Supplementary Information
For
Copper-Catalyzed Annulation of Amidines for Quinazolines Synthesis

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I. General Considerations

All commercially available compounds were purchased from Aldrich or J&K Chemical Limited. Most commercially supplied chemicals were used without further purification. ^{1}H NMR spectra were recorded at 25 ºC on a Varian 500 MHz, ^{13}C NMR spectra were recorded at 25 ºC on a Varian 125 MHz, and TMS as internal standard. The chemical shifts (δ) are given in parts per million relative to internal standard TMS (0 ppm for ^{1}H) and $CDCl_3$ (77.0 ppm for ^{13}C). Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and are uncorrected. High resolution mass spectra were recorded on Bruck microtof. Flash column chromatography was performed on silica gel 60 (particle size 300-400 mesh ASTM, purchased from Taizhou, China).

II. Synthesis of substrates

Mathod A:[1] Under an air atmosphere, a pressure flask (75 mL in volume) equipped with a stir bar was charged with the aniline (10.0 mmol, 1. 0 equiv) and the carbonitrile (12.0 mmol, 1.2 equiv). $AlCl_3$ (12.0 mmol, 1.0 equiv) was added in one portion while stirring the reaction mixture. The flask was tightly sealed with a screw cap and lowered into a preheated oil bath at 130 ℃. The reaction mixture was stirred for the indicated time, and taken out of the oil bath. The hot mixture was poured into a solution of concentrated NaOH solution (40.0 mL) in mixed water and ice (100.0 mL) and stirred for about 15 minutes. Then the mixture was extracted with CH_2Cl_2 (30.0 mL × 3). The combined organic layers were washed with brine (30.0 mL × 3), dried over anhydrous Na_2SO_4, and evaporated under vacuum. The residue was purified either by column chromatography on silica gel or by recrystallization.

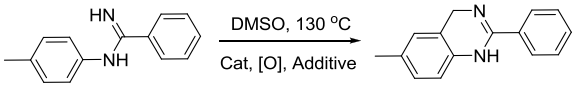
Mathod B:[2] To a solution of aniline (10.0 mmol, 1. 0 equiv) and carbonitrile (12.0 mmol) in 5.0 mL of anhydrous DMSO was added NaH (12.0 mmol, 70%, 1.2 equiv) in portions at 0 ^{o}C under a nitrogen atmosphere. The mixture was kept at 0 ℃ for 30-60 min and then stirred for the indicated time at room temperature. Ice water (10.0 mL) was added carefully to quench the reaction. The mixture was then extracted with CH_2Cl_2 (10.0 mL × 3). The combined organic layers were washed with brine (10.0 mL × 3), dried over anhydrous Na_2SO_4, and evaporated under vacuum. The residue was purified either by column chromatography on silica gel or recrystallization.

References:

1. (a) G. Brasche and S. L. Buchwald, *Angew. Chem. Int. Ed.* 2008, **47**, 1932-1934; (b) F. C. Cooper and M. W. Partridge, *J. Chem. Soc.* 1953, 255-260.
2. (a) B. Singh and J. C. Collins, *Chem. Commun.* 1971, 498-499; (b) Q. Xiao, W.-H. Wang, G. Liu, F.-K. Meng, J.-H. Chen, Z. Yang and Z.-J. Shi, *Chem. Eur. J.* 2009, **15**, 7292-7296.

III. Optimization Study for copper catalyzed Intermolecular annulation of 1a with DMSO.

Table 1 Intermolecular annulation of **1a** with DMSO.[a]



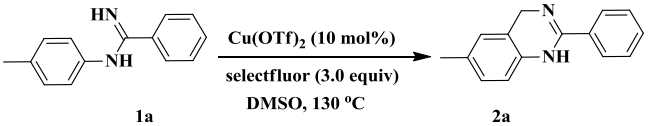
1a **2a**

Entry	Cat. (0.1 equiv)	Additive (equiv)	Oxidant (equiv)	Yield[b] (%)
1	$CuCl_2$	No	Selectfluor (2.0)	15
2	$CuSO_4$	No	Selectfluor (2.0)	20
3	$CuBr_2$	No	Selectfluor (2.0)	31
4	$Cu(OAc)_2$	No	Selectfluor (2.0)	22
5	$Cu(OTf)_2$	No	Selectfluor (2.0)	42
6	CuCl	No	Selectfluor (2.0)	22
7	CuBr	No	Selectfluor (2.0)	36
8	**$Cu(OTf)_2$**	**No**	**Selectfluor (3.0)**	**71**
9	No	No	Selectfluor (3.0)	0
10	$Cu(OTf)_2$	HOAc (5.0)	Selectfluor (3.0)	37
11	$Cu(OTf)_2$	TFA (5.0)	Selectfluor (3.0)	41
12	$Cu(OTf)_2$	phen (0.1)	Selectfluor (3.0)	60
13	$Cu(OTf)_2$	No	NFSI (3.0)	58[c]
14	$Cu(OTf)_2$	No	F^+ (3.0)[d]	n.d.[e]
15	$Cu(OTf)_2$	No	O_2	12[f]
16	$Cu(OTf)_2$	No	TBHP (3.0)	n.d[g]
17	$Cu(OTf)_2$	No	Selectfluor (3.0)	33[h]

[a]Reaction conditions: **1a** (0.3 mmol), catalyst, additive and oxidant in 2 mL DMSO at 130 °C for 2.5 hours. [b]Yield of the isolated product. [c]NFSI = *N*-fluorobenzenesulfonimide. [d]F^+ = *N*-fluoro-2,4,6-trimethylpyridinium tetrafluoroborate. [e]n.d. = not detected. [f]The reaction was performed for 4.0 hours. [g]TBHP = *tert*-butyl hydroperoxide (5.5 M in decane). [h]3.0 equiv. of DMSO was used with 2 mL CH_3CN as the solvent.

IV. General procedure for the preparation of 2

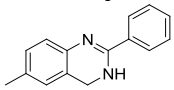
General procedure for Intermolecular annulation of amidines 1 with DMSO



1a **2a**

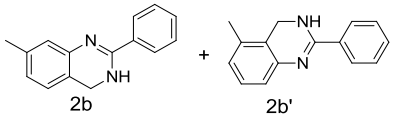
To a solution of *N*-(p-tolyl)benzimidamide or its derivatives 1a (63.0mg, 0.3 mmol, 1.0 equiv) in DMSO (2.0 mL) were added Selectfluor (318.8mg, 0.9 mmol, 3.0 equiv) and $Cu(OTf)_2$ (10.8 mg, 0.03 mmol, 0.1 equiv) in screw-cap test tube. The resulting mixture was stirred at 130 °C. The reaction was monitored by TLC until the starting material was completely consumed. The reaction mixture was diluted with CH_2Cl_2 (5.0 mL × 3) and washed with brine (5.0 mL × 3). The organic layer was dried over Na_2SO_4, and concentrated under vacuum. The residue was purified by column chromatography to give the corresponding products 2a (47.3mg, 71%) .

V. Analytical data of New Compounds:



6-methyl-2-phenyl-3,4-dihydroquinazoline (2a)

White solid. mp:74-75 °C; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.30 (s, 3H), 4.75 (s, 2H), 6.77 (s, 1H), 7.00 (s, 2H), 7.42-7.45 (m, 3H), 7.79 (d, J = 7.0 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 20.9, 44.5, 120.0, 126.1, 126.4, 128.6, 128.7, 130.6, 134.3, 135.2, 154.5. HRMS (ESI-TOF) Calcd for $C_{15}H_{14}N_2$, $[M+H]^+$ *m/z* 223.1230; Found 223.1237.

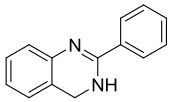


2b 2b'

7-methyl-2-phenyl-3,4-dihydroquinazoline (2b);
5-methyl-2-phenyl-3,4-dihydroquinazoline (2b') (2b/2b' = 10 : 9)

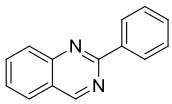
White solid. mp:76-77 °C ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.15 (s, 3H), 2.29 (s, 3H), 4.72 (s, 4H), 6.81-6.86 (m, 3H),

6.91 (m, 2H), 7.07 (t, *J* = 7.5 Hz, 1H), 7.38-7.45 (m, 6H), 7.77 (d, *J* = 7.0 Hz, 4H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 18.1, 21.1, 42.9, 44.6, 117.1, 118.7, 125.2, 125.3, 126.0, 126.4, 126.5, 127.6, 128.5, 128.8, 130.5, 130.6, 130.9, 134.1, 135.0, 135.2, 137.8, 154.4, 154.8. HRMS (ESI-TOF) Calcd for $C_{15}H_{14}N_2$, $[M+H]^+$ *m/z* 223.1230; Found 223.1236.



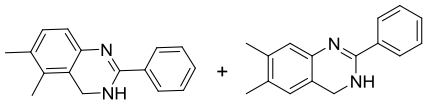
6-methyl-2-phenyl-3,4-dihydroquinazoline (2c)

White solid. mp: 79-80 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 4.76 (s, 2H), 6.94 (d, *J* = 7.5 Hz, 1H), 7.04 (t, *J* = 7.0 Hz, 1H), 7.10 (d, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.39-7.46 (m, 3H), 7.79 (d, *J* = 7.0 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 44.6, 120.1, 121.4, 124.4, 125.4, 126.5, 128.0, 128.5, 130.5, 135.1, 141.1, 154.9. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}N_2$, $[M+H]^+$ *m/z* 209.1073; Found 209.1072.



2-phenylquinazoline (2c')

Pale yellow solid; mp 97−98 °C; ^{1}H NMR (500 MHz, CDCl3): δ =7.51-7.56 (m, 3H), 7.61 (t, J = 7.5 Hz, 1H), 7.89-7.93 (m, 2H), 8.09 (d, J = 9.5 Hz, 1H), 8.62 (d, J = 7.0 Hz, 2H), 9.47 (s, 1H). ^{13}C NMR (125 MHz, CDCl3): δ = 123.6, 127.1, 127.3, 128.5, 128.6, 128.6, 130.6, 134.1, 138.0, 150.7, 160.5, 161.0. HRMS (ESI-TOF) Calcd for $C_{14}H_{10}N_2$, $[M+H]^+$207.0917 Found 207.0911.

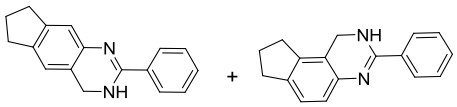


2d 2d'

5,6-dimethyl-2-phenyl-3,4-dihydroquinazoline(2d)

6,7-dimethyl-2-phenyl-3,4-dihydroquinaz- oline (2d') (2d/2d' = 1.3 : 1)

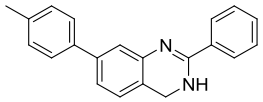
White solid. mp:136-137 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.01 (s, 3H), 2.19-2.21 (m, 6H), 4.66 (s, 2H), 4.70 (s, 2H), 6.68 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.87 (s, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.35-7.41 (m, 6H), 7.73-7.74 (m, 4H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 19.9, 20.0, 20.1, 20.8, 44.5, 48.8, 122.4, 122.7, 126.1, 126.9, 127.8, 128.3, 130.3, 131.6, 132.2, 132.9, 135.0, 137.1, 137.4, 138.1, 138.3, 145.1, 149.8, 157.0, 159.0. HRMS (ESI-TOF) Calcd for $C_{16}H_{16}N_2$, $[M+H]^+$ *m/z* 237.1386; Found 237.1385.



2e 2e'

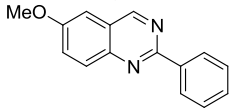
2-phenyl-4,6,7,8-tetrahydro-3H-cyclopenta[g]quinazoline (2e) 3-phenyl-2,7,8,9-tetrahydro-1H- cyclo penta[f]quinazoline (2e') (2e/2e' = 1.6 : 1)

White solid. mp:72-73 ºC ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.04-2.10 (m, 4H), 2.68-2.72 (m, 2H), 2.83-2.88 (m, 6H), 4.69 (s, 2H), 4.71 (s, 2H), 6.79 (s, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 7.02-7.04 (m, 2H), 7.36-7.43 (m, 6H), 7.79 (d, *J* = 8.0 Hz, 4H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 16.7, 19.1, 25.3, 25.5, 32.3, 32.3, 42.7, 44.7, 116.1, 117.9, 121.1, 123.3, 126.4, 126.5, 128.5, 130.4, 130.9, 135.0, 135.0, 140.4, 140.5, 140.6, 144.0, 154.2, 154.5. HRMS (ESI-TOF) Calcd for $C_{17}H_{16}N_2$, $[M+H]^+$ *m/z* 249.1386; Found 249.1392.



2-phenyl-7-*p*-tolyl-3,4-dihydroquinazoline (2f)

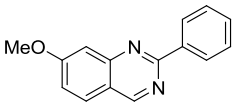
White solid. mp:124-125 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.39 (s, 3H), 4.81 (s, 2H), 6.99 (d, *J* = 7.5 Hz, 1H), 7.23-7.27 (m, 3H), 7.36 (s, 1H), 7.41-7.46 (m, 3H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.82 (m, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 21.1, 48.8, 118.9, 123.0, 125.8, 126.3, 126.5, 126.7, 128.6, 129.4, 130.6, 135.2, 137.0, 137.8, 141.1, 155.1. HRMS (ESI-TOF) Calcd for $C_{21}H_{18}N_2$, $[M+H]^+$ *m/z* 229.1543; Found 229.1561.



6-methoxy-2-phenylquinazoline (2k)

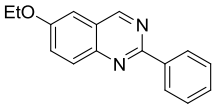
White solid. mp:81-82 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.98 (s, 3H), 7.17 (d, *J* = 2.5 Hz, 1H), 7.49-7.57 (m, 4H), 8.01 (d, *J* = 9.5 Hz, 1H), 8.57 (d, *J* = 7.5 Hz, 2H), 9.38 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 55.6 103.9, 124.3, 127.2, 128.0, 128.5, 129.9, 129.9, 133.4, 137.9, 146.8, 158.1, 158.7. HRMS (ESI-TOF) Calcd for $C_{15}H_{12}N_2O$, $[M+H]^+$

m/z 237.1022; Found 237.1019.



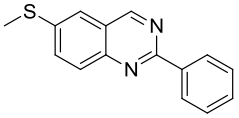
7-methoxy-2-phenylquinazoline (2l)

White solid. mp:84-85 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.99 (s, 3H), 7.22 (d, J = 2.5 Hz, 1H), 7.35 (s, 1H), 7.51 (t, J = 8.0 Hz, 3H), 7.79 (d, J = 9.0 Hz, 1H), 8.56 (d, J = 7.0 Hz, 2H), 9.29 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 55.7, 106.1, 119.1, 120.7, 128.4, 128.5, 130.4, 130.8, 138.1, 153.1, 158.9, 161.5, 164.2. HRMS (ESI-TOF) Calcd for $C_{15}H_{12}N_2O$, $[M+H]^+$ *m/z* 237.1022; Found 237.1026.



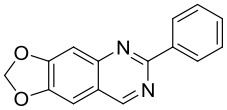
6-ethoxy-2-phenylquinazoline (2m)

White solid. mp:89-91 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.52 (t, J = 6.5 Hz, 3H), 4.19 (q, J = 6.5 Hz, 2H),7.14 (d, J = 3.0 Hz, 1H), 7.48-7.56 (m, 4H), 7.99 (d, J = 9.5 Hz, 1H), 8.57 (d, J = 8.5 Hz, 2H), 9.35 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 14.7, 64.1, 104.5, 124.5, 127.5, 128.1, 128.6, 130.1, 130.1, 138.2, 146.9, 157.6, 158.8, 159.3. HRMS (ESI-TOF) Calcd for $C_{16}H_{14}N_2O$, $[M+H]^+$ *m/z* 251.1179; Found 251.1174.



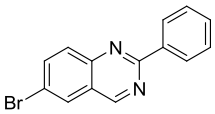
methyl(6-phenylnaphthalen-2-yl)sulfane (2n)

White solid. mp:66-67 ºC, ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.63 (s, 3H), 7.50-7.54 (m, 3H), 7.59 (d, J = 2.0 Hz, 1H), 7.76 (dd, J_1 = 2.5 Hz, J_1 = 9.0 Hz, 1H), 7.97 (d, J = 8.5 Hz, 1H), 8.58 (dd, J_1 = 1.5 Hz, J_1 = 8.0 Hz, 2H), 9.37 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 15.5, 120.9, 124.0, 128.4, 128.6, 128.7, 130.5, 133.5, 137.9, 138.9, 149,0, 158.9, 160.3. HRMS (ESI-TOF) Calcd for $C_{15}H_{12}N_2S$, $[M+H]^+$ *m/z* 253.0794, Found: 253.0795.



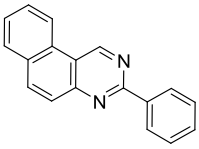
6-phenyl-[1,3]dioxolo[4,5-g]quinazoline (2o)

White solid. mp:152-153 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 6.10 (s, 2H), 7.06 (s, 1H), 7.30 (s, 1H), 7.45-7.52(m, 3H), 8.53 (d, J = 6.5 Hz, 2H), 9.13 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 101.8, 102.1, 104.9, 120.6, 128.1, 128.5, 130.1, 138.1, 148.2, 150.2, 154.0, 157.4, 159.9. HRMS (ESI-TOF) Calcd for $C_{15}H_{10}N_2O_2$, $[M+H]^+$ *m/z* 251.0815, Found: 251.0817.



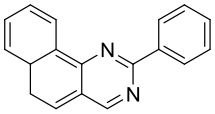
6-bromo-2-phenylquinazoline (2p)

White solid. mp:167-169 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 7.53-7.55 (m, 3H), 7.97 (d, J = 1.0 Hz, 2H), 8.10 (t, J = 1.0 Hz, 1H), 8.60-8.62 (m, 2H), 9.41 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 120.7, 124.5, 128.6, 128.7, 129.2, 130.5, 130.9, 137.6, 149.5, 159.4, 161.3. HRMS (ESI-TOF) Calcd for $C_{14}H_9BrN_2$, $[M+H]^+$ *m/z* 285.0022; Found 285.0027.



3-phenylbenzo[f]quinazoline (2q)

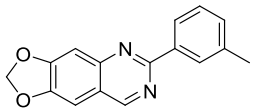
White solid. mp:182-184 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 7.52-7.60 (m, 3H), 7.74 (d, J = 9.0 Hz, 1H), 7.80-7.82 (m, 2H), 7.85 (d, J = 9.0 Hz, 1H), 7.93-7.95 (m, 1H), 8.77 (m, 2H), 9.41 (s, 1H). 9.44-9.46 (m, 1H),^{13}C NMR (125 MHz; $CDCl_3$): 120.1, 121.7, 126.9, 127.8, 128.3, 128.4, 128.6, 129.0, 130.6, 131.6, 135.6, 137.9, 152.2, 154.5, 161.9. HRMS (ESI-TOF) Calcd for $C_{18}H_{12}N_2$, $[M+H]^+$ *m/z* 257.1073; Found: 257.1074.



2-phenyl-6,6a-dihydrobenzo[h]quinazoline (2r)

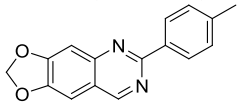
White solid. mp:137-140 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 7.53-7.58 (m, 3H), 7.71 (t, J = 7.5 Hz, 1H), 7.79 (t, J = 7.5 Hz, 1H), 7.96-7.99 (m, 2H), 8.18 (d, J = 9.5 Hz, 1H), 8.66 (d, J = 7.0 Hz, 2H), 8.75 (d, J = 8.0 Hz, 1H), 10.17 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 121.4, 122.9, 124.9, 127.4, 128.0, 128.4, 128.5, 128.6, 130.1, 130.3, 130.5, 135.5,

138.2, 150.7, 158.6, 161.0. HRMS (ESI-TOF) $C_{18}H_{12}N_2$, $[M+H]^+$ *m/z* 257.1073; Found 257.1074.



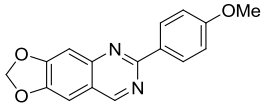
6-m-tolyl-[1,3]dioxolo[4,5-g]quinazoline (2s)

White solid. mp:157-159 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.47 (s, 3H), 6.14 (s, 2H), 7.09 (s, 1H), 7.29 (d, *J* = 7.5 Hz, 1H), 7.33 (s, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 8.32 (d, *J* = 8.5 Hz, 1H), 8.35 (s, 1H), 9.15 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 21.5, 101.8, 102.1, 104.9, 120.7, 125.3, 128.5, 128.7, 131.0, 138.1, 138.2, 148.2, 150.3, 154.1, 157.4, 160.2. HRMS (ESI-TOF) Calcd for $C_{16}H_{12}N_2O_2$, $[M+H]^+$ *m/z* 265.0972; Found 265.0974.



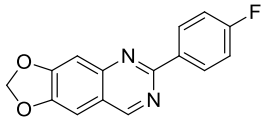
6-*p*-tolyl-[1,3]dioxolo[4,5-g]quinazoline (2t)

White solid. mp:182-184 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.42(s, 3H), 6.10 (s, 2H), 7.05 (s, 1H) 7.30 (d, *J* = 8.0 Hz, 3H), 8.42 (d, *J* = 8.0 Hz, 2H), 9.11 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): 21.4, 101.8, 102.1, 104.8, 120.5, 128.0, 129.3, 135.4, 140.3, 148.0, 150.2, 154.0, 157.3, 160.0. HRMS (ESI-TOF) calcd for $C_{16}H_{12}N_2O_2$, $[M+1]^+$ *m/z* 265.0972, found: 265.0978.



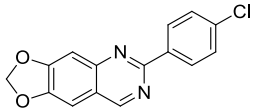
6-(4-methoxyphenyl)-[1,3]dioxolo[4,5-g]quinazoline(2u)

White solid. mp:193-195 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.87 (s, 3H), 6.12 (s, 2H), 7.00 (d, *J* = 8.5 Hz, 2H), 7.07 (s, 1H), 7.28 (s, 1H), 8.47 (d, *J* = 9.0 Hz, 2H), 9.10 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 55.3, 101.8, 102.1, 104.7, 113.8, 120.3, 129.7, 130.8, 147.9, 150.2, 154.0, 157.4, 159.8, 161.4. HRMS (ESI-TOF) Calcd for $C_{16}H_{12}N_2O_3$, $[M+H]^+$ *m/z* 281.0921; Found 281.0929.



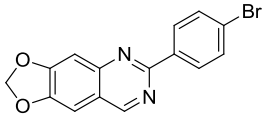
6-(4-fluorophenyl)-[1,3]dioxolo[4,5-g]quinazoline (2v)

White solid. mp:149-151 ºC; ^{1}H NMR (500 MHz; CDCl3): δ = 6.17 (s, 2H), 7.12 (s, 1H), 7.19 (t, J = 8.5 Hz, 2H), 7.32 (s, 1H), 8.53-8.56 (m, 2H), 9.15 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 101.8, 102.2, 104.9, 115.3, 115.5, 120.6, 130.1, 130.2, 134.3, 148.3, 150.2, 154.2, 157.5, 159.1, 163.4, 165.4. HRMS (ESI-TOF) Calcd for $C_{15}H_9FN_2O_2$, $[M+H]^+$ *m/z* 269.0721; Found 269.0731.



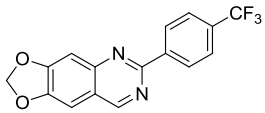
6-(4-chlorophenyl)-[1,3]dioxolo[4,5-g]quinazoline (2w)

White solid. mp:212-214 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 6.17 (s, 2H), 7.12, (s, 1H), 7.32 (s, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 8.49 (d, *J* = 8.0 Hz, 2H), 9.15 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 102.1, 102.5, 105.0, 109.9, 121.0, 128.9, 129.7, 136.4, 136.9, 148.6, 150.4, 157.7. HRMS (ESI-TOF) Calcd for $C_{15}H_9ClN_2O_2$, $[M+H]^+$ *m/z* 285.0425; Found 285.0434.



6-(4-bromophenyl)-[1,3]dioxolo[4,5-g]quinazoline (2x)

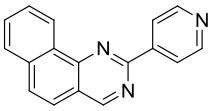
White solid. mp:142-144 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 6.18, (s, 2H), 7.12 (s, 1H), 7.32 (s, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 8.42 (d, *J* = 9.0 Hz, 2H), 9.15 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 101.9, 102.3, 104.9, 120.8, 124.9, 129.8, 131.7, 137.1, 148.5, 150.2, 154.3, 157.5, 159.1. HRMS (ESI-TOF) Calcd for $C_{15}H_9BrN_2O_2$, $[M+H]^+$ *m/z* 328.9920; Found 328.9929.



6-(4-(trifluoromethyl)phenyl)-[1,3]dioxolo[4,5-g]quinazoline (2y)

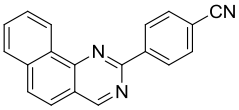
White solid. mp:77-78 ºC; ^{1}H NMR (500 MHz; CDCl3): δ = 6.19 (s, 2H), 7.15, (s, 1H), 7.35 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 8.66 (d, *J* = 8.0 Hz, 2H), 9.18 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 101.8, 102.3, 105.0, 121.1, 125.4, 125.4, 128.4, 141.4, 148.7, 150.2, 154.4, 157.5, 158.5. HRMS (ESI-TOF) Calcd for $C_{16}H_9F_3N_2O_2$, $[M+H]^+$ *m/z* 319.0689,

Found 319.0686.



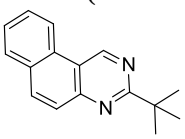
2-(pyridin-4-yl)benzo[h]quinazoline (2z)

White solid. mp:165-167 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 7.77 (d, J = 8.5 Hz, 1H), 7.82-7.85 (m, 2H), 7.92 (d, J = 8.5 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 8.57-8.58 (m, 2H), 8.85 (d, J = 4.5 Hz, 2H), 9.41 (t, J = 4.5 Hz, 1H), 9.43 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 122.3, 122.7, 124.8, 127.7, 128.1, 129.6, 130.0, 130.5, 135.5, 145.4, 150.5, 150.7, 158.8, 158.9. HRMS (ESI-TOF) Calcd for $C_{17}H_{11}N_3$, C17H11N3[M+H]$^+$ *m/z* 258.1026, Found 258.1032.



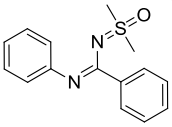
4-(benzo[h]quinazolin-2-yl)benzonitrile (2aa)

White solid. mp:215-217 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 7.76 (d, J = 9.0 Hz, 1H), 7.82-7.84 (m, 4H), 7.91 (d, J = 9.0 Hz, 1H), 7.96-7.97 (m, 1H), 8.85 (d, J = 8.5 Hz, 2H), 9.38-9.40 (m, 1H), 9.42 (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 113.7, 119.0, 121.9, 122.8, 124.8, 127.7, 128.2, 128.9, 129.5, 130.1, 130.5, 132.4, 135.5, 142.3, 150.7, 158.7, 159.0. HRMS (ESI-TOF) Calcd for $C_{19}H_{11}N_3$, [M+H]$^+$ *m/z* 282.1026, Found 282.1033.



3-*tert*-butylbenzo[f]quinazoline (2ab)

White solid. mp:141-144 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.54 (s, 9H), 7.67 (d, J = 7.5 Hz, 1H), 7.73 (d, J = 7.5 Hz, 1H), 7.86 (d, J = 9.5 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 8.12 (d, J = 9.0 Hz, 1H), 8.68 (d, J = 8.5 Hz, 1H), 10.05, (s, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 29.8, 39.5, 119.2, 121.6, 127.0, 127.4, 127.6, 128.1, 128.7, 128.9, 131.5, 135.1, 151.6, 154.0. HRMS (ESI-TOF) Calcd for $C_{16}H_{16}N_2$, [M+H]$^+$ *m/z* 236.1386; Found 236.1387.

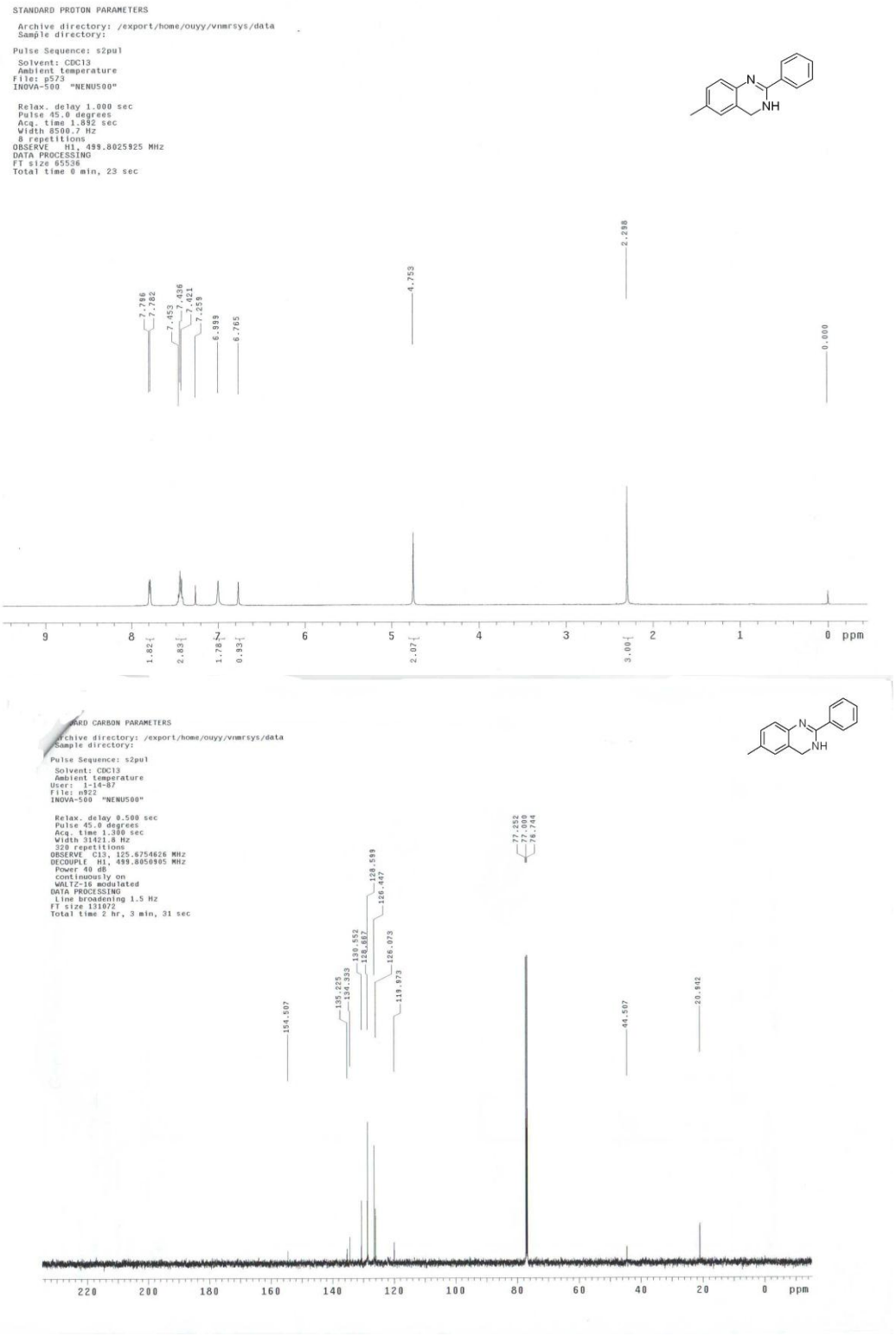


sulfoxyimine (3)

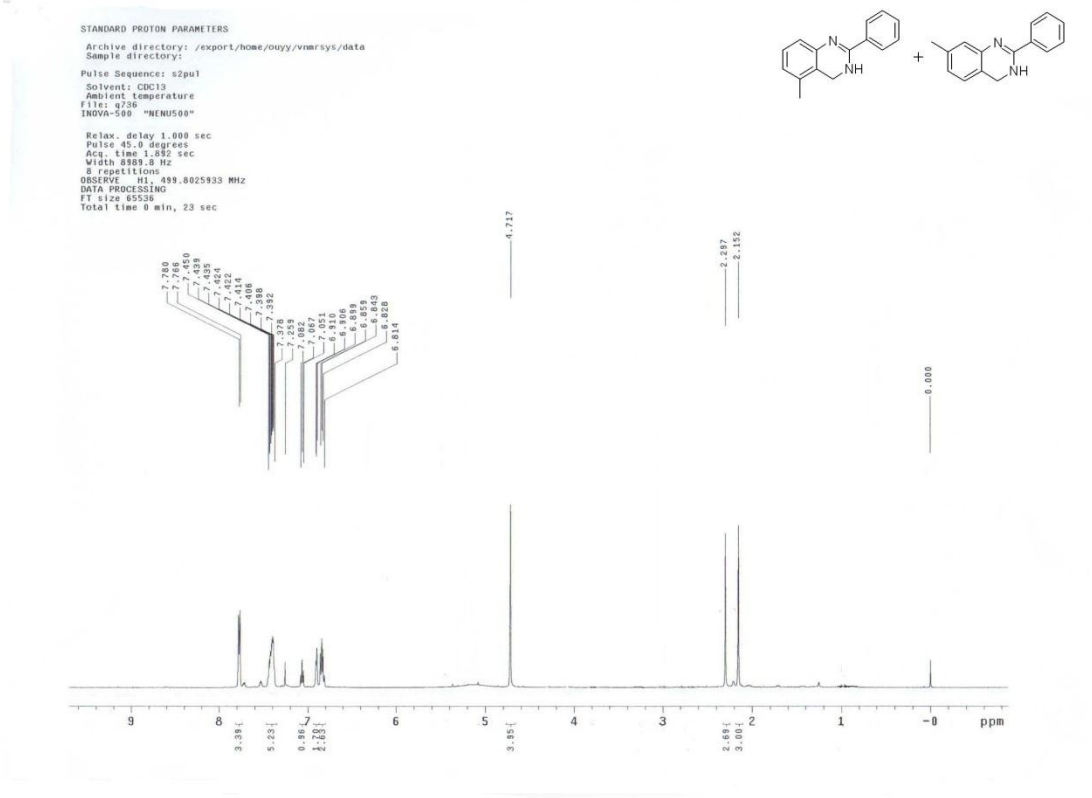
Yellow solid. mp:140-142 ºC; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.43 (s, 6H), 6.67 (d, J = 7.5 Hz, 2H), 6.89 (d, J = 7.5 Hz, 1H), 7.11 (t, J = 7.5 Hz, 2H), 7.17 (t, J = 7.5 Hz, 2H), 7.21 (d, J = 7.0 Hz, 1H), 7.32 (d, J = 7.0 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 41.5, 122.0, 122.1, 127.7, 128.5, 129.0, 129.4, 135.3, 150.0, 160.4. HRMS (ESI-TOF) Calcd for $C_{15}H_{16}N_2OS$, [M+H]$^+$ *m/z* 273.1056; Found 273.1064.

VI. ^{1}H and ^{13}C Spectra of New Compounds

Product 2a



Product 2b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Solvent: CDCl3
Ambient temperature
File: q736
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Relax. delay 1.000 sec
Pulse 45.0 degrees
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8 repetitions
OBSERVE H1, 499.8025933 MHz
DATA PROCESSING
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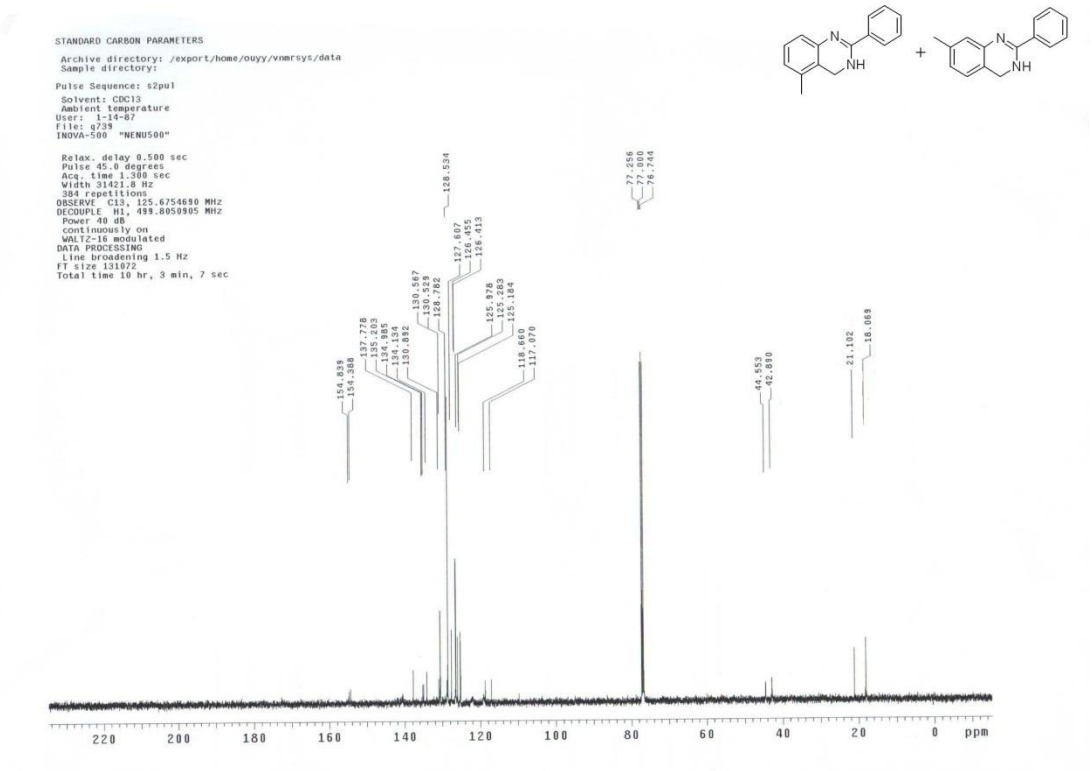
Total time 0 min, 23 sec
ppm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Sample directory:
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Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: q739
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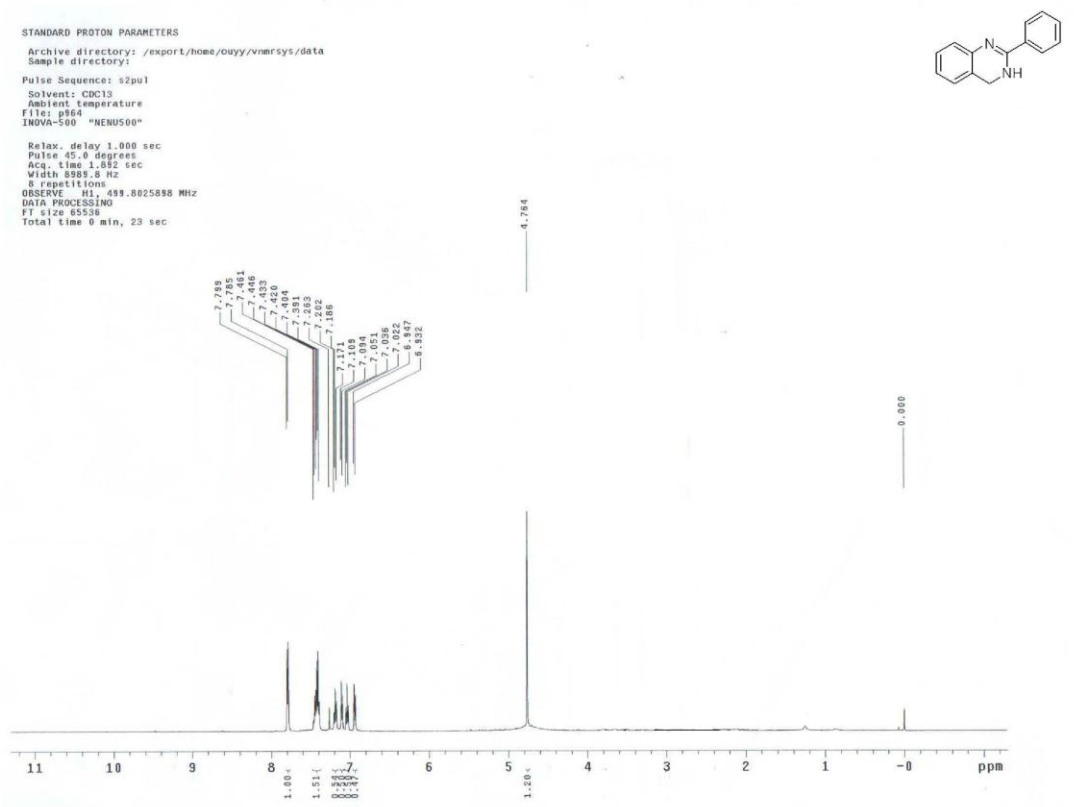
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
384 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 10 hr, 3 min, 7 sec
ppm

Product 2c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Solvent: CDCl3
Ambient temperature
File: p864
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Pulse 45.0 degrees
Acq. time 1.852 sec
Width 8989.8 Hz
8 repetitions
OBSERVE H1, 499.8825898 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
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7.446
7.433
7.420
7.404
7.381
7.283
7.282
7.186
7.178
7.108
7.094
7.051
7.038
7.022
6.947
6.932
4.764
0.000
11
10
9
8
7
6
5
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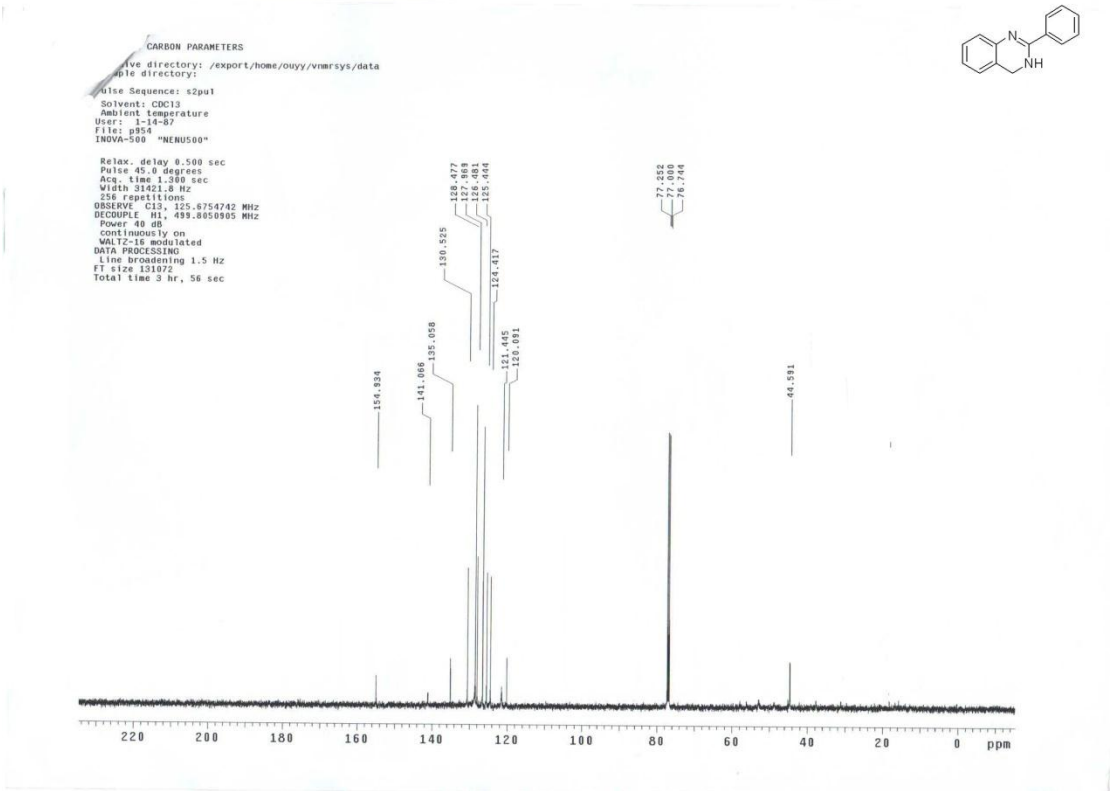
N
NH


CARBON PARAMETERS
ive directory: /export/home/ouyy/vnmrsys/data
ple directory:
ulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: p954
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754742 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
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127.681
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130.525
124.417
121.445
120.091
135.058
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154.934
77.432
77.000
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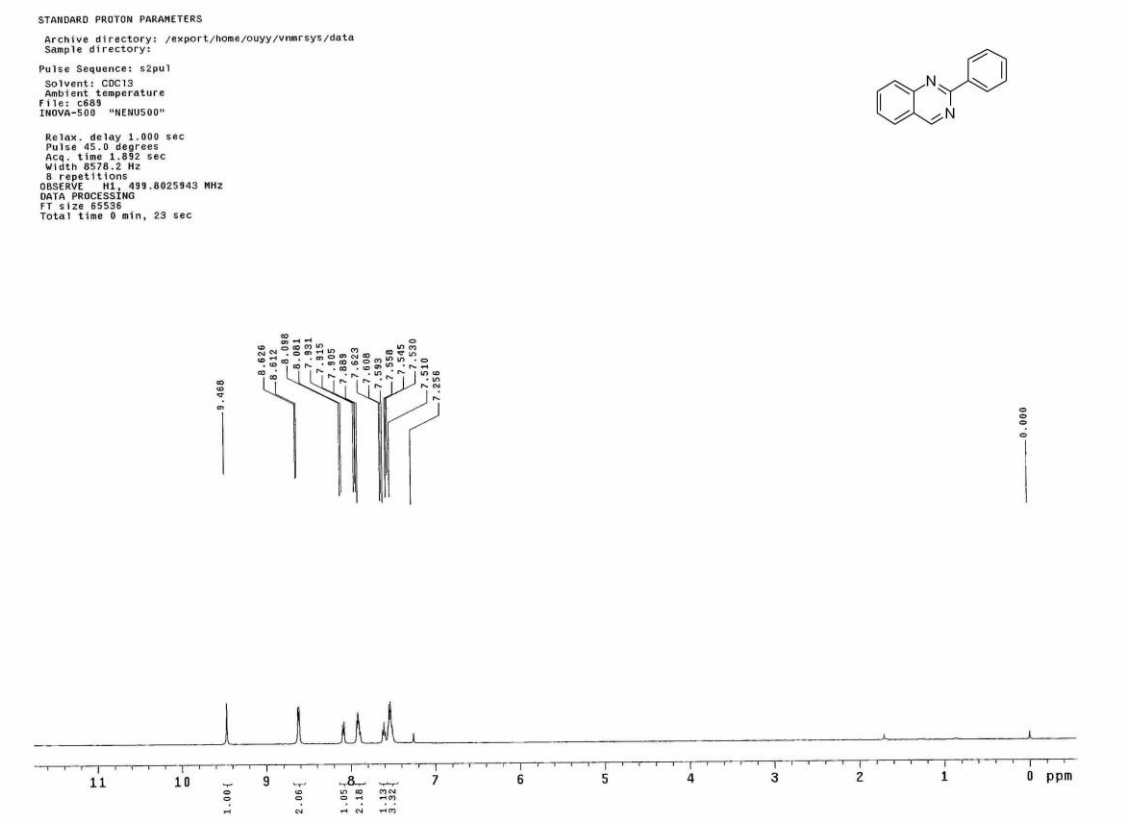
180
160
140
120
100
80
60
40
20
0
ppm
N
NH

Product 2c'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Solvent: CDCl3
Ambient temperature
File: c689
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Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025943 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.468
8.626
8.612
8.088
8.081
7.931
7.915
7.695
7.688
7.623
7.608
7.593
7.550
7.545
7.530
7.510
7.256
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11
10
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3
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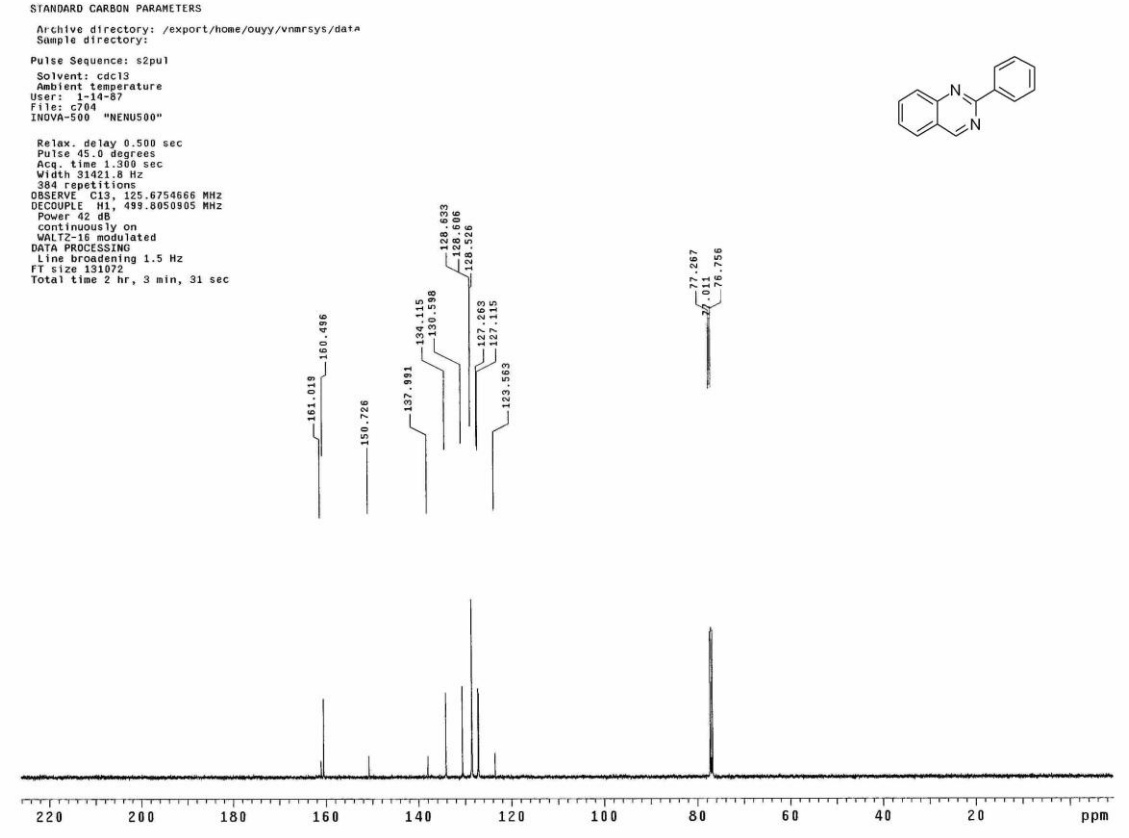
3.32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Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: c704
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
384 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
161.019
160.496
150.726
137.991
134.115
130.598
128.693
128.606
128.528
127.263
127.115
123.563
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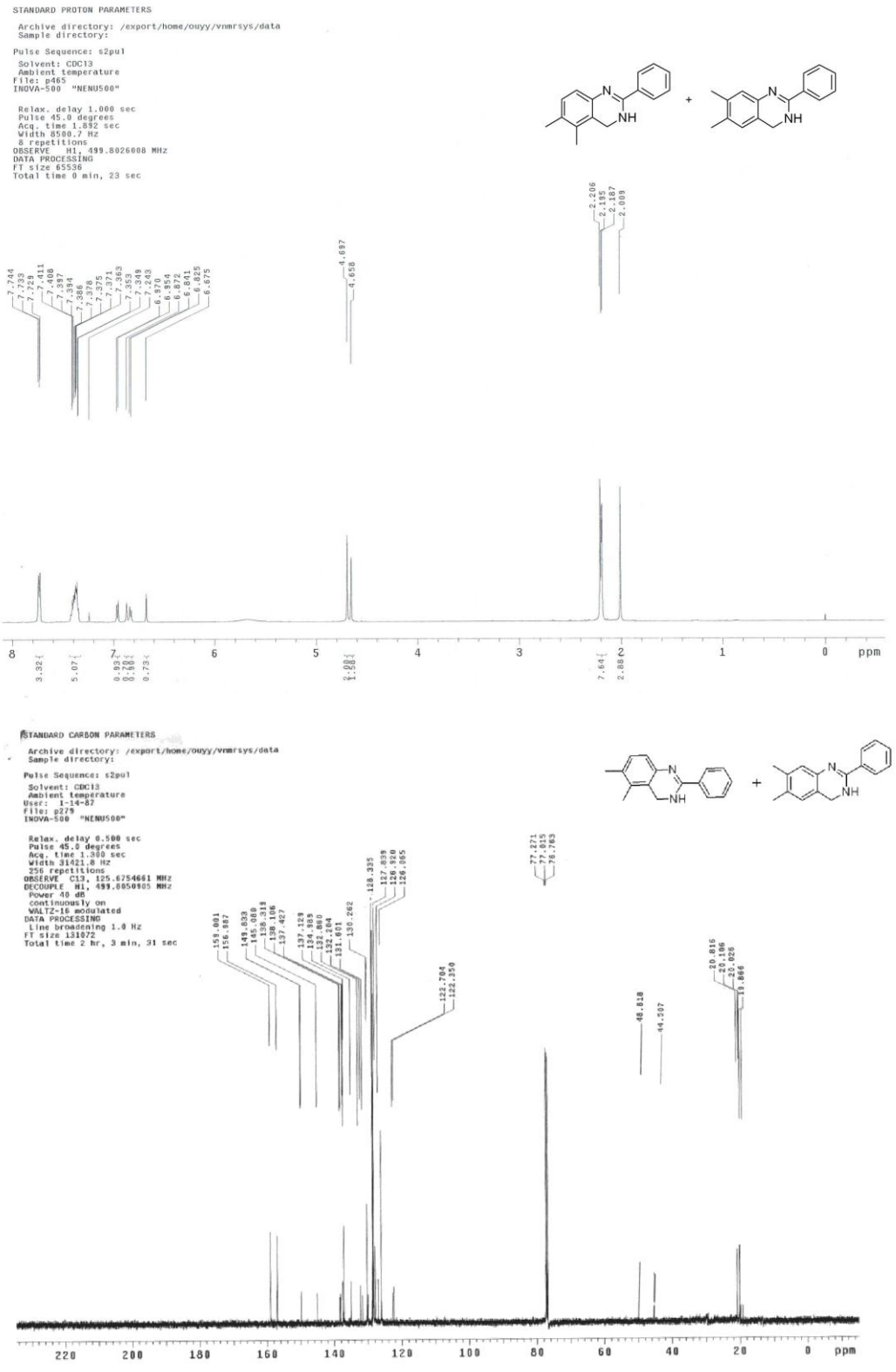
77.011
76.756
220
200
180
160
140
120
100
80
60
40
20
ppm

Product 2d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Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p465
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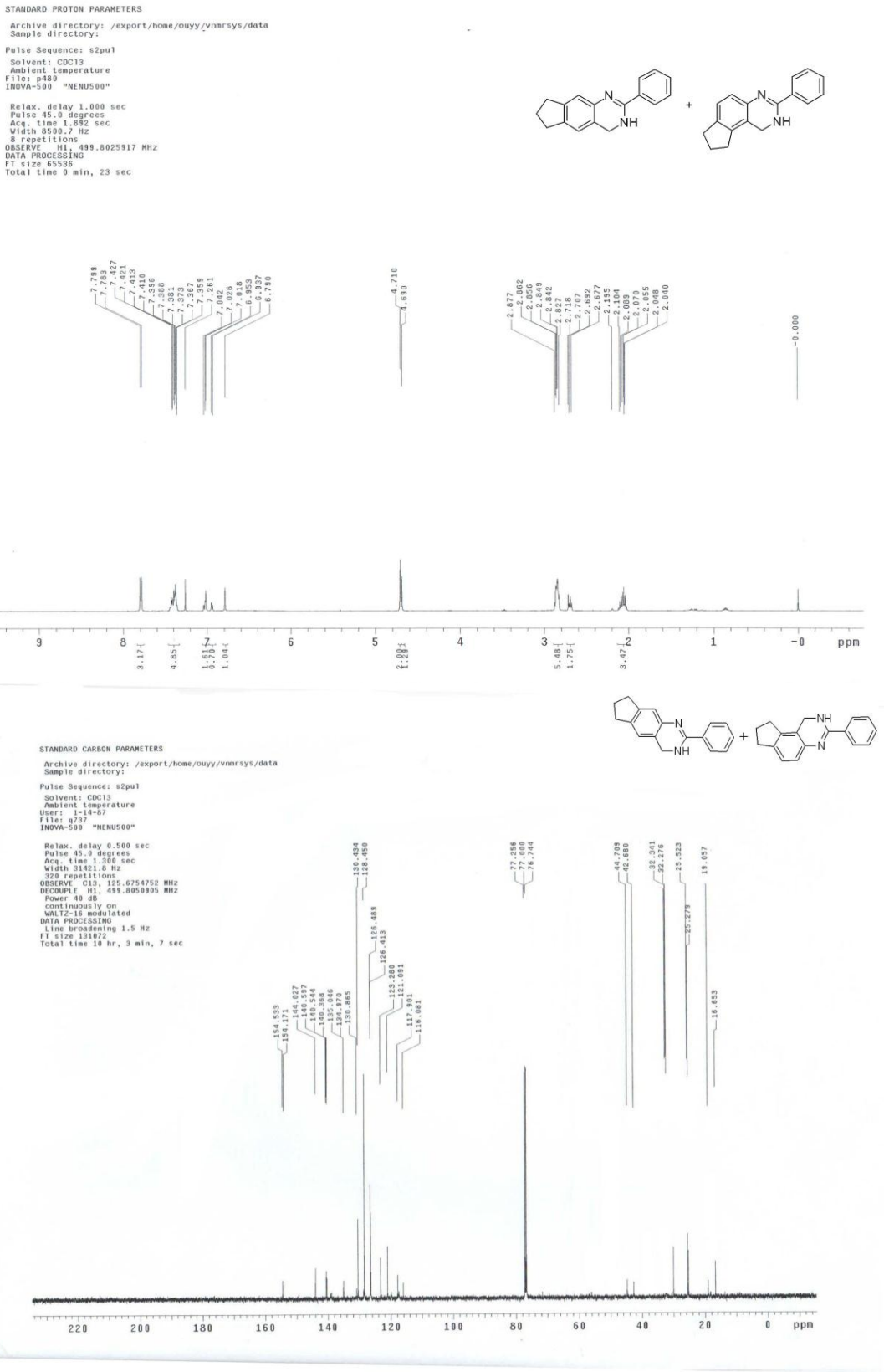
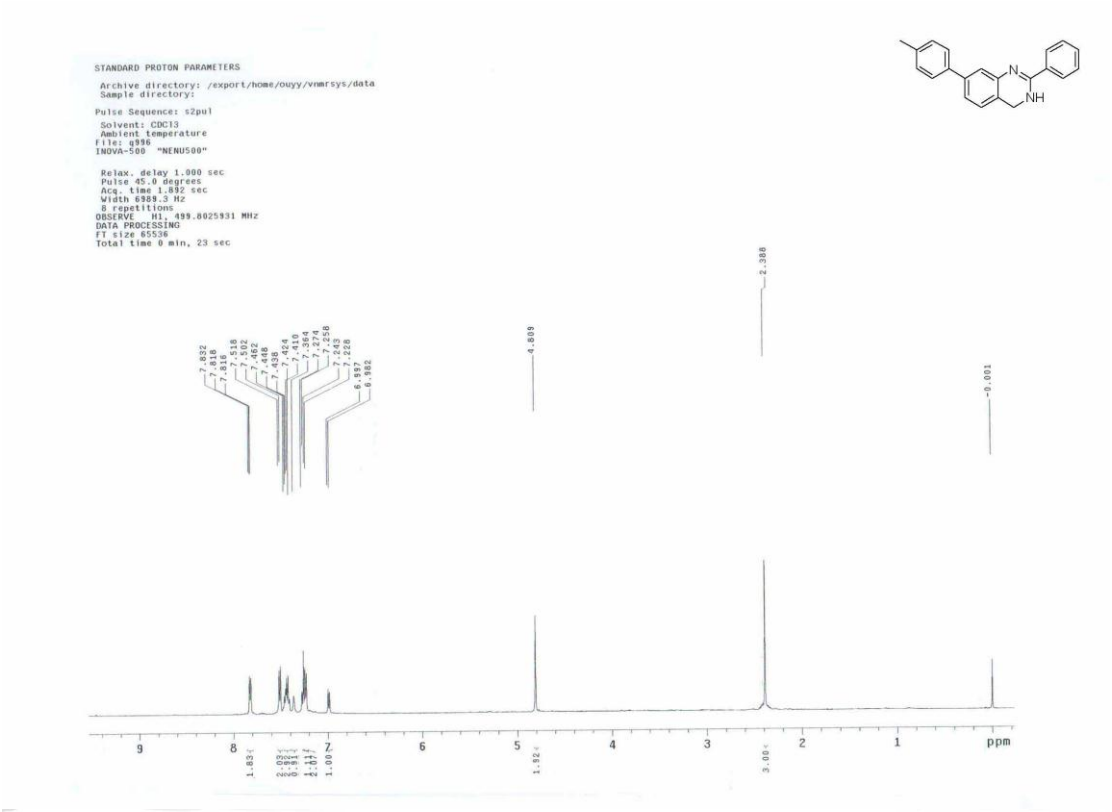
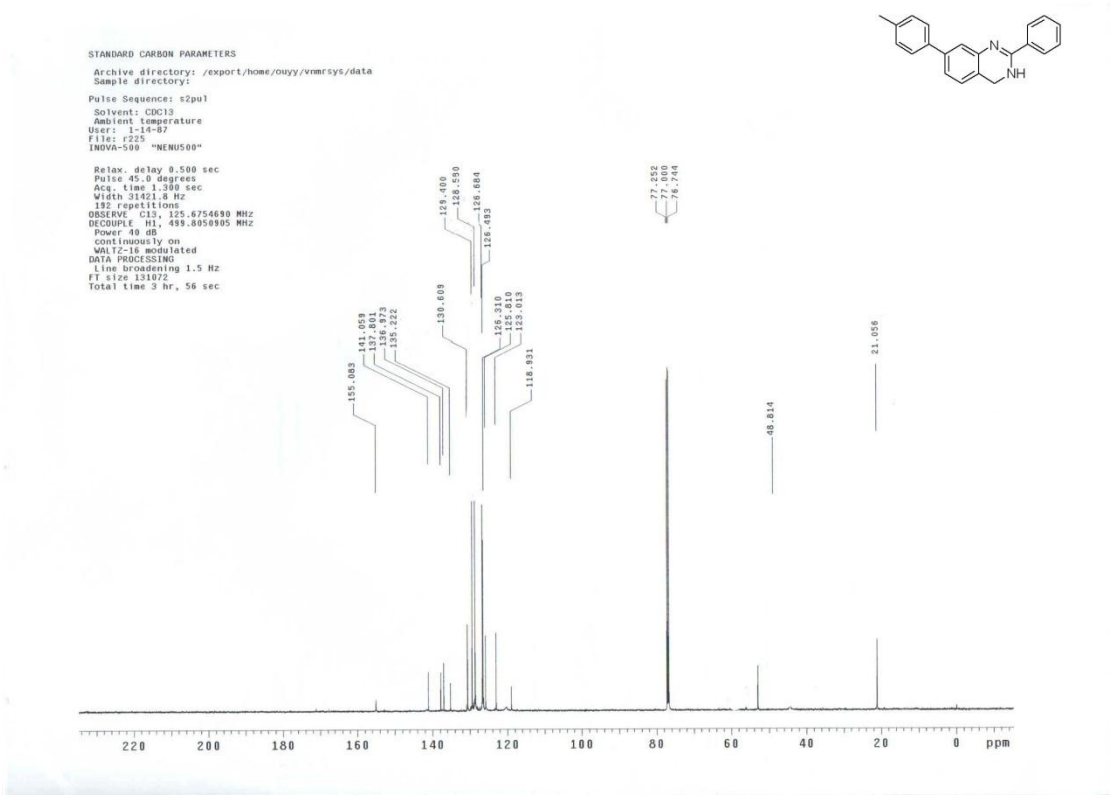
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8026008 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: p279
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
ppm

Product 2e

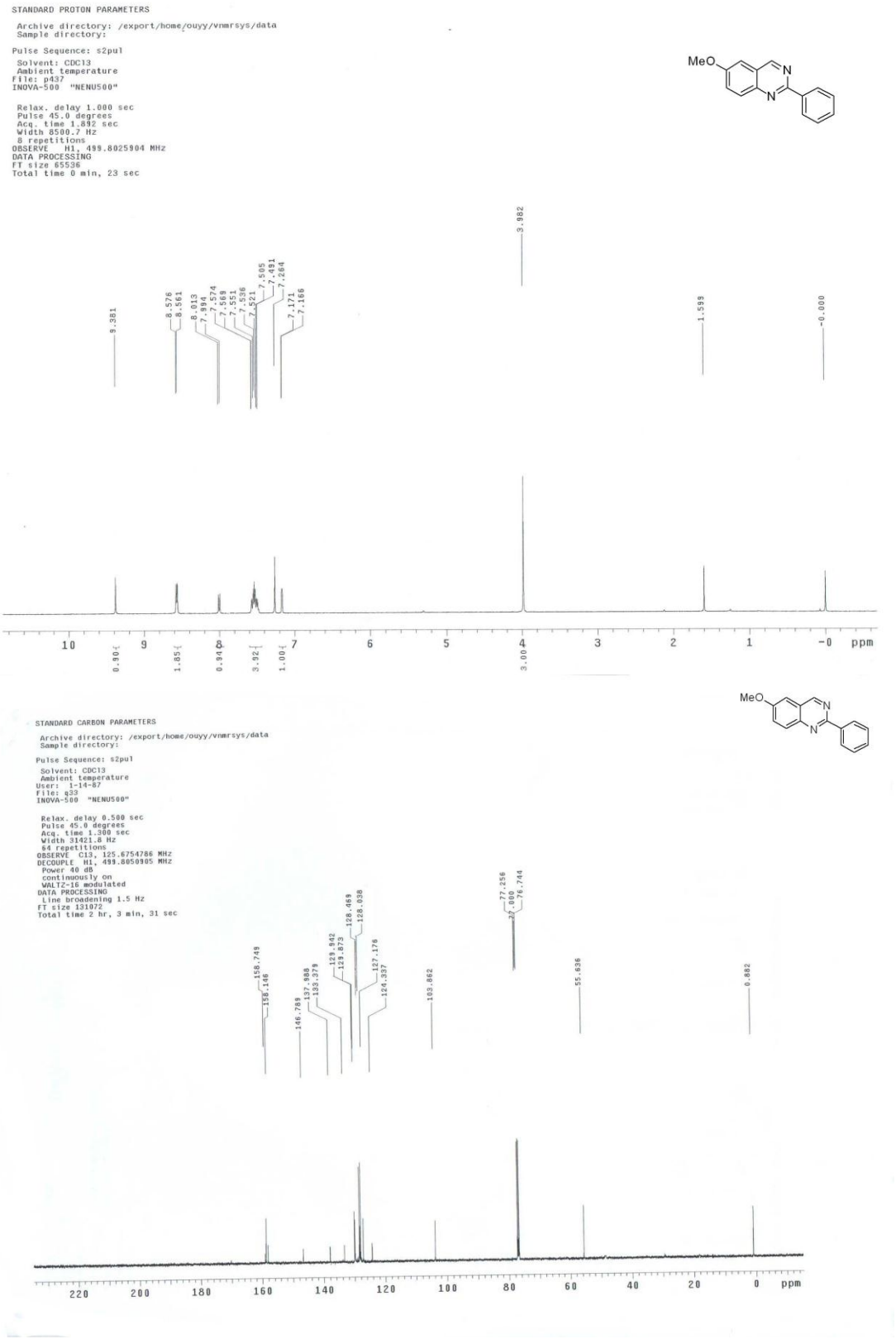

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p480
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.852 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025917 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: g737
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
320 repetitions
OBSERVE C13, 125.6754752 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 10 hr, 3 min, 7 sec
ppm

Product 2f

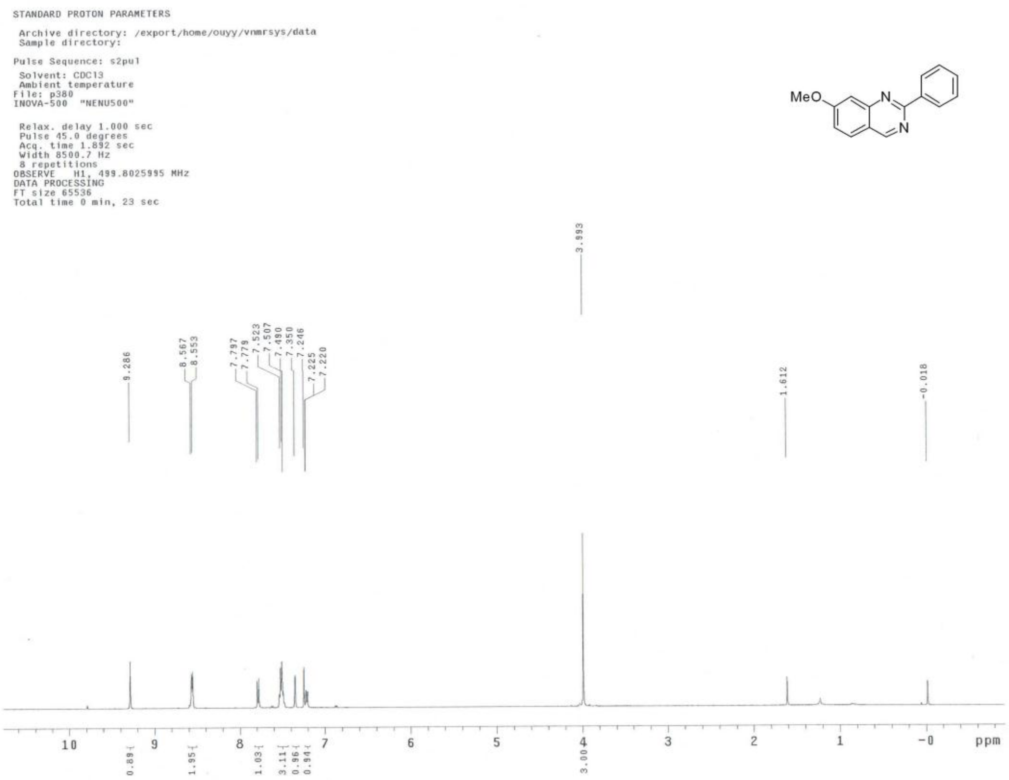

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g996
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 6988.3 Hz
8 repetitions
OBSERVE H1, 499.8025931 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.832
7.818
7.518
7.502
7.462
7.438
7.424
7.414
7.364
7.274
7.258
7.248
7.228
6.987
6.982
4.809
2.388
0.001
ppm

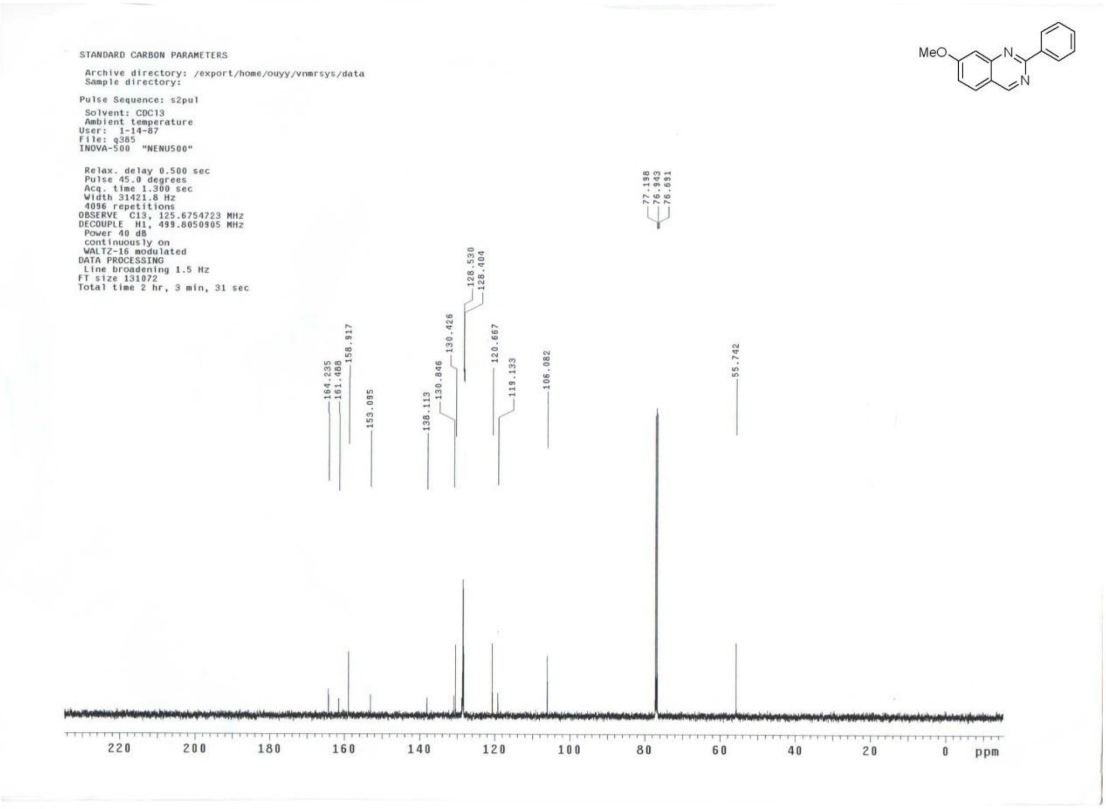

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: r225
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
155.083
141.059
137.801
136.973
135.222
130.609
129.400
128.590
128.084
128.493
126.310
125.610
123.013
118.931
77.252
77.000
76.744
48.814
21.056
ppm

Product 2k

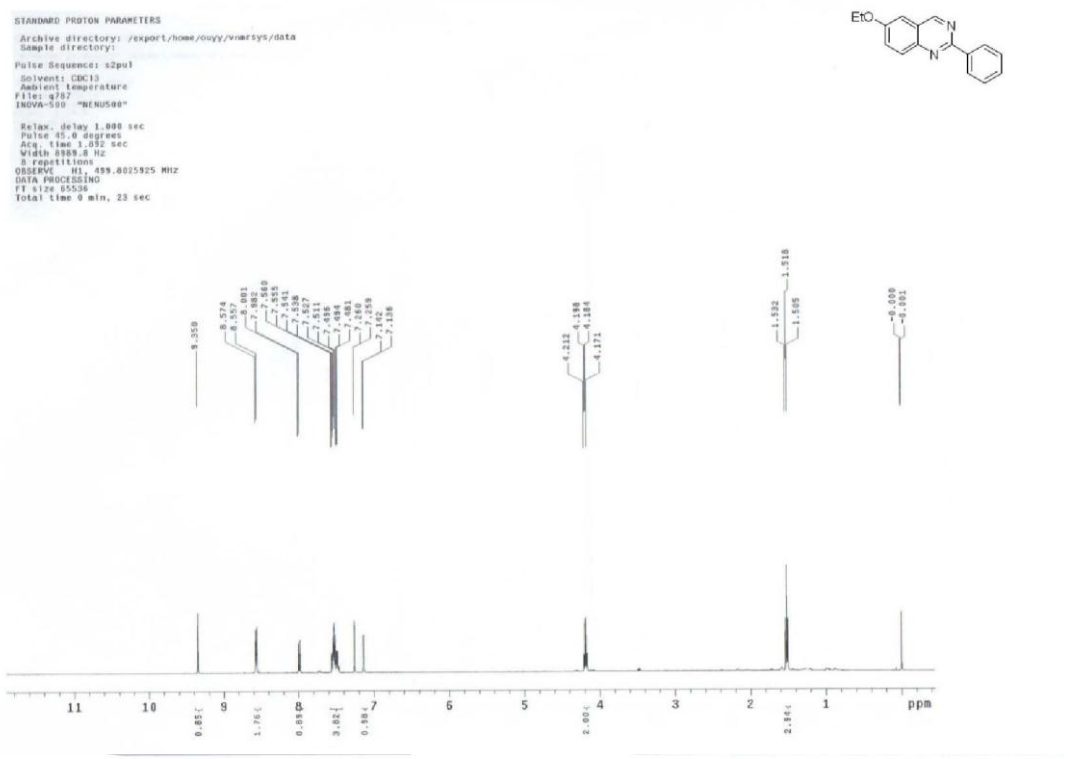

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p437
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025904 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
MeO
9.381
8.576
8.561
8.013
7.994
7.574
7.569
7.551
7.536
7.521
7.505
7.491
7.264
7.171
7.166
3.982
1.599
0.000
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.90
1.85
0.94
3.92
1.00
3.00
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: q33
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754786 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
MeO
158.749
156.140
146.789
137.988
133.379
129.942
129.873
128.469
128.038
127.176
124.357
103.862
77.256
77.000
76.744
55.636
0.882
220
200
180
160
140
120
100
80
60
40
20
0
ppm

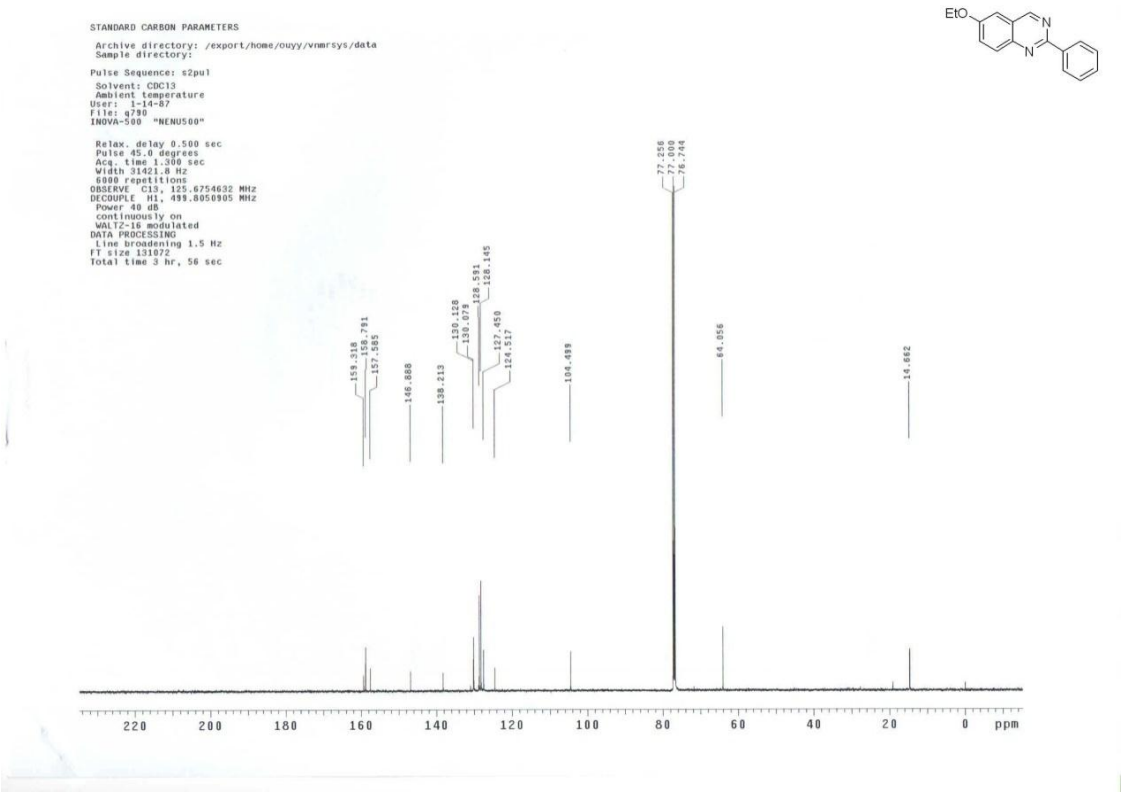
Product 2l


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p380
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025995 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
MeO
N
N
ppm

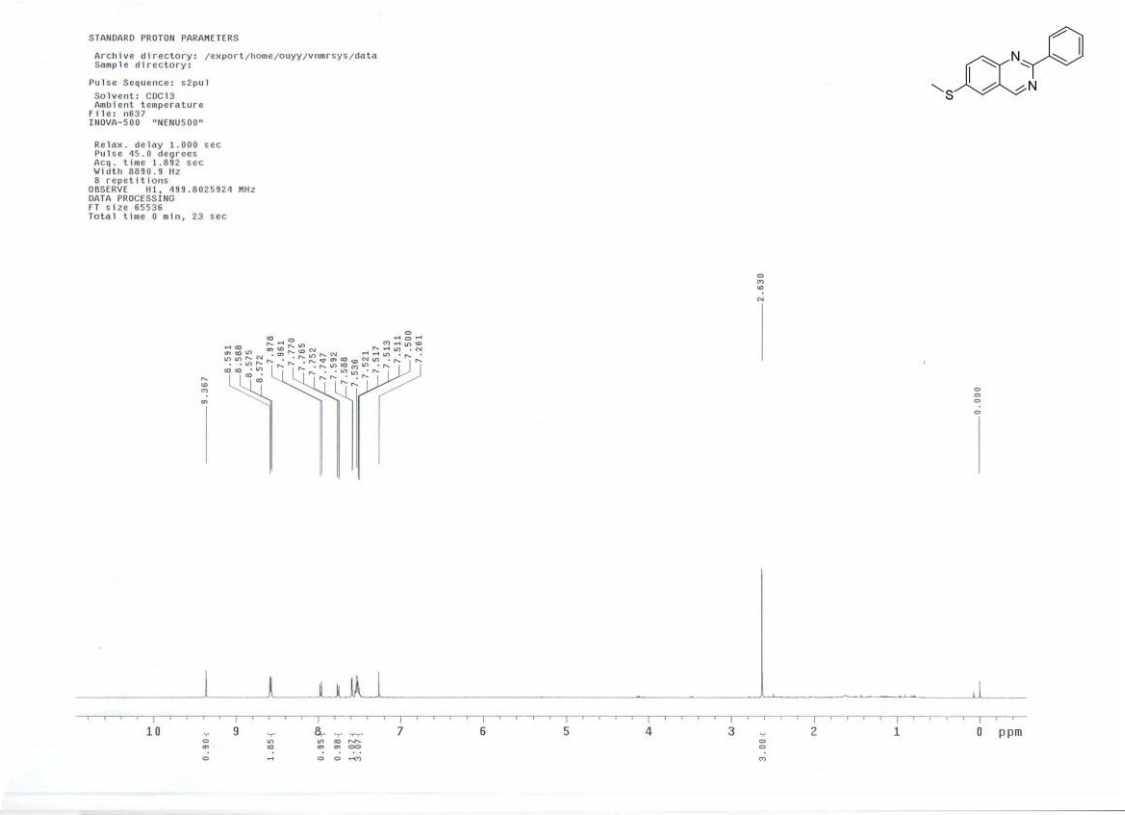

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: q385
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4096 repetitions
OBSERVE C13, 125.6754723 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
MeO
N
N
ppm

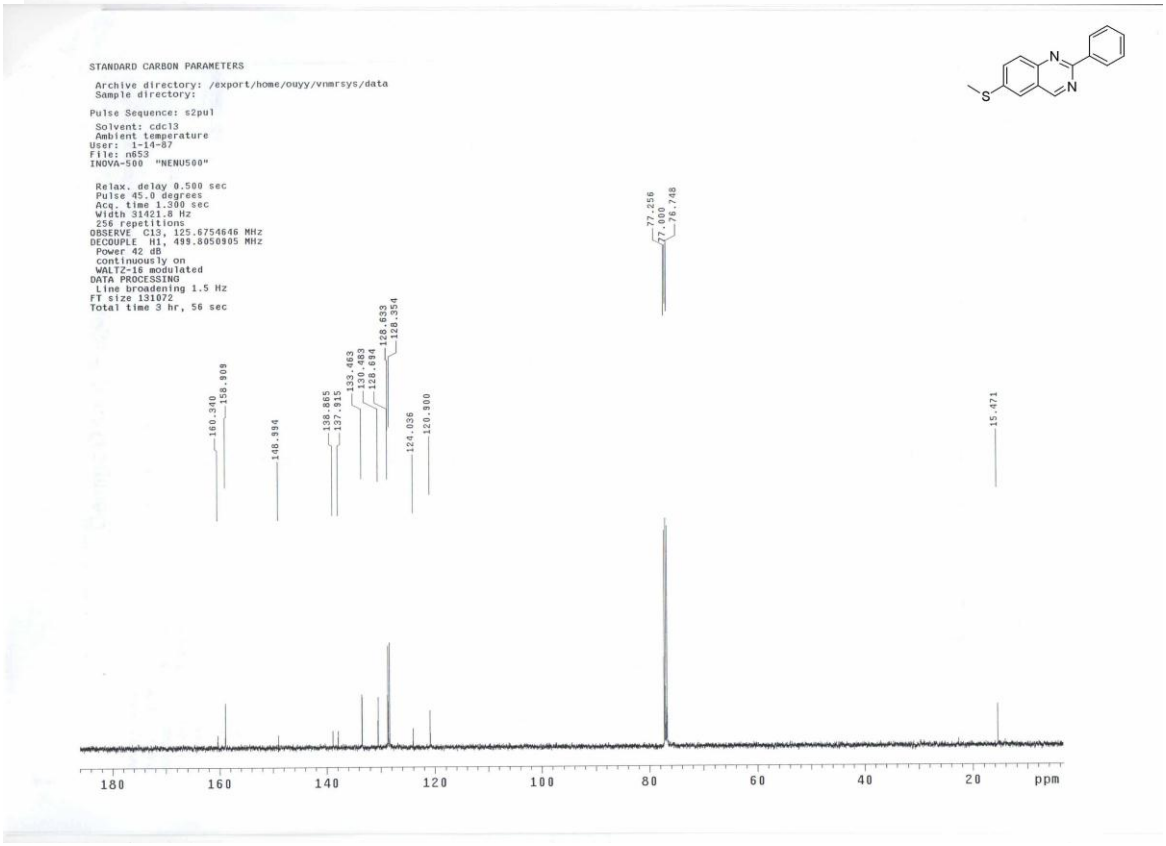
Product 2m


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: q787
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8989.8 Hz
8 repetitions
OBSERVE H1, 499.8025925 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
EtO
N
N
ppm

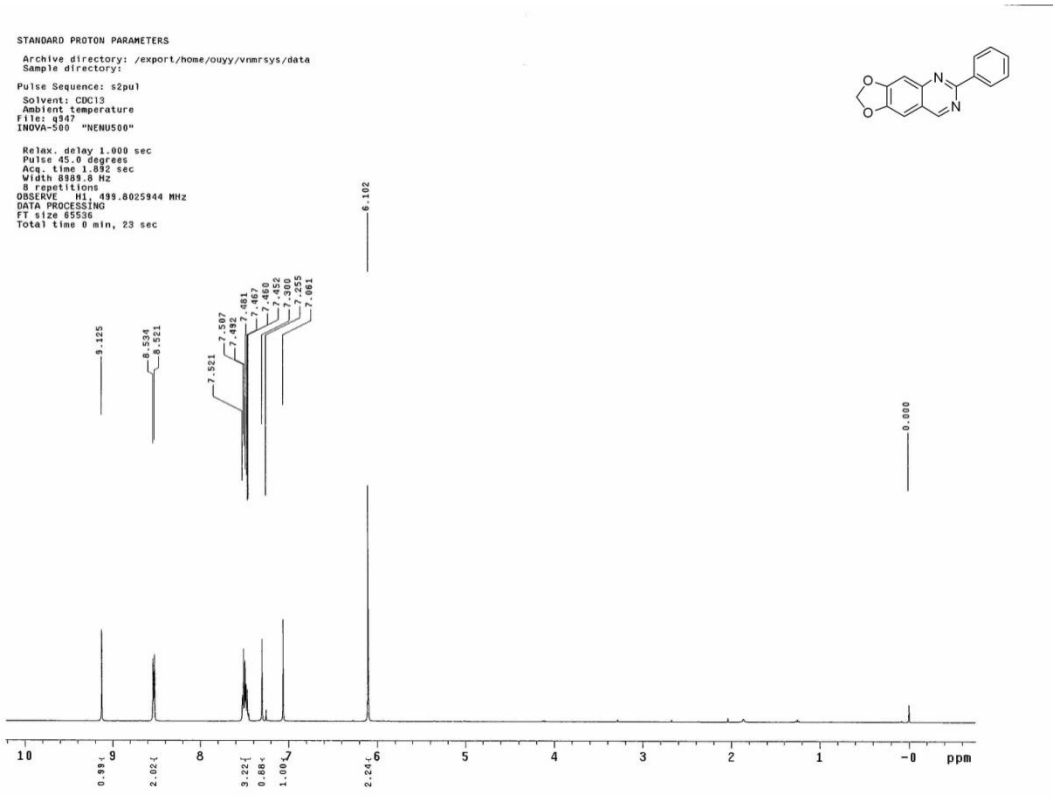

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: Y-14-87
File: q790
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
6000 repetitions
OBSERVE C13, 125.6754632 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
EtO
N
N
ppm

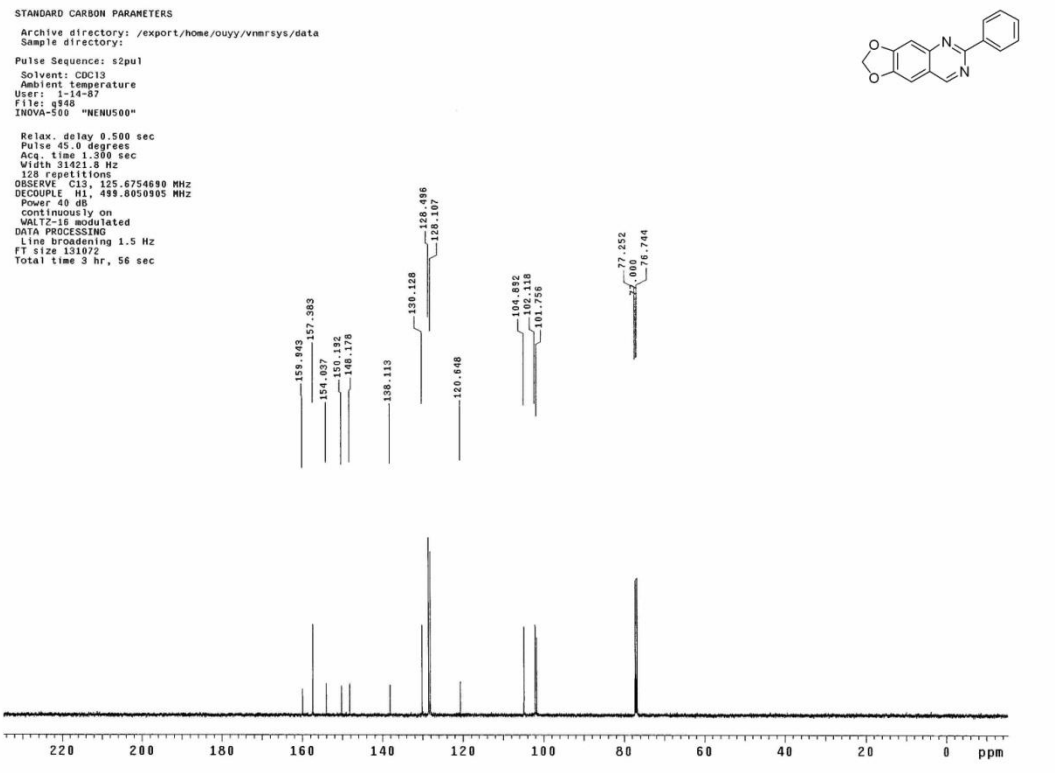
Product 2n


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: n837
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8850.9 Hz
8 repetitions
OBSERVE H1, 499.8025924 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.367
8.591
8.588
8.575
8.572
7.978
7.961
7.770
7.765
7.752
7.747
7.592
7.588
7.586
7.521
7.517
7.513
7.511
7.500
7.261
2.630
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm

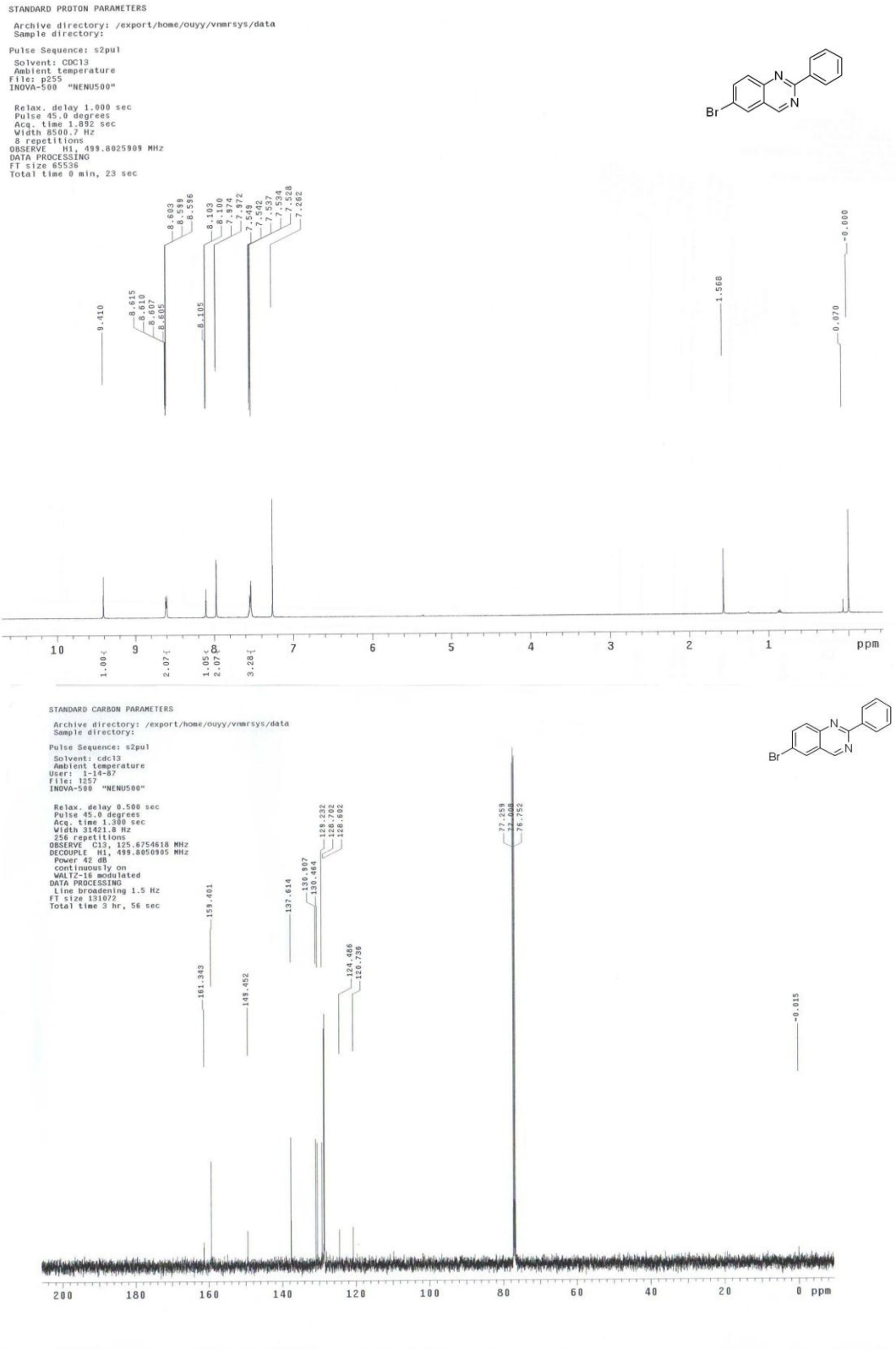

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: n653
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754646 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
160.340
158.909
148.394
138.865
137.915
133.463
130.483
128.694
128.633
128.354
124.036
120.900
77.256
77.000
76.748
15.471
180
160
140
120
100
80
60
40
20
ppm

Product 2o


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: q947
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8889.8 Hz
8 repetitions
OBSERVE H1, 499.8025944 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.125
8.534
8.521
7.587
7.492
7.481
7.467
7.460
7.452
7.300
7.255
7.081
7.521
6.102
0.000
ppm

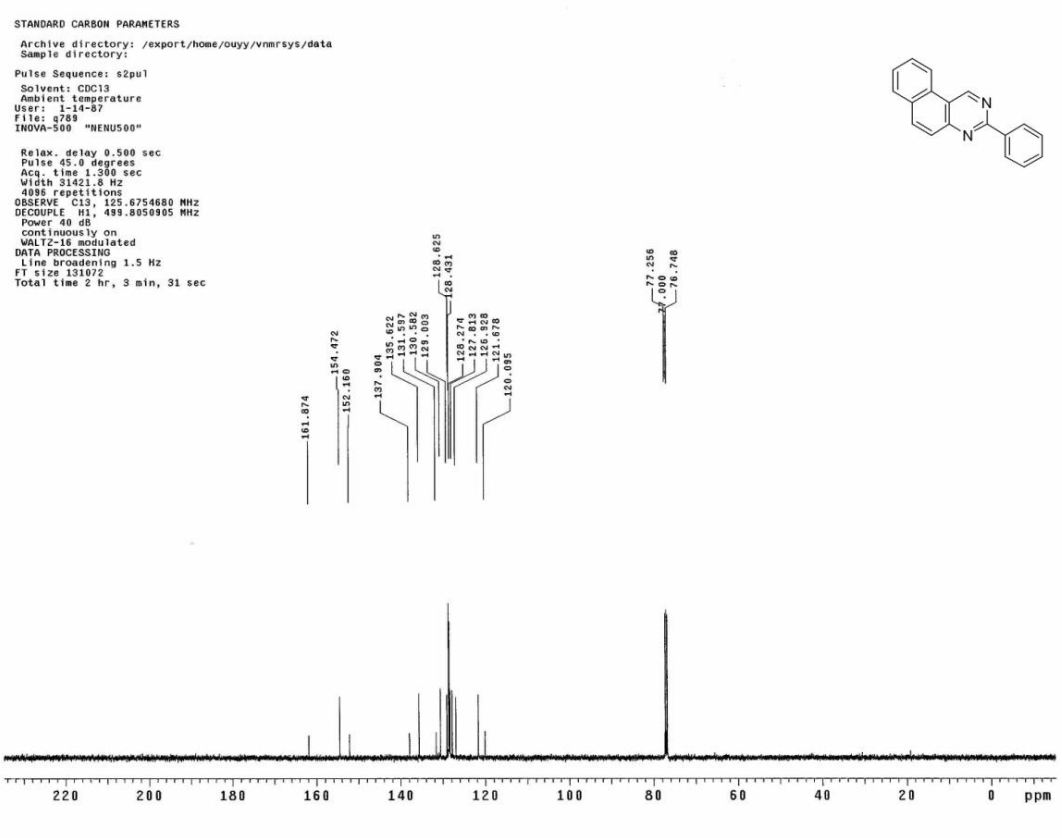

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: q948
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050305 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
159.943
157.303
154.837
151.192
148.178
138.113
130.128
128.496
128.107
120.648
104.892
102.118
101.756
77.252
77.000
76.744
ppm

Product 2p

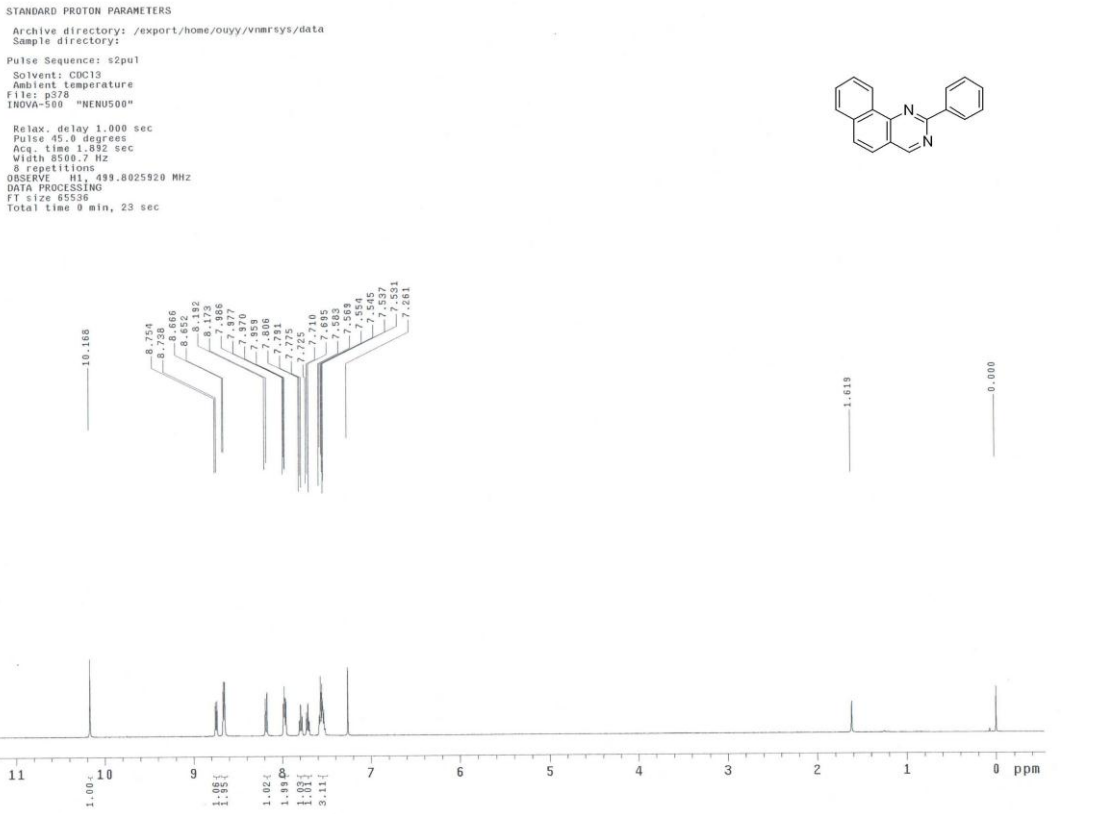

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p255
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025909 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.410
8.615
8.610
8.607
8.605
8.603
8.599
8.596
8.105
8.103
8.100
7.977
7.972
7.549
7.542
7.537
7.534
7.268
7.262
1.568
0.000
0.000
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1257
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754618 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
159.401
161.343
149.452
137.614
130.807
130.464
128.232
128.702
128.602
124.486
123.758
77.359
77.000
76.752
-0.015
ppm

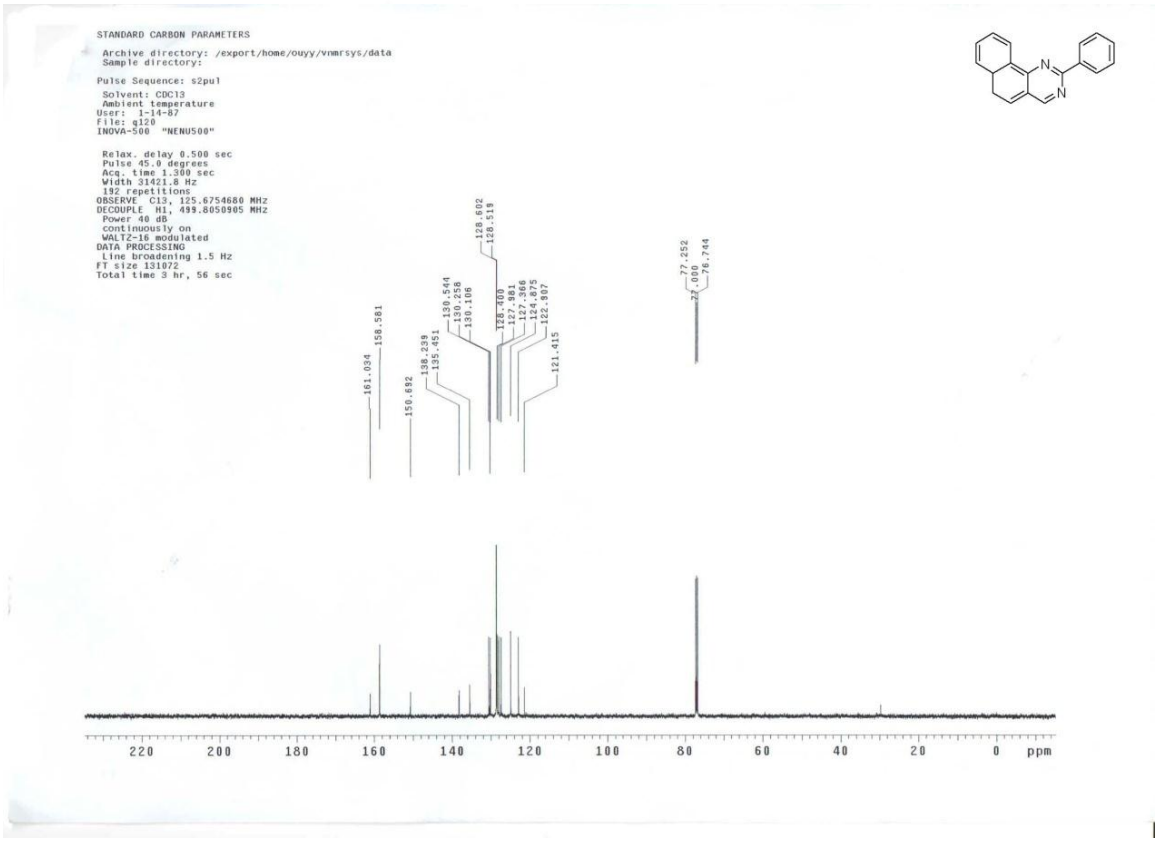
Product 2q


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p379
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025935 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.459
9.455
9.449
9.441
9.410
8.773
8.770
8.765
7.950
7.943
7.932
7.864
7.846
7.824
7.815
7.810
7.806
7.804
7.800
7.751
7.733
7.600
7.588
7.584
7.568
7.552
7.539
7.524
7.257
1.610
0.000
10
9
8
7
6
5
4
3
2
1
ppm

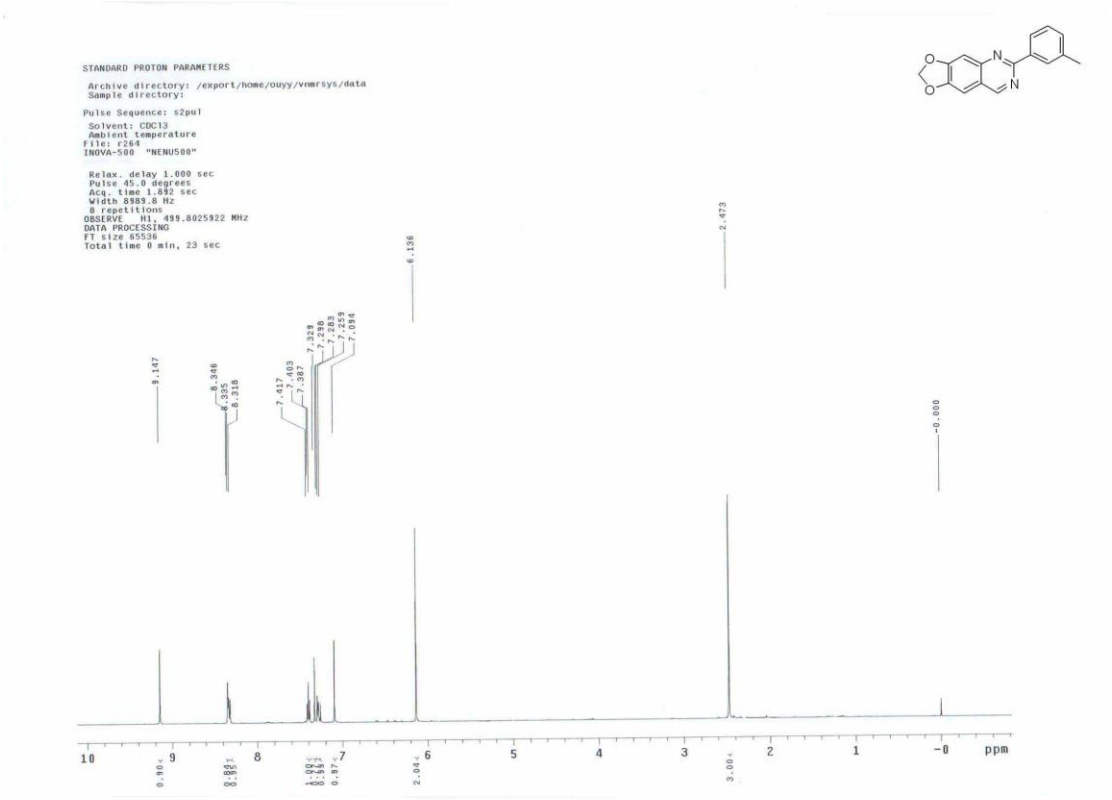

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: a789
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4096 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
161.874
154.472
152.160
137.904
135.622
131.597
130.082
129.003
128.625
128.431
128.274
127.813
126.838
121.678
120.095
77.256
77.000
76.748
220
200
180
160
140
120
100
80
60
40
20
0
ppm

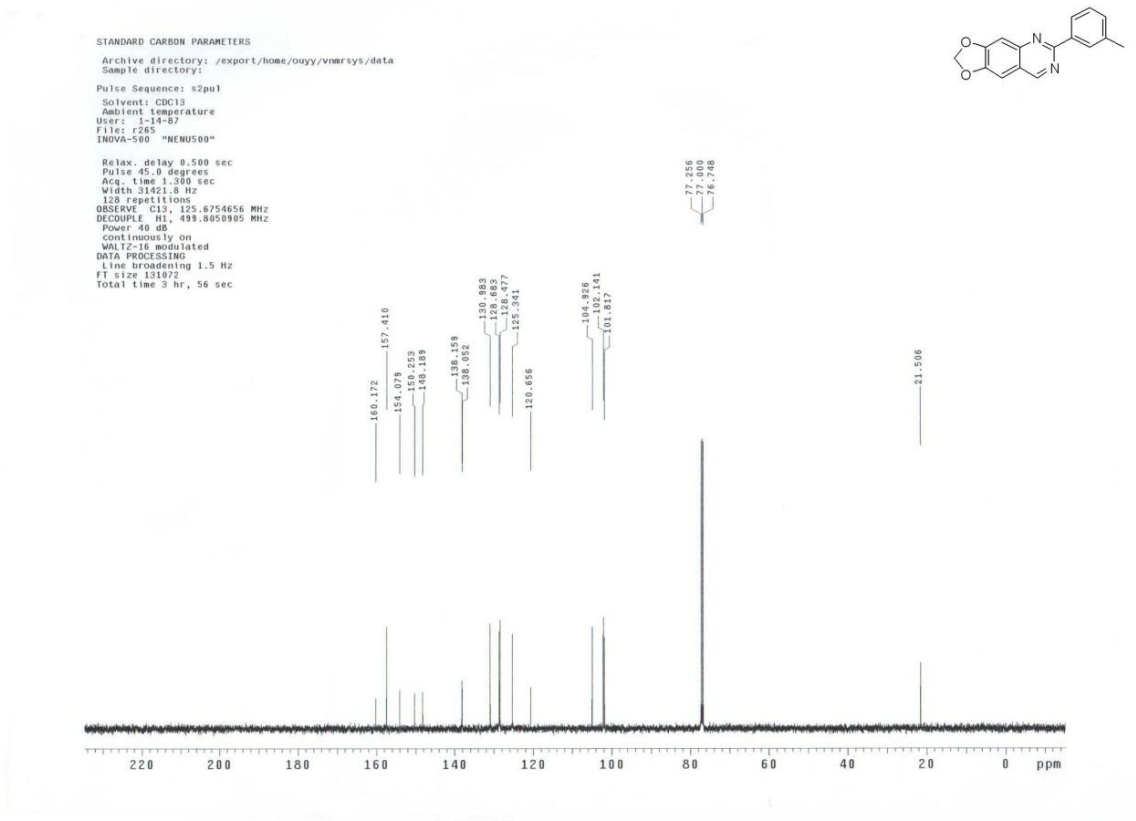
Product 2r


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p378
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025920 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
10.168
8.754
8.738
8.666
8.652
8.192
8.178
7.986
7.977
7.970
7.959
7.806
7.791
7.775
7.725
7.710
7.695
7.563
7.558
7.554
7.545
7.537
7.531
7.261
1.619
0.000
11
10
9
8
7
6
5
4
3
2
1
0 ppm

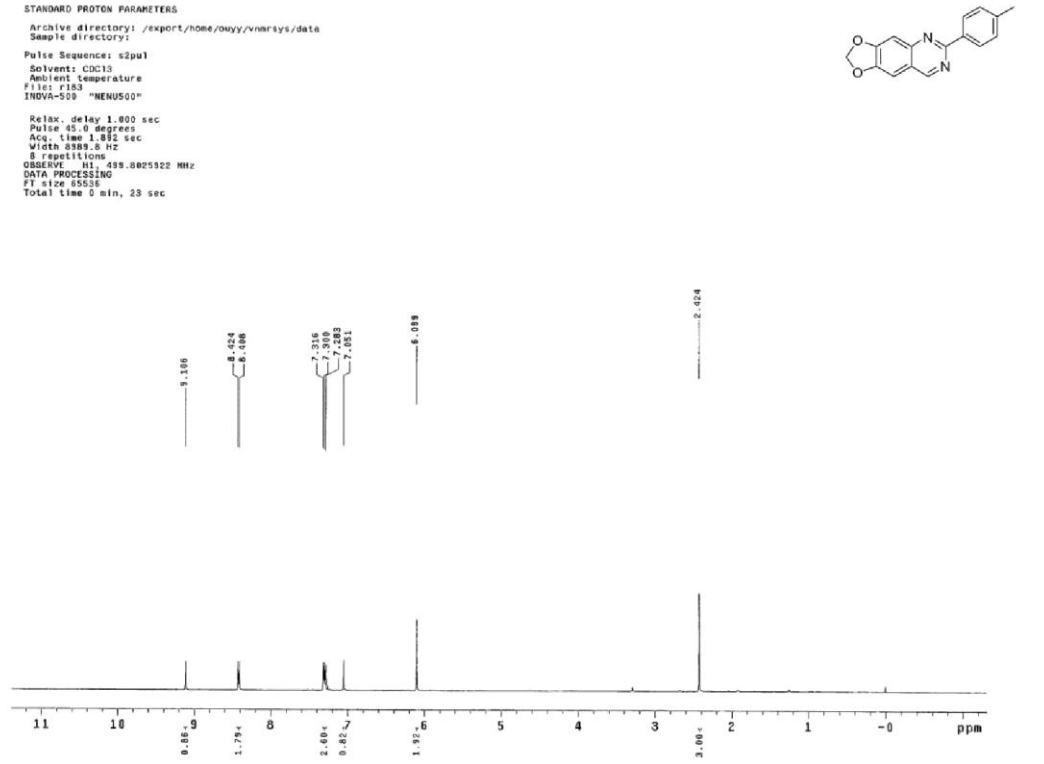

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: g120
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
161.034
158.581
150.692
138.239
135.451
130.544
130.258
130.168
128.602
128.519
128.060
127.981
127.368
124.875
122.907
121.415
77.252
77.000
76.744
220
200
180
160
140
120
100
80
60
40
20
0 ppm

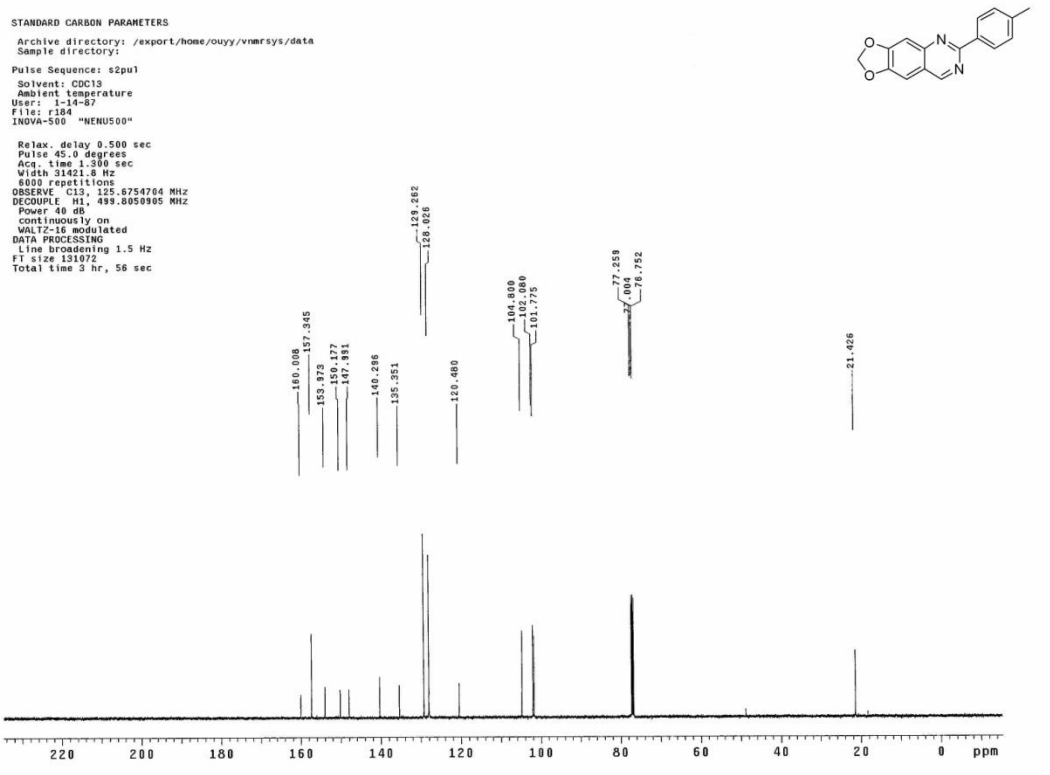
Product 2s


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r264
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8889.8 Hz
8 repetitions
OBSERVE H1, 499.8025922 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.147
8.346
8.335
8.318
7.417
7.403
7.387
7.328
7.286
7.283
7.259
7.094
6.136
2.473
0.000
ppm

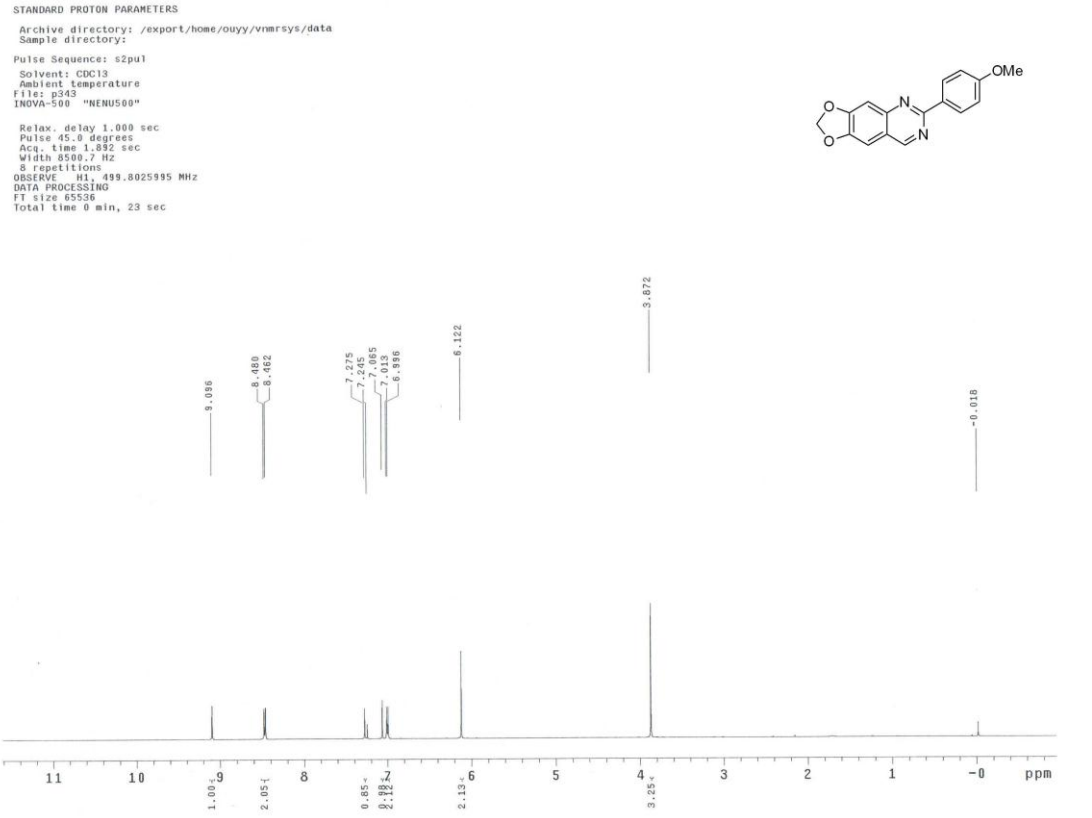

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: r265
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.256
77.000
76.748
160.172
157.410
154.079
150.253
148.189
138.159
138.052
130.983
128.683
128.477
125.341
120.656
104.926
102.141
101.817
21.506
ppm

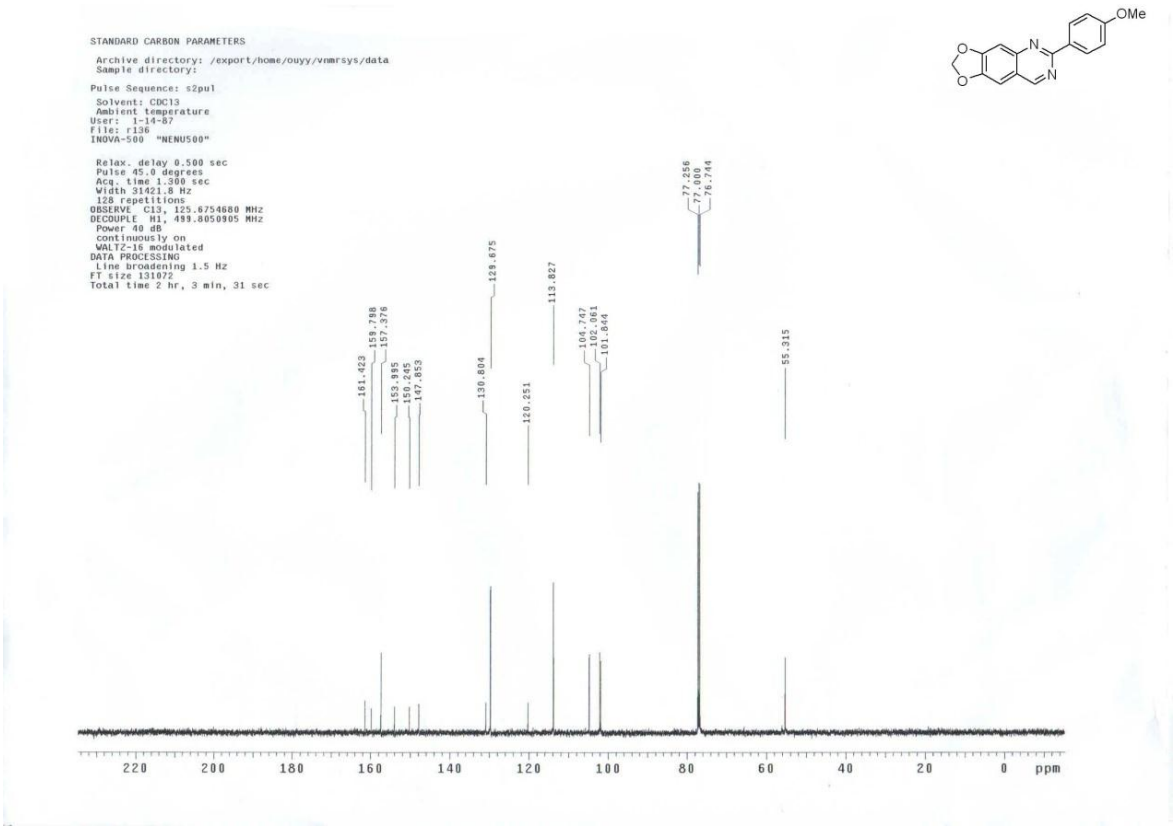
Product 2t


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r183
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.812 sec
Width 8389.8 Hz
8 repetitions
OBSERVE H1, 499.8025922 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.106
8.624
8.606
7.316
7.300
7.283
7.051
6.059
2.424
11
10
9
8
7
6
5
4
3
2
1
-0
ppm

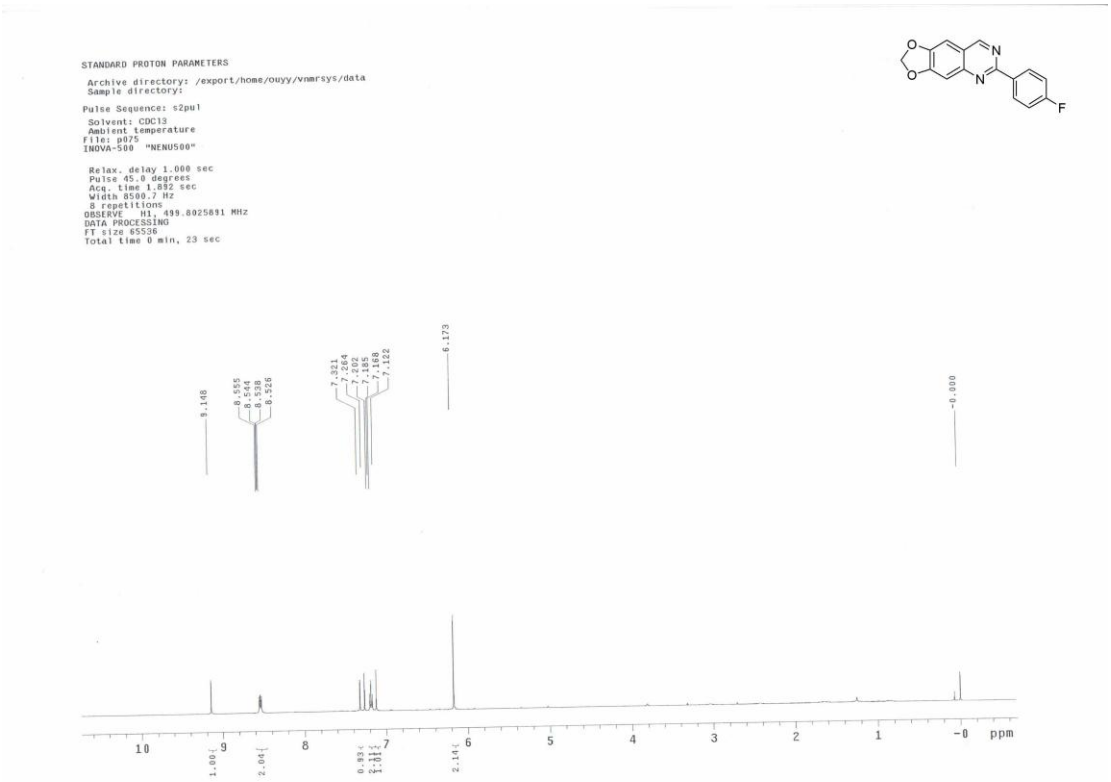

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: r184
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
6000 repetitions
OBSERVE C13, 125.6754704 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
160.008
157.345
153.873
150.127
147.981
140.286
135.951
129.262
128.026
120.480
104.800
102.080
101.775
77.259
77.004
76.752
21.426
220
200
180
160
140
120
100
80
60
40
20
0
ppm

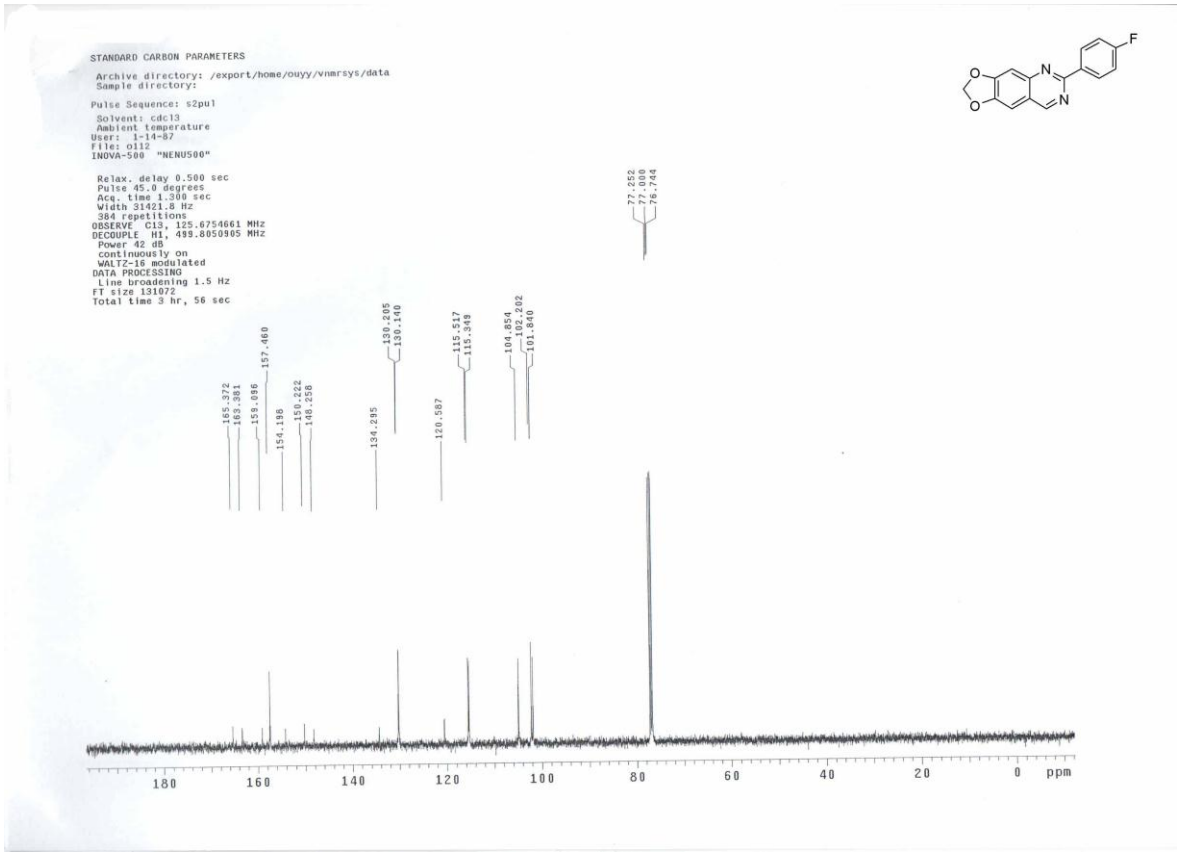
Product 2u


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p343
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025995 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
OMe
9.056
8.480
8.462
7.275
7.245
7.085
7.013
6.986
6.122
3.672
-0.018
ppm

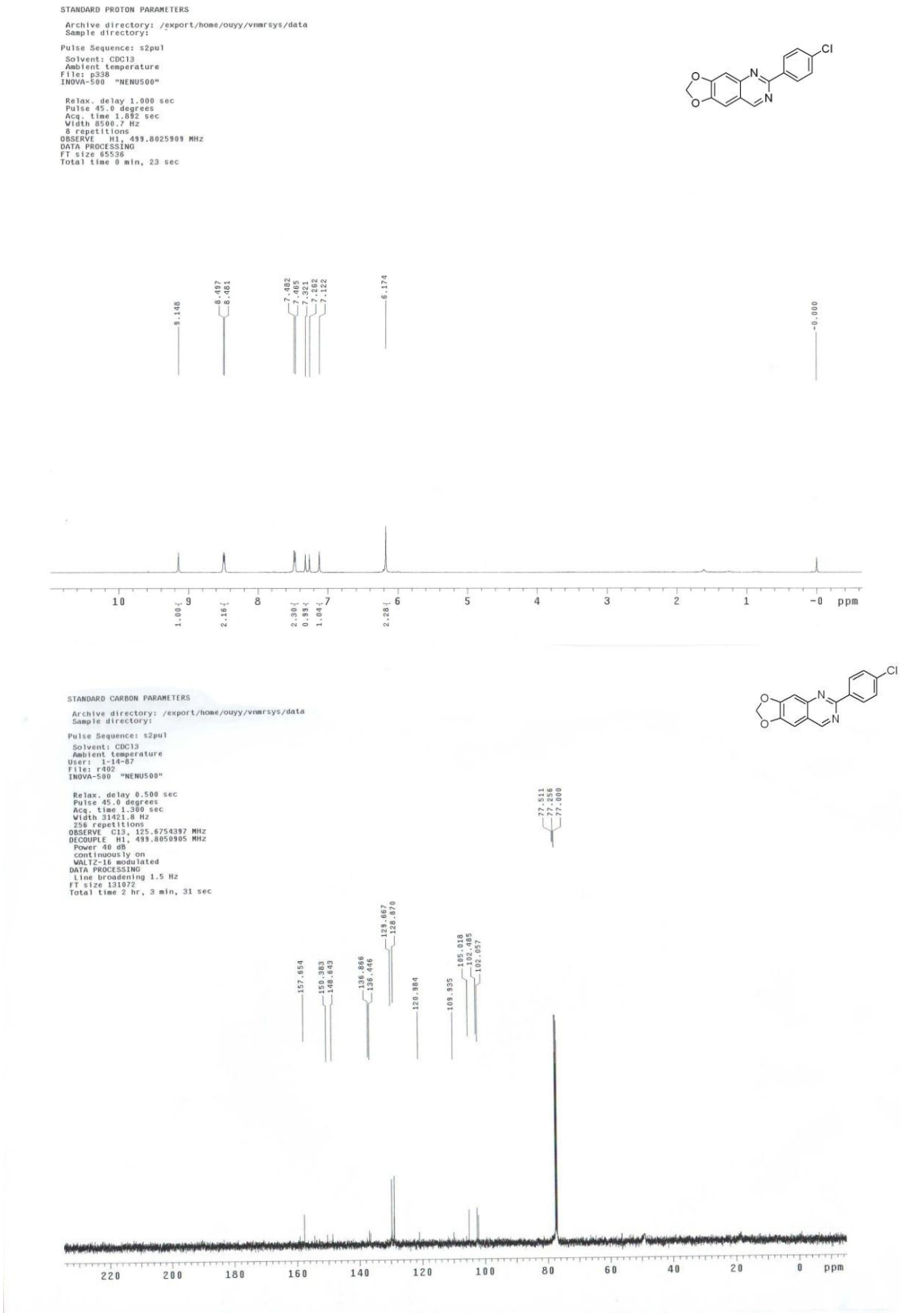

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: r136
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
OMe
161.423
159.788
157.376
153.985
150.245
147.853
130.804
129.675
120.251
113.827
104.747
103.061
101.644
77.256
77.000
76.744
55.315
ppm

Product 2v

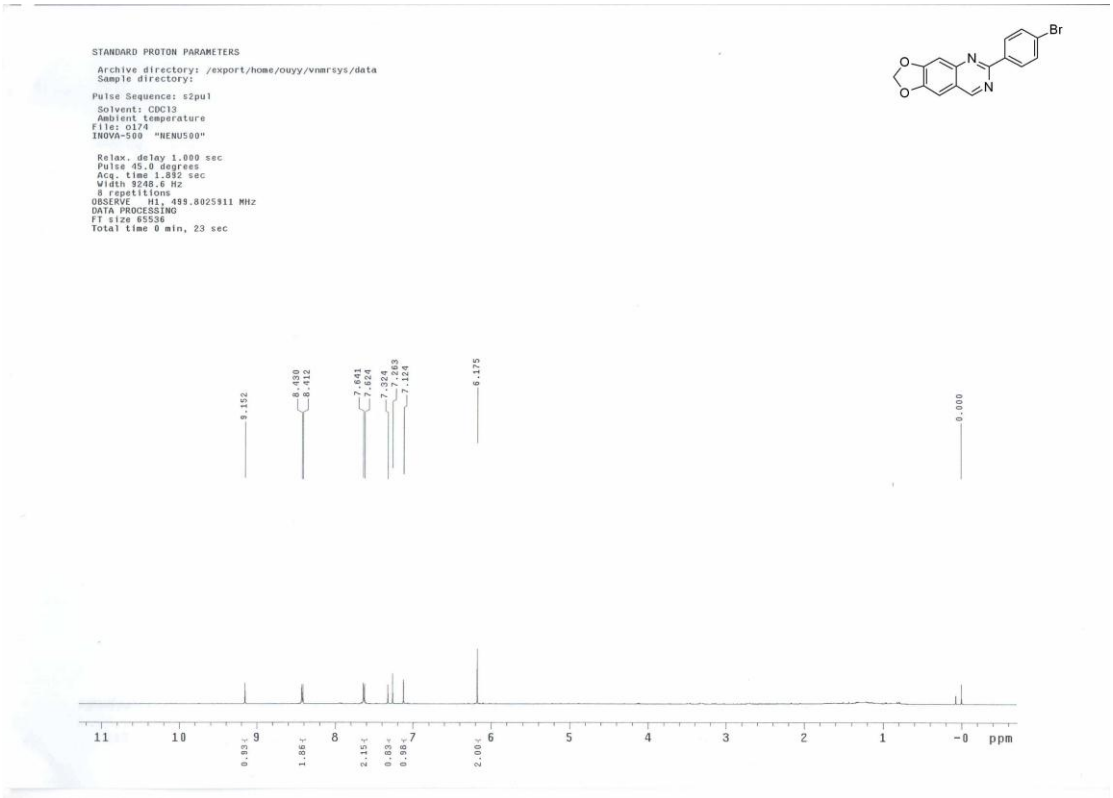

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p075
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025891 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.148
8.556
8.544
8.538
8.526
7.301
7.284
7.282
7.265
7.168
7.122
6.173
-0.000
10
9
8
7
6
5
4
3
2
1
-0
ppm

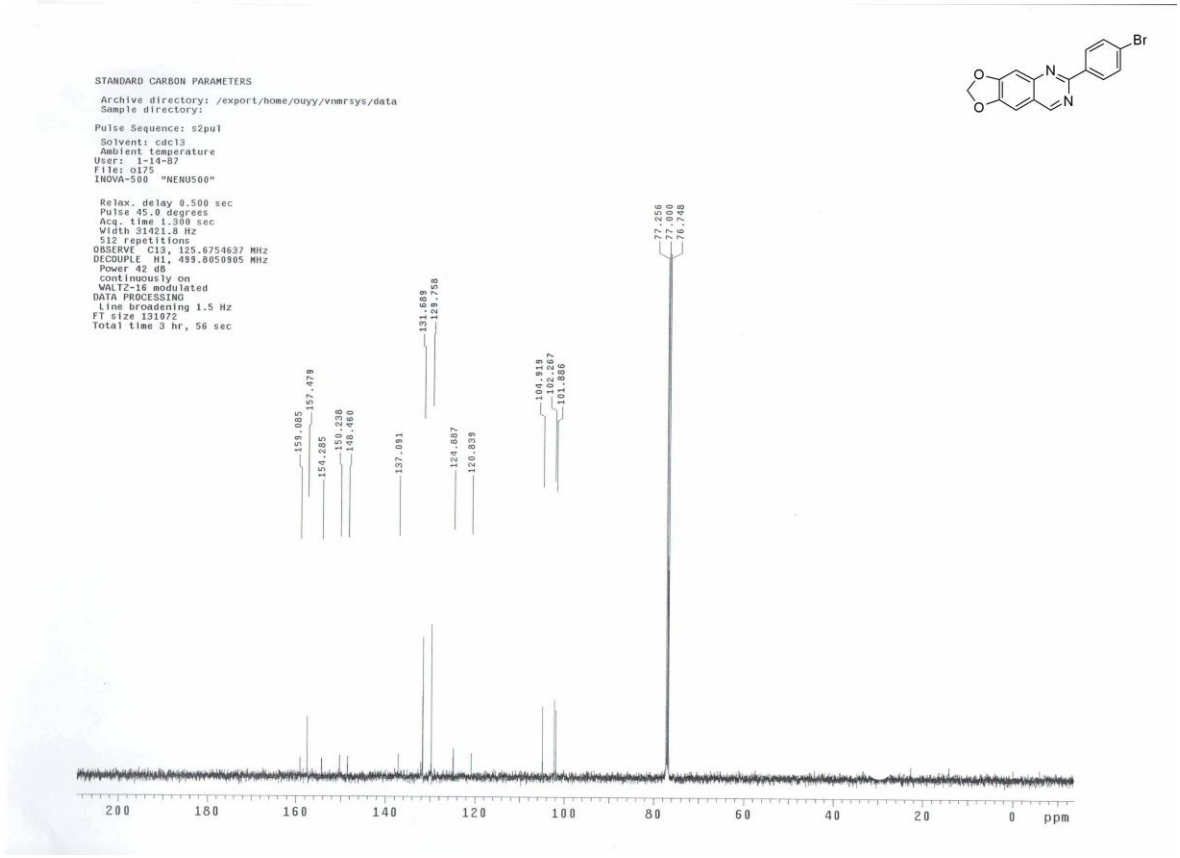

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: o112
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
384 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.252
77.000
76.744
165.372
163.381
159.086
157.460
154.196
150.222
148.256
134.295
130.205
130.140
120.587
115.517
115.349
104.854
102.202
101.840
180
160
140
120
100
80
60
40
20
0
ppm

Product 2w

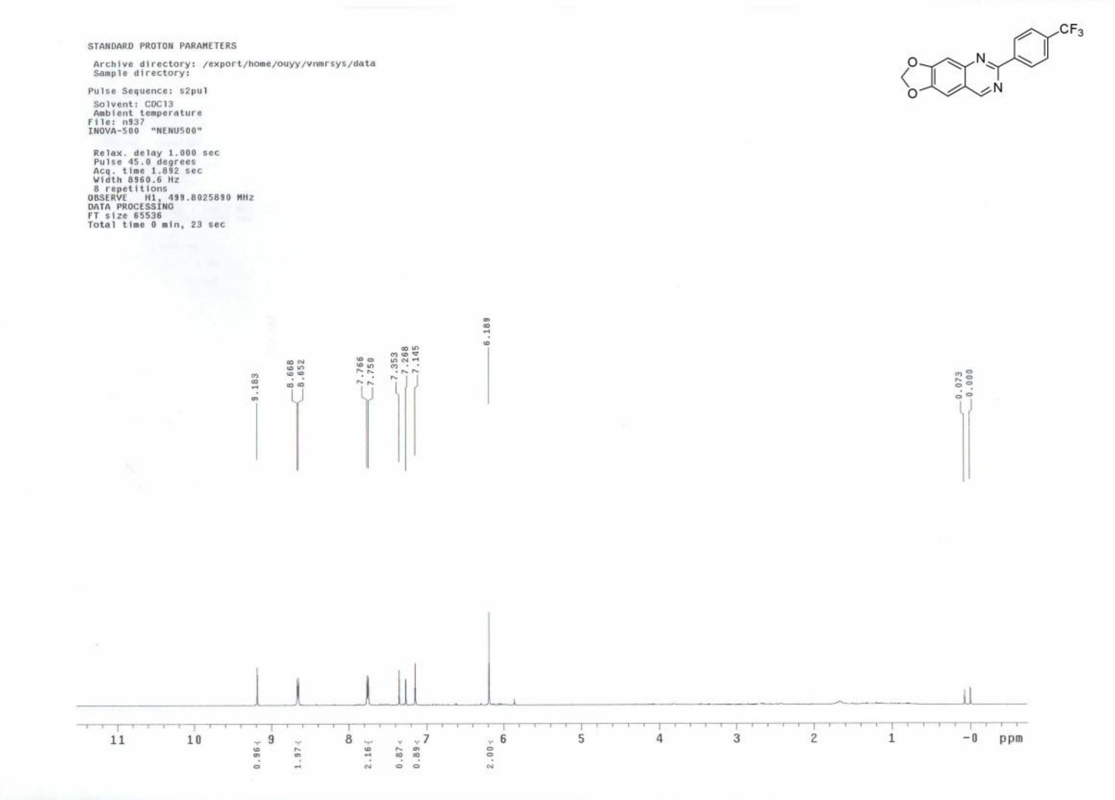

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p338
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025909 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
Cl
N
O
O
N
9.148
8.497
8.481
7.482
7.465
7.321
7.262
7.122
6.174
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.16
2.30
0.93
1.04
2.28
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: r402
INOVA-500 "NENUS00"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754397 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
77.511
77.256
77.000
157.654
150.383
148.643
136.866
136.446
129.667
128.870
120.984
109.935
105.018
102.485
102.067
220
200
180
160
140
120
100
80
60
40
20
0
ppm

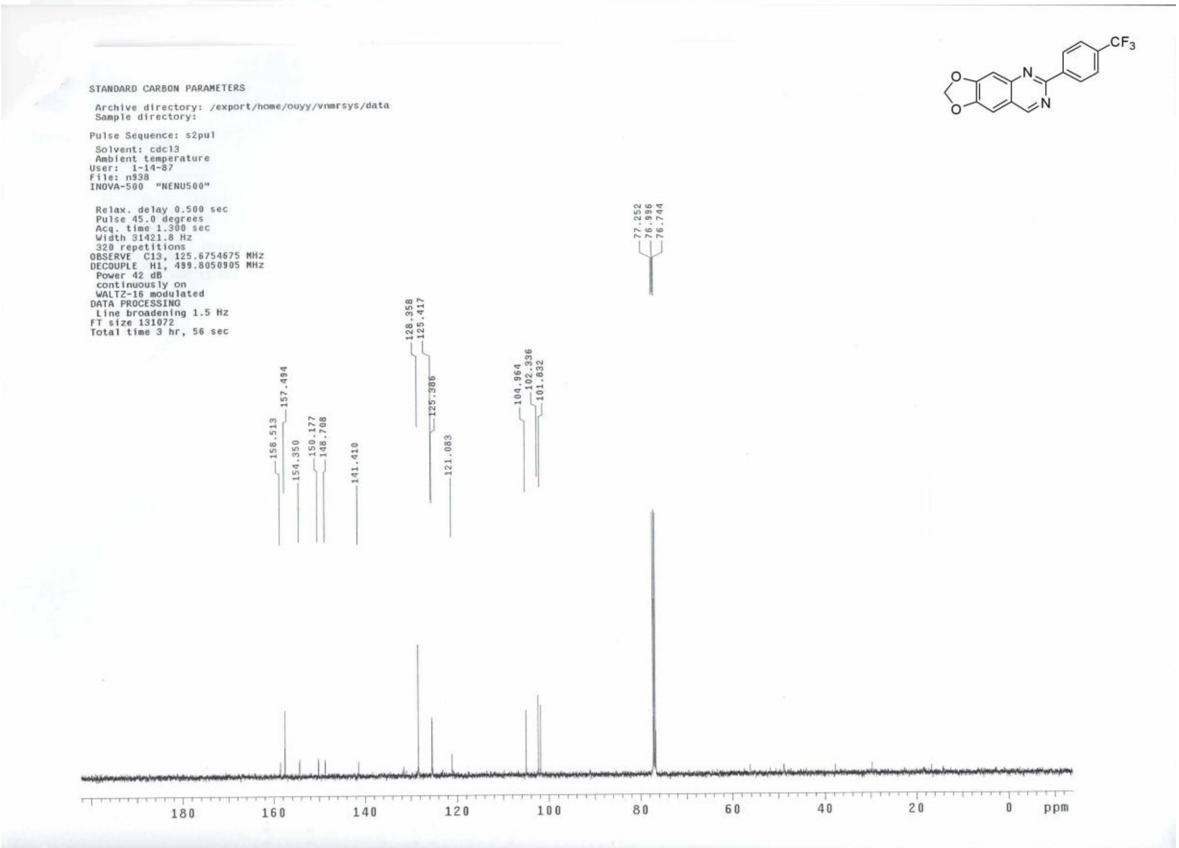
Product 2x


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: o174
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 9248.6 Hz
8 repetitions
OBSERVE H1, 499.8025911 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
Br
9.152
8.430
8.412
7.641
7.624
7.324
7.263
7.184
6.175
0.000
ppm

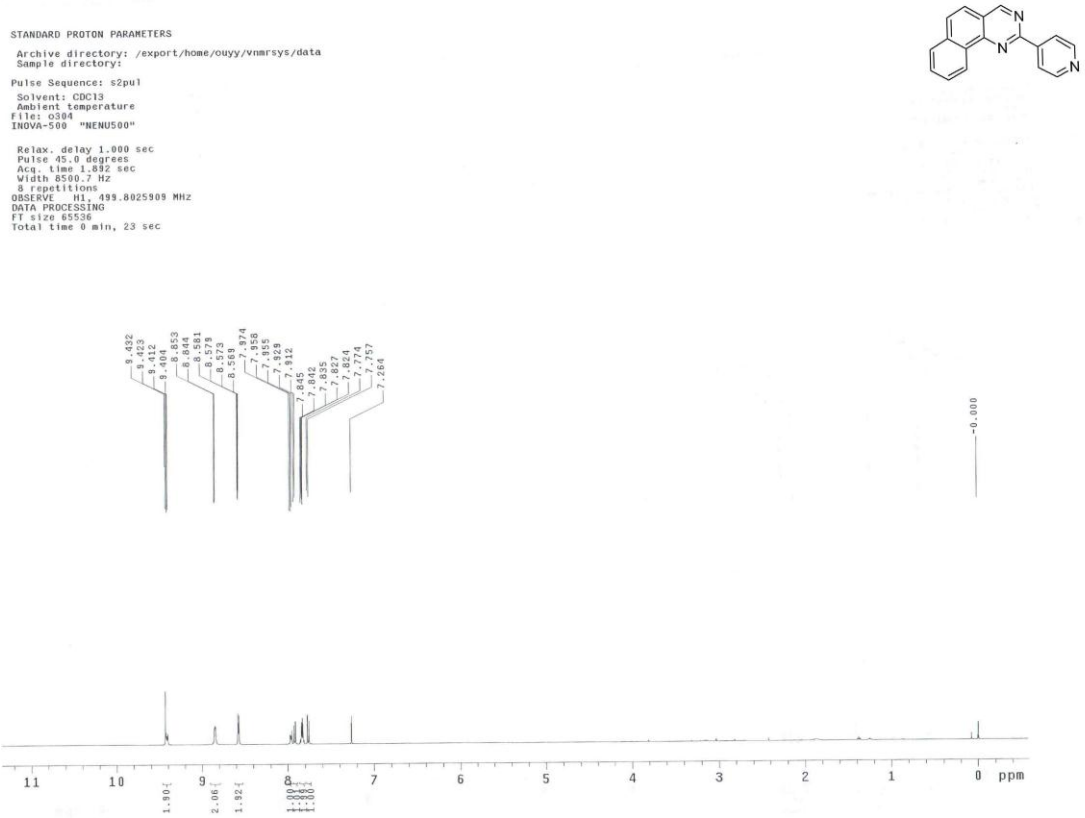

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: o175
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
512 repetitions
OBSERVE C13, 125.6754637 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
Br
159.085
157.479
154.285
150.238
148.460
137.091
131.689
128.758
124.687
120.839
104.919
102.267
101.886
77.256
77.000
76.748
ppm

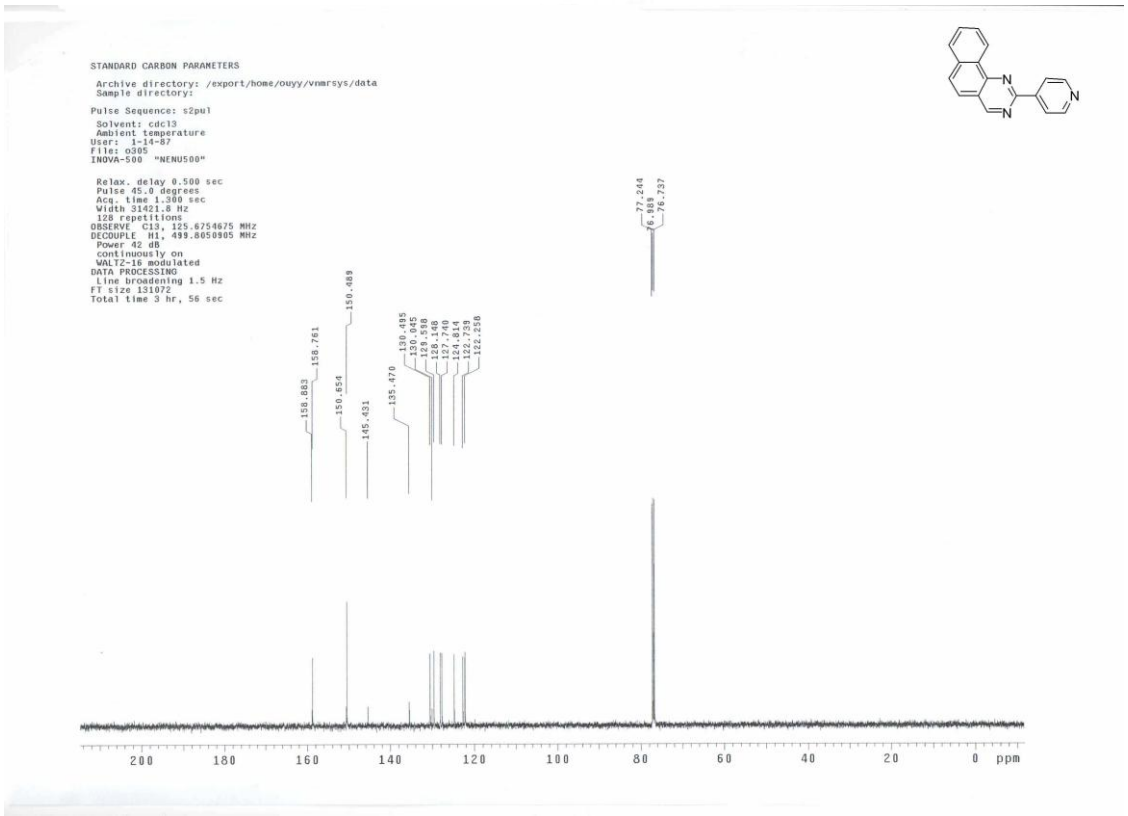
Product 2y


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: n937
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8960.6 Hz
8 repetitions
OBSERVE H1, 499.8025890 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
CF3
O
O
N
N
9.183
8.668
8.652
7.766
7.750
7.353
7.268
7.145
6.189
0.073
0.000
0.96
1.97
2.16
0.87
0.89
2.00
ppm

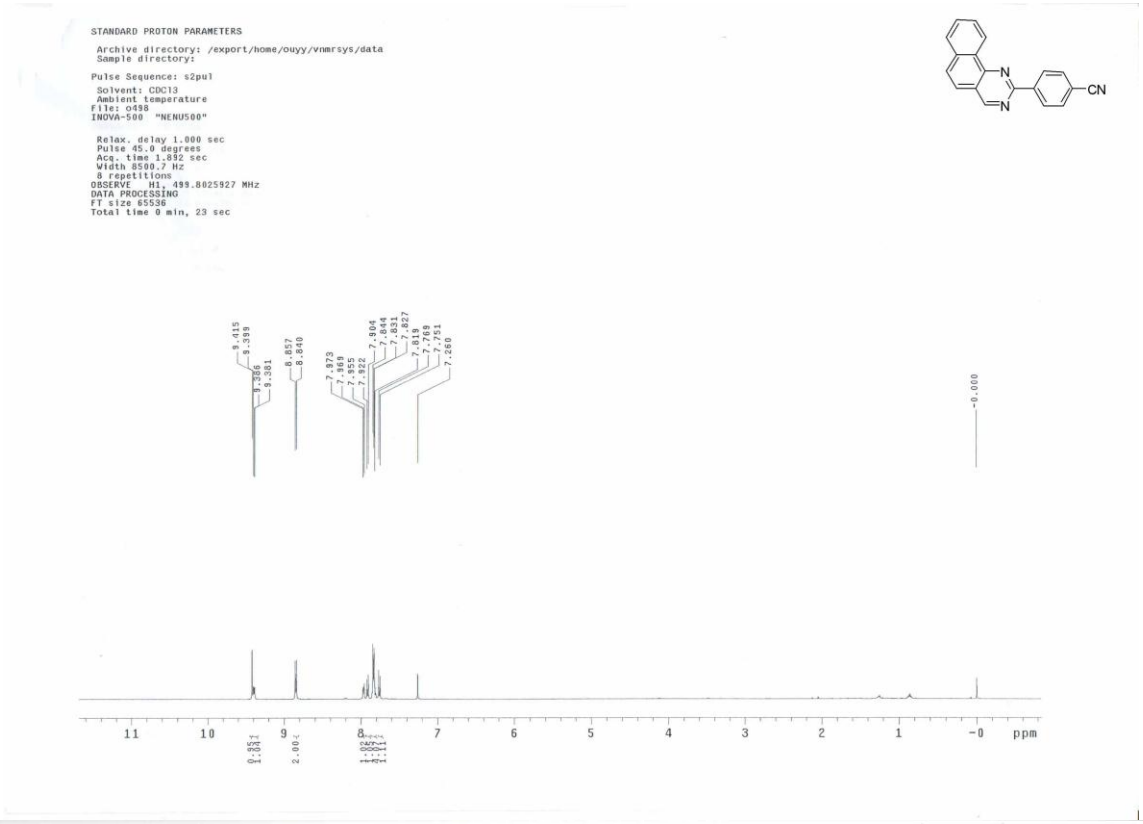

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: n938
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
320 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
CF3
O
O
N
N
158.513
157.494
154.350
150.177
148.708
141.410
128.358
125.417
125.386
121.083
104.864
102.336
101.832
77.252
76.996
76.744
ppm

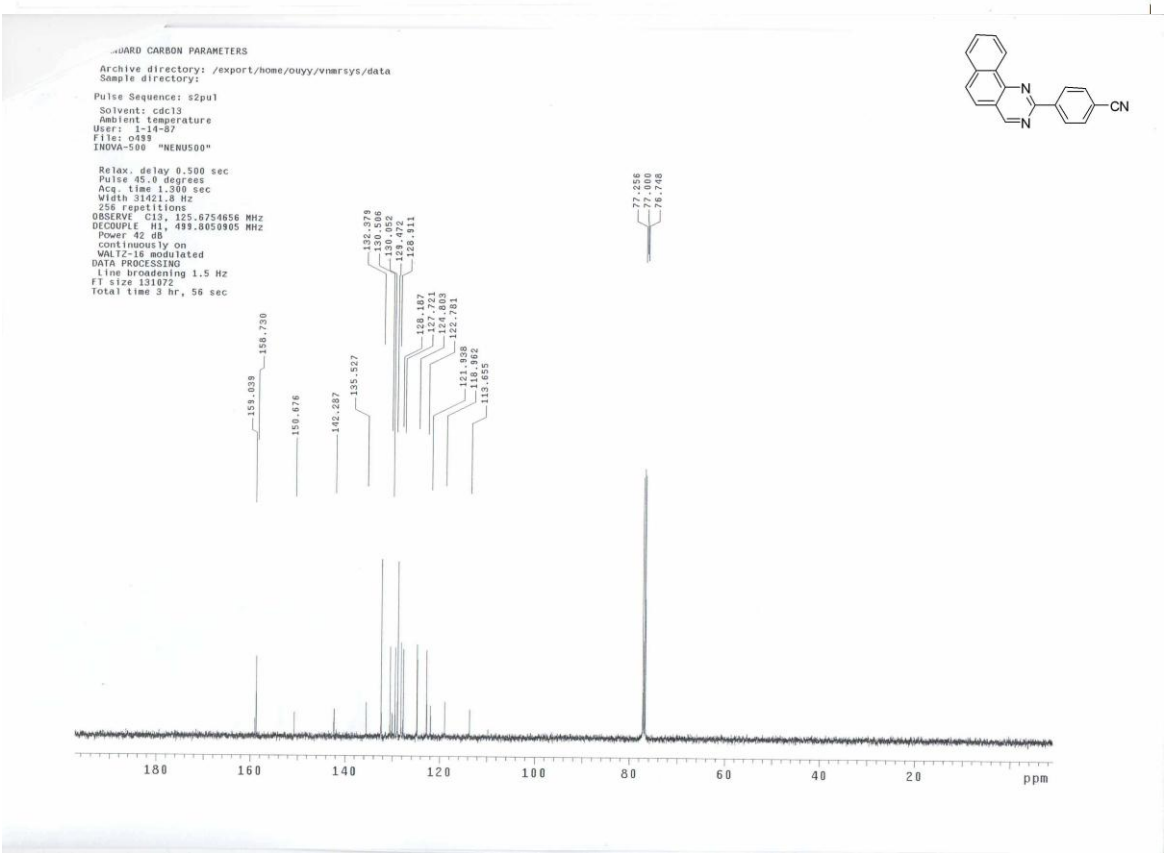
Product 2z


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: o304
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025909 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
9.432
9.423
9.412
9.404
8.853
8.844
8.581
8.578
8.573
8.569
7.974
7.956
7.955
7.938
7.912
7.845
7.842
7.835
7.827
7.824
7.774
7.757
7.284
-0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.80
2.06
1.92
1.00
1.00
1.00

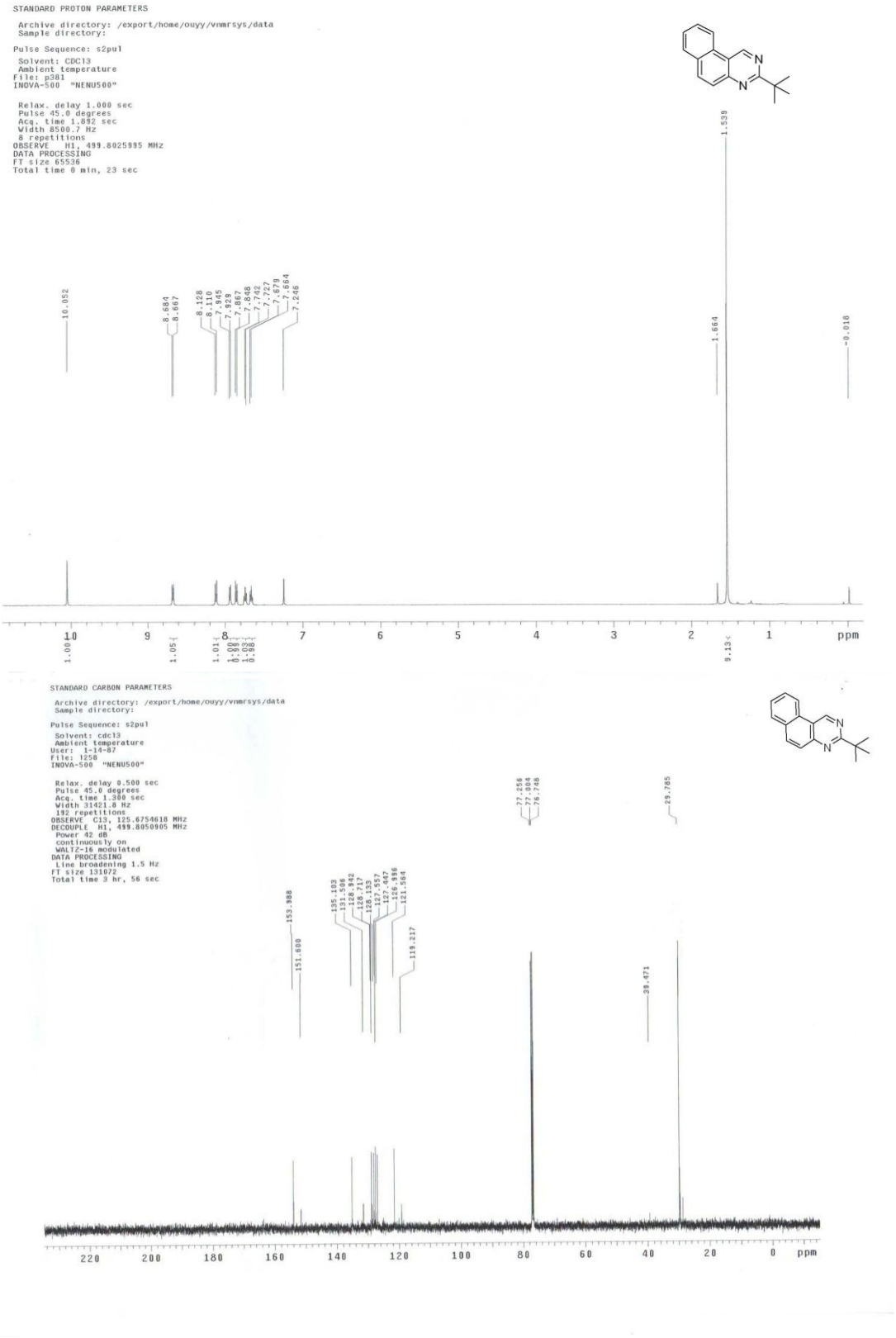

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: o305
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.244
76.981
76.737
158.883
158.761
150.654
150.489
145.431
135.470
130.485
130.055
129.598
128.148
127.740
124.864
122.739
122.256
200
180
160
140
120
100
80
60
40
20
0
ppm

Product 2aa

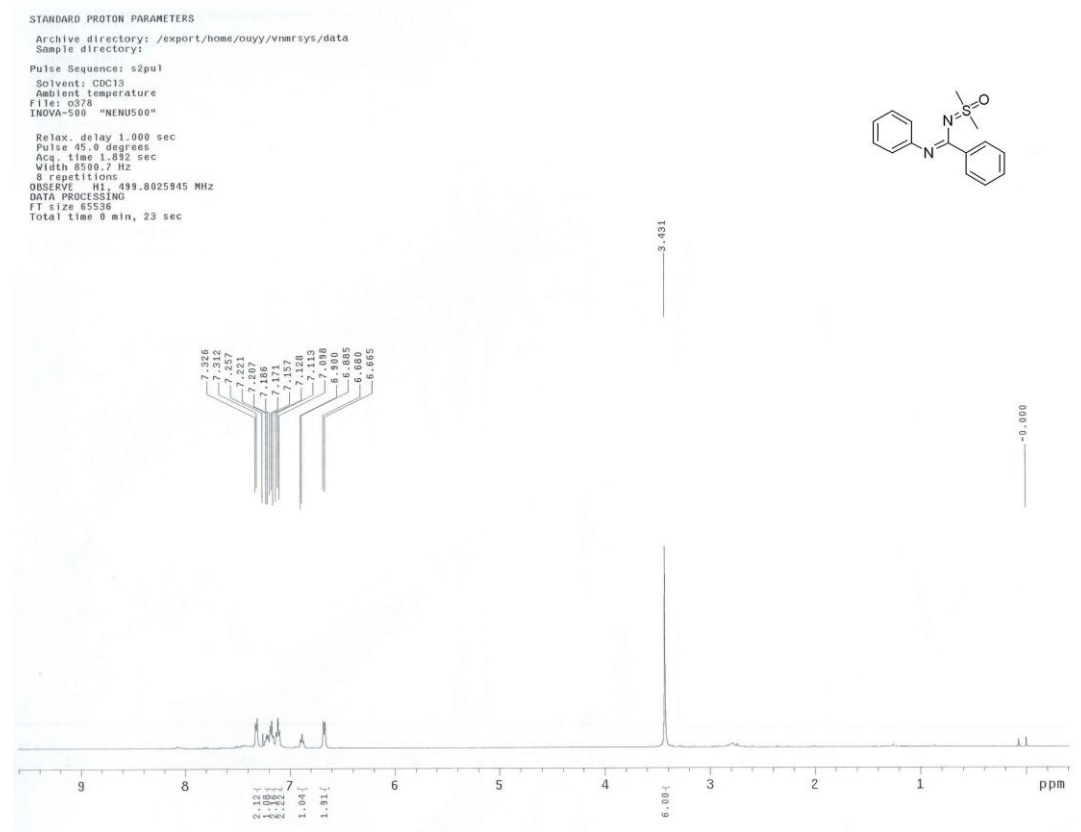

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: o498
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025927 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
CN
ppm

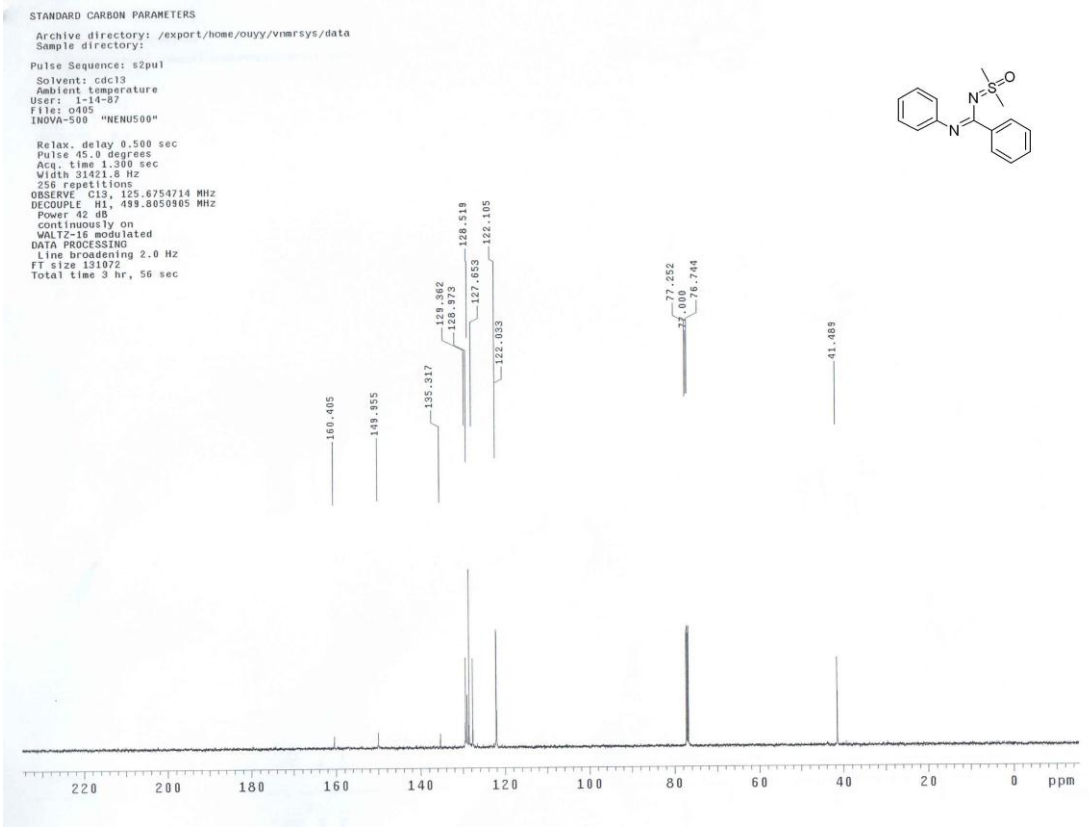

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: o489
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
CN
ppm

Product 2ab

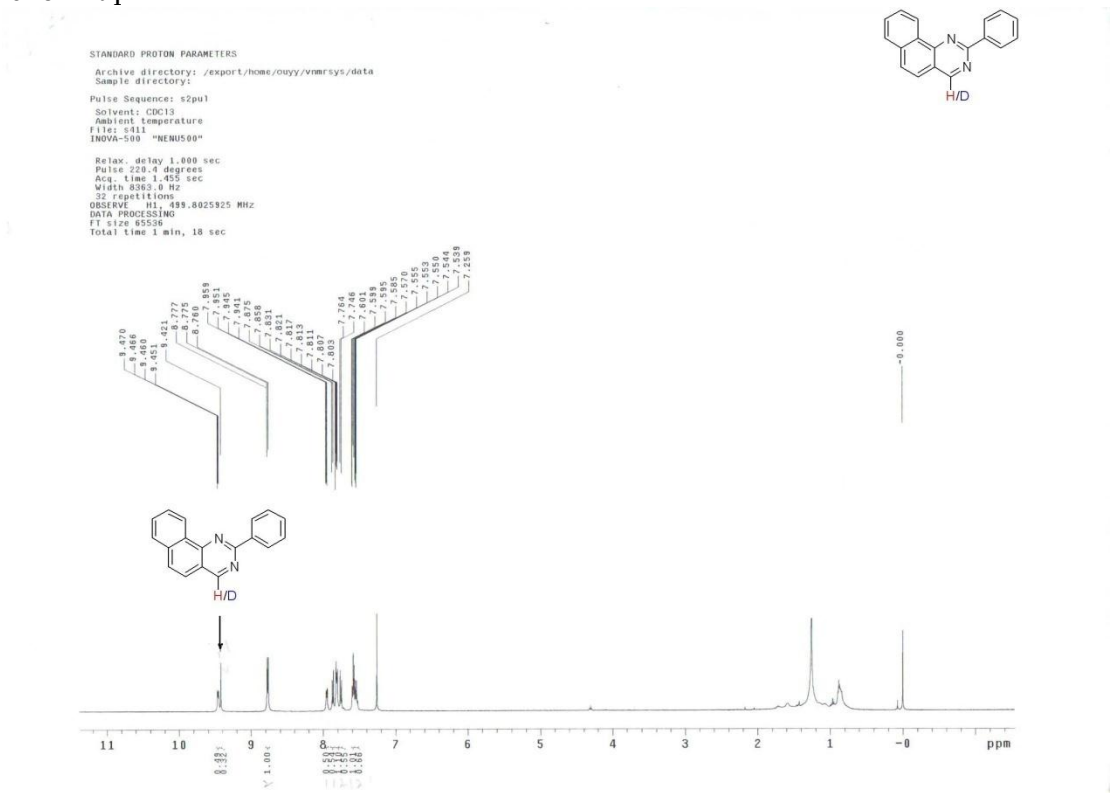

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: p381
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.692 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025995 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
10.052
8.684
8.667
8.128
8.111
7.945
7.929
7.867
7.848
7.742
7.722
7.679
7.664
7.246
1.539
1.664
-0.018
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1258
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754618 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
153.988
151.600
135.103
131.596
128.942
128.717
128.153
127.557
127.447
126.986
121.568
119.217
77.256
77.004
76.748
39.471
29.785
ppm

Product 3

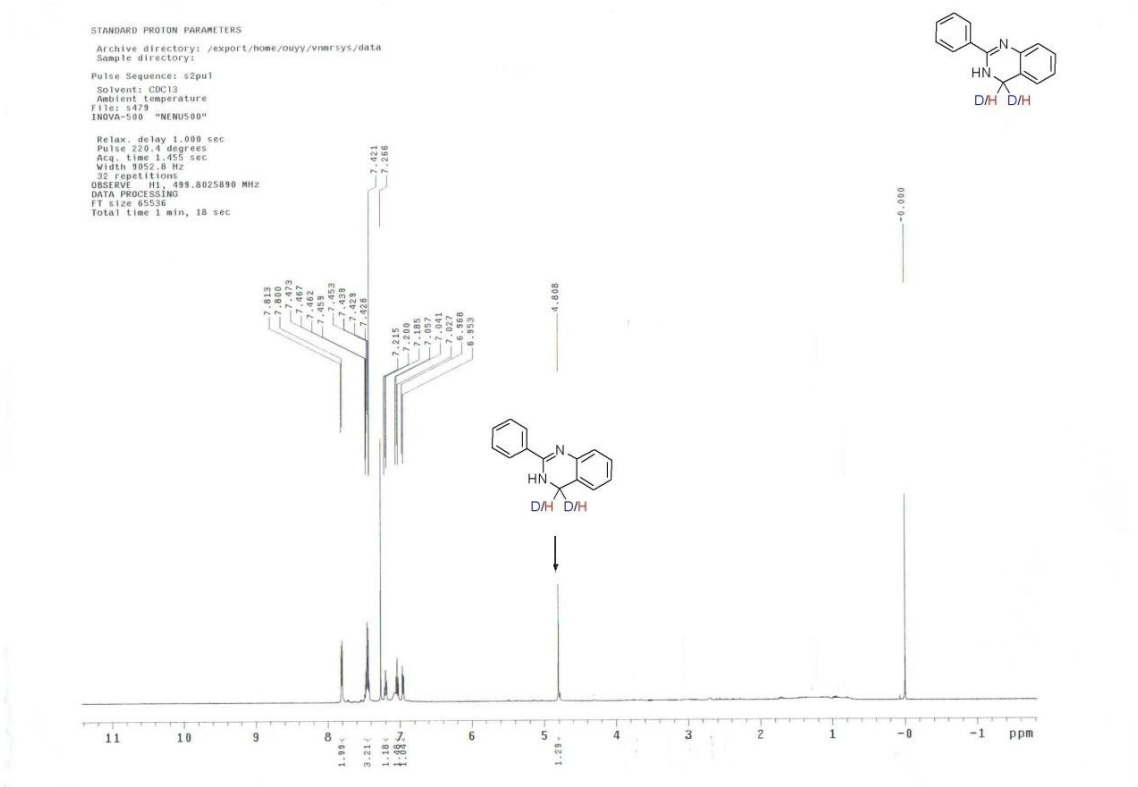

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: o378
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025945 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.326
7.312
7.257
7.221
7.207
7.186
7.171
7.157
7.128
7.113
7.098
6.900
6.855
6.680
6.665
3.431
-0.000
2.12
1.00
2.02
1.04
1.91
6.00
9
8
7
6
5
4
3
2
1
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: o405
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754714 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 3 hr, 56 sec
160.405
149.955
135.317
129.362
128.973
128.519
127.653
122.105
122.033
77.252
77.000
76.744
41.489
220
200
180
160
140
120
100
80
60
40
20
0
ppm

Product 2r and 2r-d_1



Product 2c and 2c-d_1



VII. Structrue analysis X-Ray Crystallography of 2a

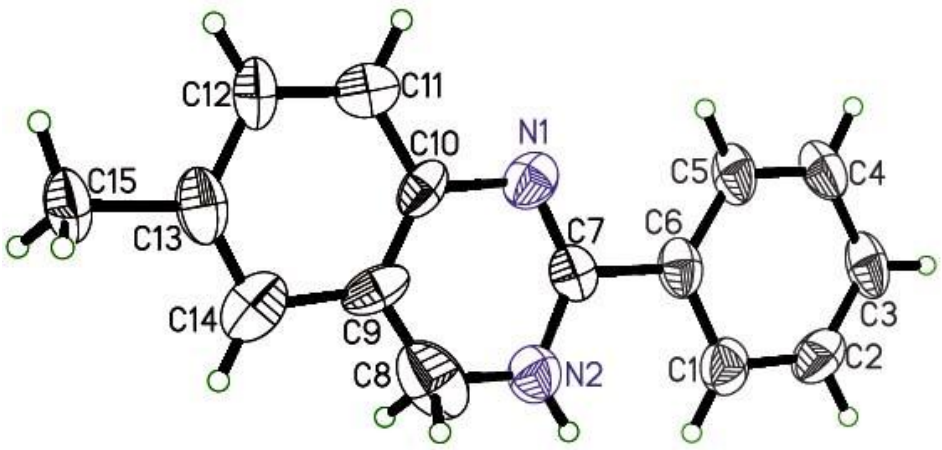


Table 1. Crystal data and structure refinement for i41a.

Identification code	i41a
Empirical formula	C15 H14 N2
Formula weight	222.28
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	?, ?
Unit cell dimensions	a = 14.4293(16) A alpha = 90 deg. b = 14.4293(16) A beta = 90 deg. c = 22.345(5) A gamma = 90 deg.
Volume	4652.3(13) A^3
Z, Calculated density	16, 1.269 Mg/m^3
Absorption coefficient	0.076 mm^-1
F(000)	1888
Crystal size	? x ? x ? mm
Theta range for data collection	1.68 to 25.05 deg.
Limiting indices	-17<=h<=17, -17<=k<=9, -24<=l<=26
Reflections collected / unique	13088 / 2059 [R(int) = 0.0606]
Completeness to theta = 25.00	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2059 / 0 / 155
Goodness-of-fit on F^2	1.107
Final R indices [I>2sigma(I)]	R1 = 0.2096, wR2 = 0.3168
R indices (all data)	R1 = 0.2669, wR2 = 0.3383
Extinction coefficient	0.00000(6)

Largest diff. peak and hole 0.618 and -0.417 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for i41a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	10876(7)	3711(6)	-471(4)	76(3)
N(2)	11097(7)	3782(7)	563(5)	81(3)
C(7)	11374(7)	3735(7)	2(5)	60(3)
C(10)	9895(7)	3733(6)	-365(6)	61(3)
C(6)	12402(7)	3732(7)	-81(6)	69(3)
C(9)	9576(9)	3757(7)	181(6)	71(4)
C(5)	12843(6)	3697(8)	-630(6)	75(3)
C(4)	13771(8)	3670(8)	-710(6)	84(4)
C(3)	14342(8)	3706(9)	-198(7)	87(4)
C(11)	9323(9)	3693(9)	-840(6)	86(4)
C(12)	8374(8)	3706(8)	-755(6)	82(4)
C(13)	8031(8)	3737(7)	-163(7)	81(4)
C(1)	12966(9)	3743(8)	447(6)	80(4)
C(2)	13924(9)	3741(9)	346(6)	84(4)
C(14)	8544(10)	3785(9)	320(7)	96(4)
C(15)	6955(7)	3774(10)	-102(6)	97(4)
C(8)	10166(12)	3790(10)	630(8)	121(6)

Table 3. Bond lengths [A] and angles [deg] for i41a.

N(1)-C(7)	1.278(13)
N(1)-C(10)	1.435(14)
N(2)-C(8)	1.352(16)
N(2)-C(7)	1.317(14)
N(2)-H(2)	0.8600
C(7)-C(6)	1.495(14)
C(10)-C(9)	1.306(15)
C(10)-C(11)	1.344(15)
C(6)-C(1)	1.433(15)
C(6)-C(5)	1.382(15)
C(9)-C(8)	1.317(19)
C(9)-C(14)	1.521(18)
C(5)-C(4)	1.352(14)
C(5)-H(5)	0.9300
C(4)-C(3)	1.411(17)
C(4)-H(4)	0.9300
C(3)-C(2)	1.358(16)
C(3)-H(3)	0.9300
C(11)-C(12)	1.382(15)
C(11)-H(11)	0.9300
C(12)-C(13)	1.413(17)
C(12)-H(12)	0.9300
C(13)-C(14)	1.311(17)
C(13)-C(15)	1.560(15)
C(1)-C(2)	1.400(16)
C(1)-H(1)	0.9300
C(2)-H(2)	0.9300
C(14)-H(14)	0.9300
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(7)-N(1)-C(10)	114.7(10)

C(8)-N(2)-C(7)	114.1(12)
C(8)-N(2)-H(2)	123.0
C(7)-N(2)-H(2)	123.0
N(1)-C(7)-N(2)	128.1(10)
N(1)-C(7)-C(6)	117.1(11)
N(2)-C(7)-C(6)	114.8(11)
C(9)-C(10)-C(11)	121.4(12)
C(9)-C(10)-N(1)	120.1(10)
C(11)-C(10)-N(1)	118.4(12)
C(1)-C(6)-C(5)	118.0(10)
C(1)-C(6)-C(7)	117.5(11)
C(5)-C(6)-C(7)	124.5(11)
C(10)-C(9)-C(8)	119.0(14)
C(10)-C(9)-C(14)	122.5(11)
C(8)-C(9)-C(14)	118.4(13)
C(4)-C(5)-C(6)	125.1(12)
C(4)-C(5)-H(5)	117.4
C(6)-C(5)-H(5)	117.4
C(5)-C(4)-C(3)	118.0(12)
C(5)-C(4)-H(4)	121.0
C(3)-C(4)-H(4)	121.0
C(4)-C(3)-C(2)	117.9(11)
C(4)-C(3)-H(3)	121.0
C(2)-C(3)-H(3)	121.0
C(12)-C(11)-C(10)	120.0(13)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	118.4(13)
C(11)-C(12)-H(12)	120.8
C(13)-C(12)-H(12)	120.8
C(14)-C(13)-C(12)	125.1(13)
C(14)-C(13)-C(15)	119.2(13)
C(12)-C(13)-C(15)	115.6(12)
C(2)-C(1)-C(6)	115.3(12)
C(2)-C(1)-H(1)	122.3
C(6)-C(1)-H(1)	122.3
C(1)-C(2)-C(3)	125.7(12)
C(1)-C(2)-H(2)	117.2
C(3)-C(2)-H(2)	117.2
C(13)-C(14)-C(9)	112.5(13)
C(13)-C(14)-H(14)	123.8
C(9)-C(14)-H(14)	123.8
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(2)-C(8)-C(9)	123.9(15)
N(2)-C(8)-H(8A)	106.4
C(9)-C(8)-H(8A)	106.4
N(2)-C(8)-H(8B)	106.4
C(9)-C(8)-H(8B)	106.4
H(8A)-C(8)-H(8B)	106.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for i41a.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	78(7)	66(6)	83(7)	11(5)	-20(5)	-3(5)
N(2)	66(6)	91(7)	86(7)	-10(6)	6(5)	0(6)

C(7)	62(6)	40(5)	80(8)	0(5)	12(6)	6(5)
C(10)	66(7)	35(5)	84(8)	6(5)	-28(6)	-7(5)
C(6)	51(6)	64(7)	93(9)	21(6)	0(6)	0(5)
C(9)	104(10)	39(5)	69(8)	-10(5)	-36(7)	7(6)
C(5)	34(5)	91(8)	99(9)	20(7)	7(6)	6(5)
C(4)	61(7)	98(9)	91(9)	26(7)	20(7)	0(7)
C(3)	41(6)	99(9)	121(11)	27(9)	17(7)	2(6)
C(11)	96(10)	94(9)	70(8)	-3(7)	-9(7)	1(8)
C(12)	46(6)	87(9)	114(11)	0(8)	11(7)	-11(6)
C(13)	68(8)	49(6)	127(12)	12(7)	18(8)	-5(6)
C(1)	84(8)	66(7)	90(9)	6(6)	-2(7)	-16(6)
C(2)	77(8)	87(9)	89(9)	-1(7)	-29(7)	-5(7)
C(14)	92(10)	77(9)	117(11)	-9(8)	-29(9)	3(7)
C(15)	49(7)	127(11)	114(11)	3(9)	21(7)	-6(7)
C(8)	140(15)	78(10)	144(16)	-8(10)	61(13)	12(10)