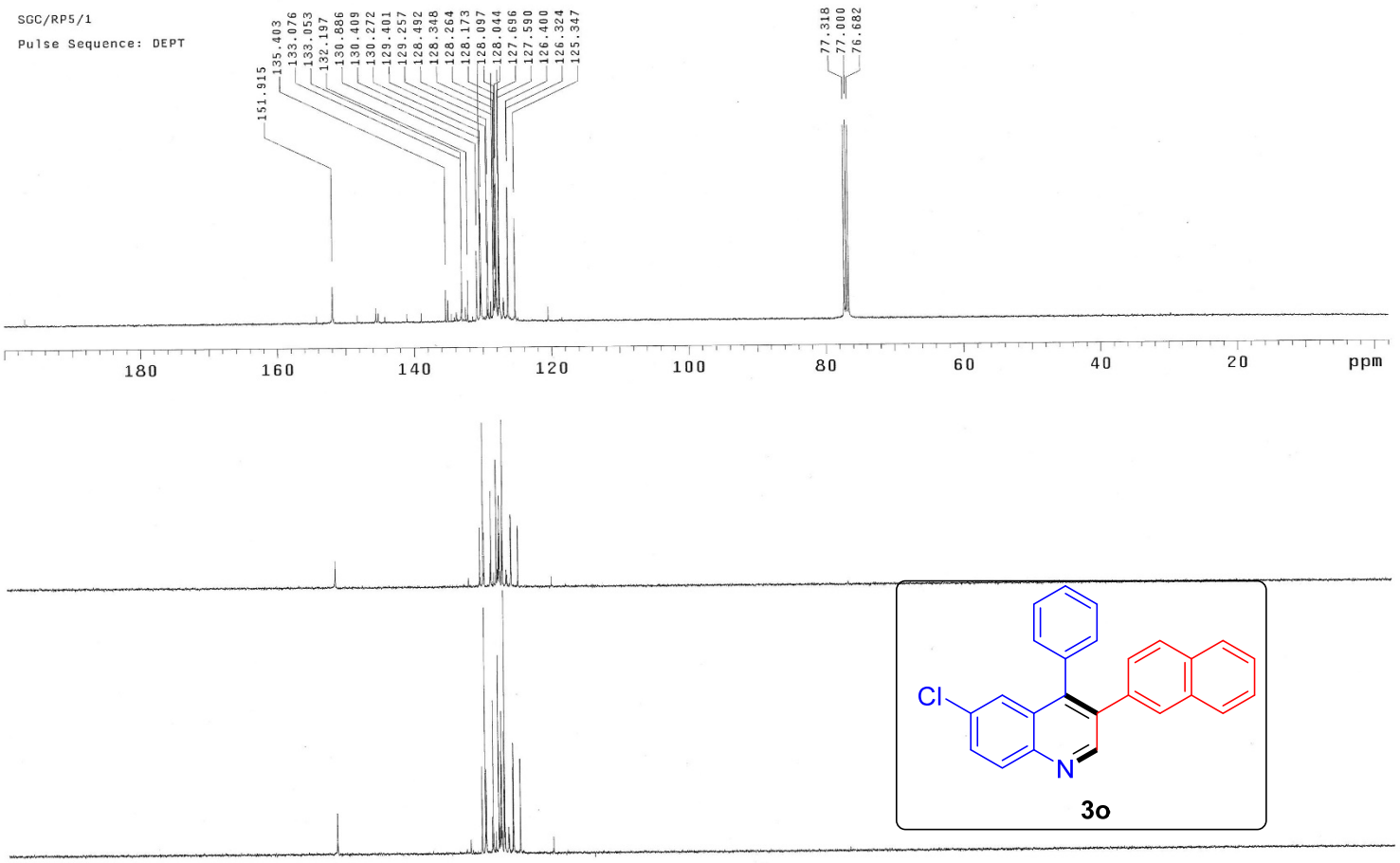
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 5 2015
Solvent: CDCl3
Ambient temperature
Total 20480 repetitions



3o

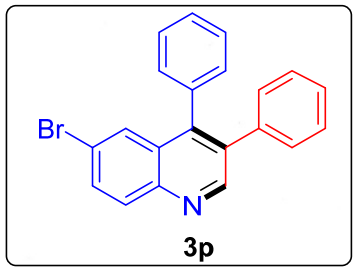



SGC/RP5/1
Pulse Sequence: DEPT
151.915
135.403
133.076
133.053
132.197
130.886
130.409
130.272
129.401
129.257
128.492
128.348
128.264
128.173
128.097
128.044
127.686
127.590
126.400
126.324
125.347
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Cl
N
3o

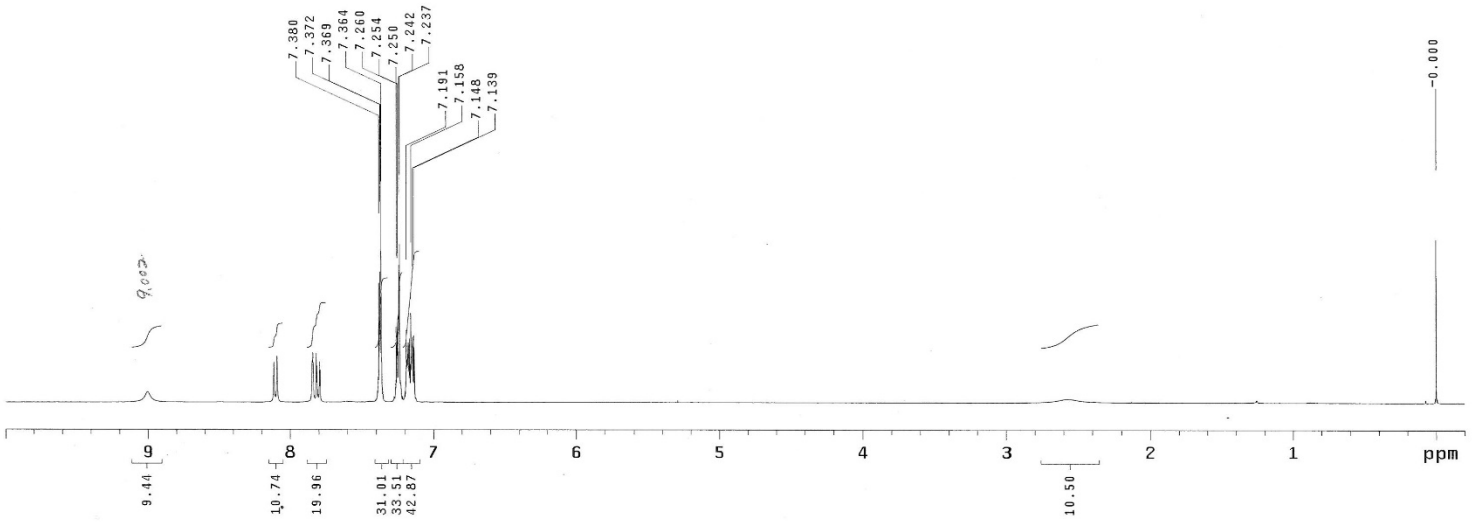
SGC/RP5/Br-final

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jun 3 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



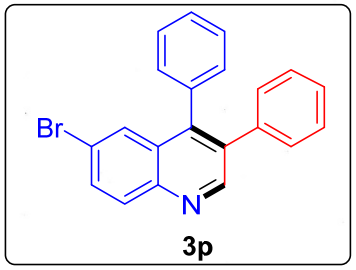
3p



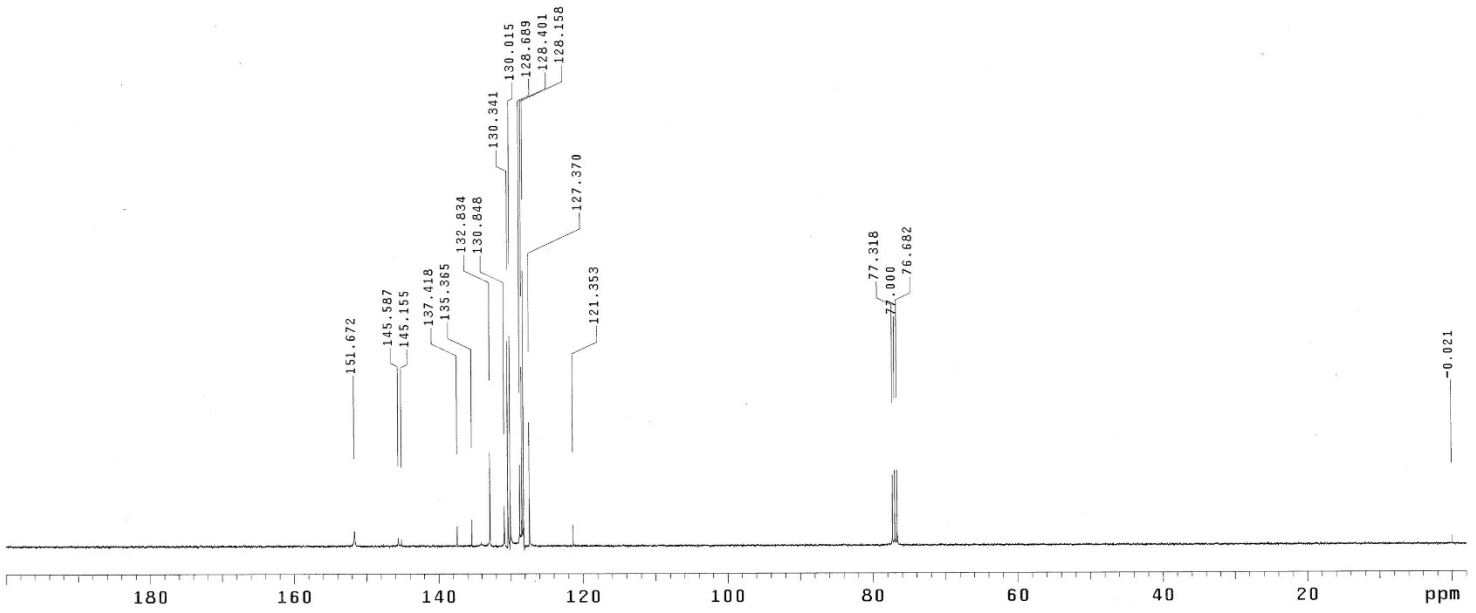
SGC/RP5/Br-final

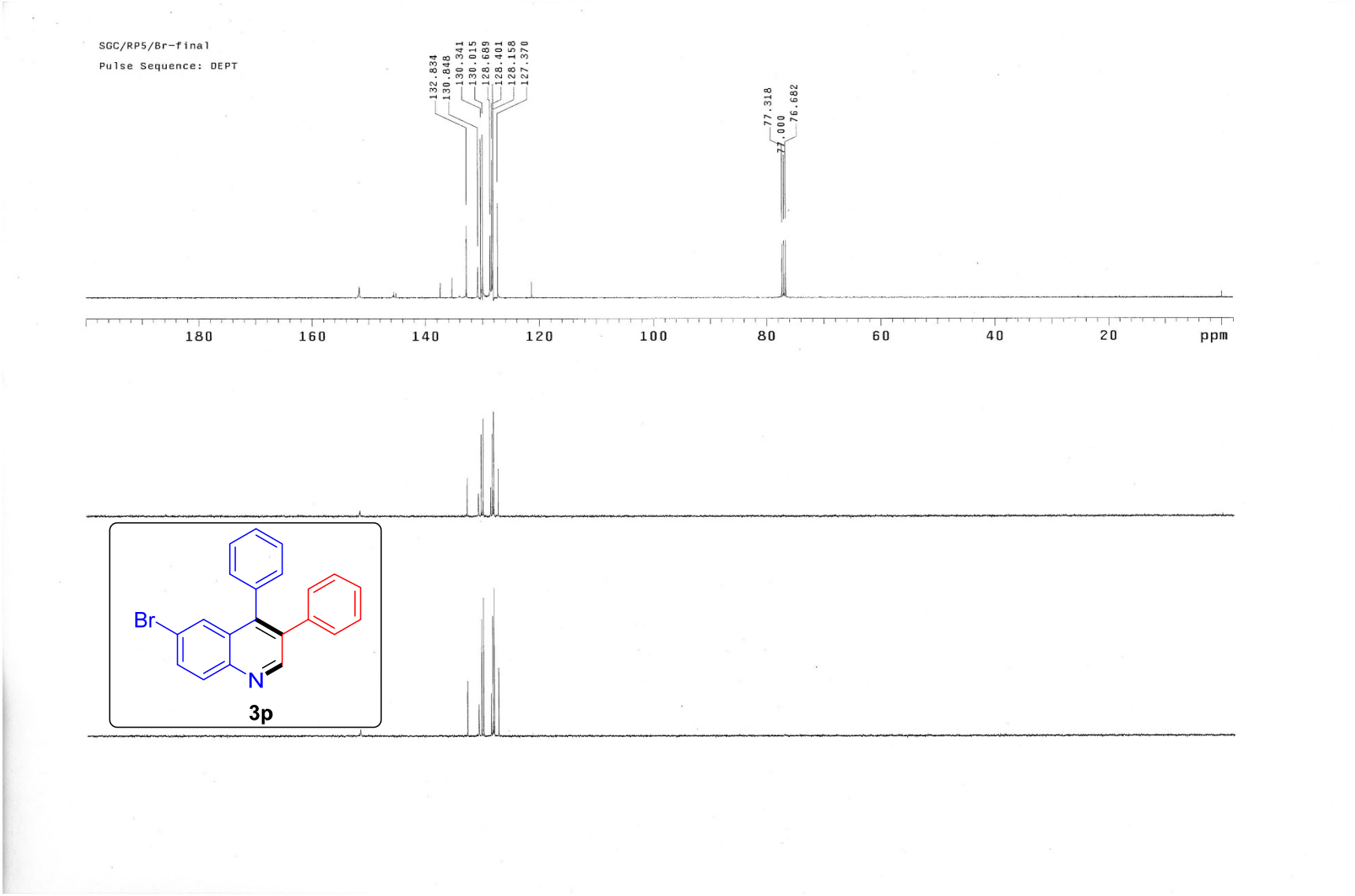
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jun 3 2015
Solvent: CDCl3
Ambient temperature
Total 4112 repetitions



3p

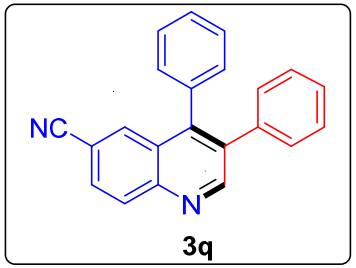



SGC/RP5/Br-final
Pulse Sequence: DEPT
132.834
130.848
130.341
130.015
128.689
128.401
128.158
127.370
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Br
N
3p

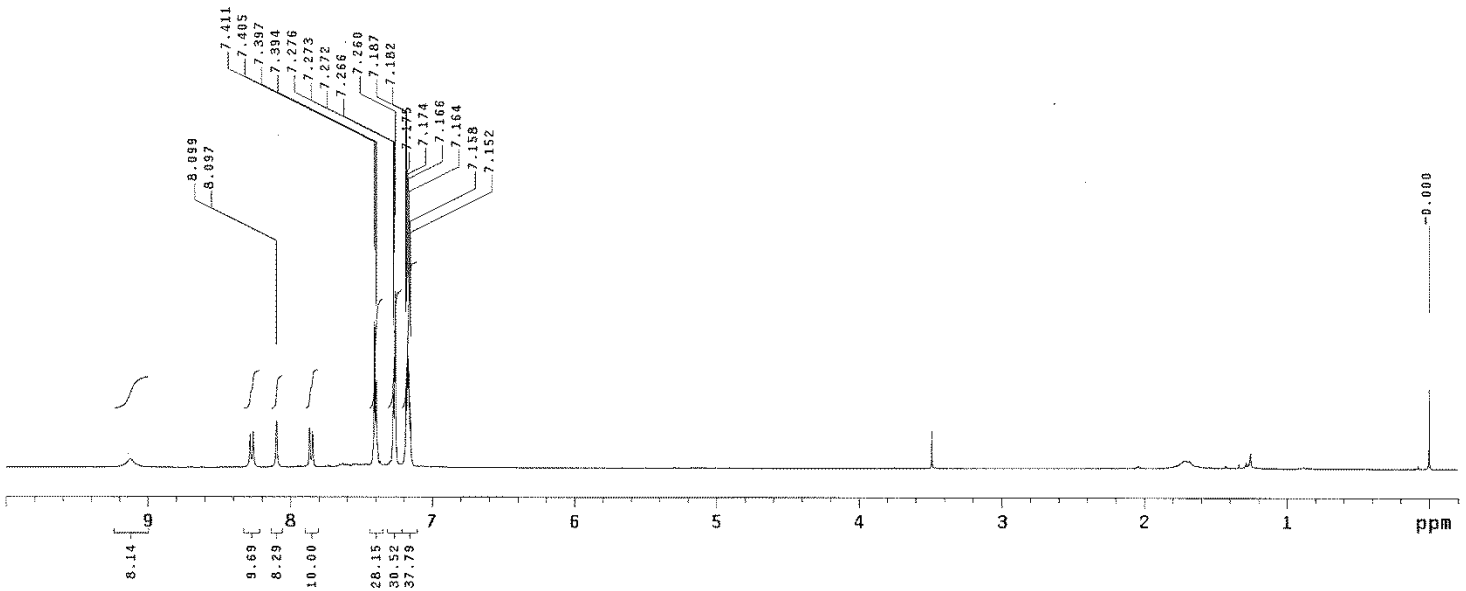
SGC/P-5/Quin

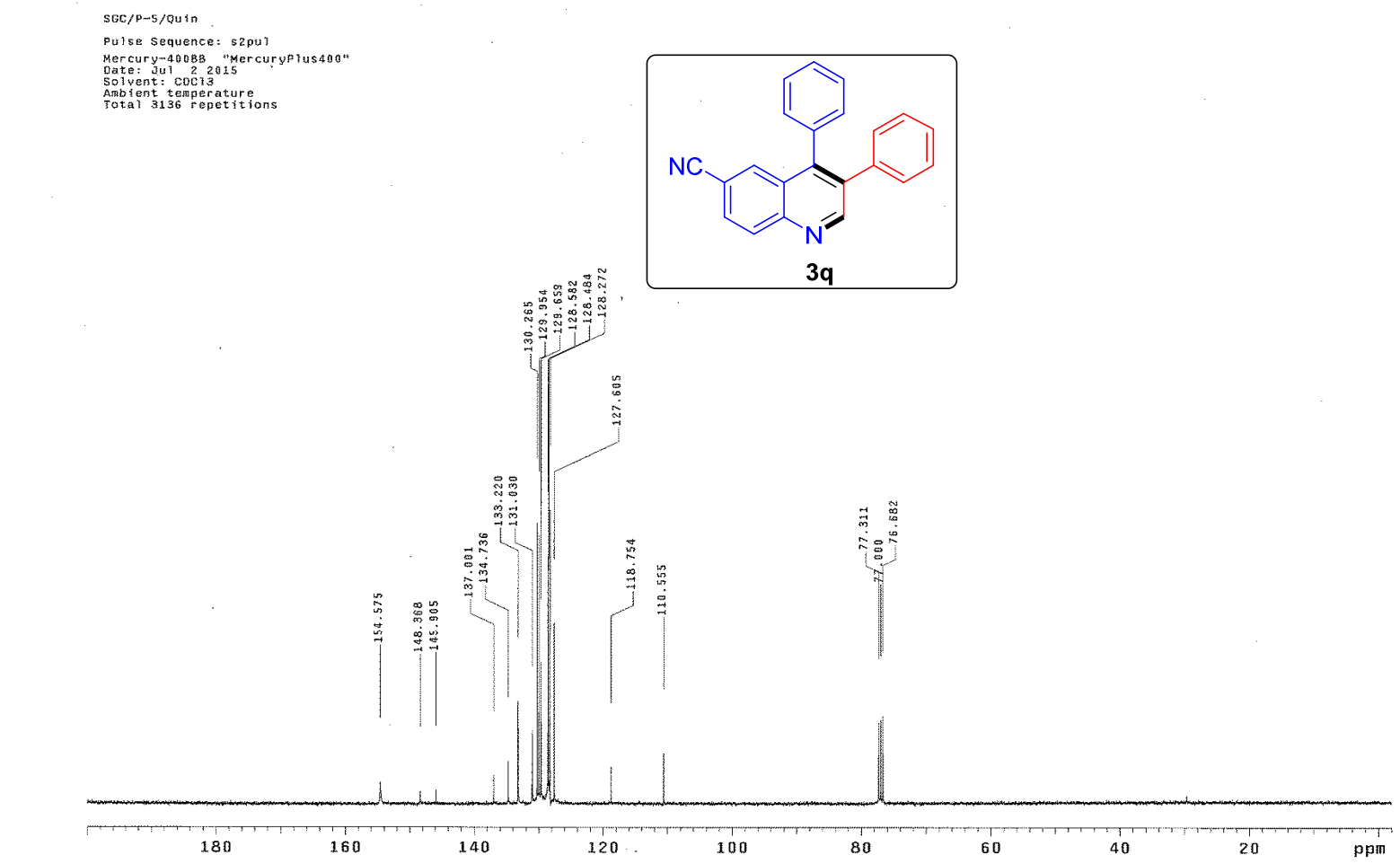
Pulse Sequence: s2pul

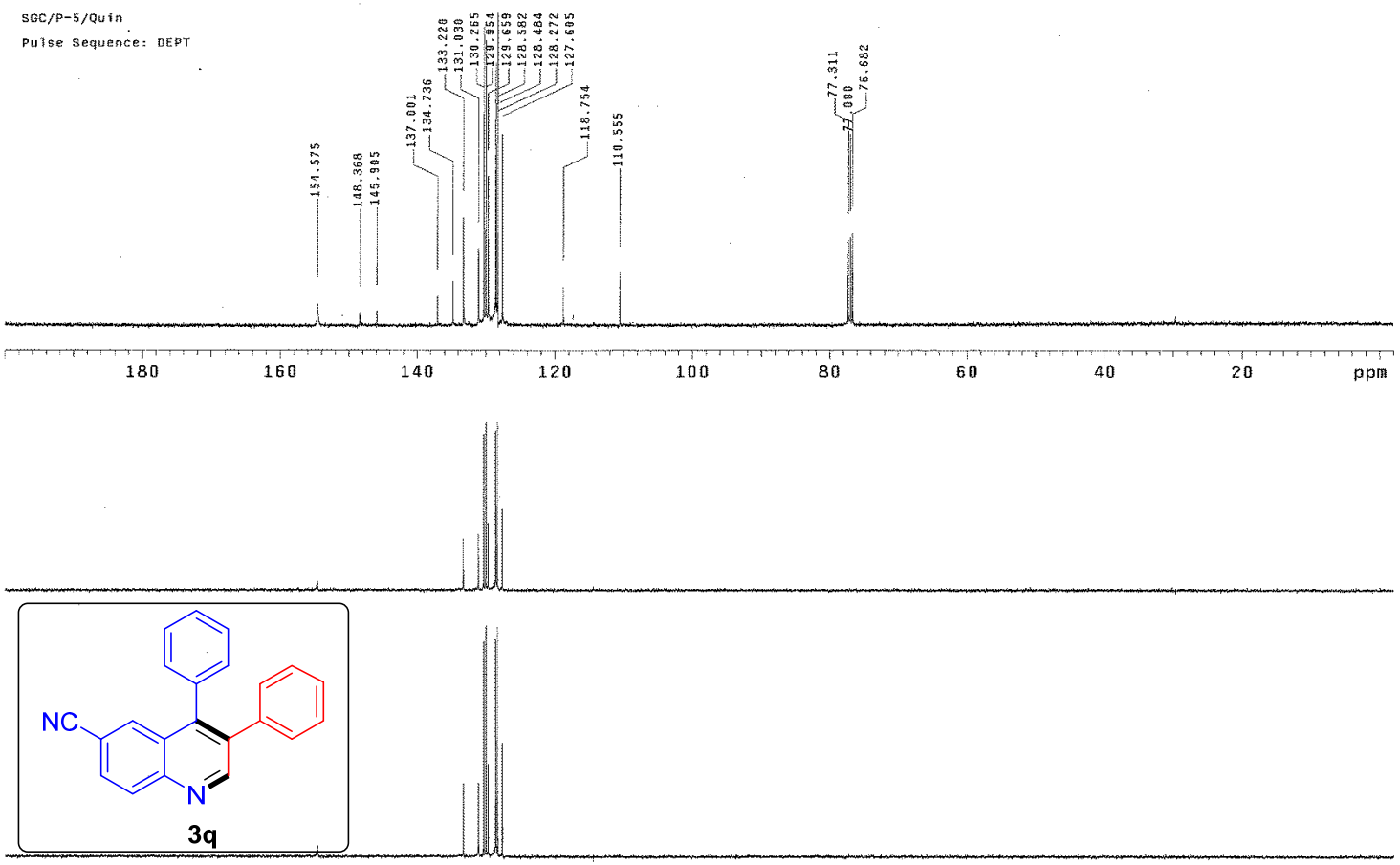
Mercury-400BB "MercuryPlus400"
Date: Jul 2 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



3q



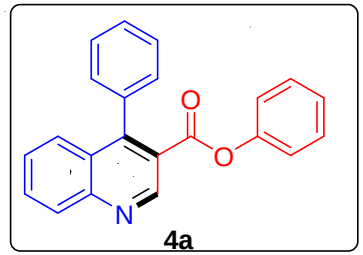

SGC/P-5/Quin
Pulse Sequence: s2pul
Mercury-400BB "MercuryPlus400"
Date: Jul 2 2015
Solvent: CDCl3
Ambient temperature
Total 3136 repetitions
NC
N
3q
154.575
148.368
145.905
137.001
134.736
133.220
131.030
130.265
129.954
129.659
128.582
128.484
128.272
127.605
118.754
110.555
77.311
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm


SGC/P-5/Quin
Pulse Sequence: DEPT
154.575
148.368
145.905
137.001
134.736
133.220
131.030
130.265
129.954
129.659
128.582
128.484
128.272
127.695
118.754
110.555
77.311
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
NC
N
3q

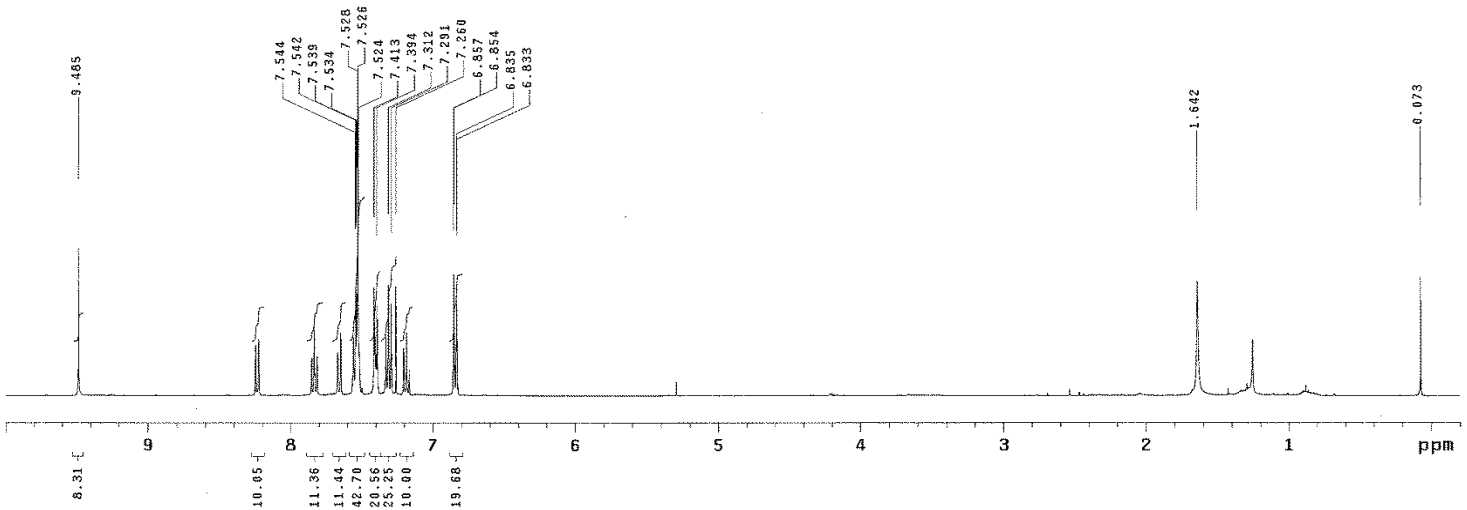
SGC/P-5/Q-Ester

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



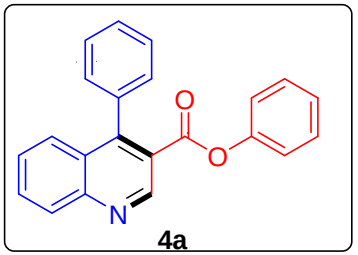
4a



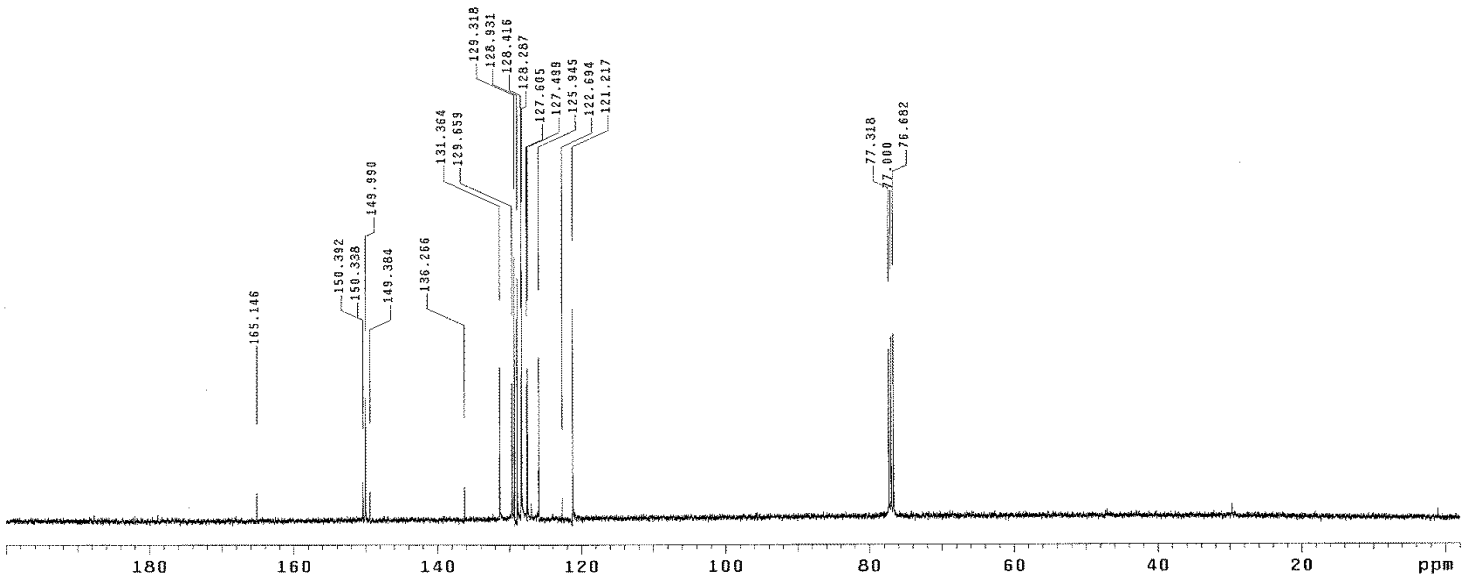
SGC/P-5/Q-Ester

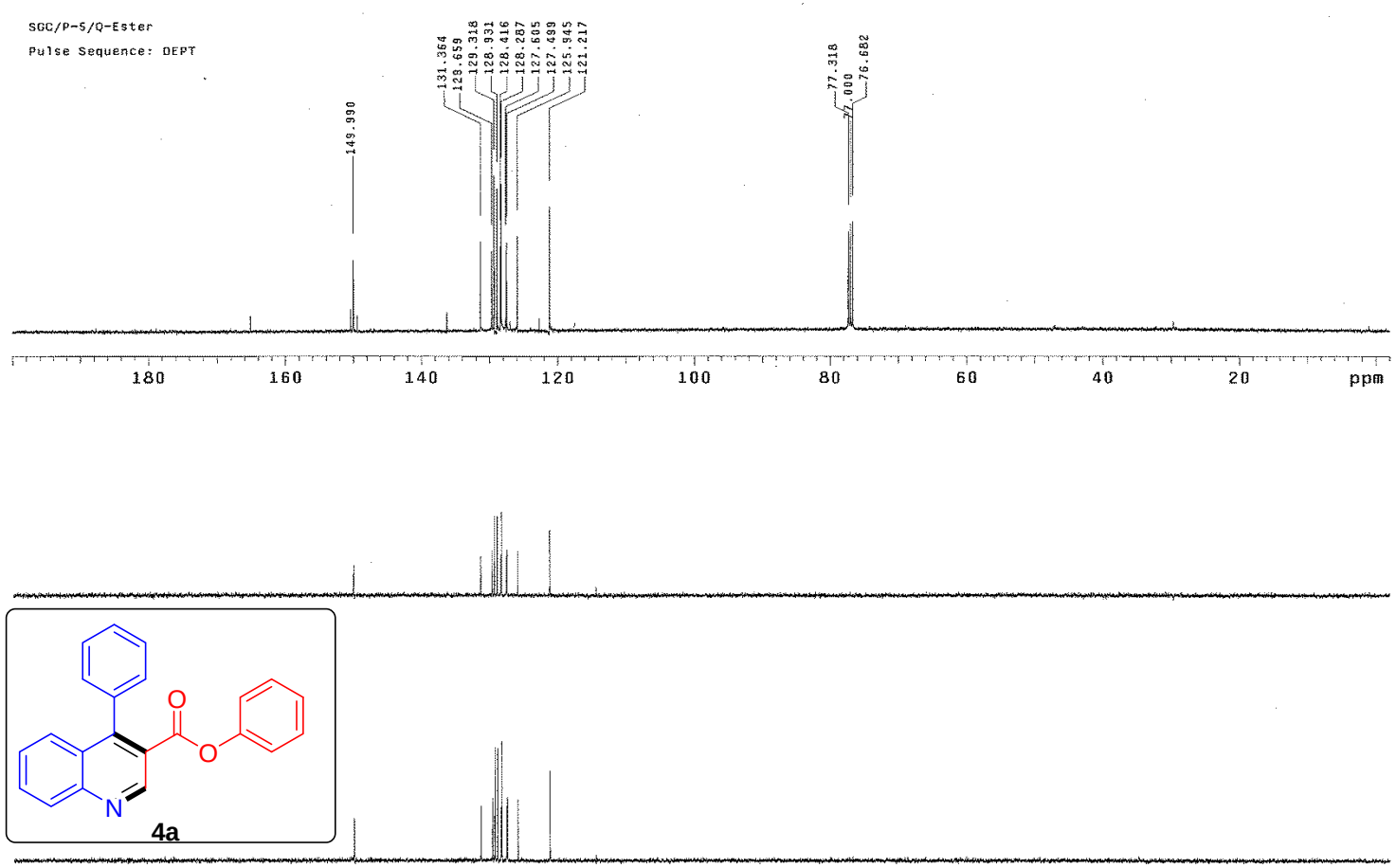
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 4112 repetitions



4a

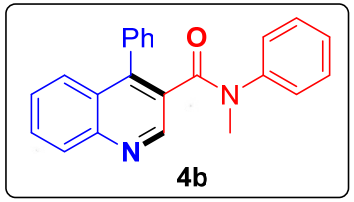



SGC/P-S/Q-Ester
Pulse Sequence: DEPT
149.930
131.364
129.659
129.318
128.931
128.416
128.287
127.605
127.499
125.945
121.217
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
O
O
N
4a

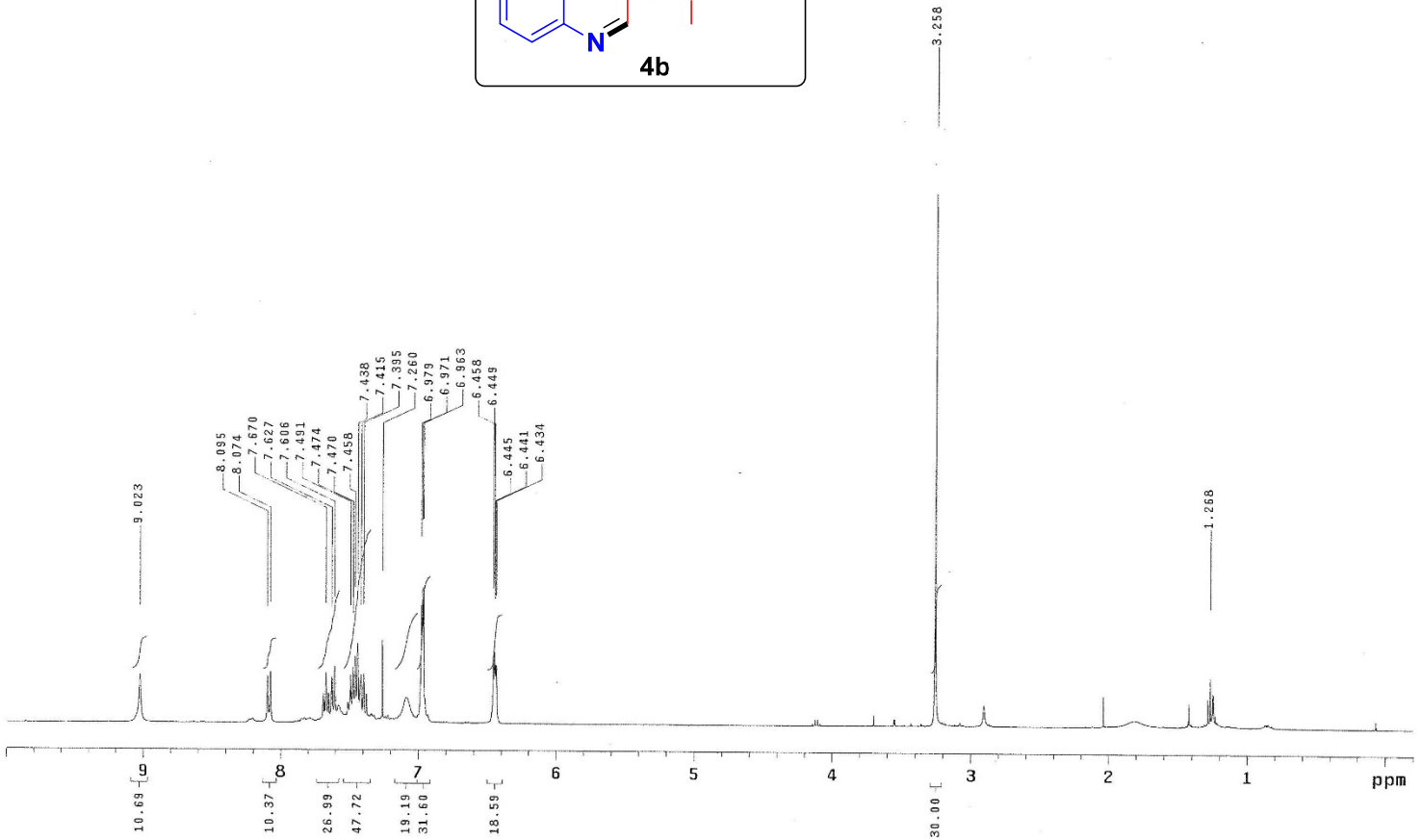
SGC/P-5/7

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 8 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



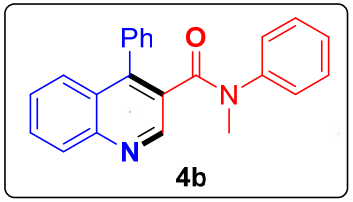
4b



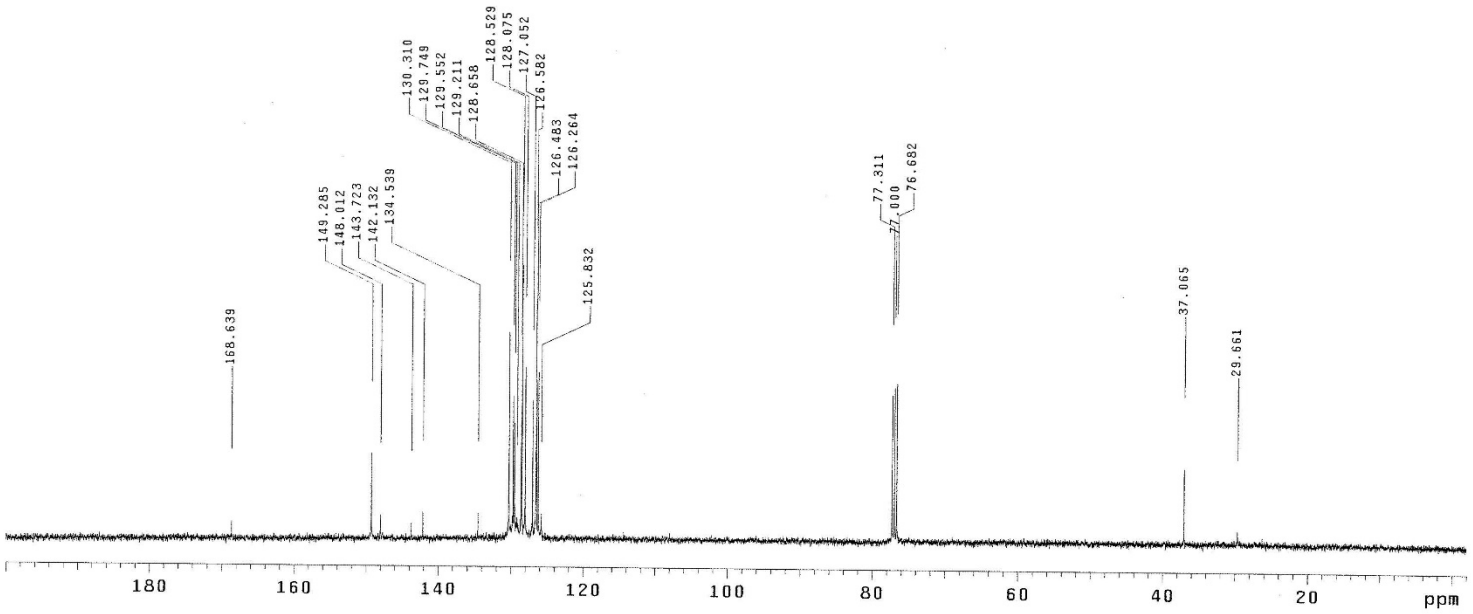
SGC/P-5/7

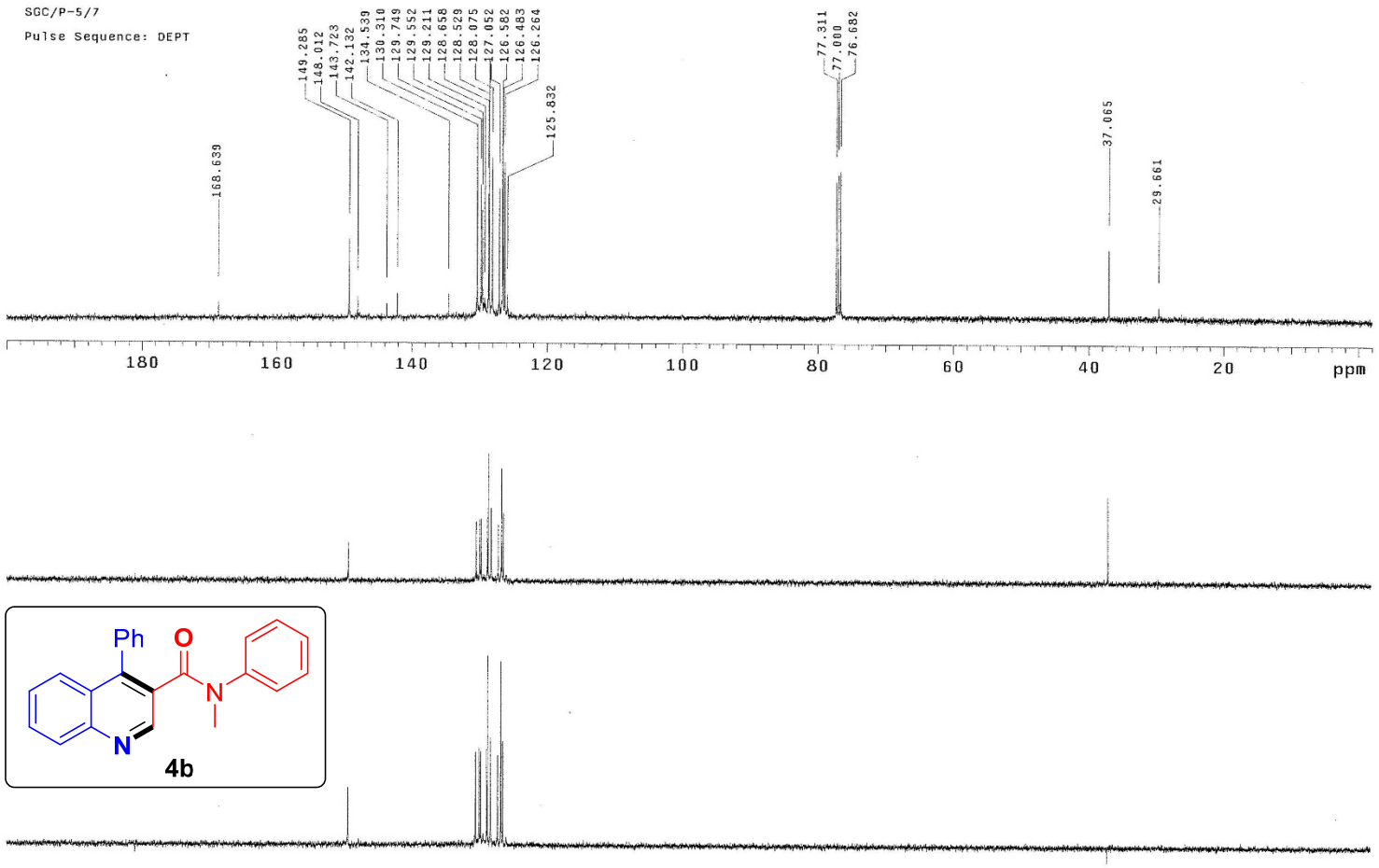
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 8 2015
Solvent: CDCl3
Ambient temperature
Total 2272 repetitions



4b

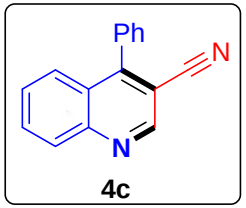



SGC/P-5/7
Pulse Sequence: DEPT
149.285
148.012
143.723
142.132
134.539
130.310
129.749
129.552
129.211
128.658
128.529
128.075
127.052
126.582
126.483
126.264
125.832
168.639
77.311
77.000
76.682
37.065
29.661
180
160
140
120
100
80
60
40
20
ppm
Ph
O
N
N
4b

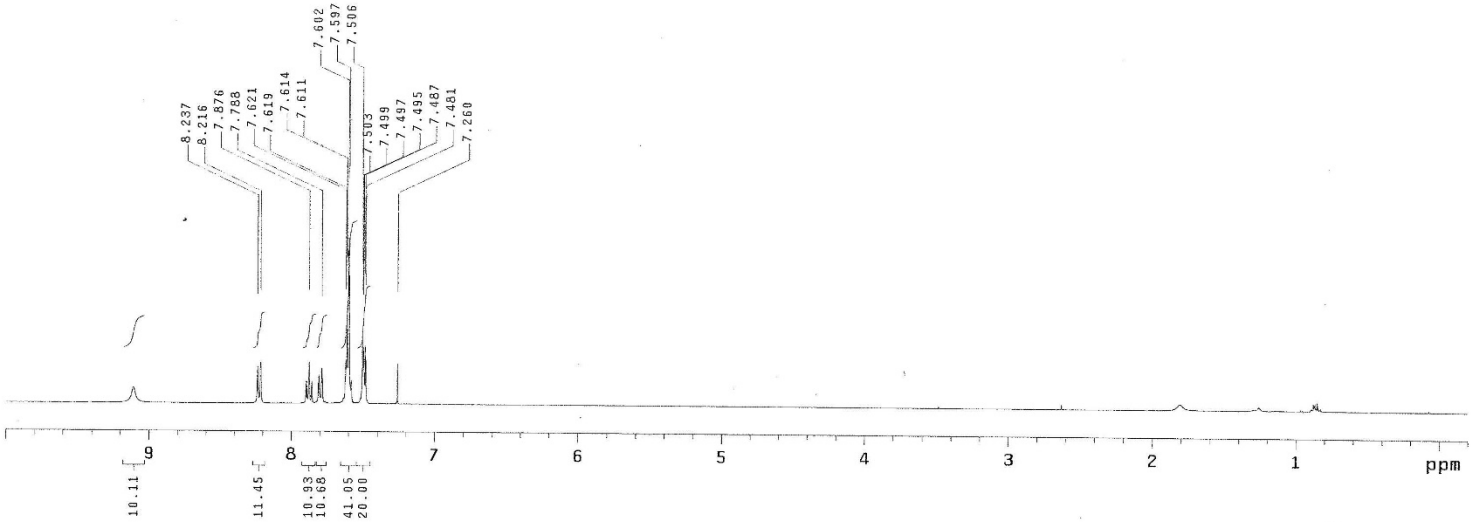
SGC/P-5/Q-1

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 27 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



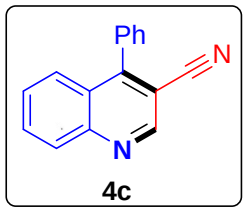
4c



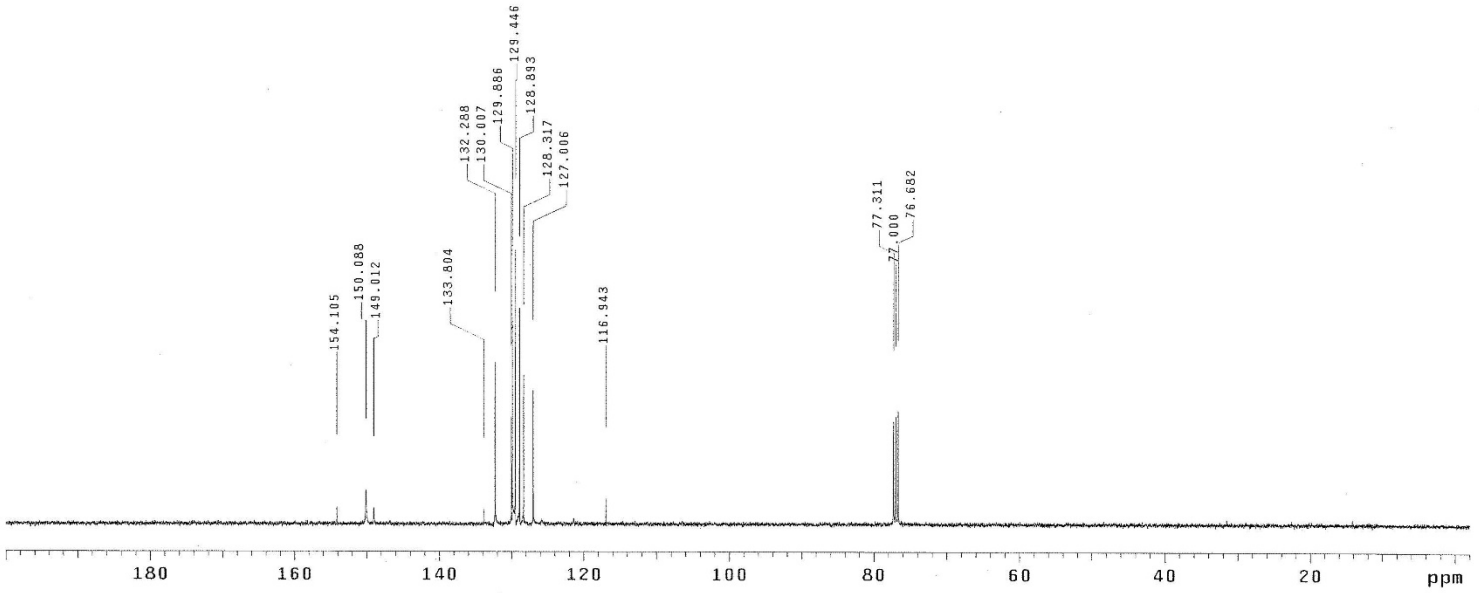
SGC/P-5/Q-1

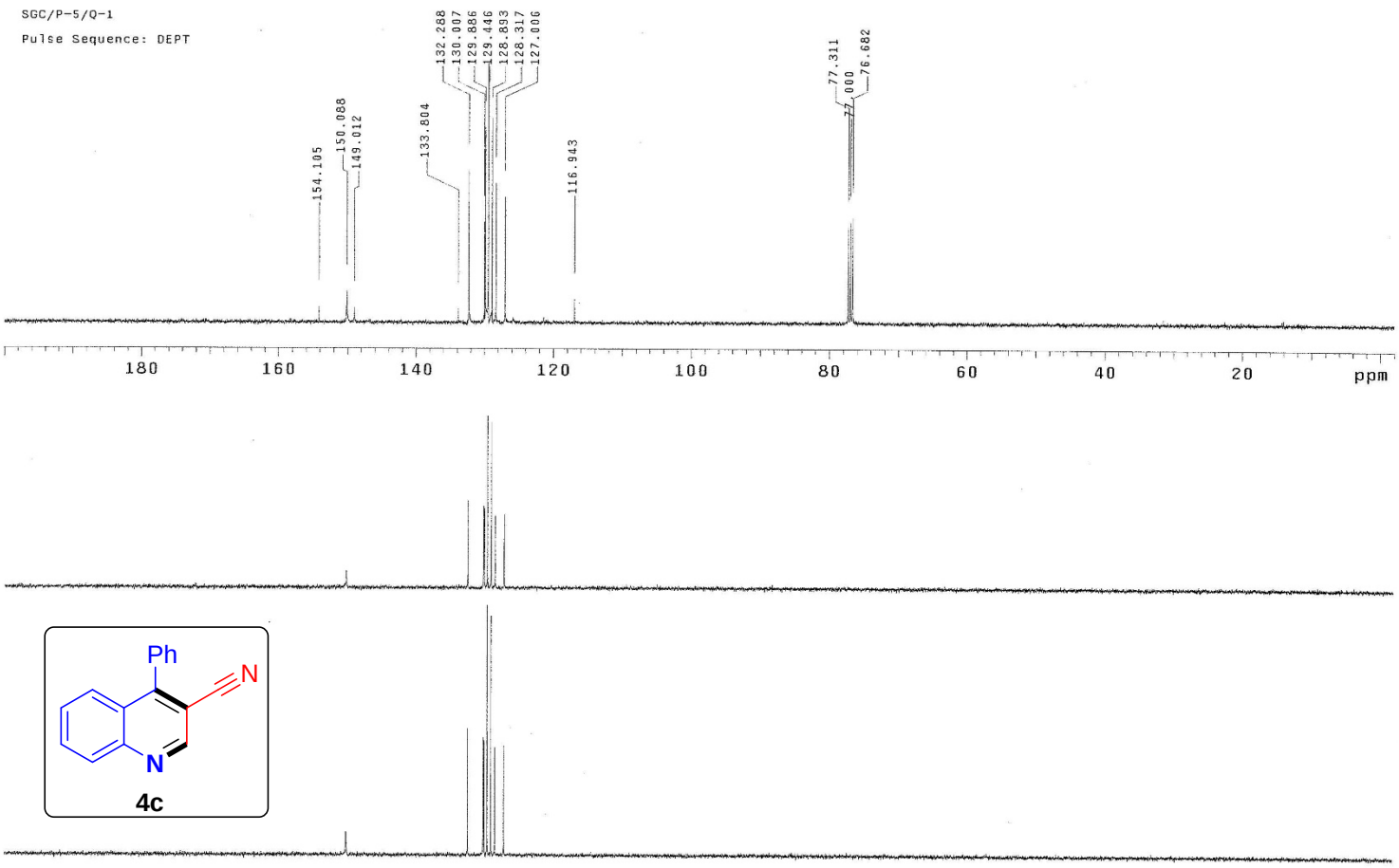
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 27 2015
Solvent: CDCl3
Ambient temperature
Total 3456 repetitions



4c

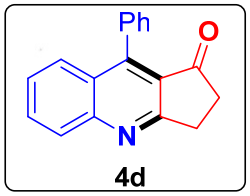



SGC/P-5/Q-1
Pulse Sequence: DEPT
154.105
150.088
149.012
133.804
132.288
130.007
129.886
129.446
128.833
128.317
127.006
116.943
77.311
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Ph
N
N
4c

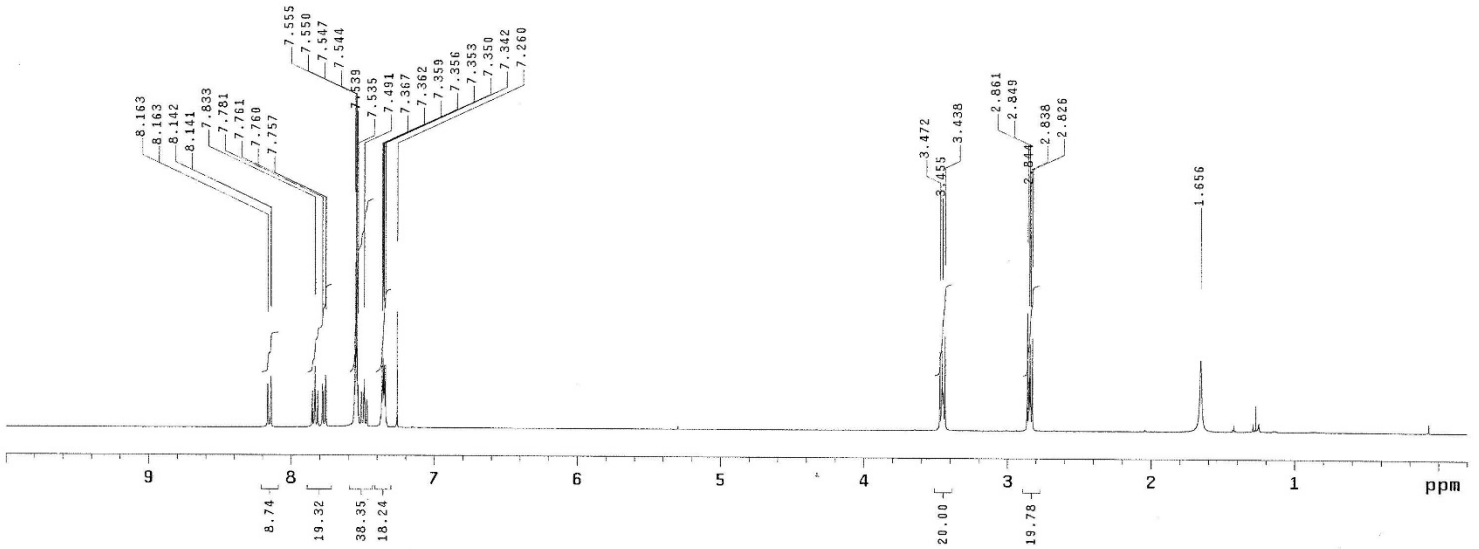
SGC/RP5/3

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 7 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



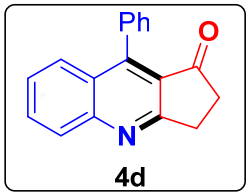
4d



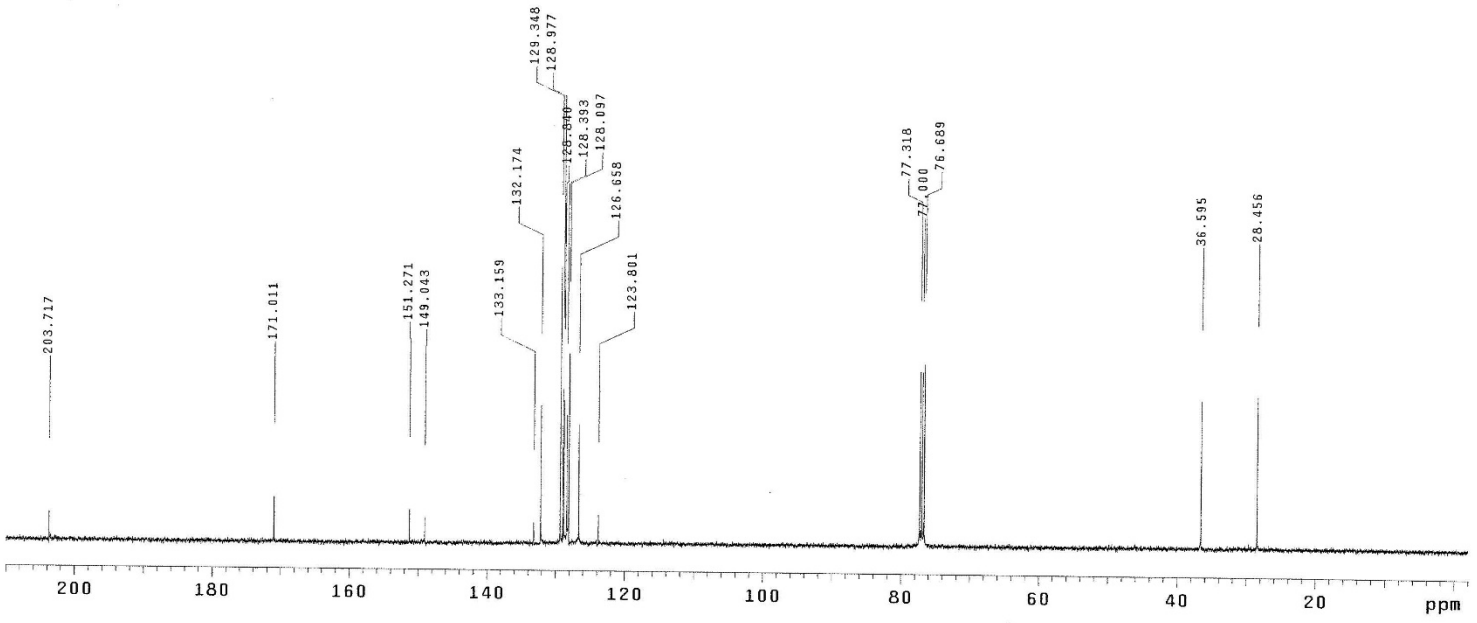
SGC/RP5/3

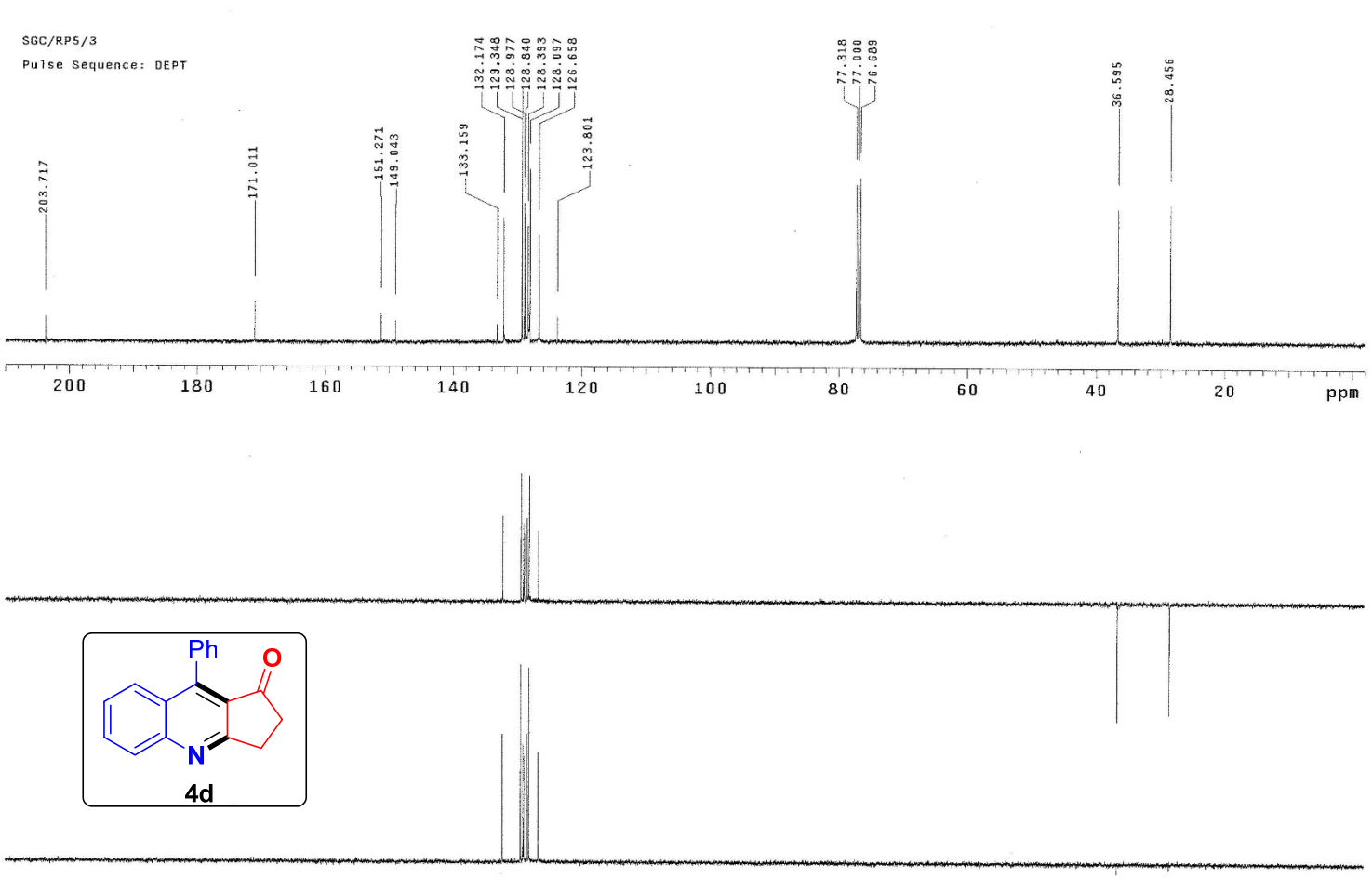
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jan 7 2015
Solvent: CDCl3
Ambient temperature
Total 6272 repetitions



4d

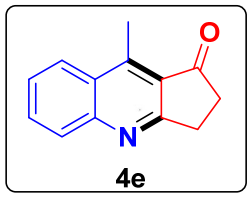



SGC/RP5/3
Pulse Sequence: DEPT
203.717
171.011
151.271
149.043
133.159
132.174
129.348
128.977
128.840
128.393
128.097
126.658
123.801
77.318
77.000
76.689
36.595
28.456
200
180
160
140
120
100
80
60
40
20
ppm
Ph
O
N
4d

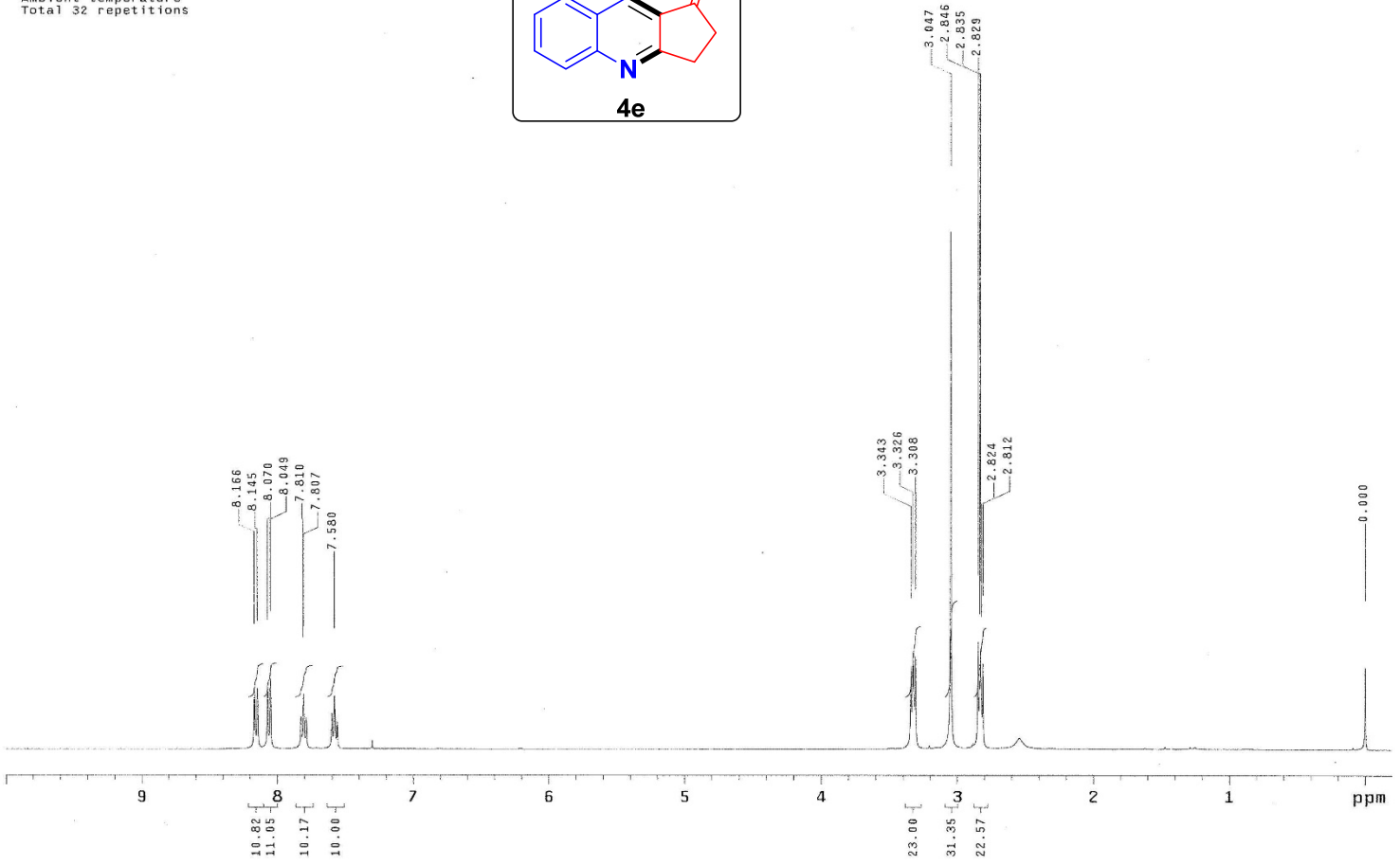
SGC/RP5/Q-10

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 29 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



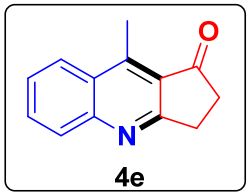
4e



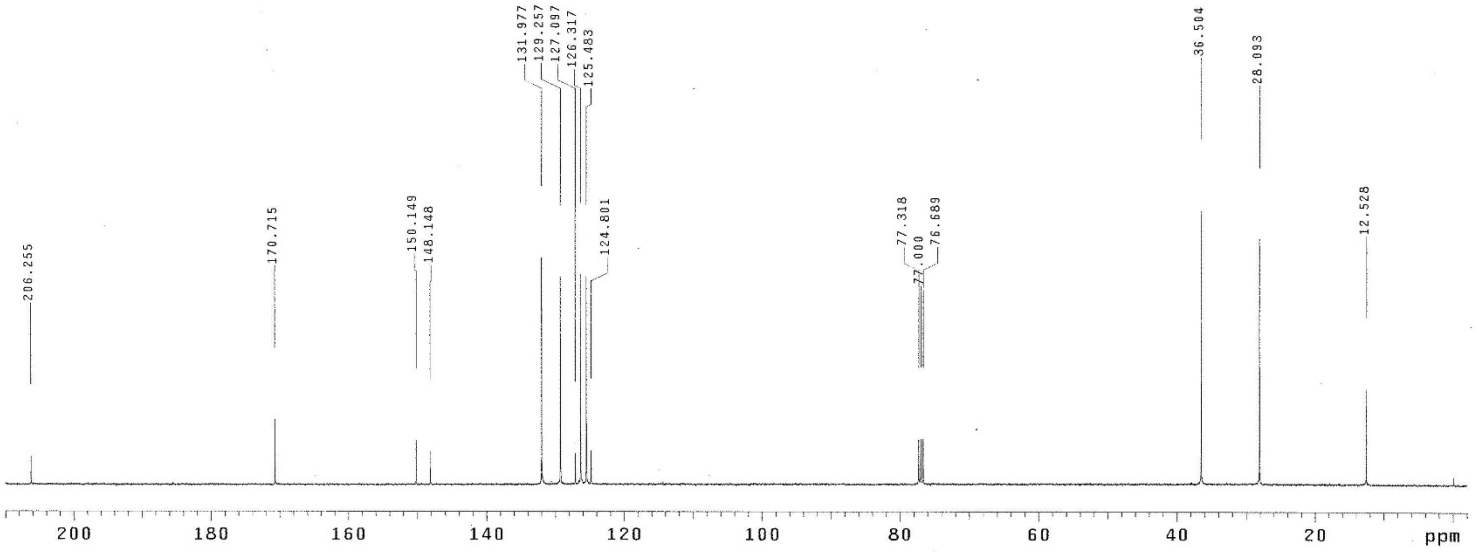
SGC/RP5/Q-10

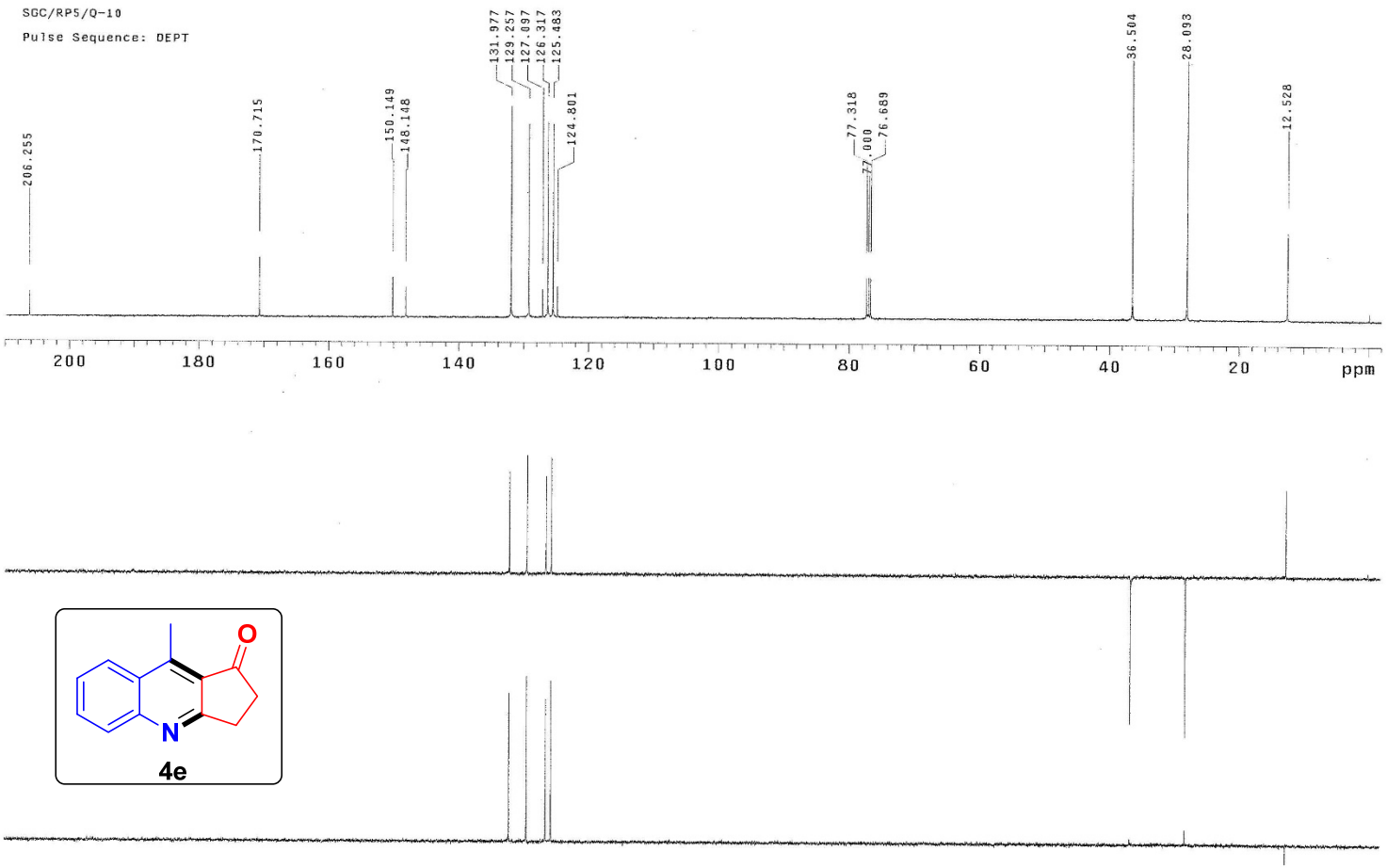
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 29 2015
Solvent: CDCl3
Ambient temperature
Total 20480 repetitions



4e

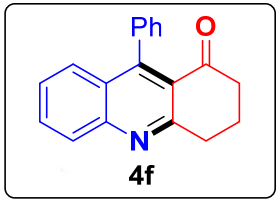



SGC/RP5/Q-10
Pulse Sequence: DEPT
206.255
170.715
150.149
148.148
131.977
129.257
127.097
126.317
125.483
124.801
77.318
77.000
76.689
36.504
28.093
12.528
200
180
160
140
120
100
80
60
40
20
ppm
O
N
4e

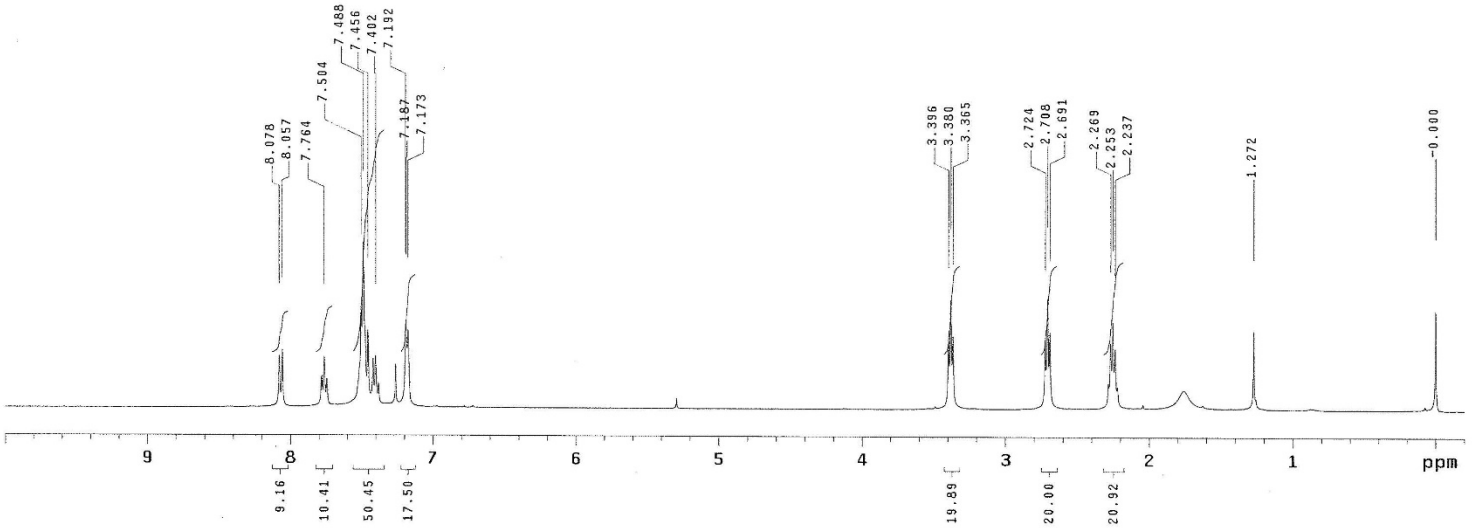
SGC/P-5/Q-14

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 12 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



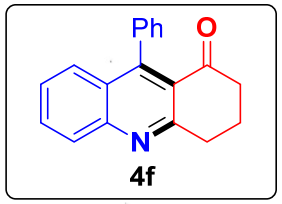
4f



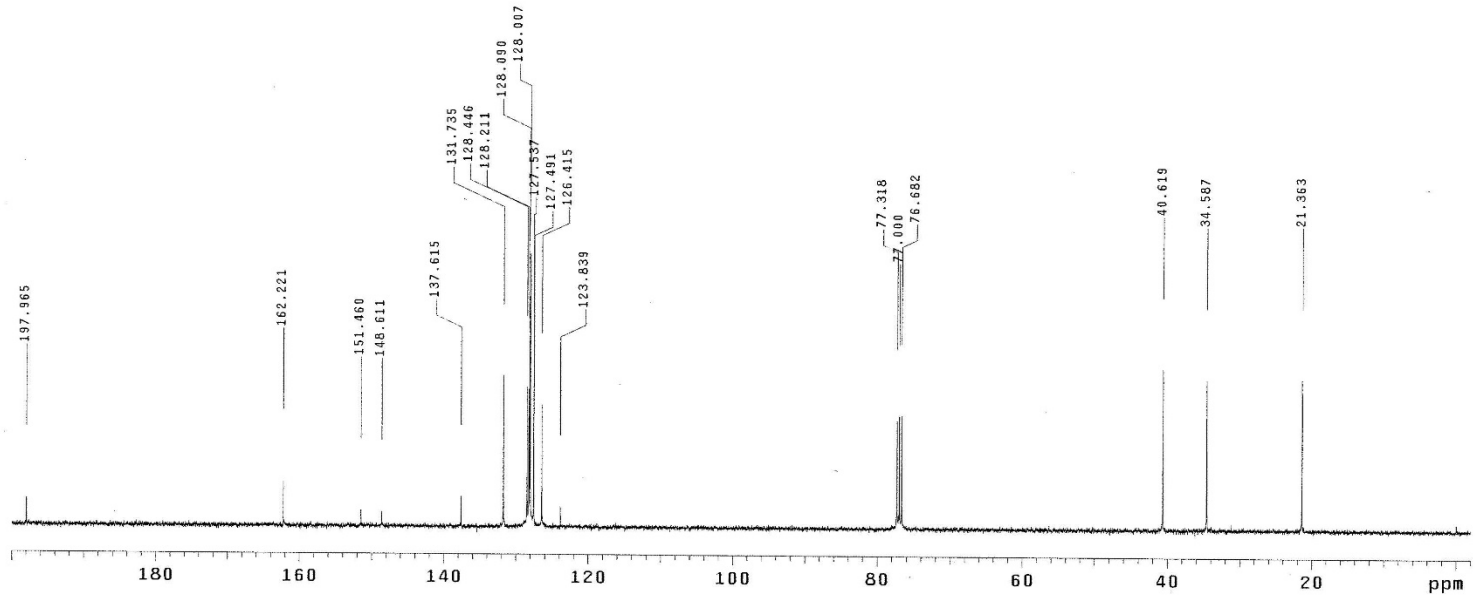
SGC/P-5/Q-14

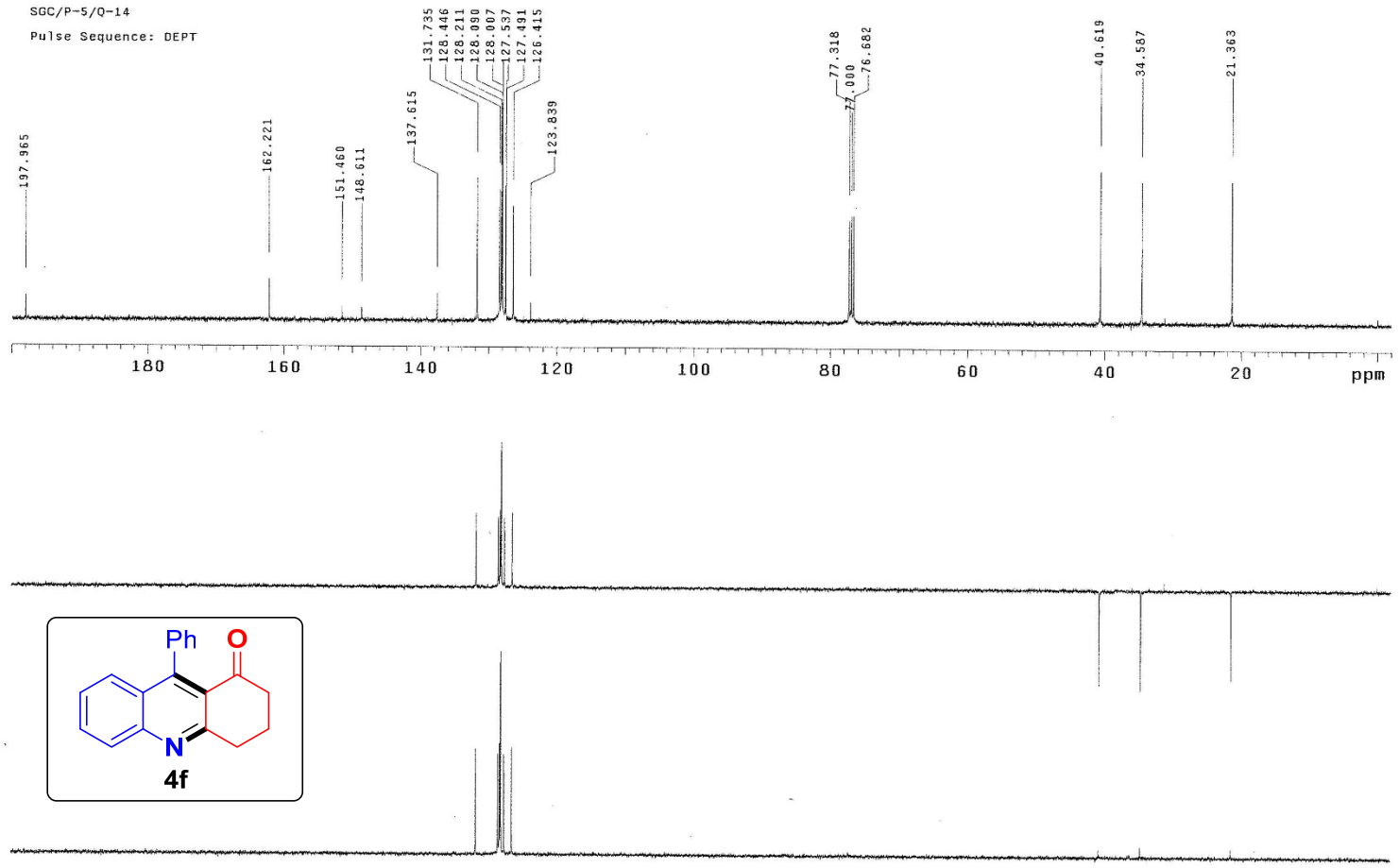
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 12 2015
Solvent: CDCl3
Ambient temperature
Total 5136 repetitions



4f

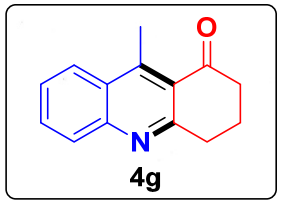



SGC/P-5/Q-14
Pulse Sequence: DEPT
197.965
162.221
151.460
148.611
137.615
131.735
128.446
128.211
128.090
128.007
127.537
127.491
126.415
123.839
77.318
77.000
76.682
40.619
34.587
21.363
180
160
140
120
100
80
60
40
20
ppm
Ph
O
N
4f

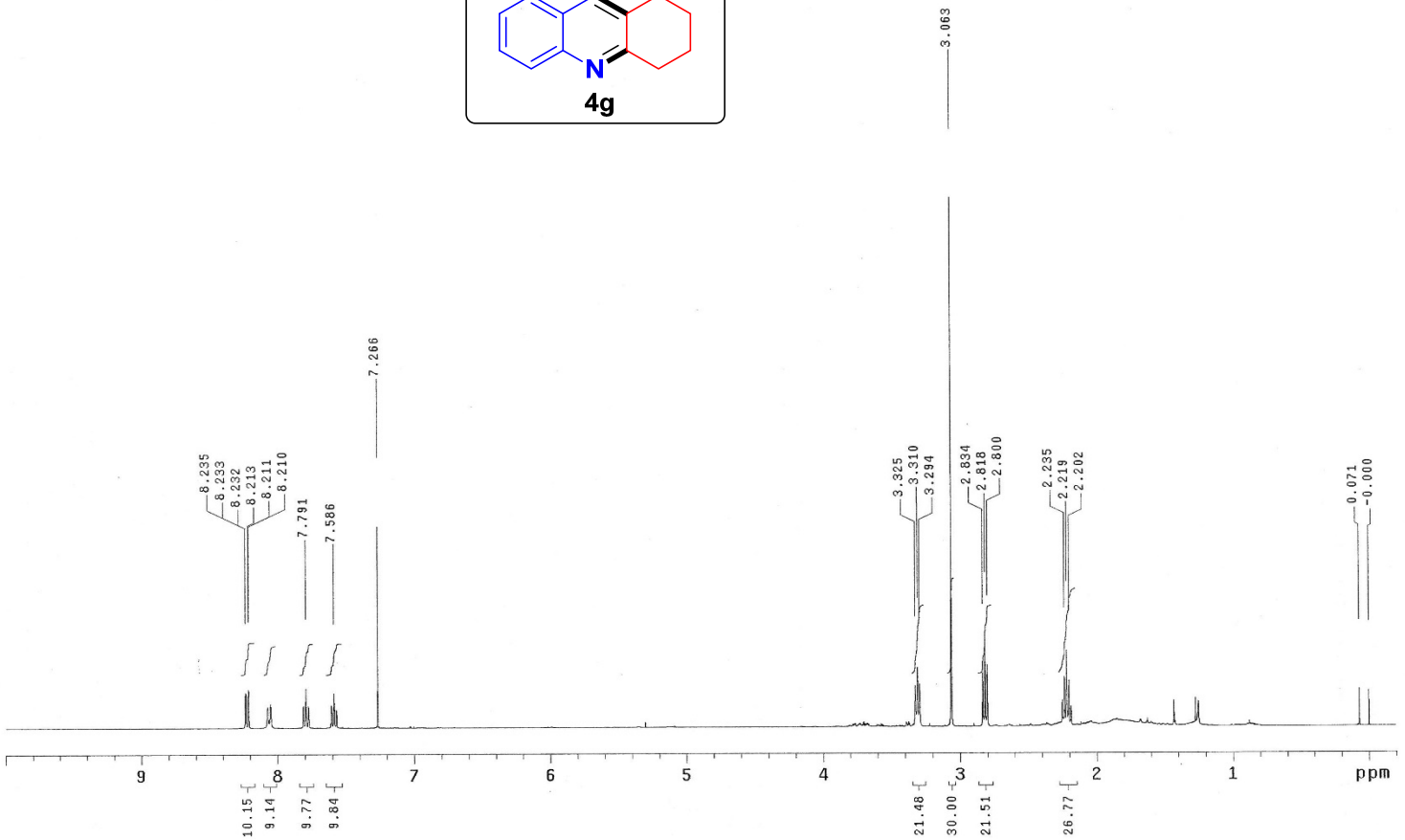
SGC/P-5/butene

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 25 2015
Solvent: CDCl3
Ambient temperature
Total 532 repetitions



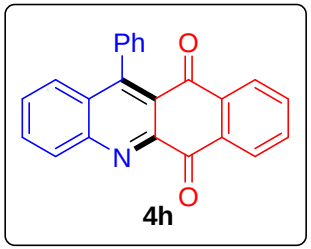
4g



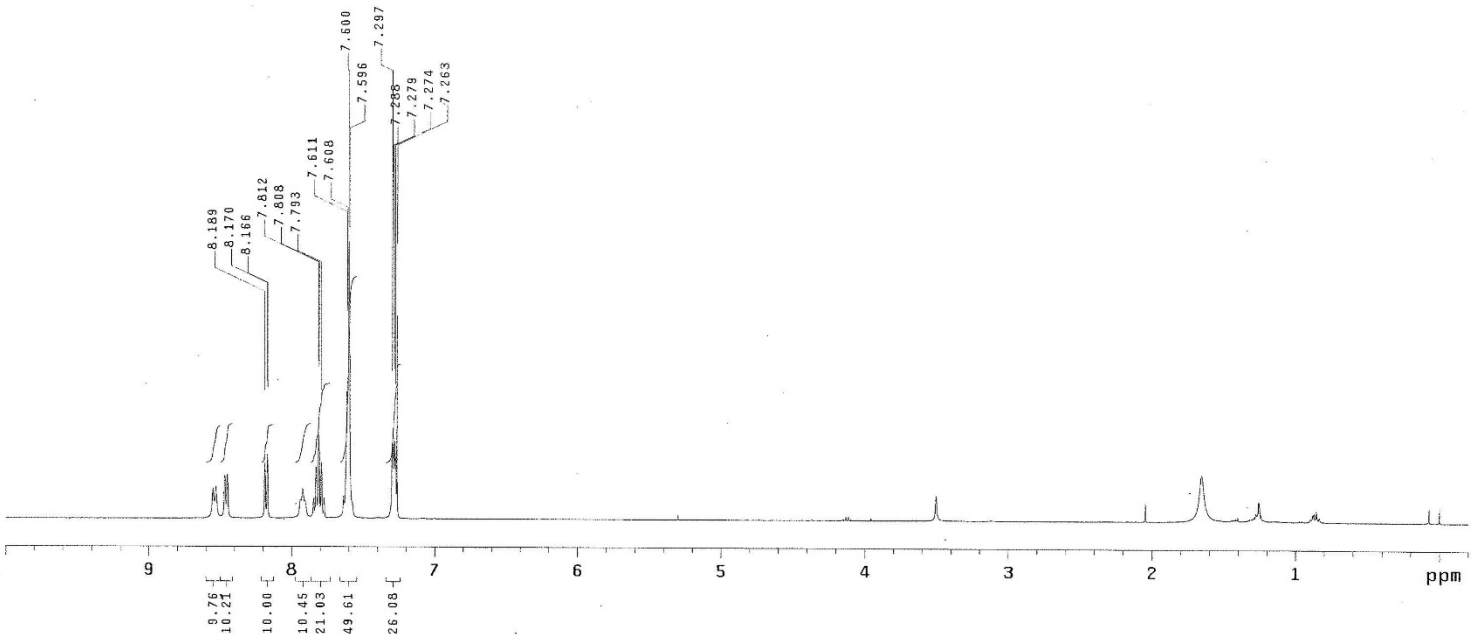
SGC/P-5/Q-2

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 27 2015
Solvent: CDCl3
Ambient temperature
Total 48 repetitions



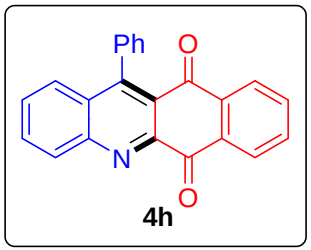
4h



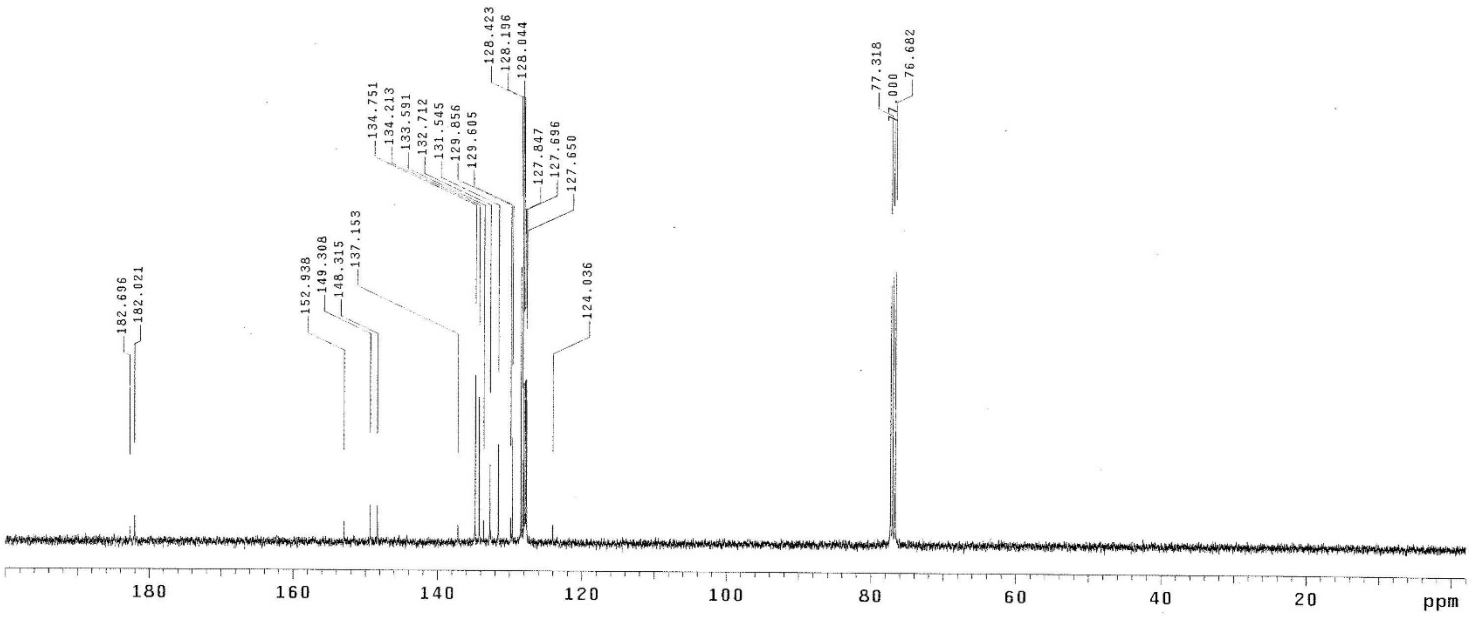
SGC/P-5/Q-2

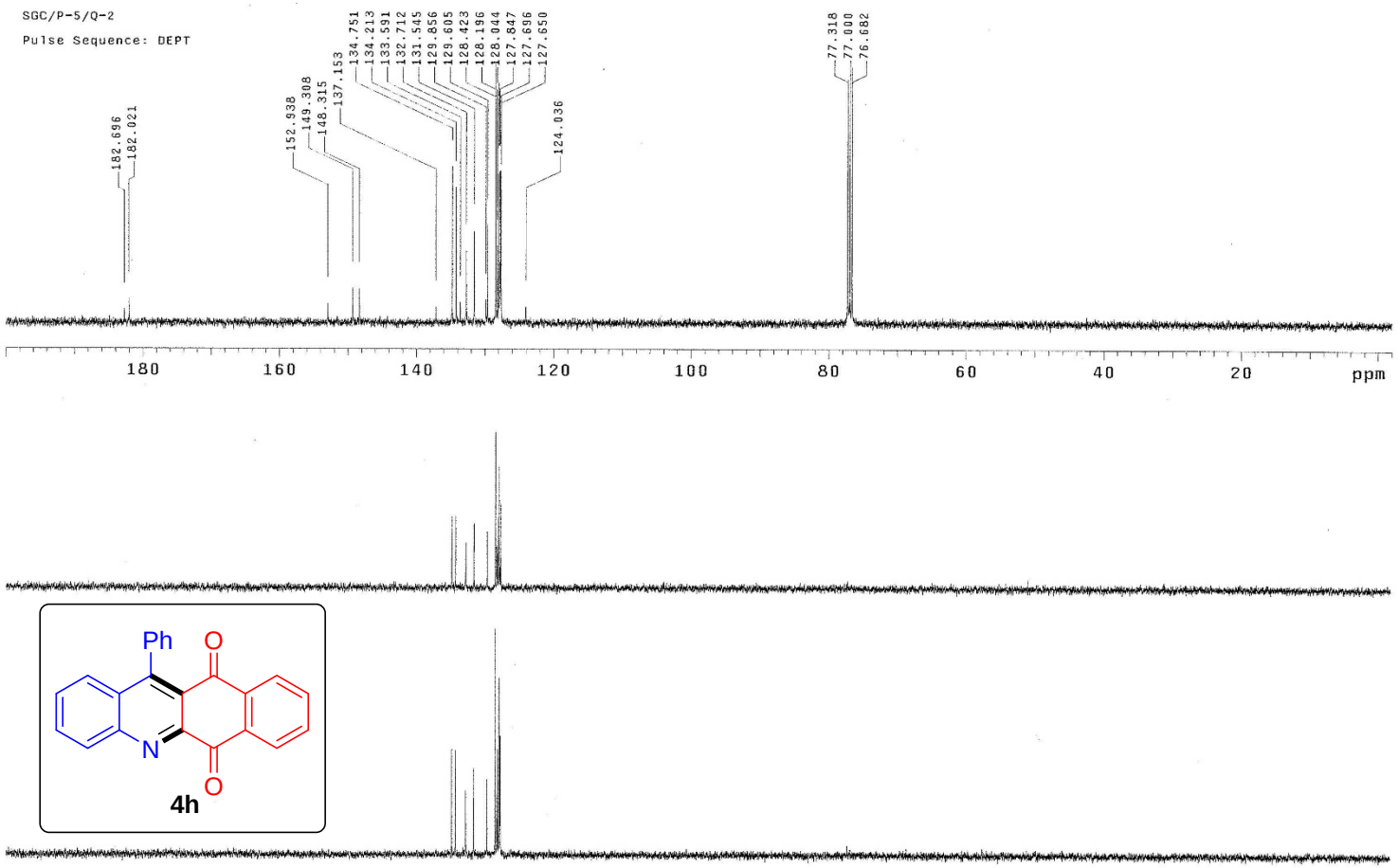
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 27 2015
Solvent: CDCl3
Ambient temperature
Total 3504 repetitions



4h

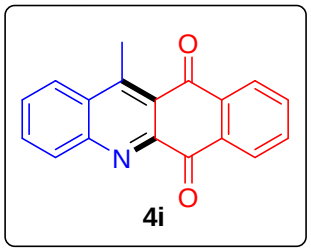



SGC/P-5/Q-2
Pulse Sequence: DEPT
182.696
182.021
152.938
149.308
148.315
137.153
134.751
134.213
133.591
132.712
131.545
129.856
129.605
128.423
128.196
128.044
127.847
127.696
127.650
124.036
77.318
77.000
76.682
180
160
140
120
100
80
60
40
20
ppm
Ph
O
N
O
4h

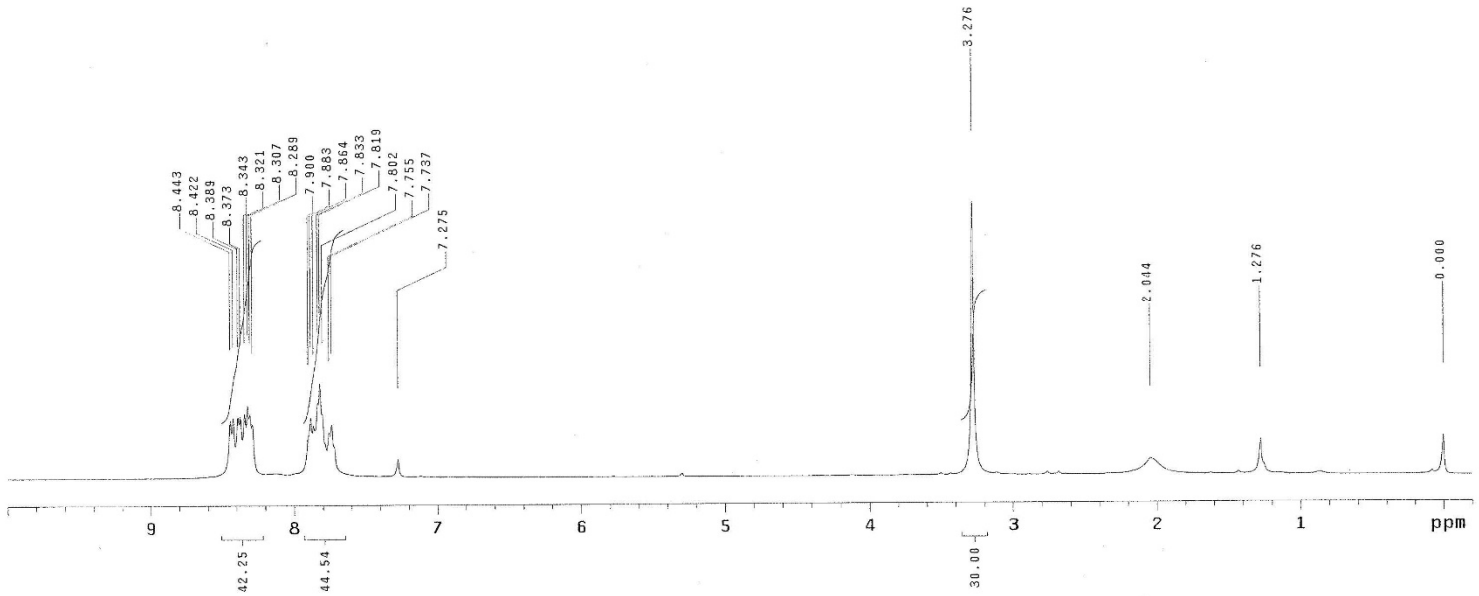
SGC/P-5/Q-3

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 11 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



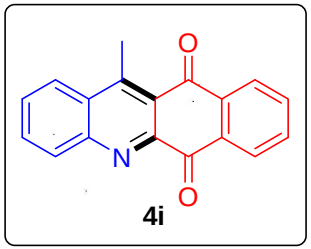
4i



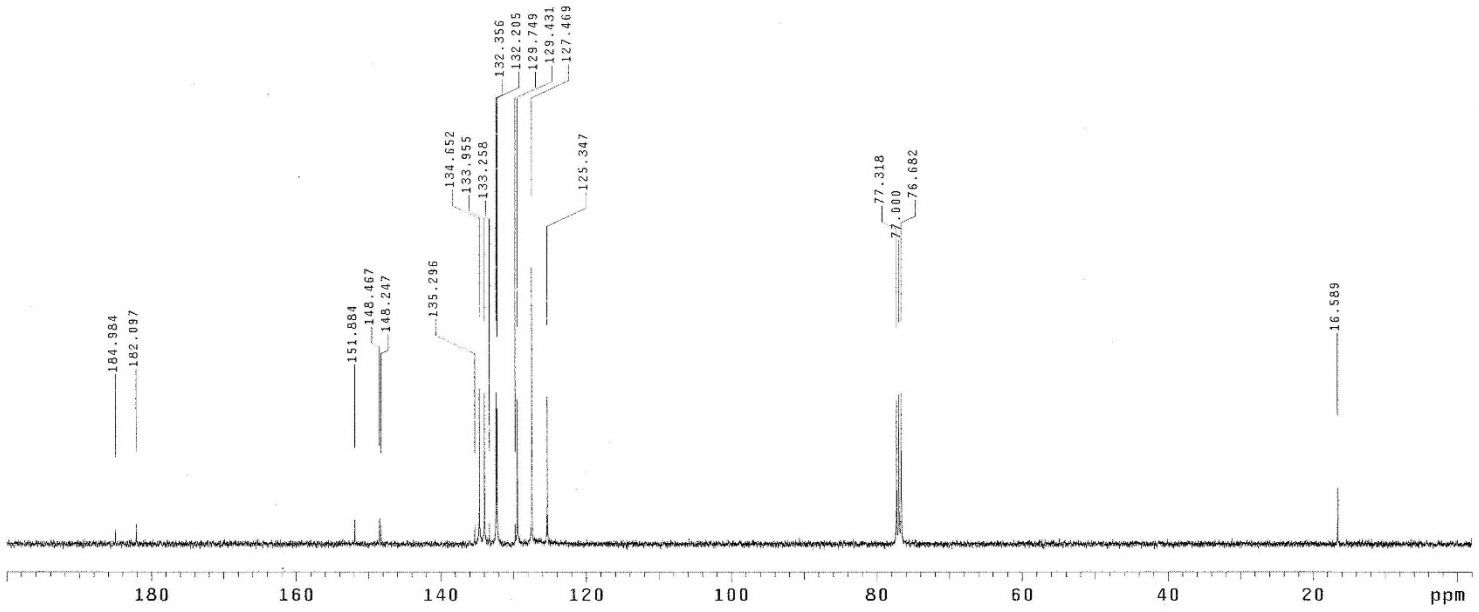
SGC/P-5/Q-3

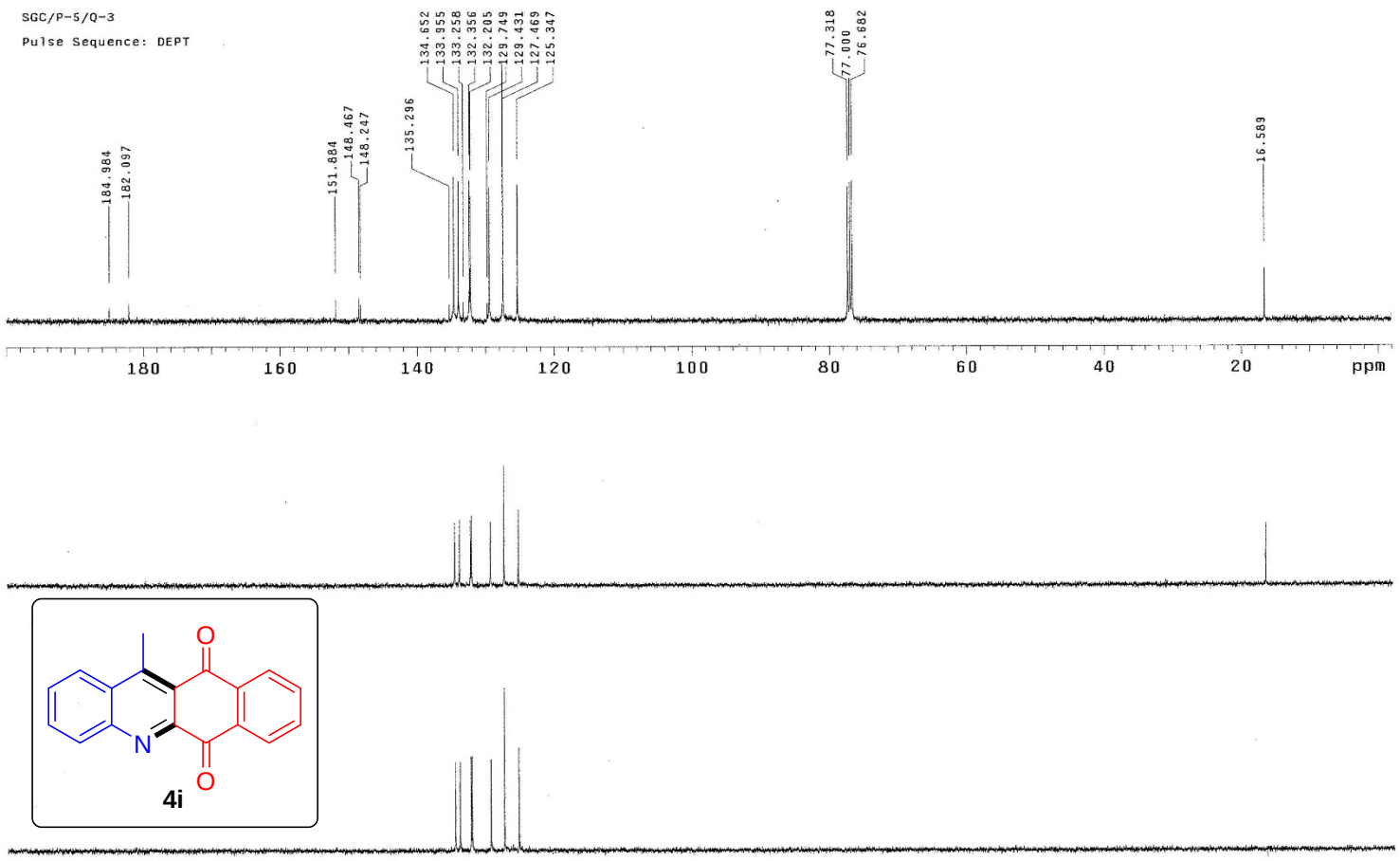
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: May 11 2015
Solvent: CDCl3
Ambient temperature
Total 3008 repetitions



4i

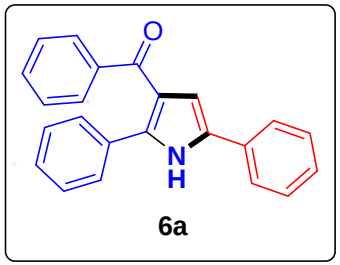



SGC/P-5/Q-3
Pulse Sequence: DEPT
184.984
182.097
151.884
148.467
148.247
135.296
134.652
133.955
133.258
132.356
132.205
129.749
129.431
127.469
125.347
77.318
77.000
76.682
16.589
180
160
140
120
100
80
60
40
20
ppm
O
N
O
4i

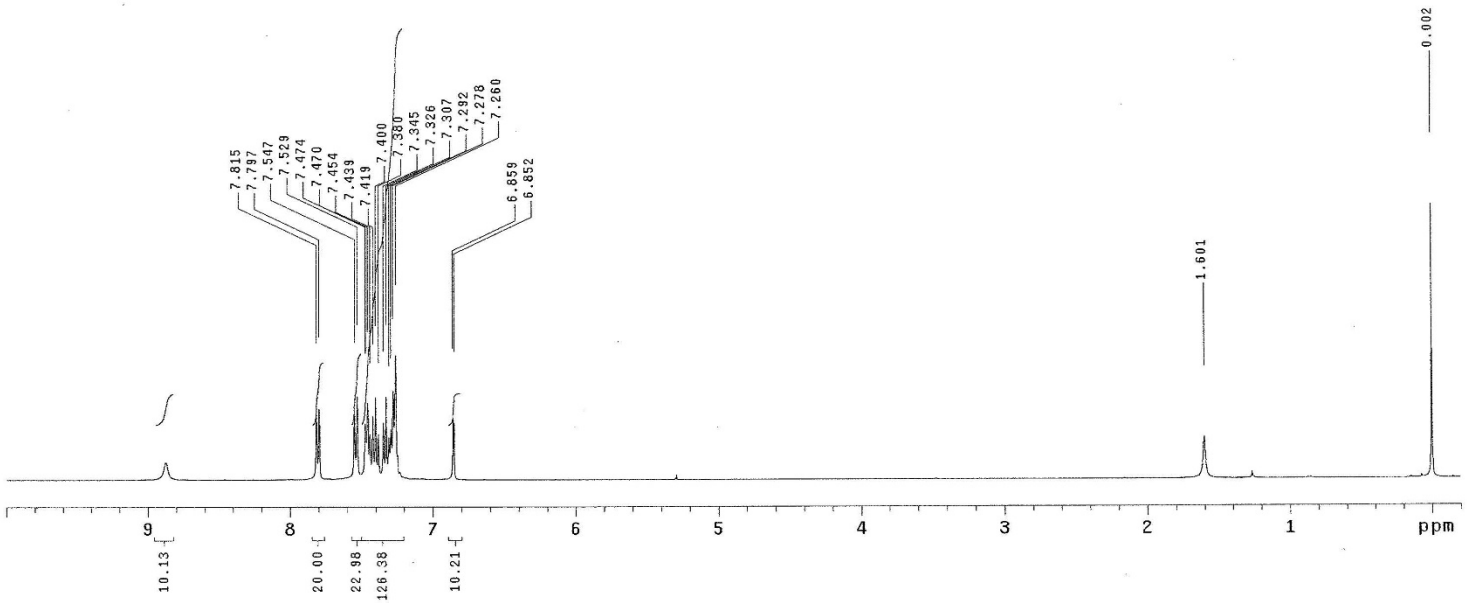
SGC/P-5/P-Ph

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



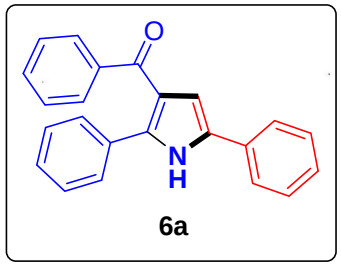
6a



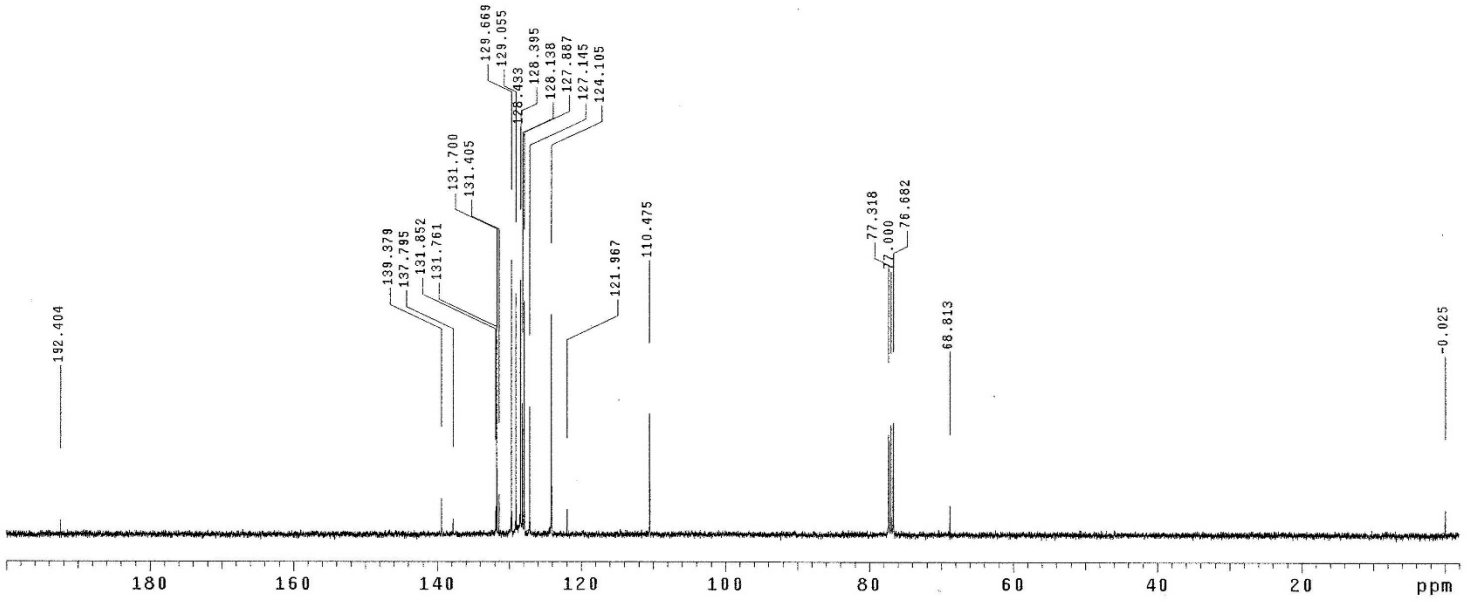
SGC/P-5/P-Ph

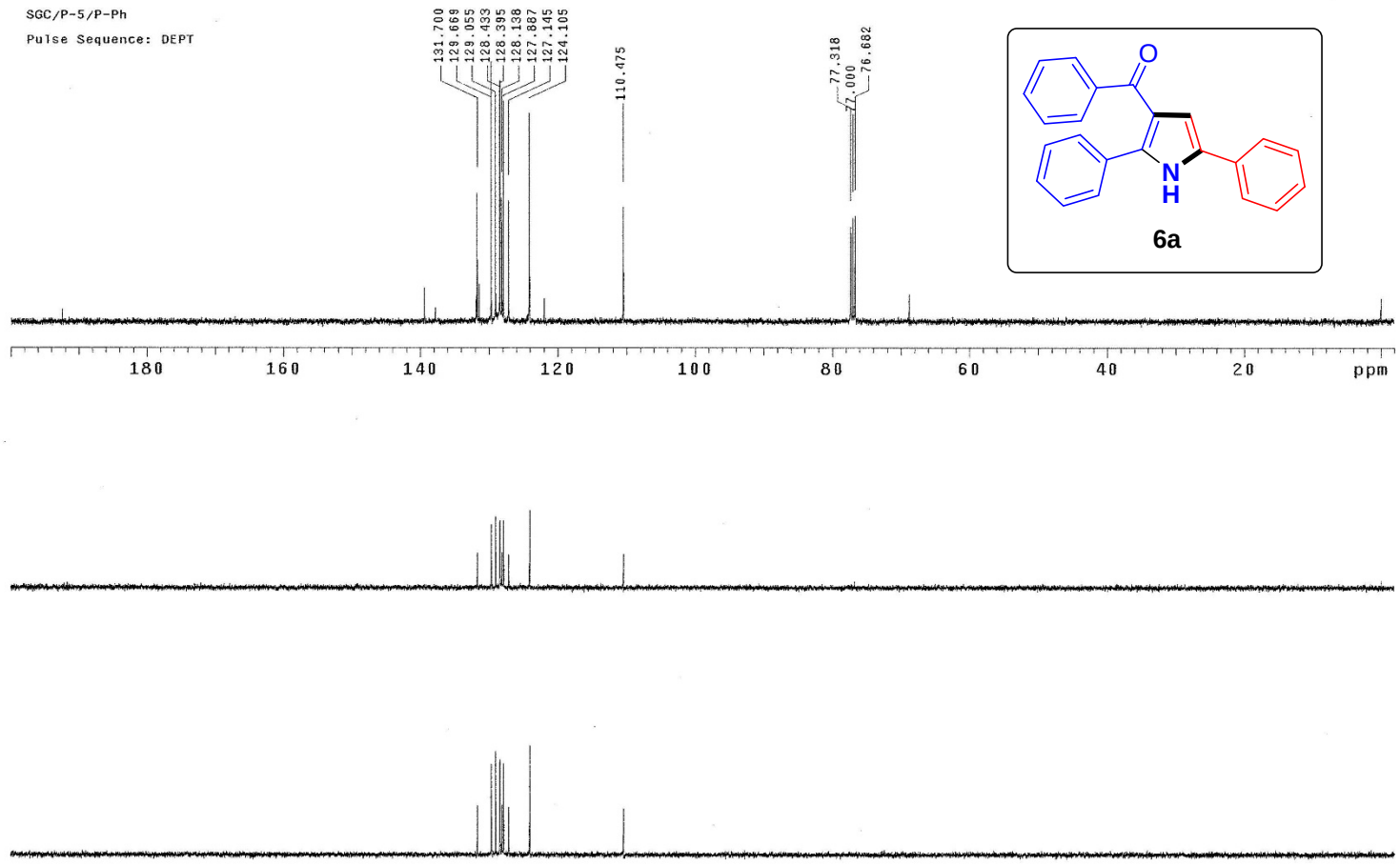
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 4720 repetitions



6a

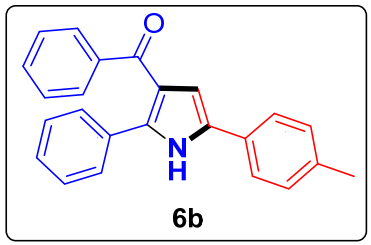



SGC/P-5/P-Ph
Pulse Sequence: DEPT
131.700
129.669
129.055
128.433
128.395
128.138
127.887
127.145
124.105
110.475
77.318
77.000
76.682
O
N
H
6a
180
160
140
120
100
80
60
40
20
ppm

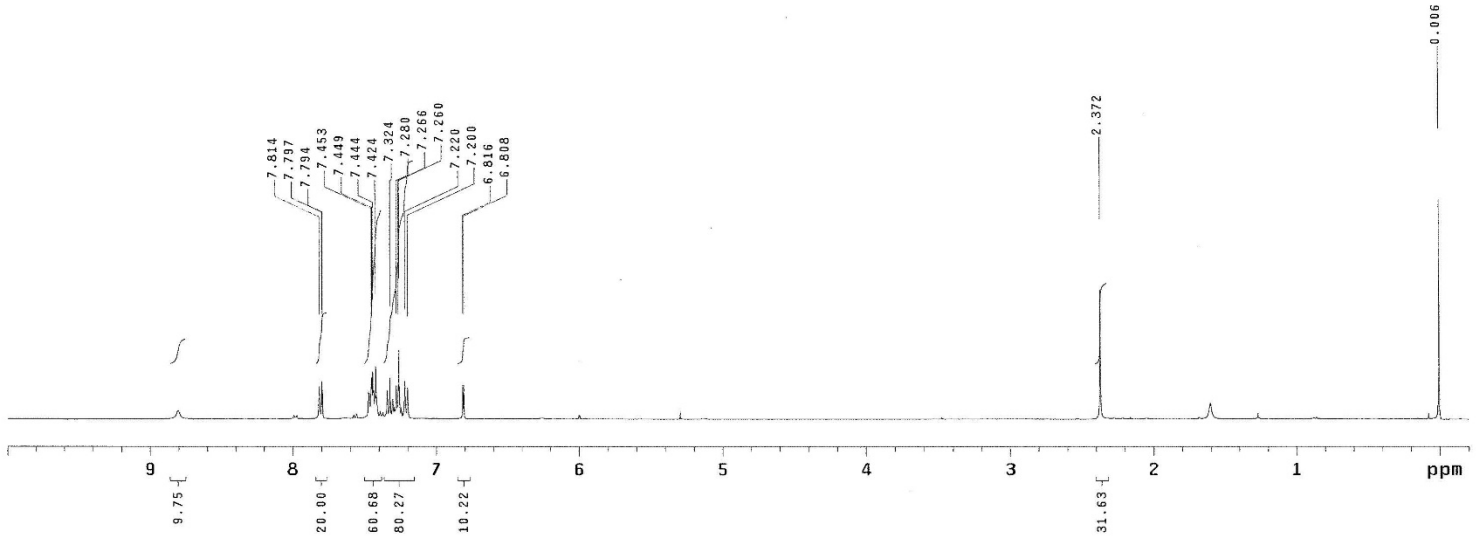
SGC/P-5/P-Me

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
File: M0097-19
Total 32 repetitions



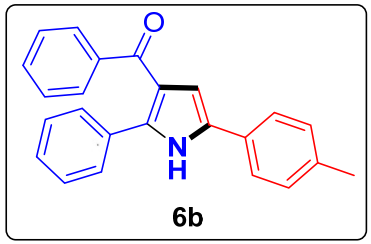
6b



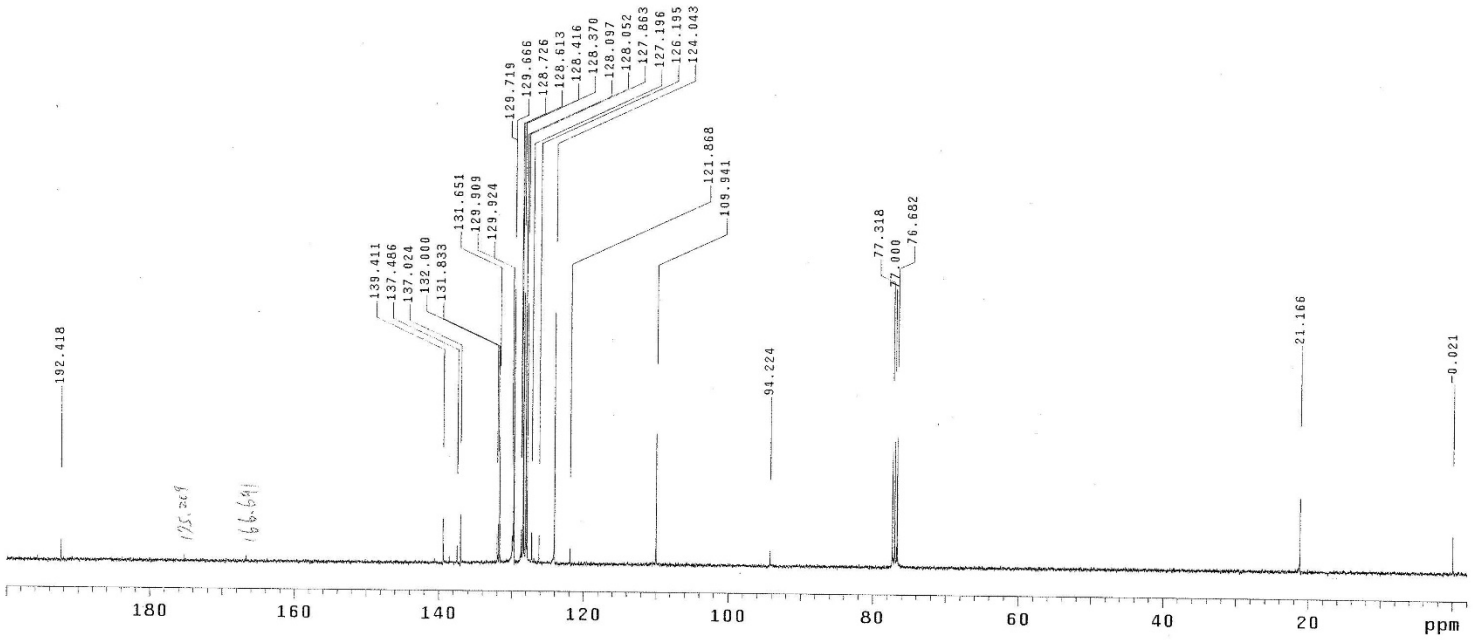
SGC/P-5/P-Me

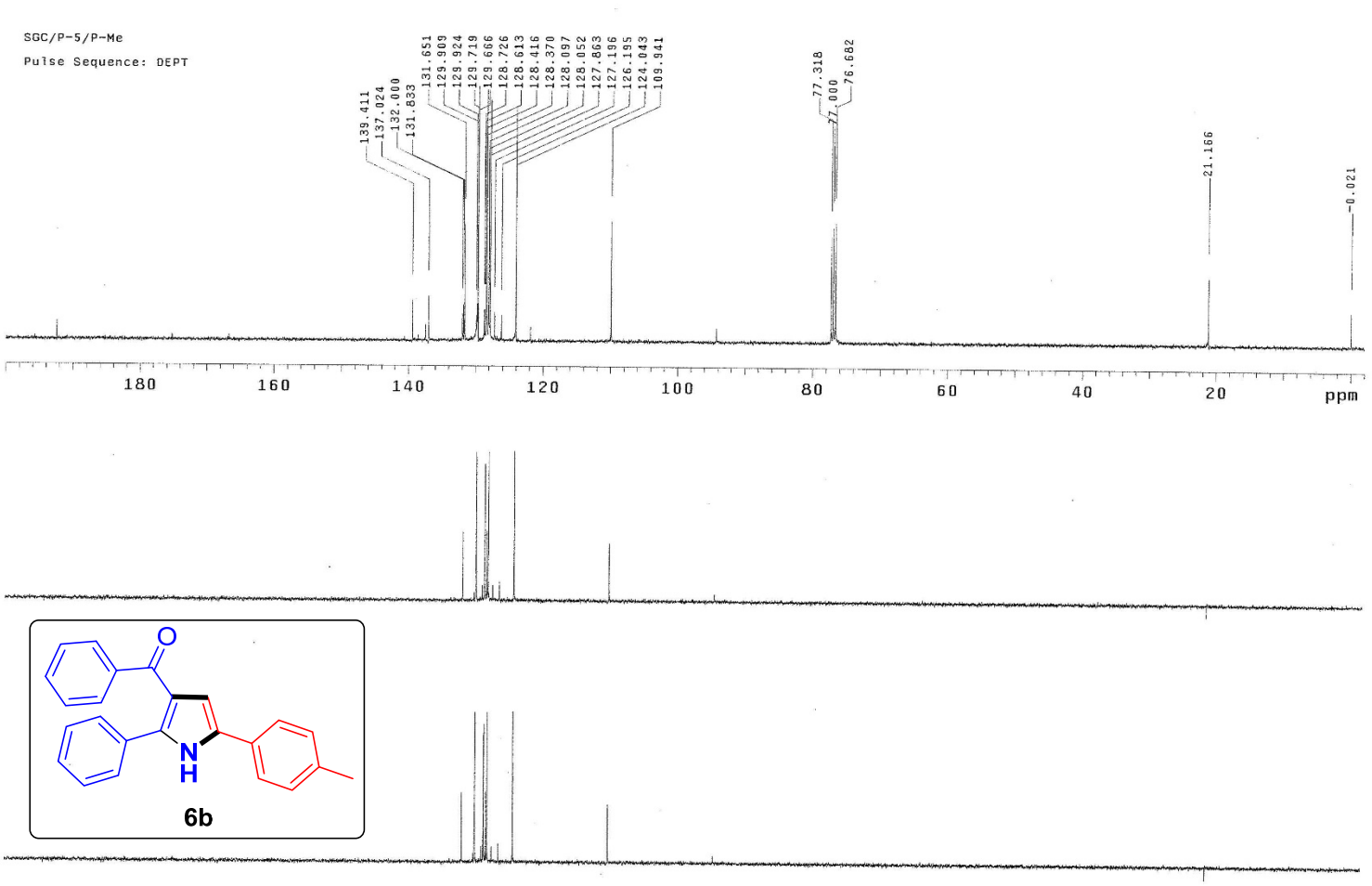
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 6544 repetitions



6b

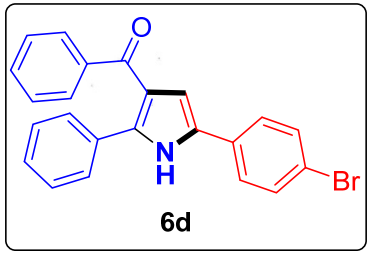



SGC/P-5/P-Me
Pulse Sequence: DEPT
139.411
137.024
132.000
131.833
131.651
129.909
129.924
129.719
129.666
128.726
128.613
128.416
128.370
128.097
128.052
127.863
127.196
126.195
124.043
109.941
77.318
77.000
76.682
21.166
0.021
180
160
140
120
100
80
60
40
20
ppm
O
N
H
6b

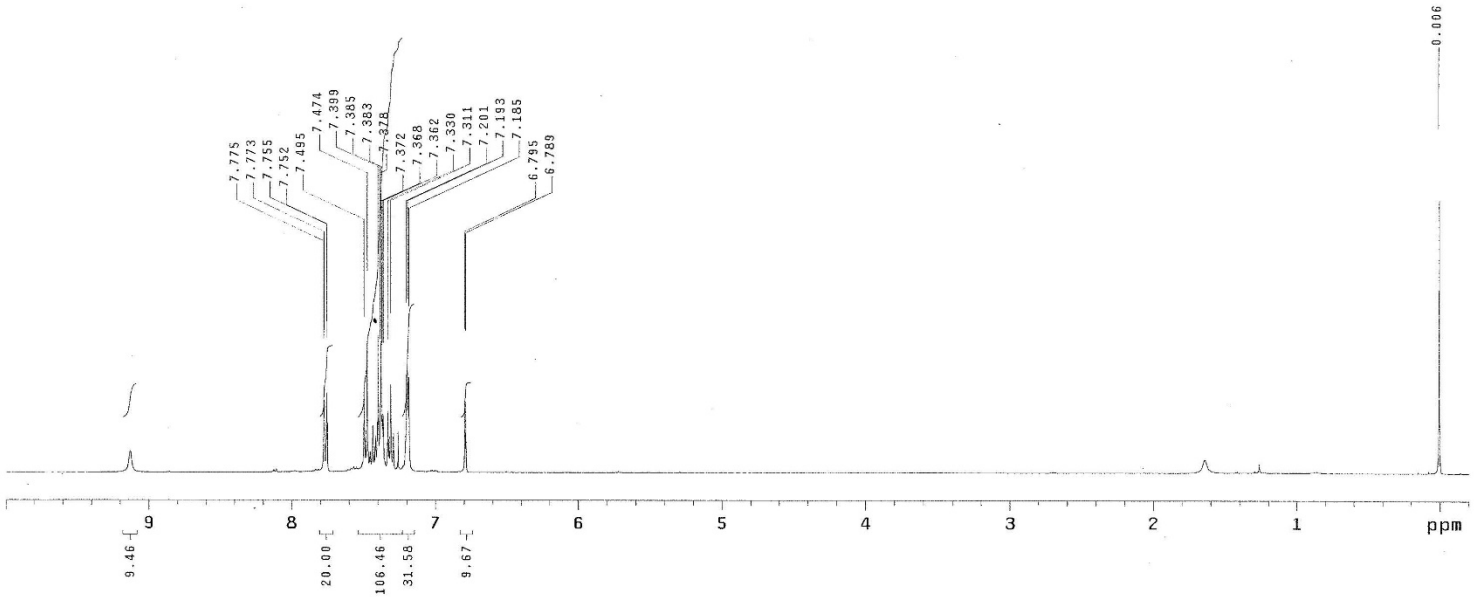
SGC/P-5/P-Br

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



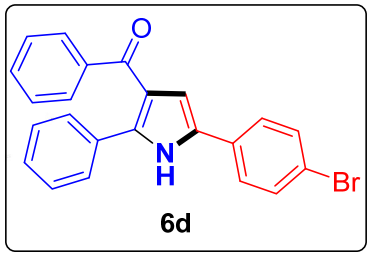
6d



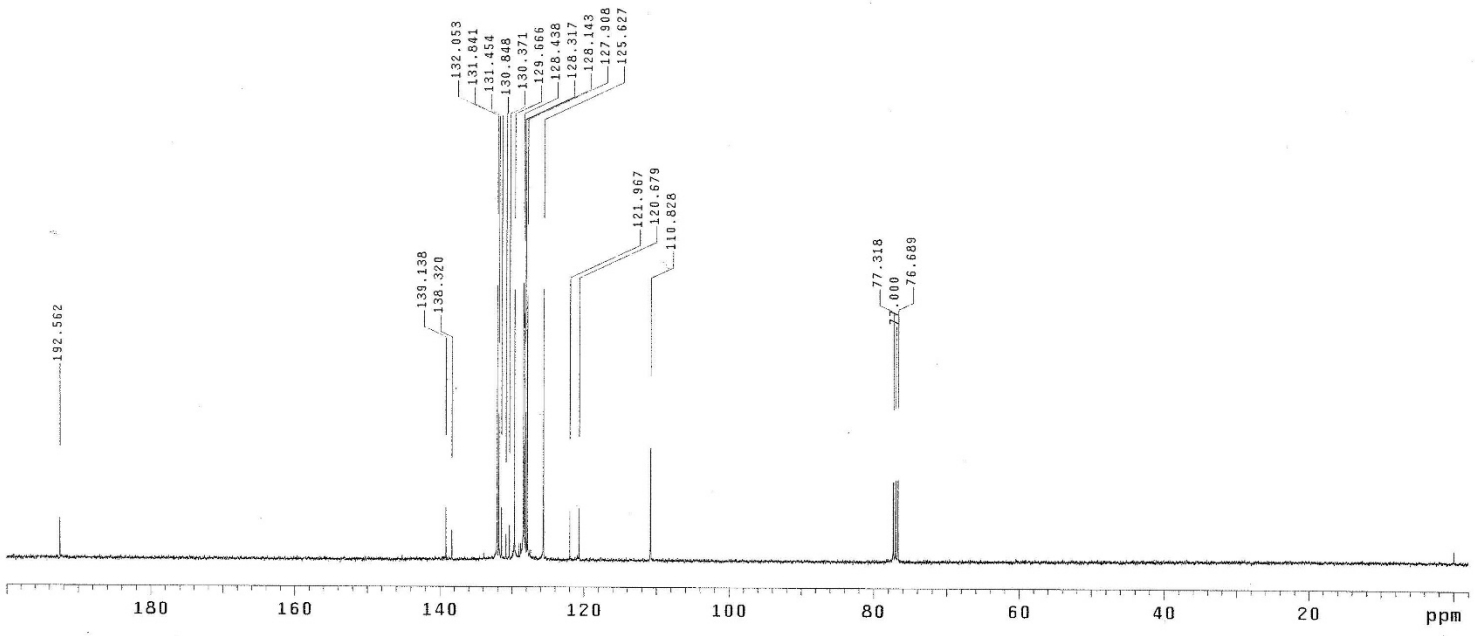
SGC/P-5/P-Br

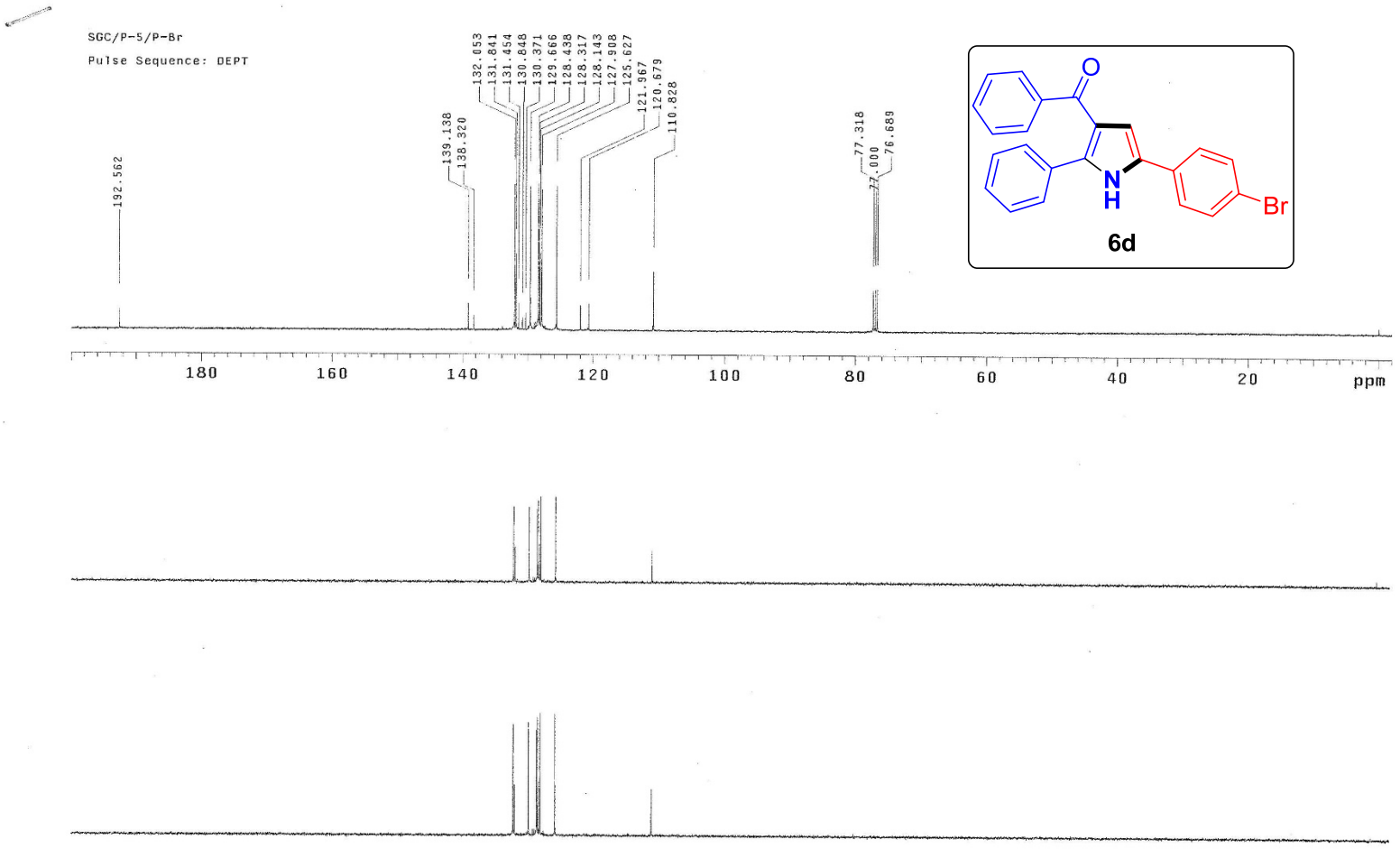
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 20480 repetitions



6d

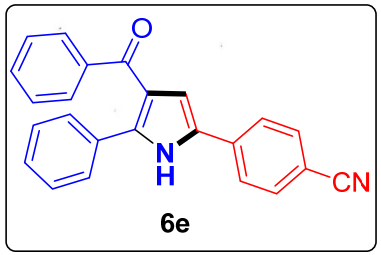



SGC/P-5/P-Br
Pulse Sequence: DEPT
192.562
139.138
138.320
132.053
131.841
131.454
130.848
130.371
129.666
128.438
128.317
128.143
127.908
125.627
121.967
120.679
110.828
77.318
77.000
76.689
O
N
H
Br
6d
180
160
140
120
100
80
60
40
20
ppm

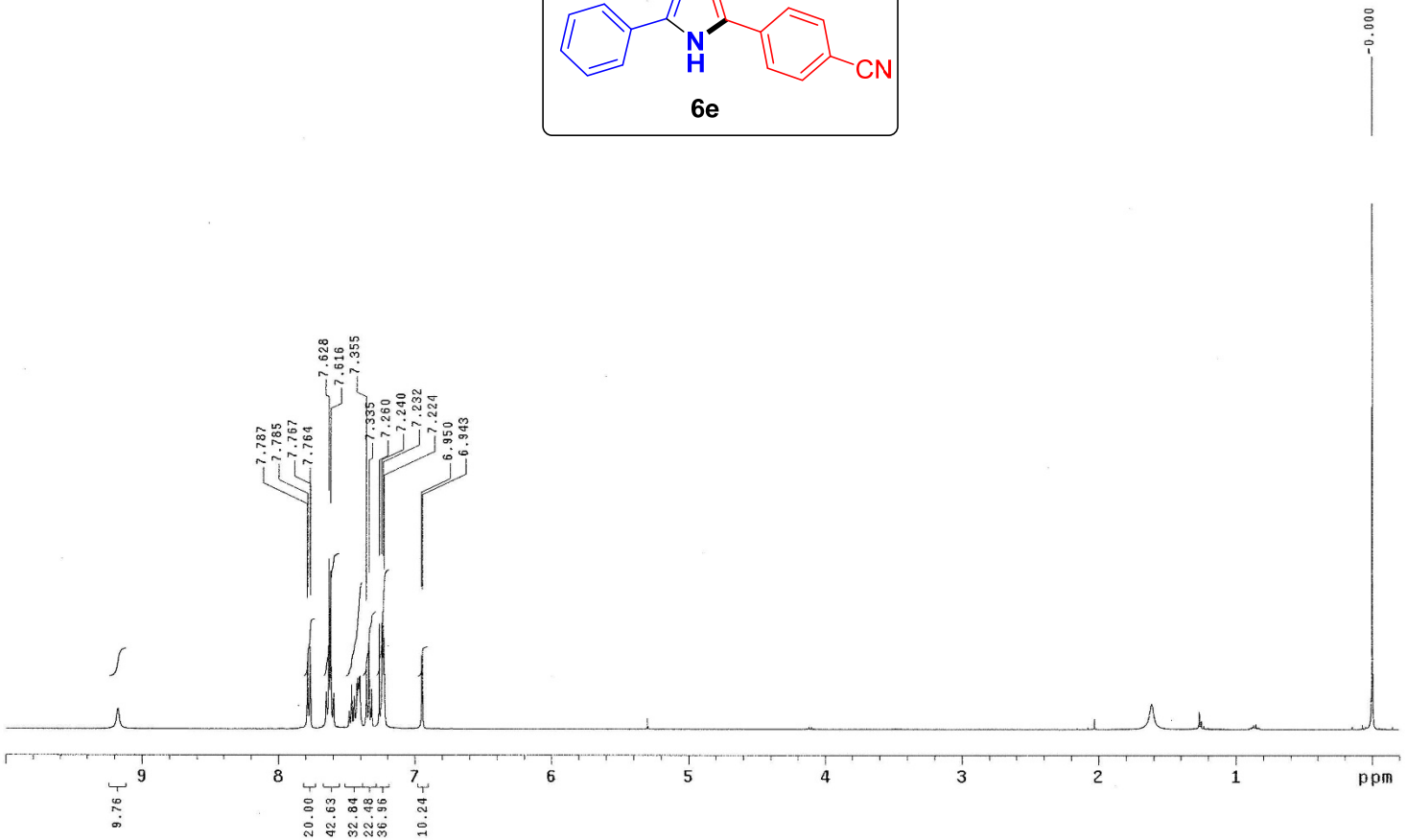
SGC/P-5/P-CN

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



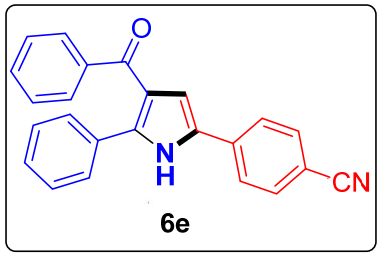
6e



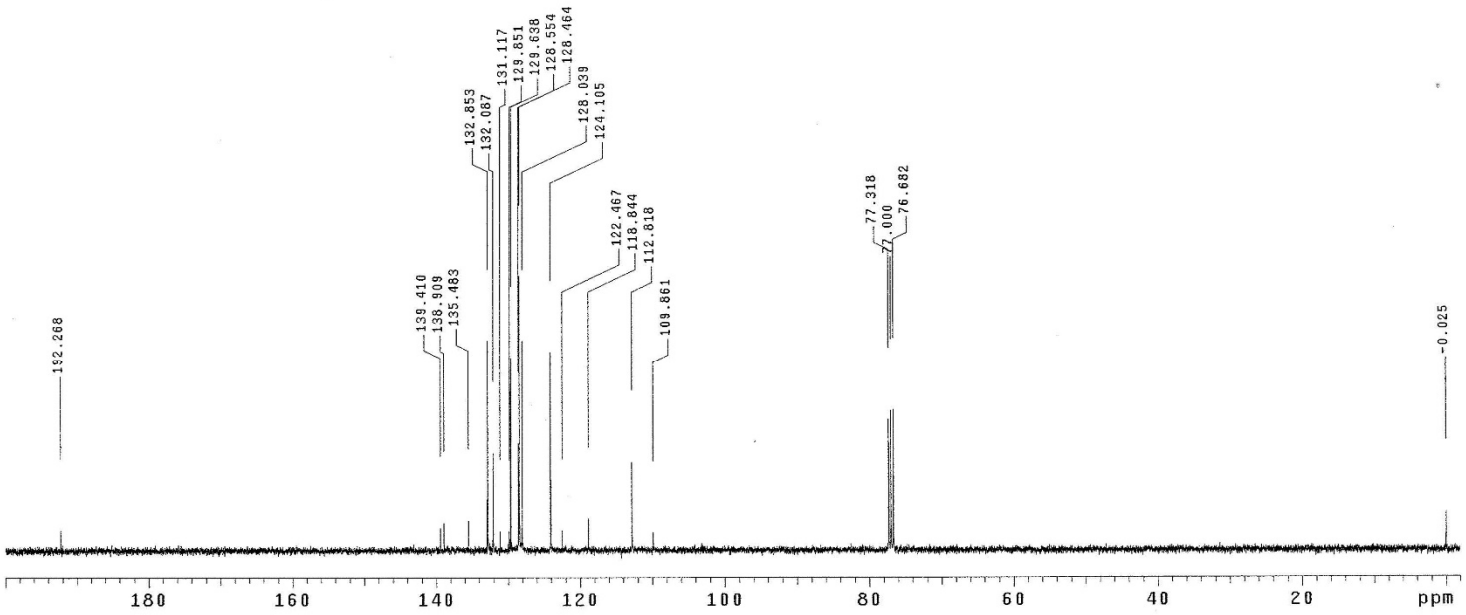
SGC/P-5/P-CN

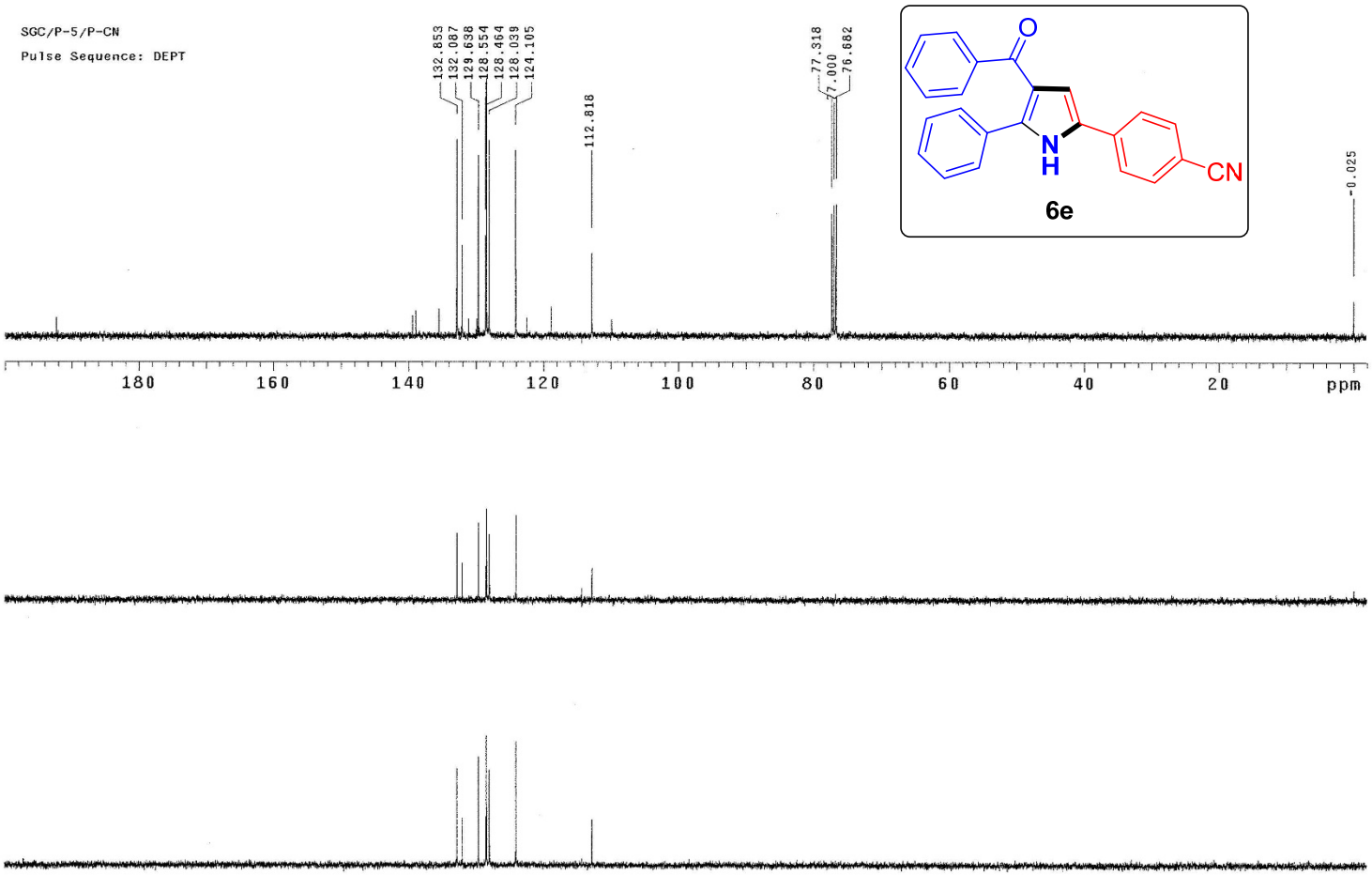
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 3376 repetitions



6e



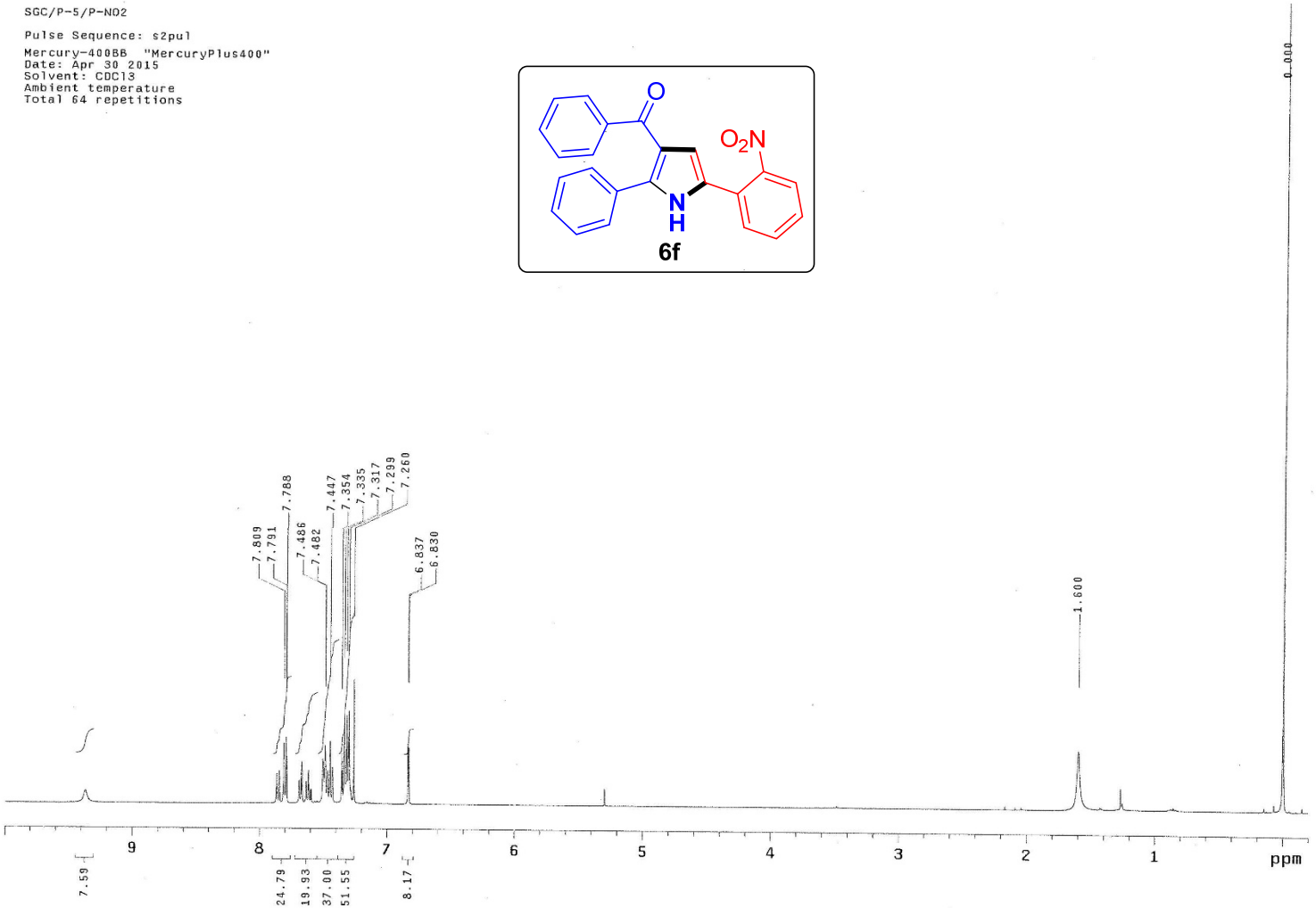

SGC/P-5/P-CN
Pulse Sequence: DEPT
132.853
132.087
129.638
128.554
128.464
128.039
124.105
112.818
77.318
77.000
76.682
-0.025
O
N
H
CN
6e
180
160
140
120
100
80
60
40
20
ppm

SGC/P-5/P-NO2

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

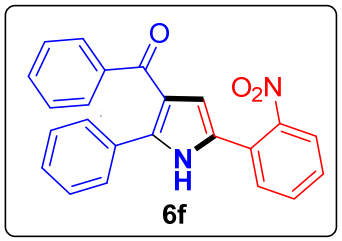
6f



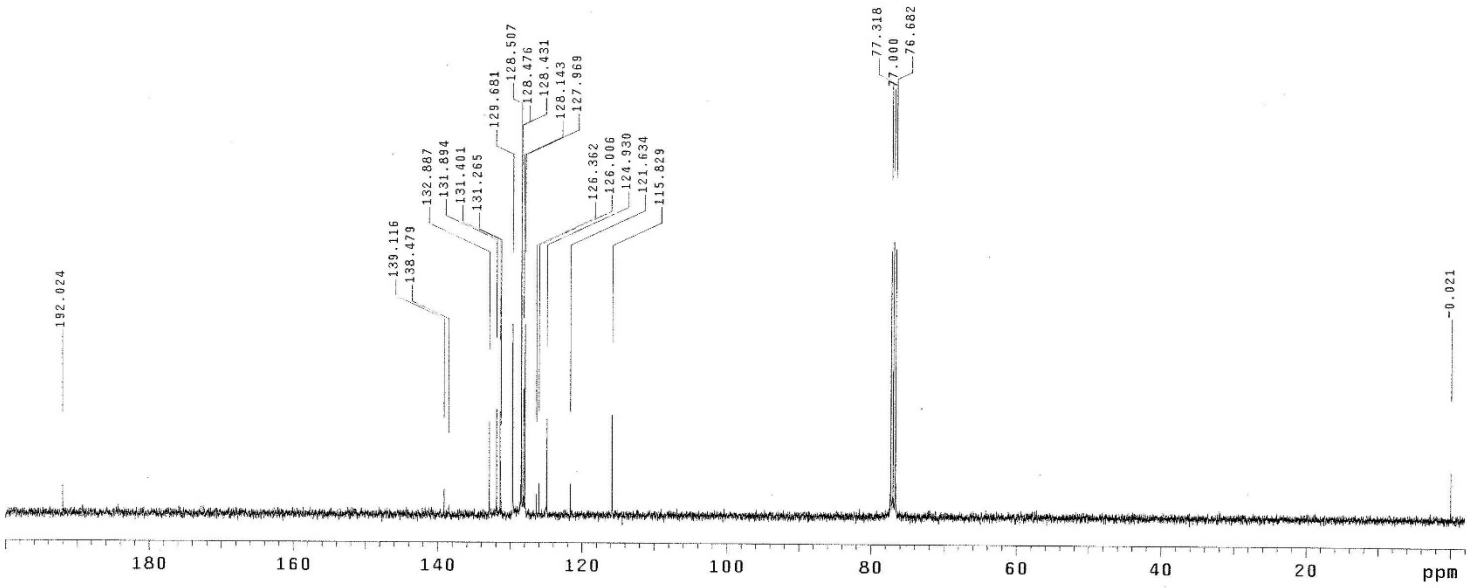
SGC/P-5/P-NO2

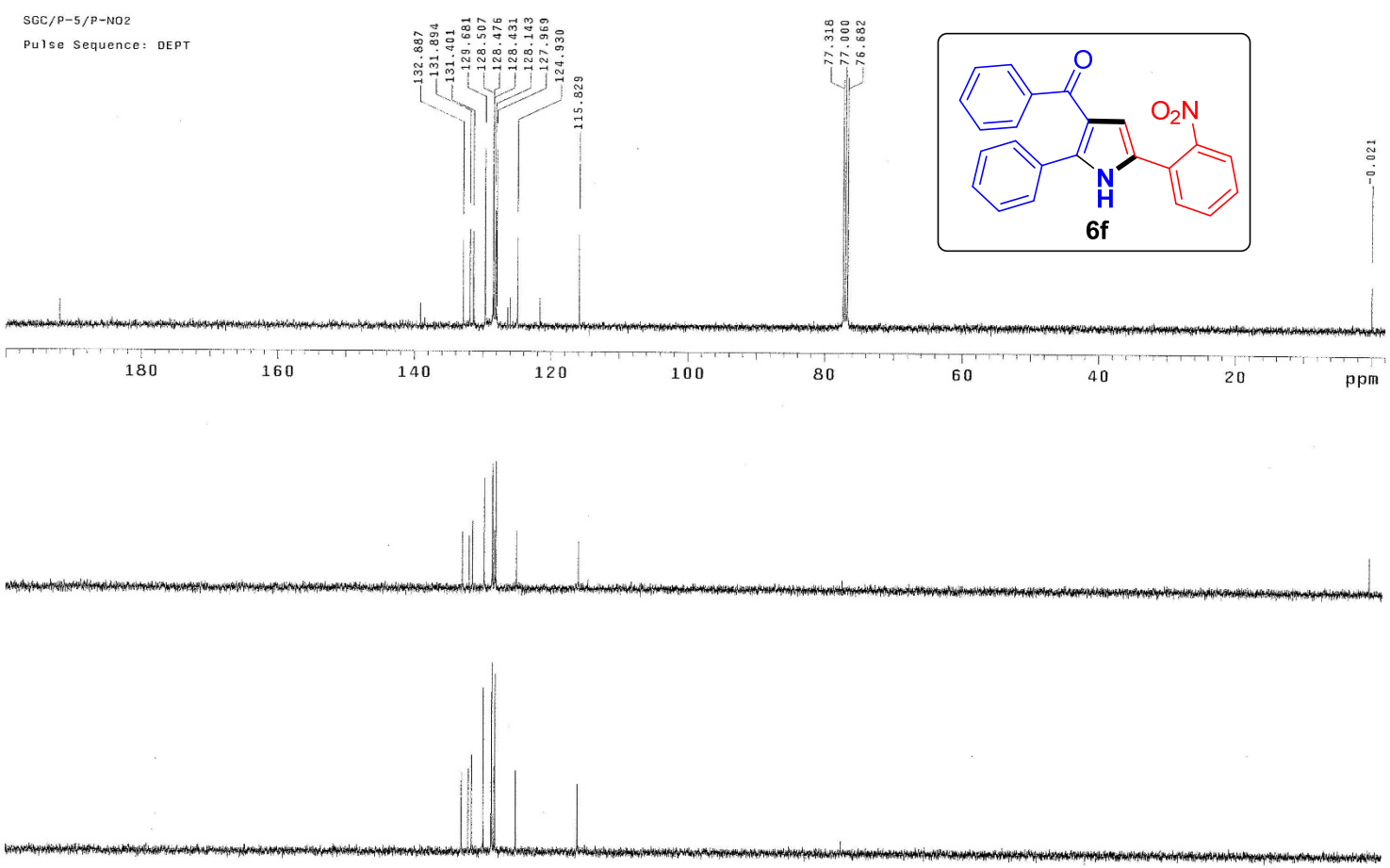
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 4464 repetitions



6f

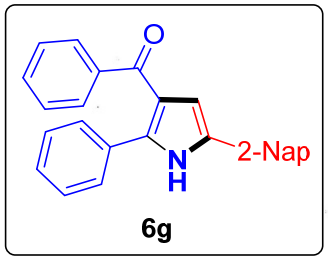



SGC/P-5/P-NO2
Pulse Sequence: DEPT
132.887
131.894
131.401
129.681
128.507
128.476
128.431
128.143
127.969
124.930
115.829
77.318
77.000
76.682
0.021
O
O2N
N
H
6f
180
160
140
120
100
80
60
40
20
ppm

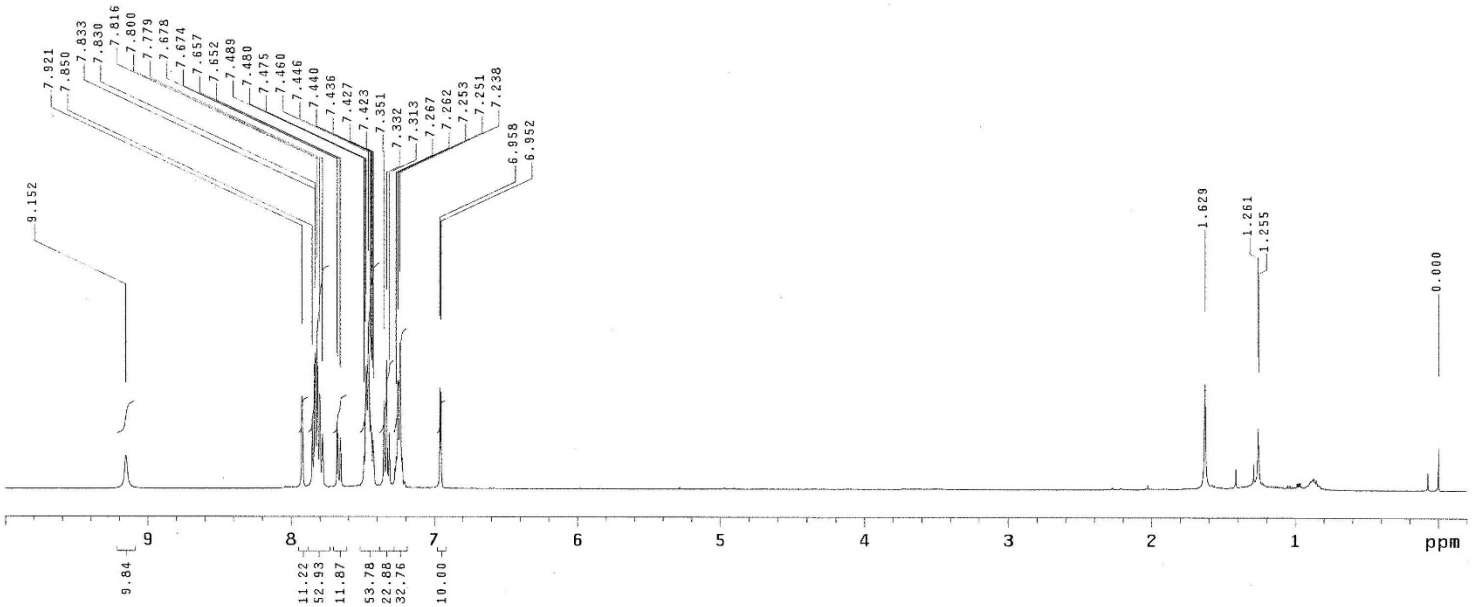
SGC/P-5/P-2

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Apr 1 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



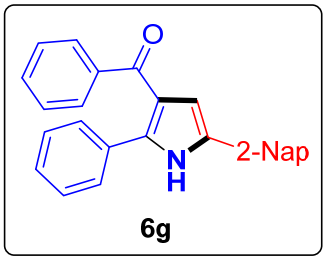
6g



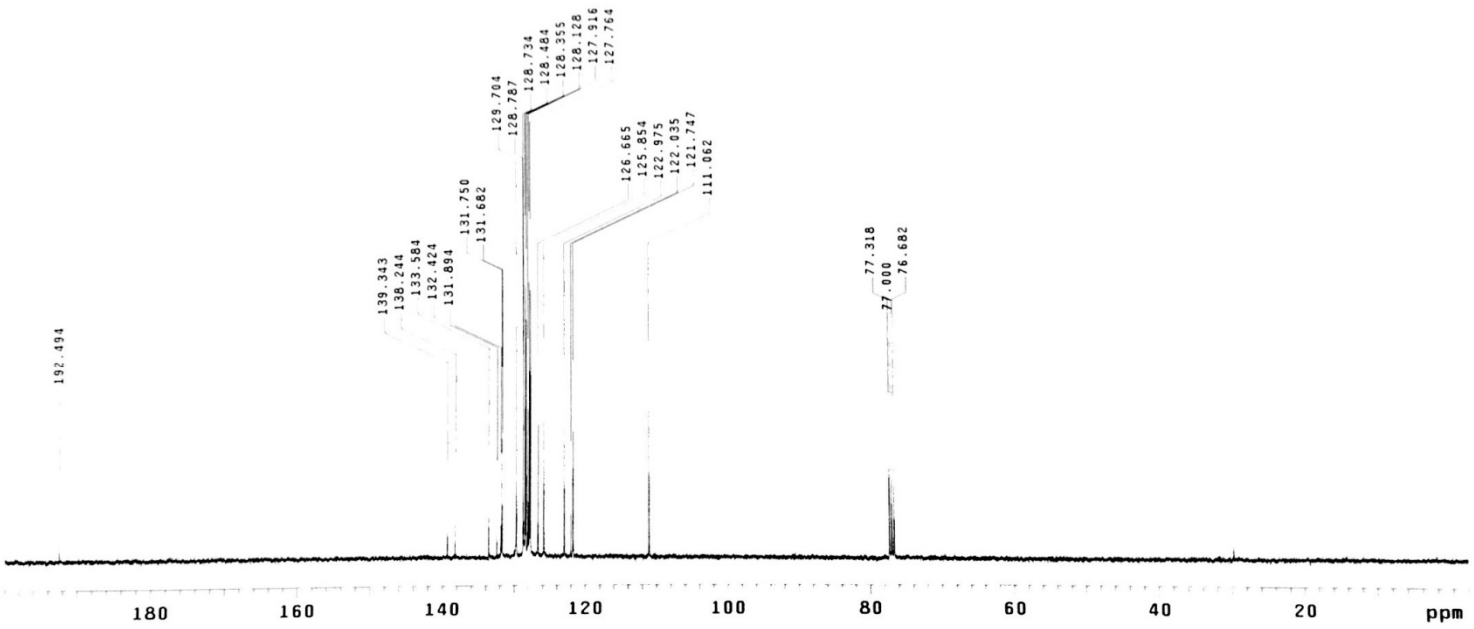
SGC/P-5/P-2

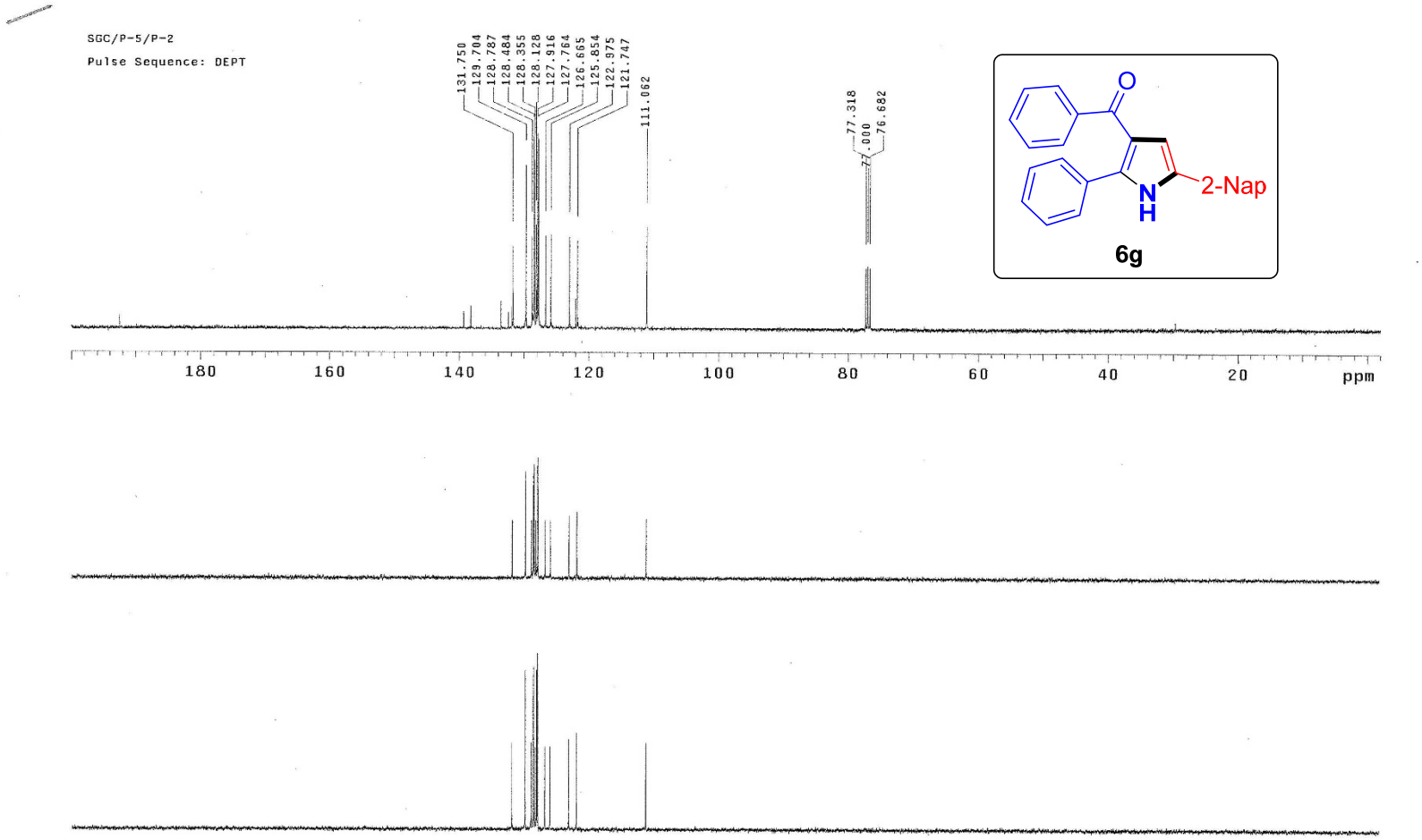
Pulse Sequence: s2pul

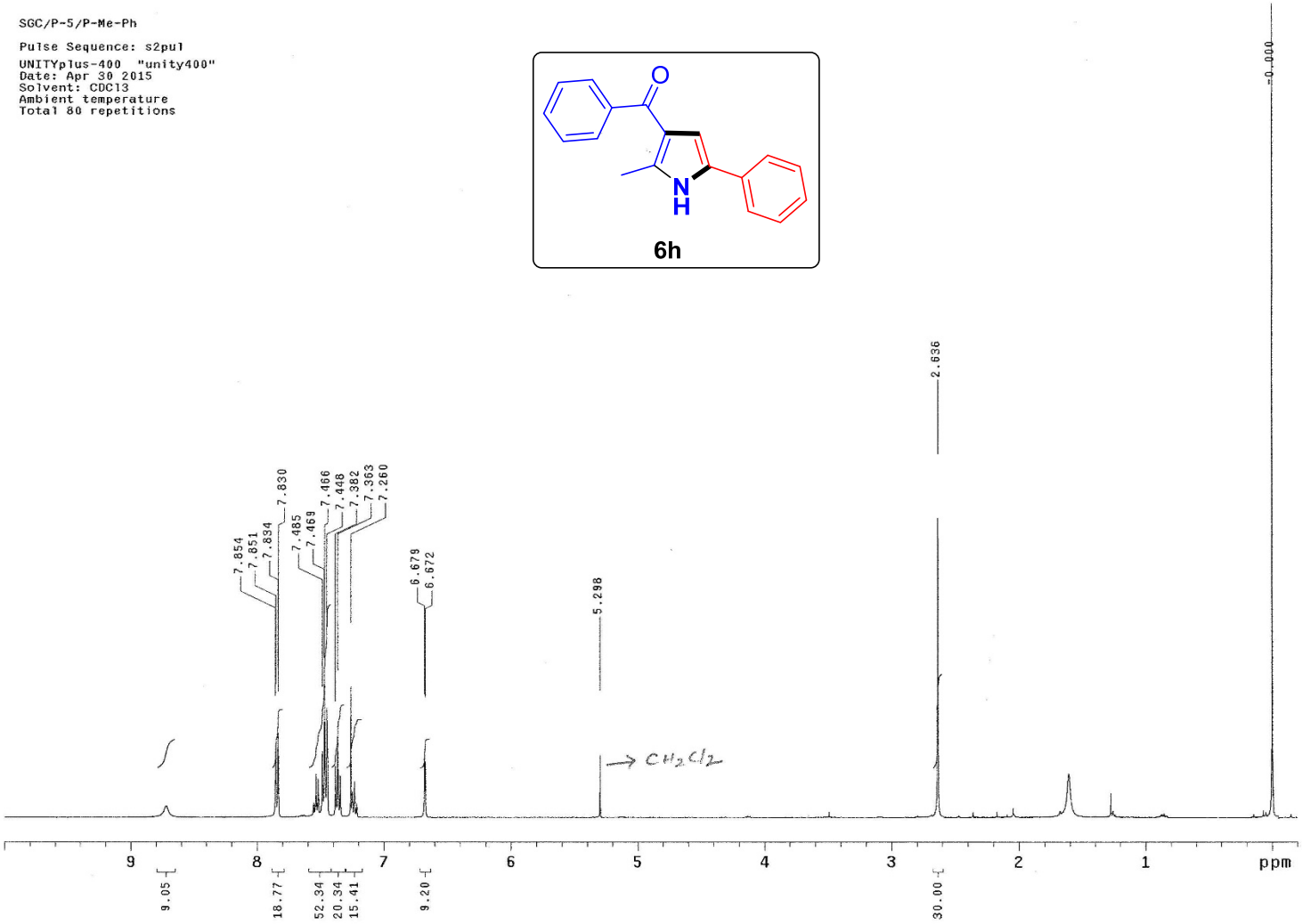
Mercury-400BB "MercuryPlus400"
Date: Apr 1 2015
Solvent: CDCl3
Ambient temperature
File: M0075-8
Total 1472 repetitions



6g



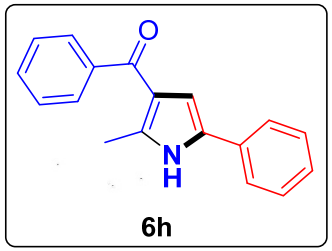

SGC/P-5/P-2
Pulse Sequence: DEPT
131.750
129.704
128.787
128.484
128.355
128.128
127.916
127.764
126.665
125.854
122.975
121.747
111.062
77.318
77.000
76.682
O
N
H
2-Nap
6g
180
160
140
120
100
80
60
40
20
ppm


SGC/P-5/P-Me-Ph
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 80 repetitions
O
N
H
6h
7.854
7.851
7.834
7.830
7.485
7.469
7.466
7.448
7.382
7.363
7.260
6.679
6.672
5.298
2.636
0.000
→ CH2Cl2
9
8
7
6
5
4
3
2
1
ppm
9.05
18.77
52.34
20.34
15.41
9.20
30.00

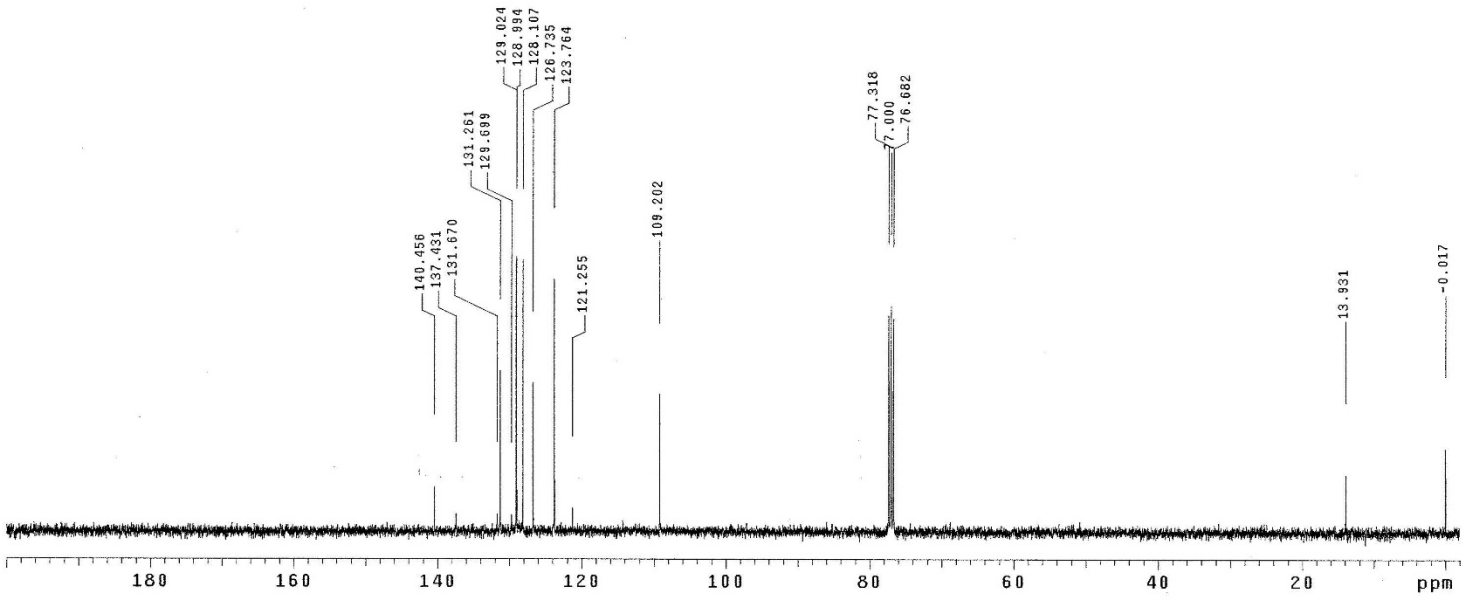
SGC/P-5/P-Me-Ph

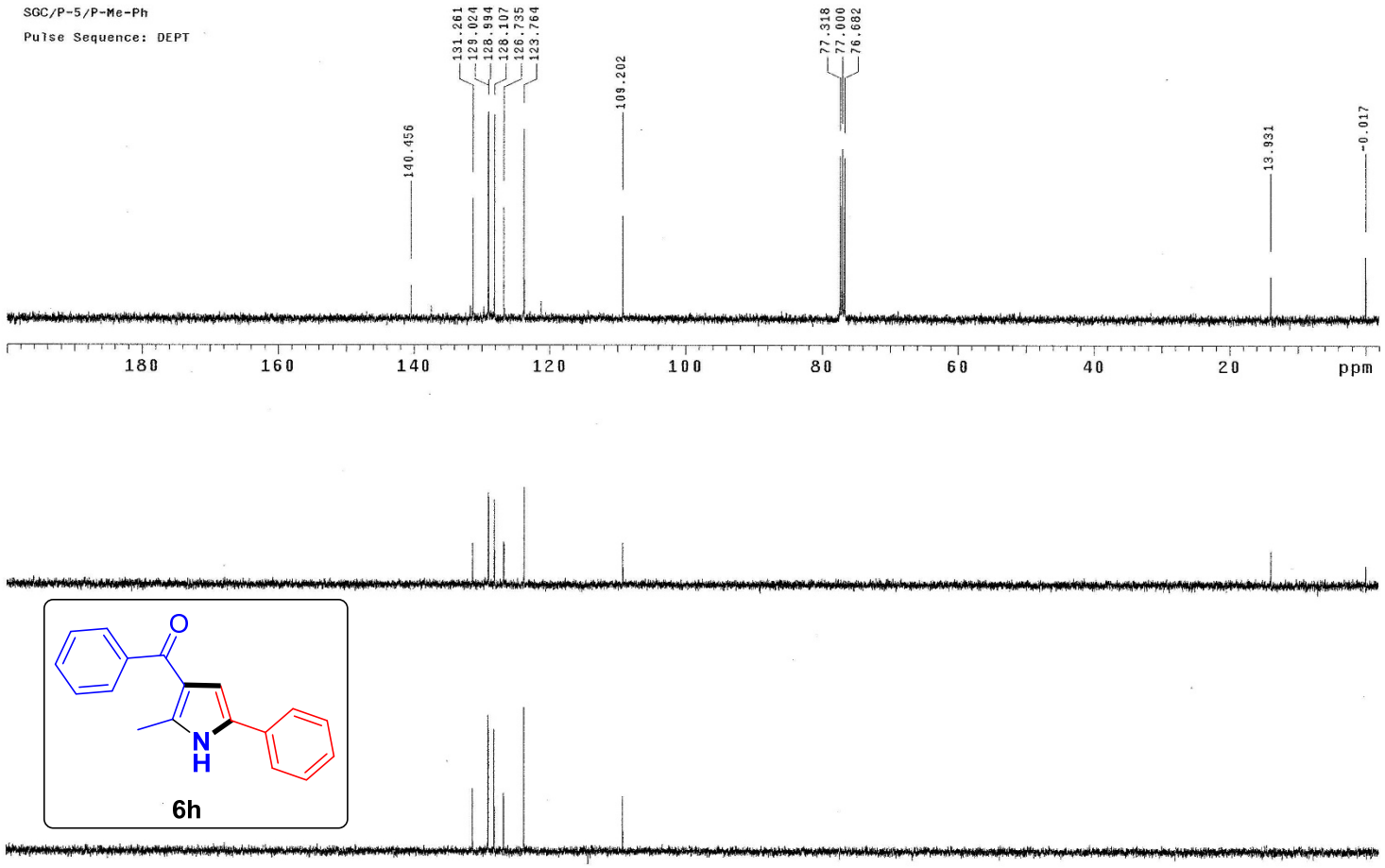
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 30 2015
Solvent: CDCl3
Ambient temperature
Total 6592 repetitions



6h

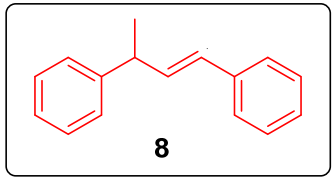



SGC/P-5/P-Me-Ph
Pulse Sequence: DEPT
131.261
129.024
128.994
128.107
126.735
123.764
140.456
109.202
77.318
77.000
76.682
13.931
-0.017
180
160
140
120
100
80
60
40
20
ppm
O
N
H
6h

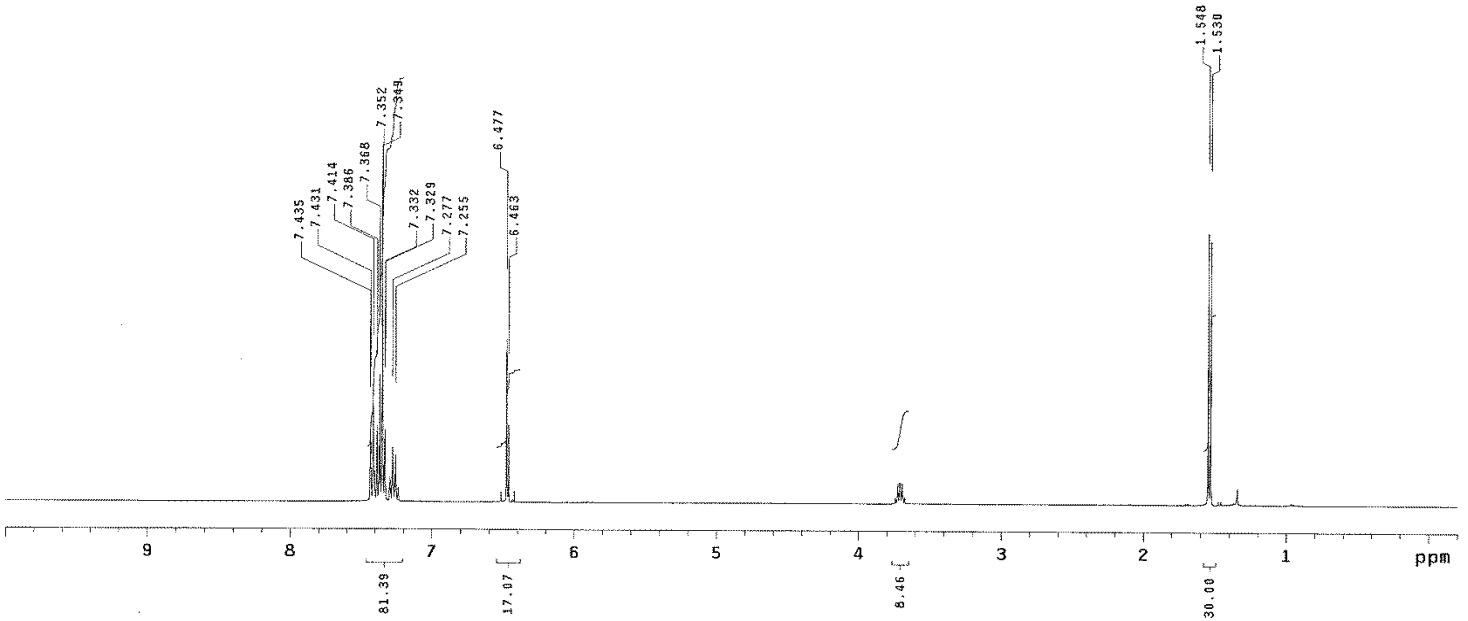
SGC/P-5/Dimer

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



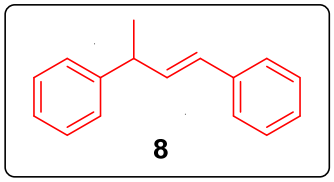
8



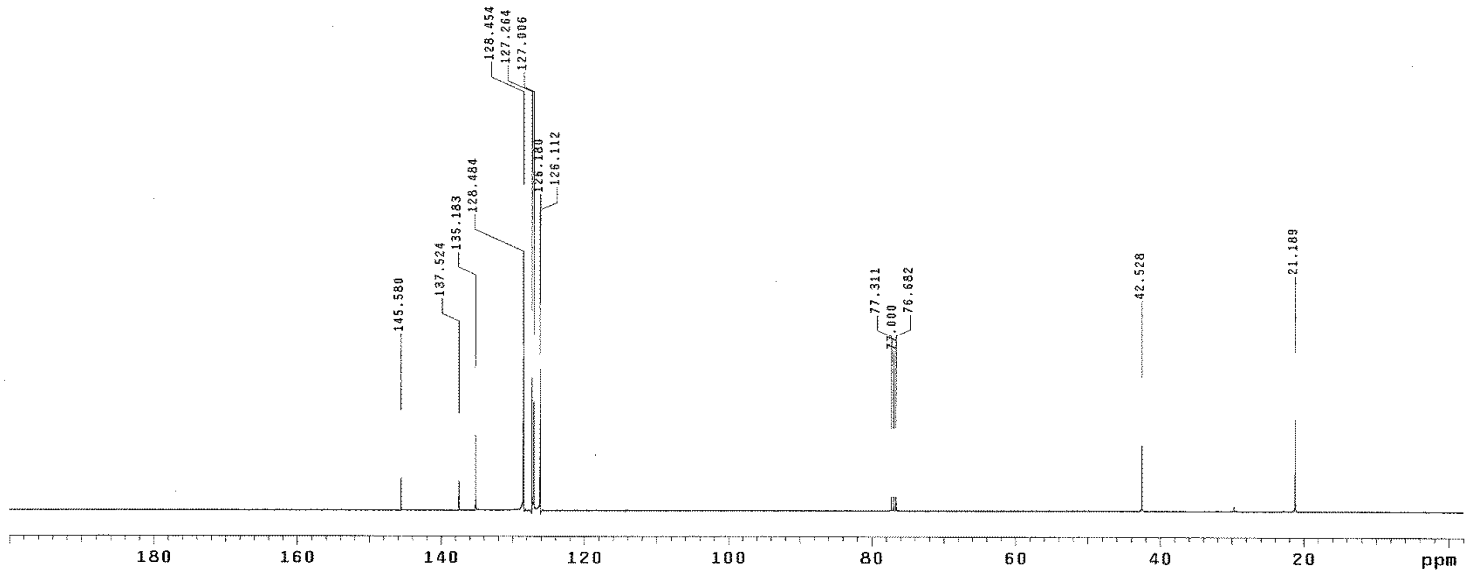
SGC/P-5/Dimer

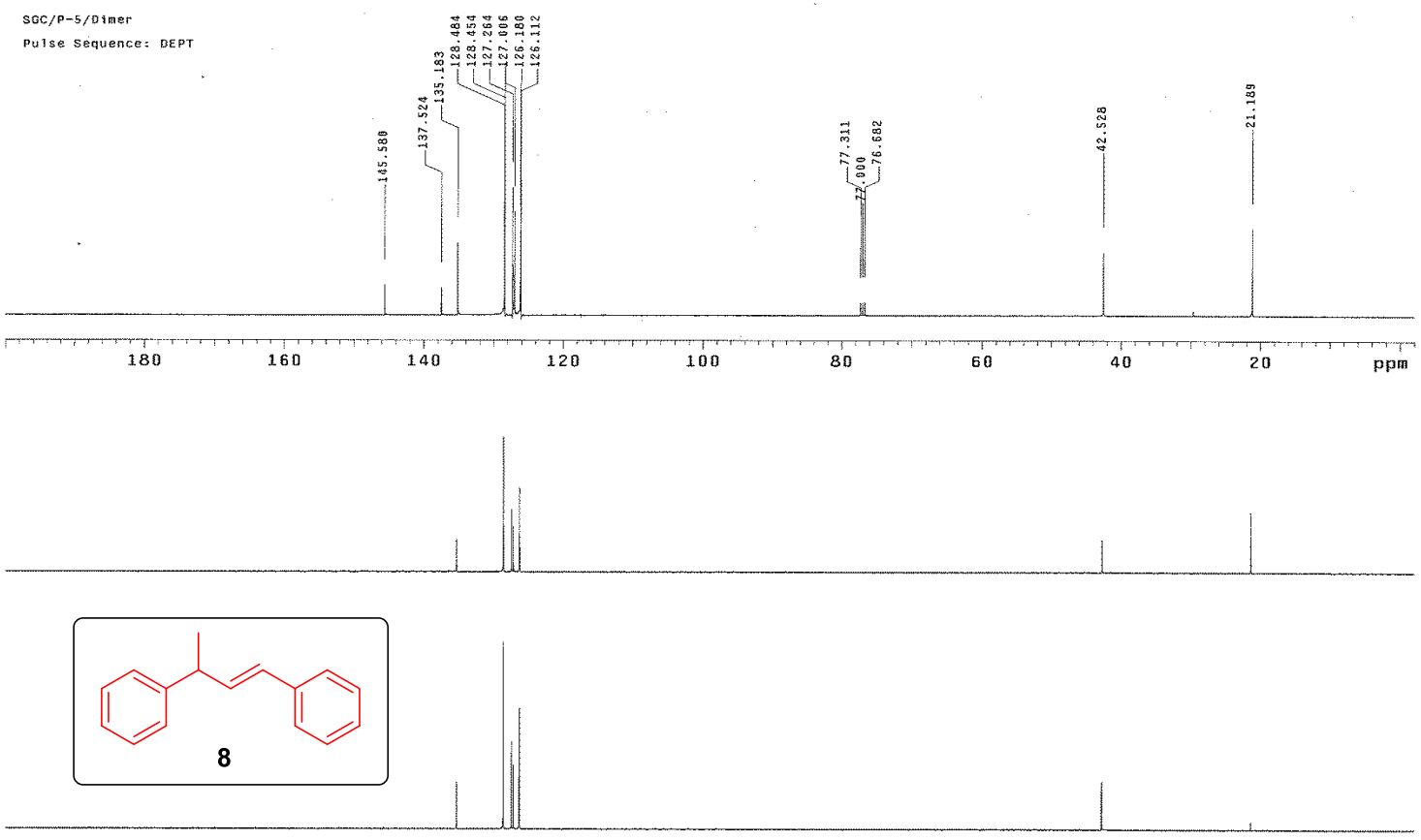
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 20480 repetitions



8

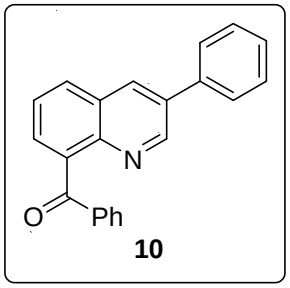



SGC/P-5/Dimer
Pulse Sequence: DEPT
145.580
137.524
135.183
128.484
128.454
127.264
127.006
126.180
126.112
77.311
77.000
76.682
42.528
21.189
180
160
140
120
100
80
60
40
20
ppm
8

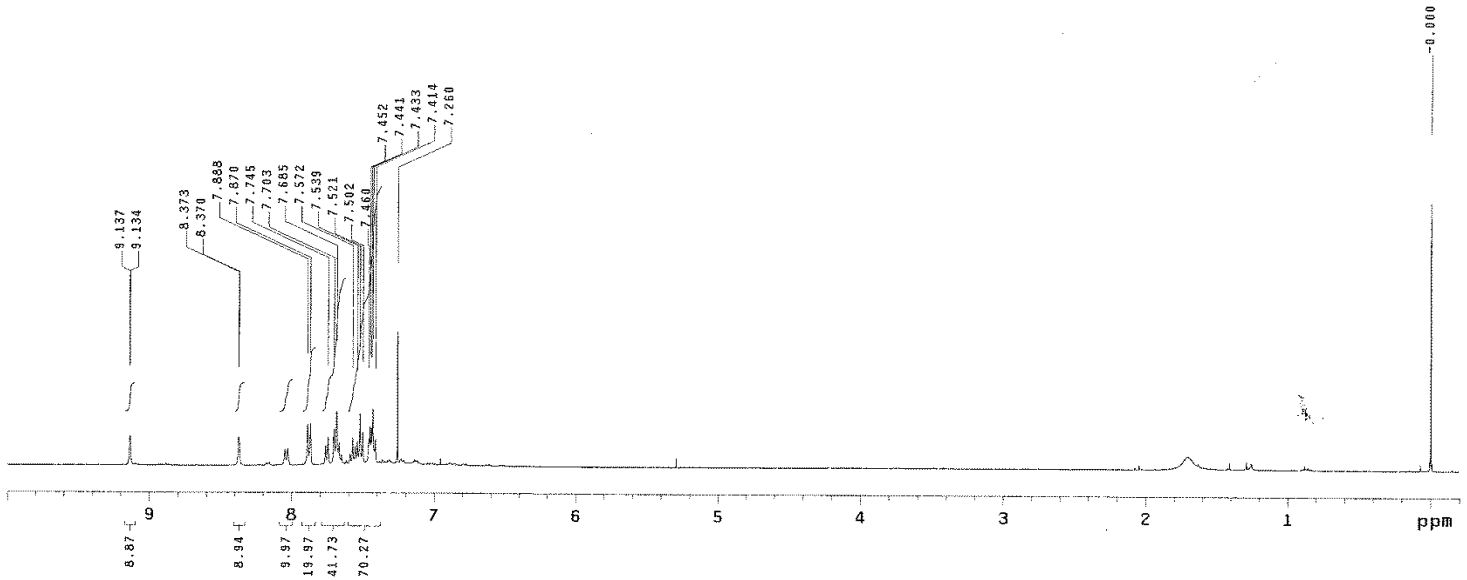
SGC/RPS/CHO

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jun 3 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



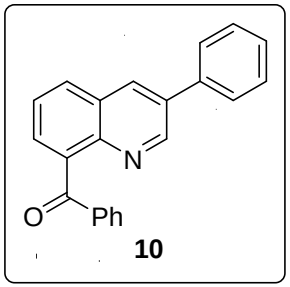
10



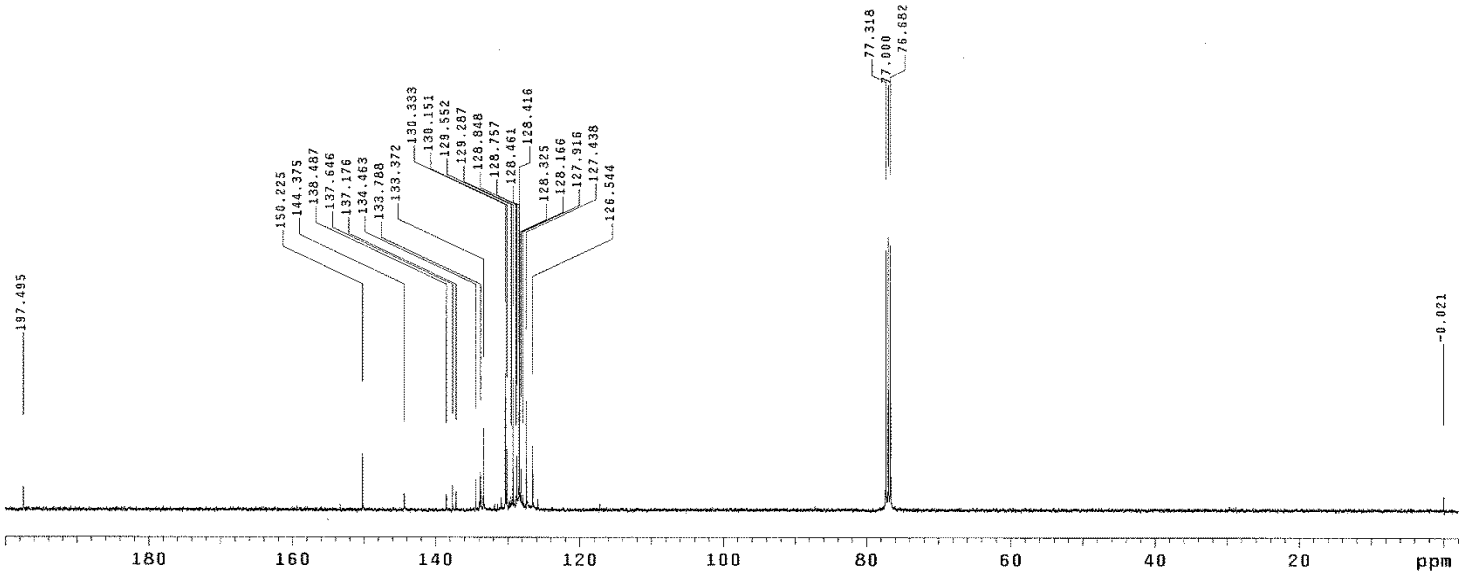
SGC/RP5/CHO

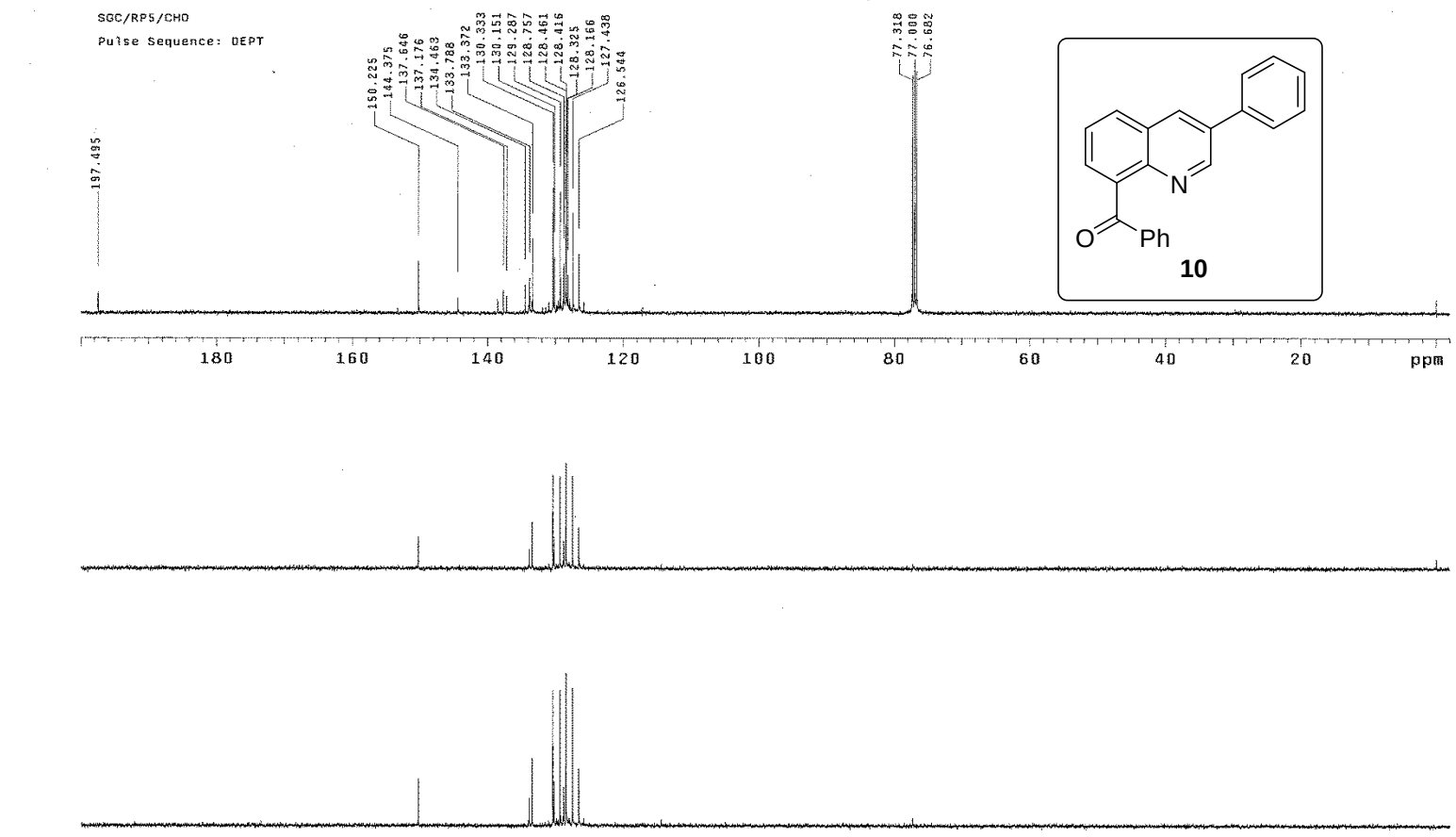
Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"
Date: Jun 4 2015
Solvent: CDCl3
Ambient temperature
Total 10400 repetitions



10

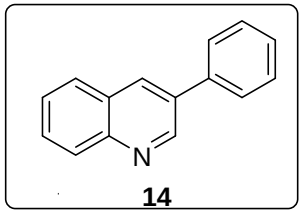



SGC/RP5/CHO
Pulse Sequence: DEPT
197.495
150.225
144.375
137.646
137.176
134.463
133.788
133.372
130.333
130.151
129.287
128.757
128.461
128.416
128.325
128.166
127.438
126.544
77.318
77.000
76.682
N
O
Ph
10
180
160
140
120
100
80
60
40
20
ppm

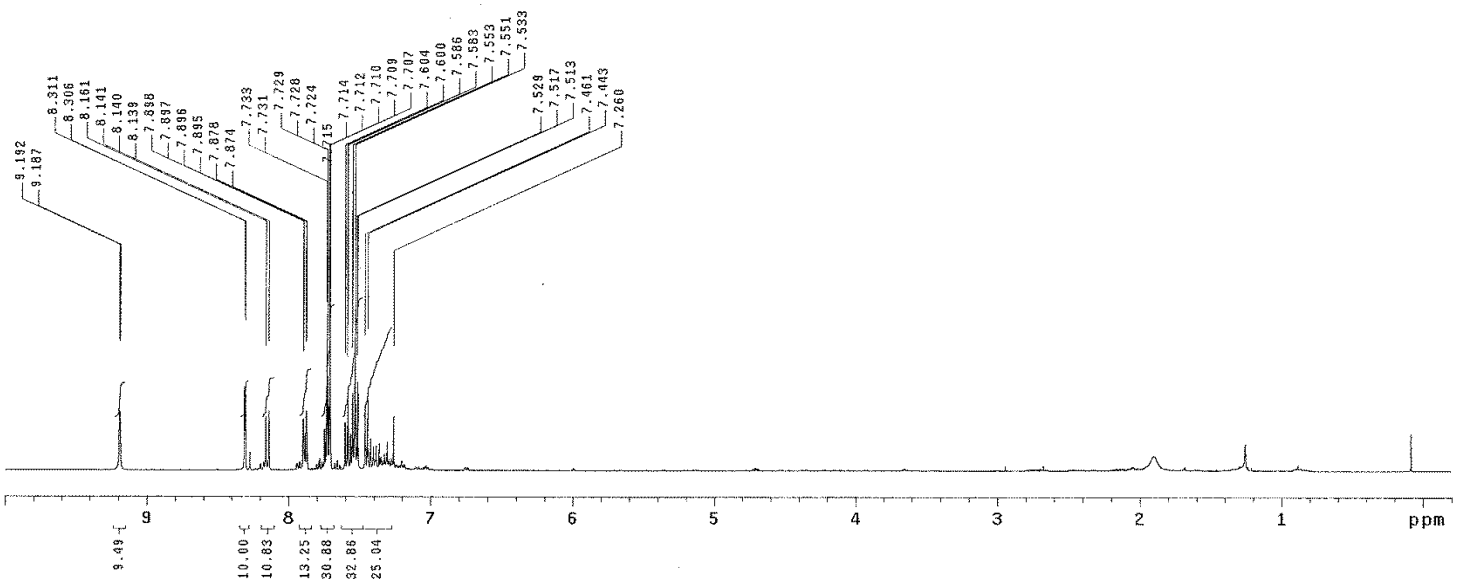
SGC/P-5/3Aguin

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



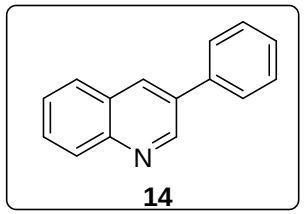
14



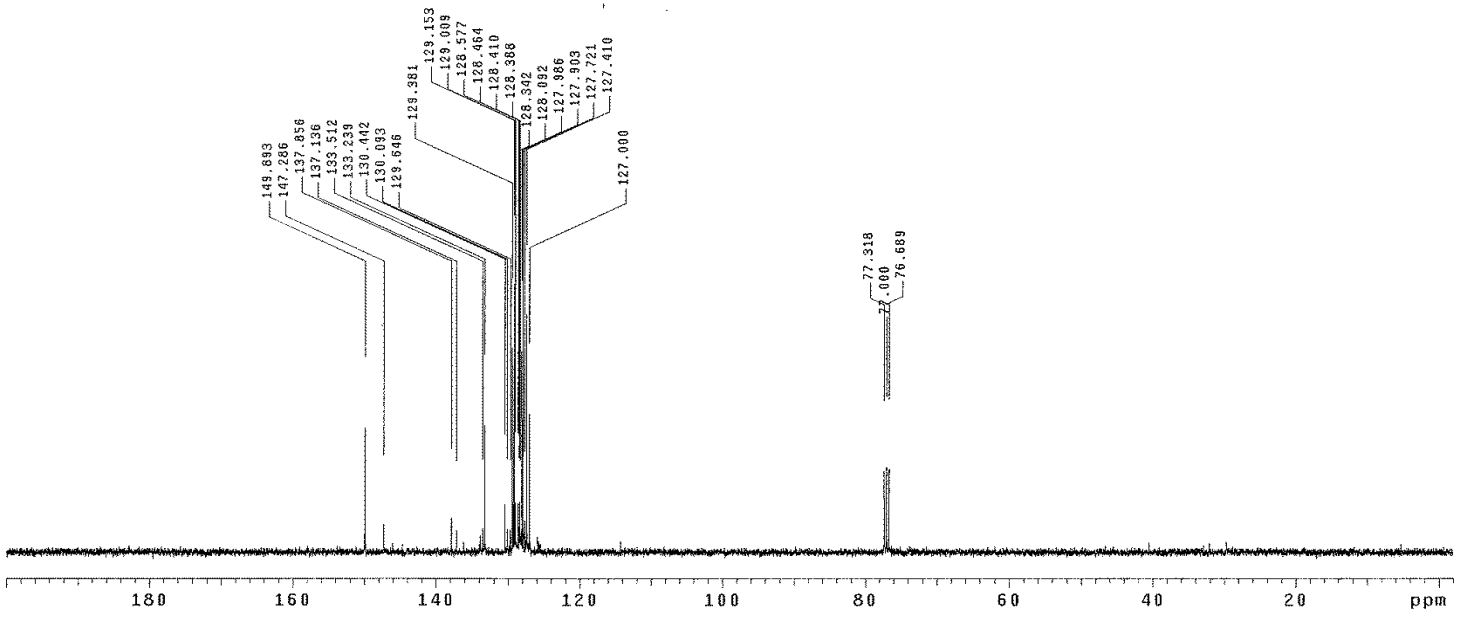
SGC/P-5/3Aguin

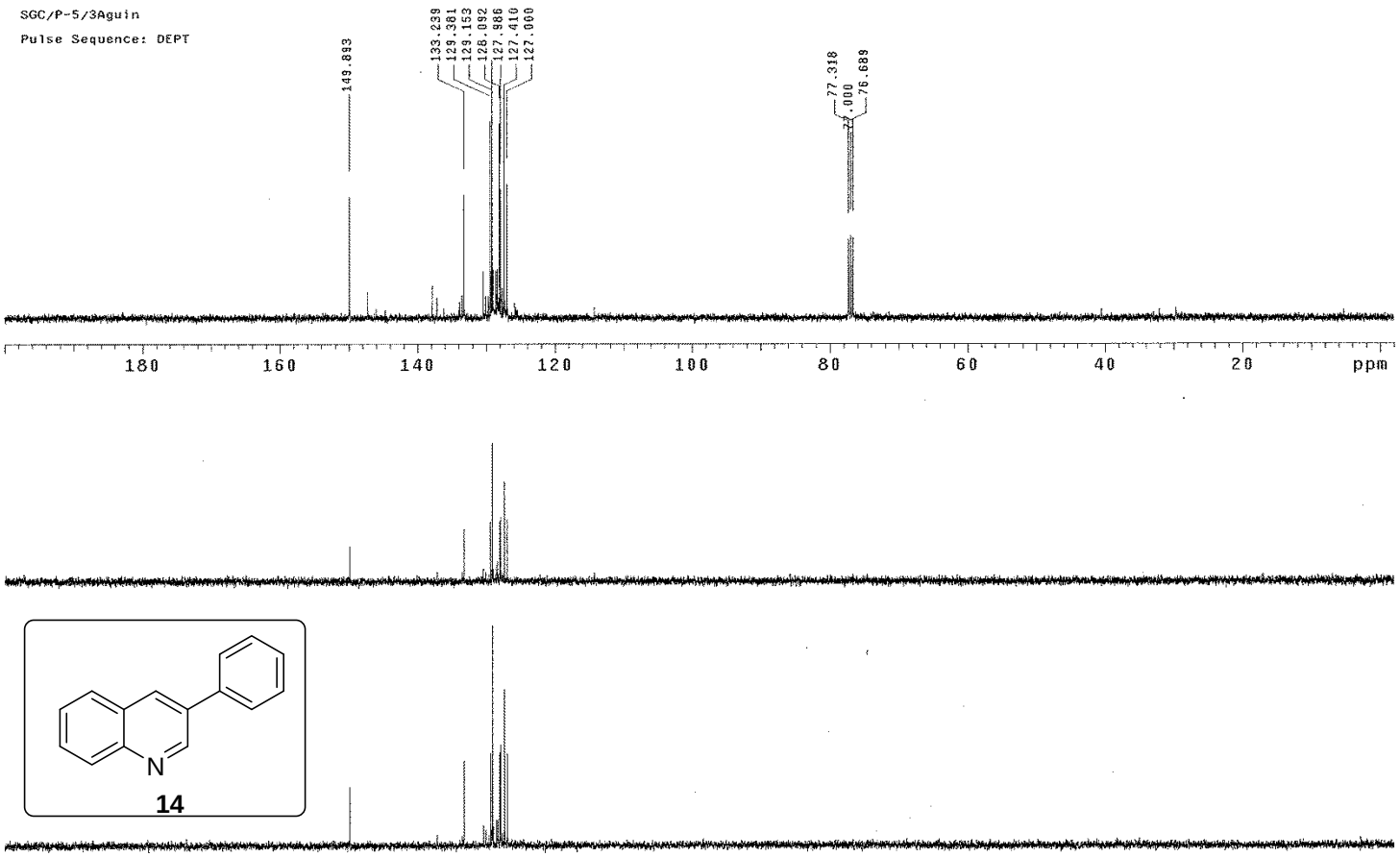
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 20 2015
Solvent: CDCl3
Ambient temperature
Total 1840 repetitions



14




SGC/P-5/3Aguin
Pulse Sequence: DEPT
149.893
133.239
129.381
129.153
128.092
127.986
127.410
127.060
77.318
77.000
76.689
180
160
140
120
100
80
60
40
20
ppm
N
14