

Supporting Information

**Metal Free Cycloaddition to Synthesize
Naphtho[2,3-d][1,2,3]triazole-4,9-diones**

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1. General Information

Experimental Details: All reagents and starting materials were obtained from commercial sources and used as received. All dry solvents were purified using a solvent purification system. All reactions were performed under an atmosphere of argon unless otherwise mentioned. Brine refers to a saturated solution of sodium chloride. Aluminum-backed plates precoated with silica gel 60F254 were used for thin layer chromatography and were visualized with a UV lamp. Melting points are uncorrected. ^1H NMR and ^{13}C NMR spectra were recorded in 400 MHz instrument using CDCl_3 as a solvent. ^1H NMR chemical shifts are referenced to TMS (0 ppm) or CDCl_3 (7.26 ppm). ^{13}C NMR was referenced to CDCl_3 (77.0 ppm). Multiplicities were denoted as (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or overlap of nonequivalent resonances, integration). Mass spectra and high resolution mass spectra (HRMS) were obtained by electron impact at 70 eV in an ion trap. Flash column chromatography was carried out over silica gel 60 (230-400 mesh).

NP-TMA

Pulse Sequence: s2pu1

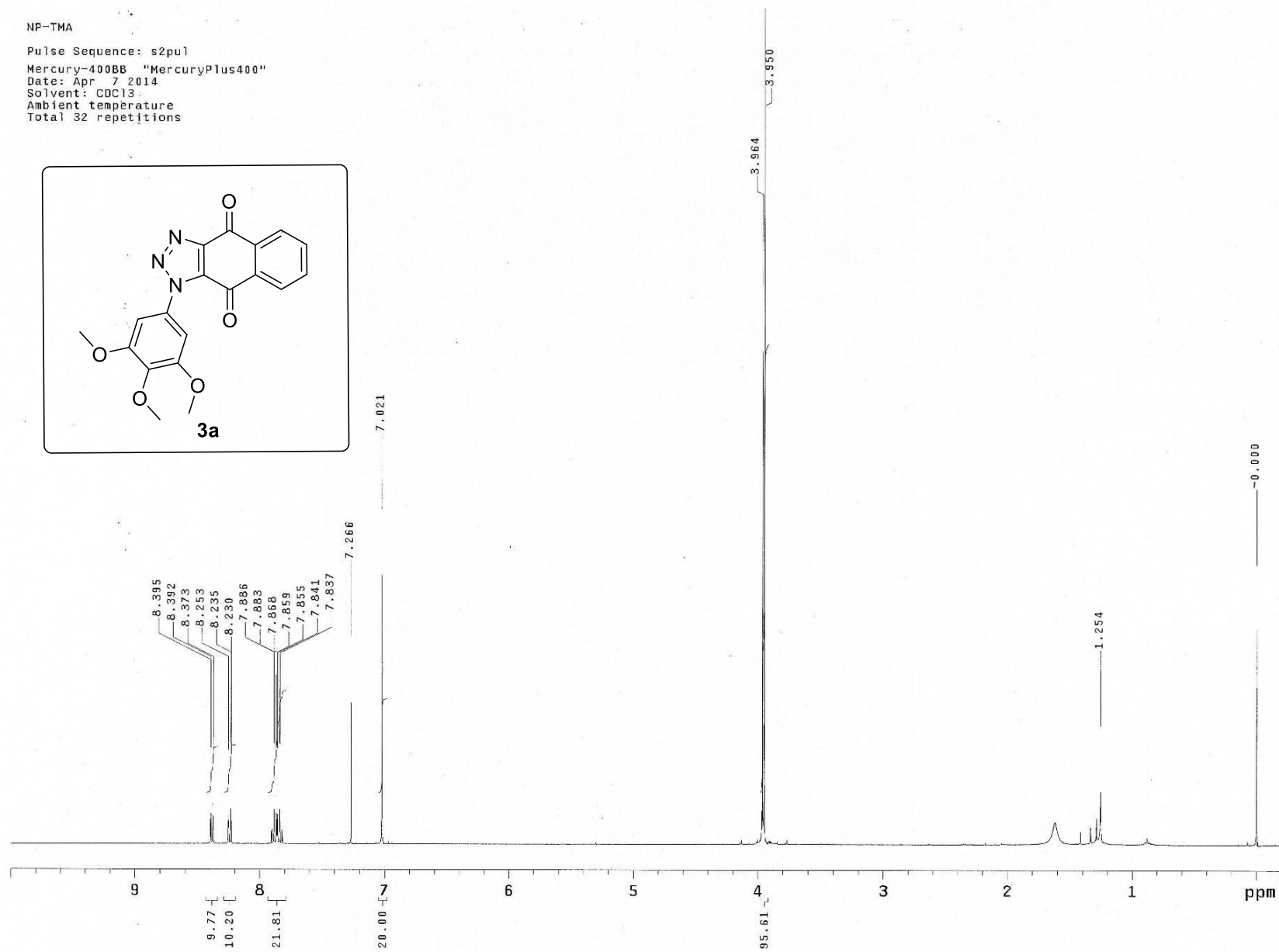
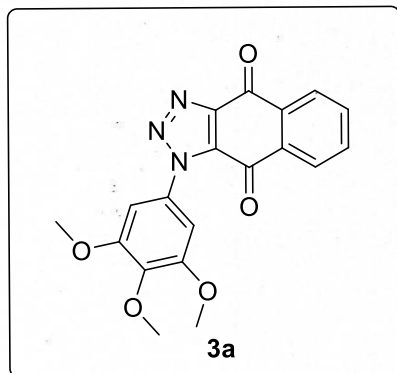
Mercury-400BB "MercuryPlus400"

Date: Apr 7 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



NP-TMA

Pulse Sequence: s2pu1

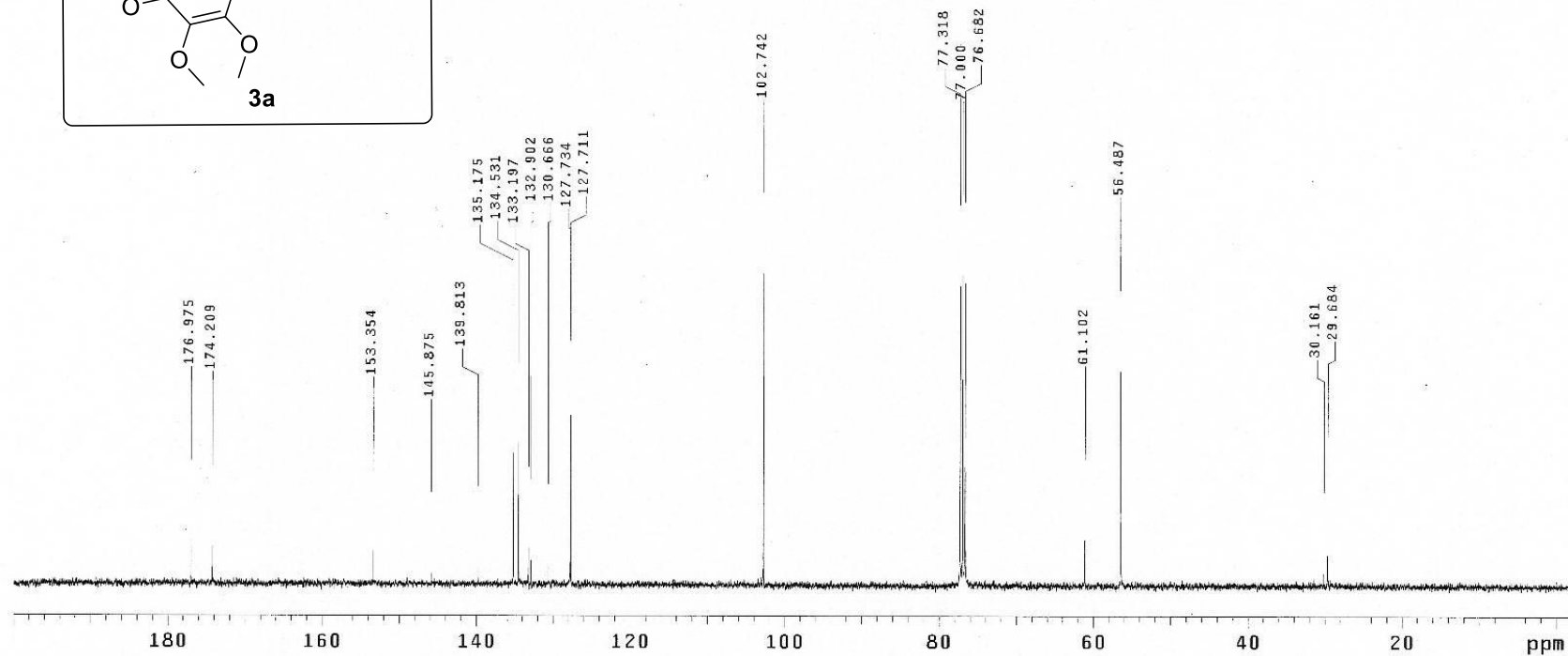
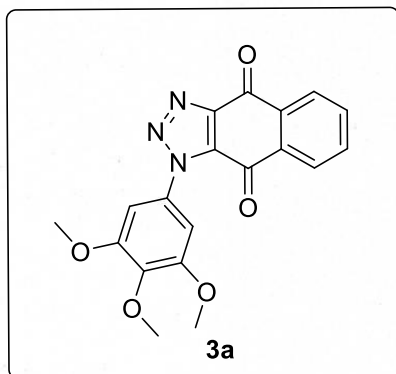
Mercury-400BB "MercuryPlus400"

Date: Apr 7 2014

Solvent: CDCl₃

Ambient temperature

Total 5728 repetitions



NP-4OMe

Pulse Sequence: s2pu1

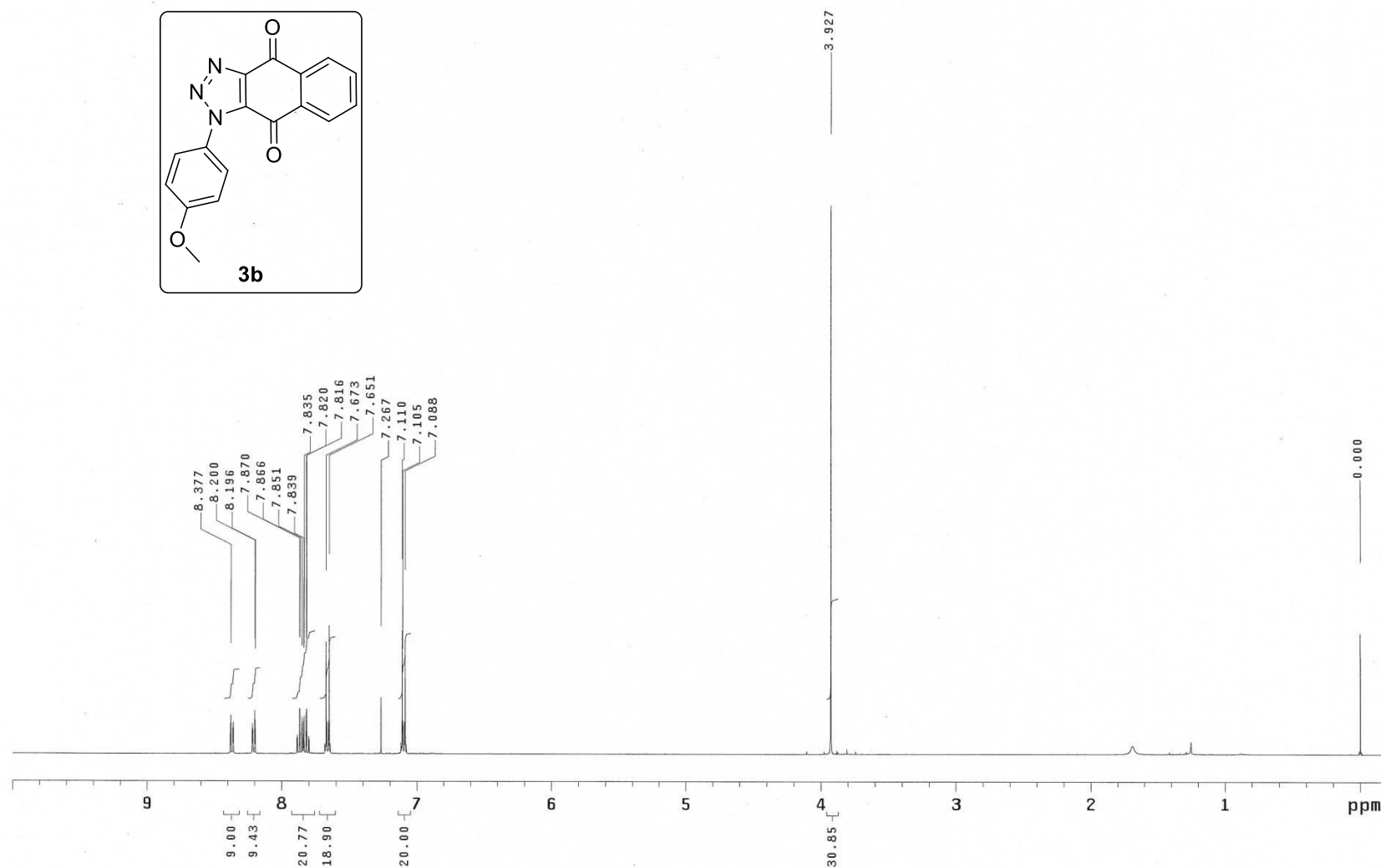
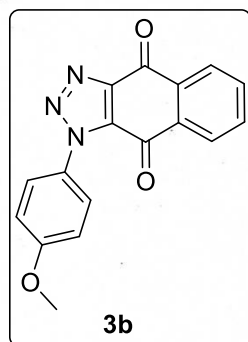
Mercury-400BB "MercuryPlus400"

Date: Mar 26 2014

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



NP-40Me

Pulse Sequence: s2pu1

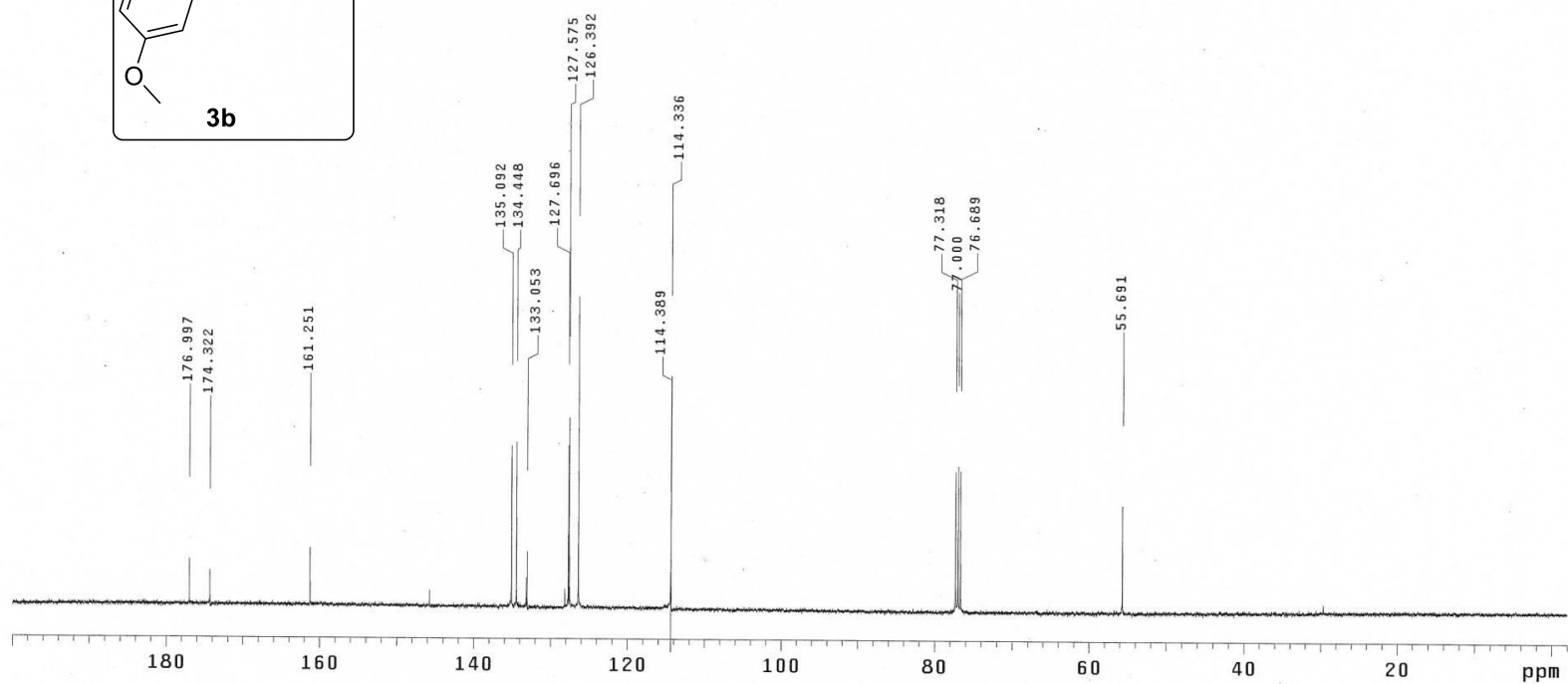
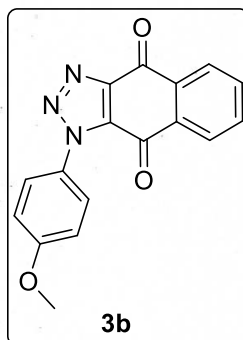
Mercury-400BB "MercuryPlus400"

Date: Mar 26 2014

Solvent: CDCl₃

Ambient temperature

Total 4752 repetitions



NP-3OMe

Pulse Sequence: s2pu1

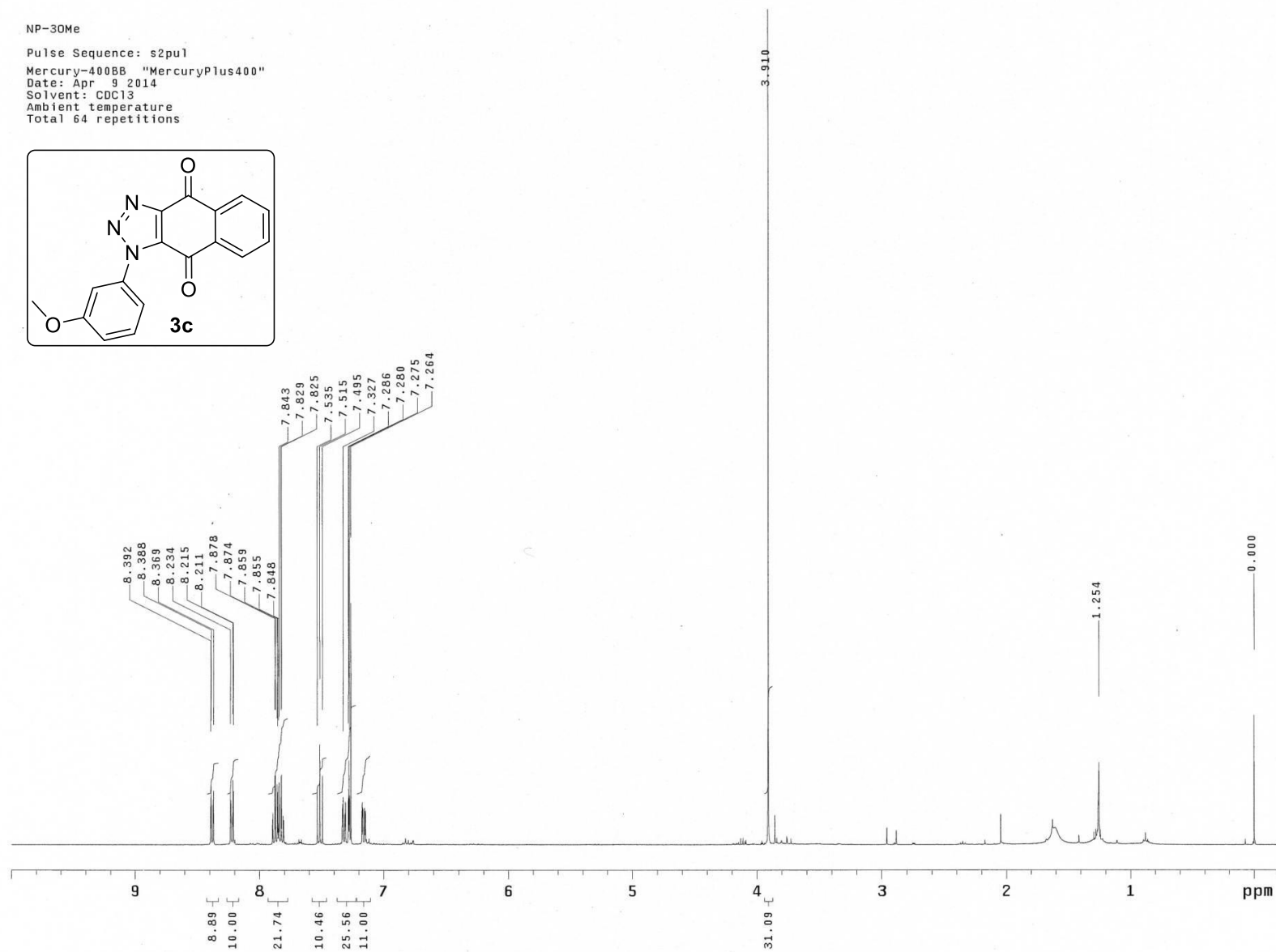
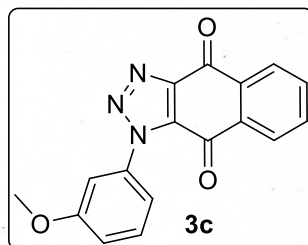
Mercury-400BB "MercuryPlus400"

Date: Apr 9 2014

Solvent: CDCl3

Ambient temperature

Total 64 repetitions



NP-30Me

Pulse Sequence: s2pu1

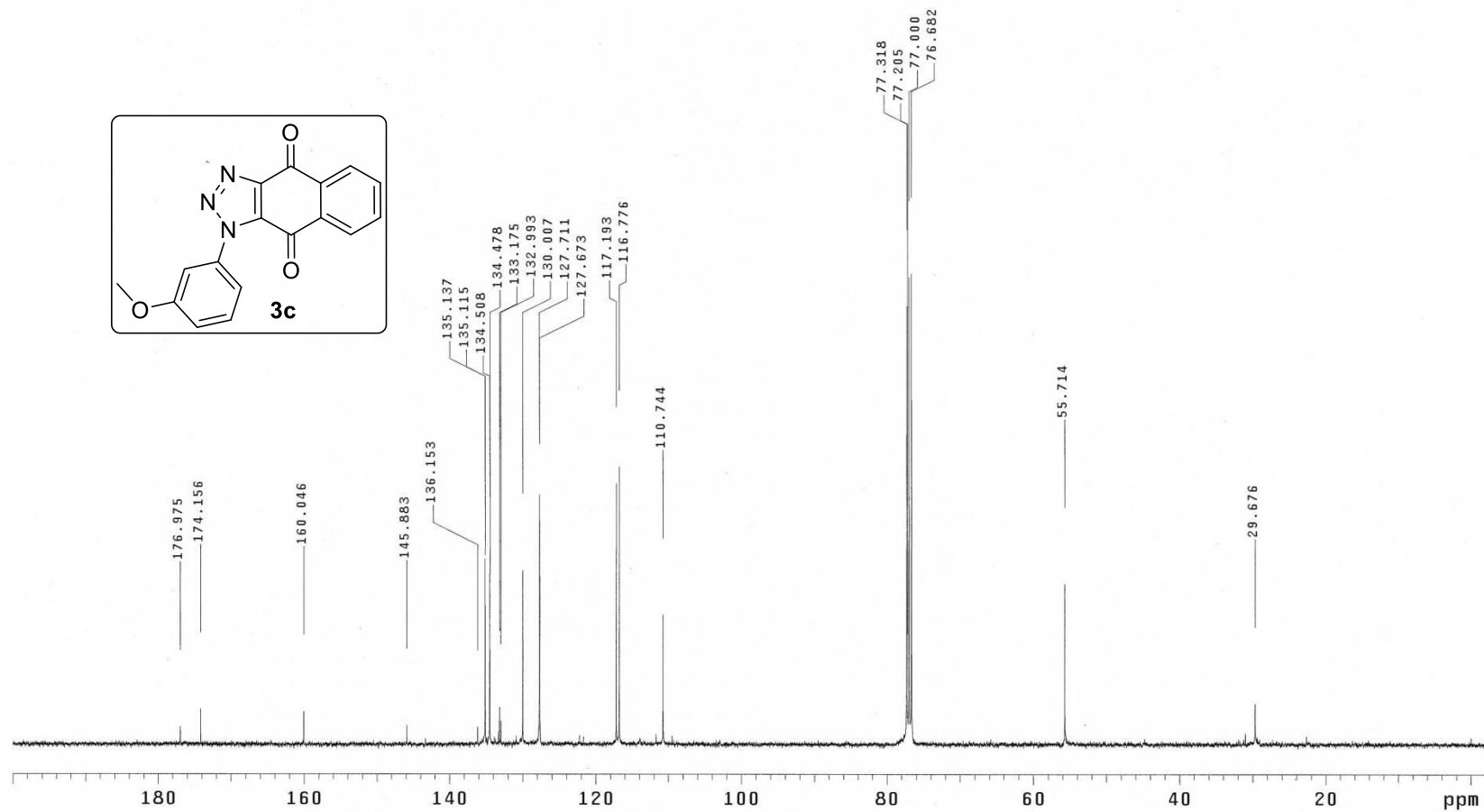
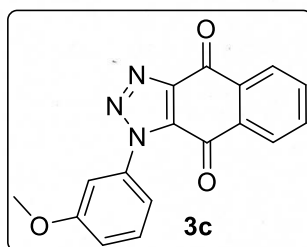
Mercury-400BB "MercuryPlus400"

Date: Apr 9 2014

Solvent: CDCl₃

Ambient temperature

Total 64000 repetitions



NP-20Me

Pulse Sequence: s2pu1

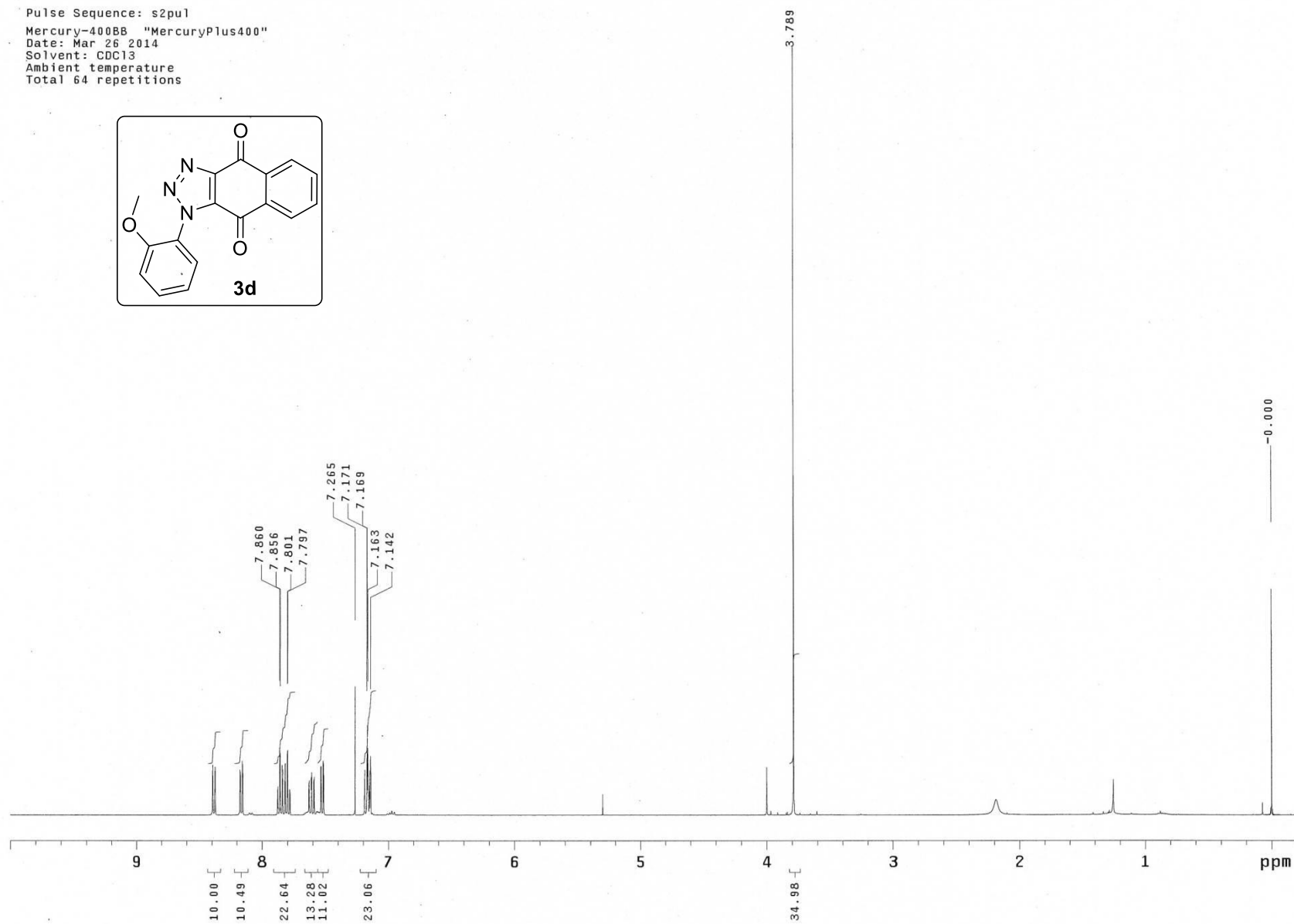
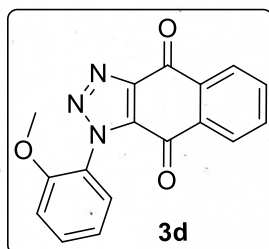
Mercury-400BB "MercuryPlus400"

Date: Mar 26 2014

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



NP-4Me

Pulse Sequence: s2pu1

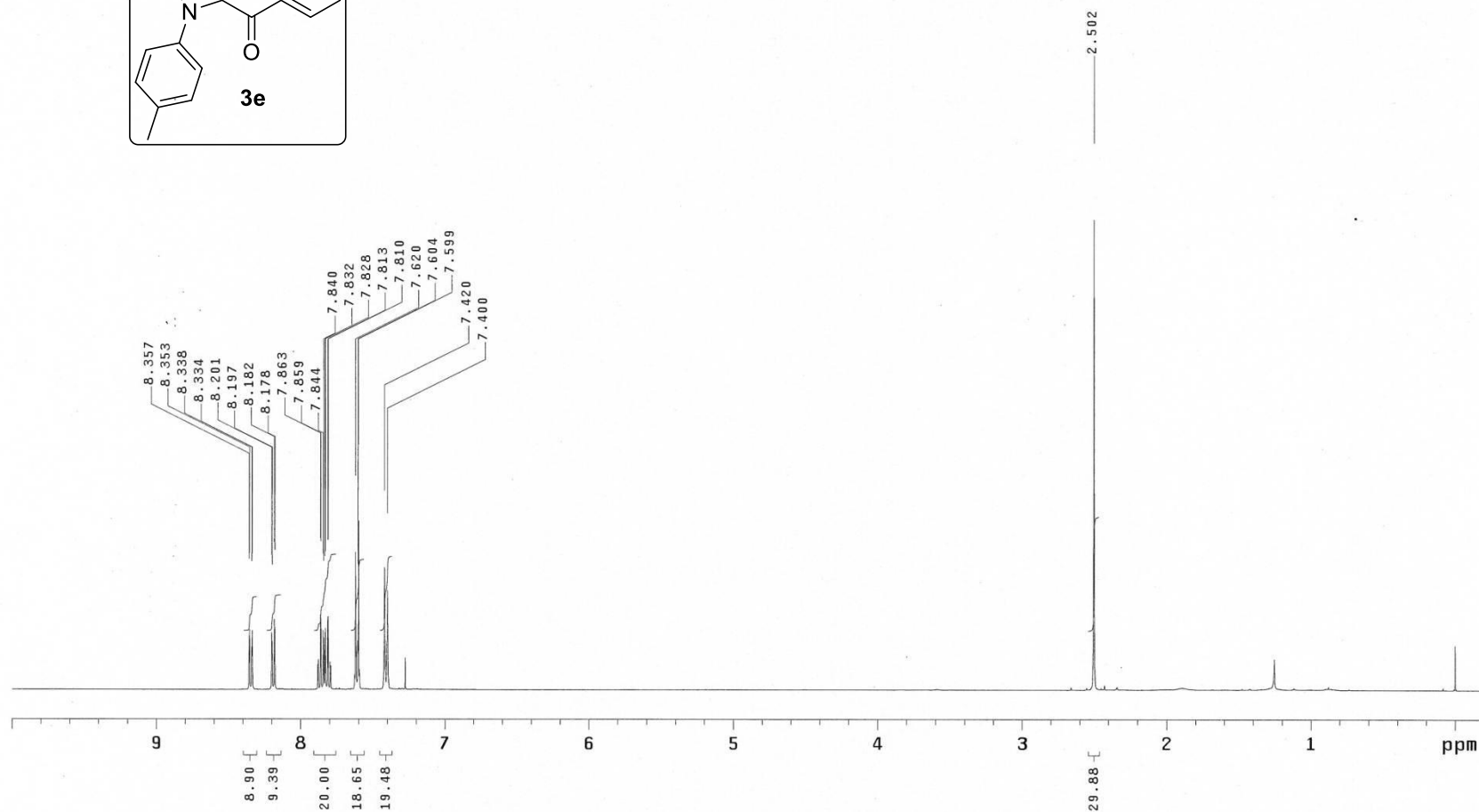
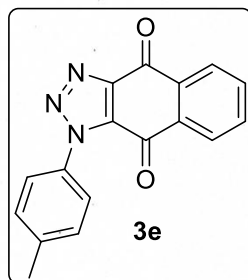
Mercury-400BB "MercuryPlus400"

Date: Apr 7 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



NP-4Me

Pulse Sequence: s2pu1

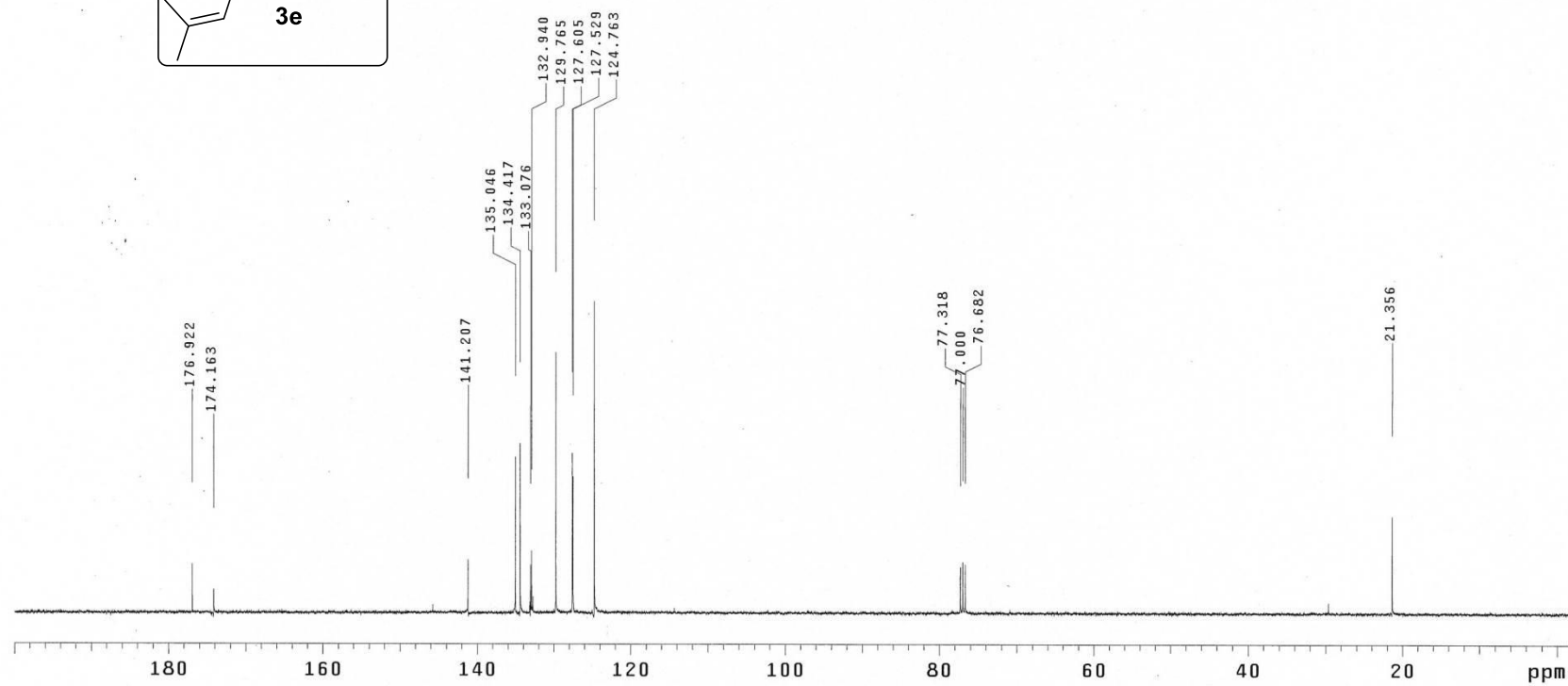
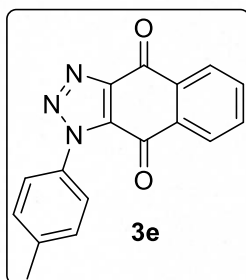
Mercury-400BB "MercuryPlus400"

Date: Apr 7 2014

Solvent: CDCl₃

Ambient temperature

Total 480 repetitions



NP-Ph

Pulse Sequence: s2pu1

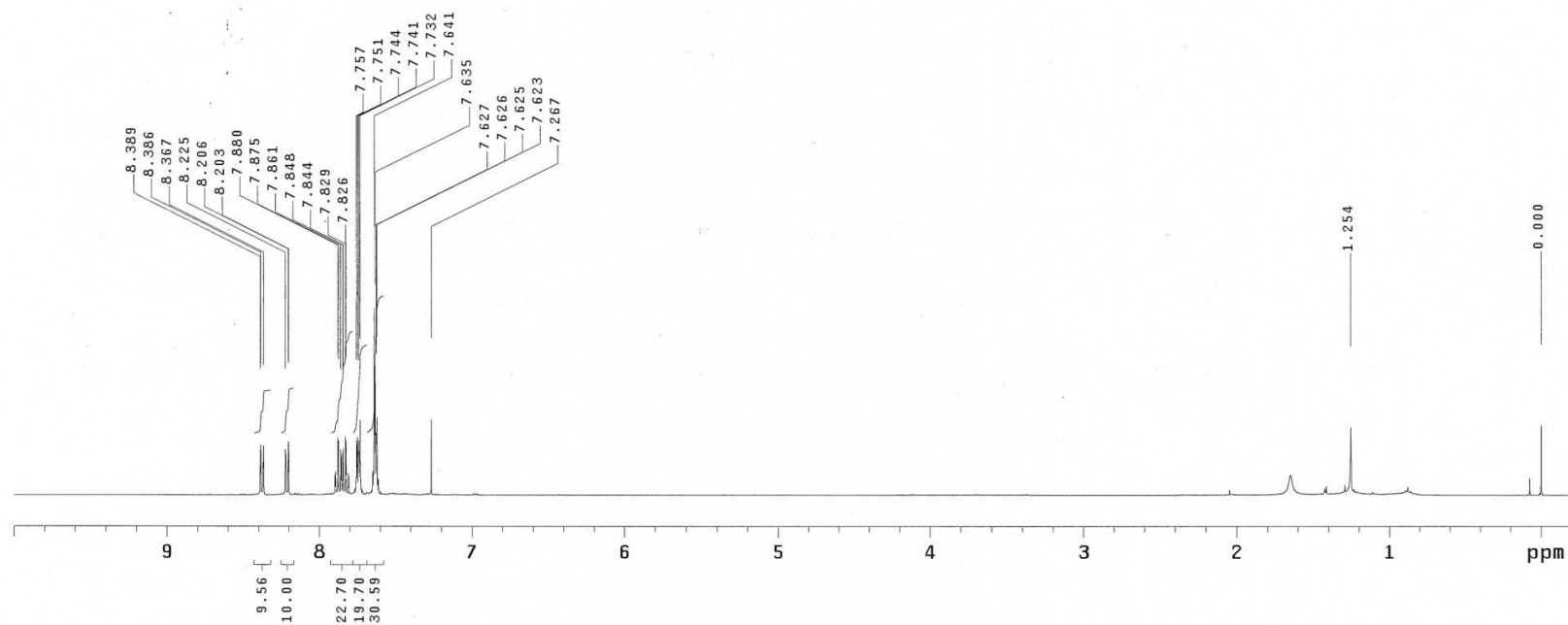
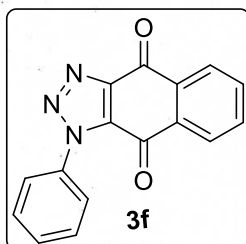
Mercury-400BB "MercuryPlus400"

Date: Mar 26 2014

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



NP-Ph

Pulse Sequence: s2pu1

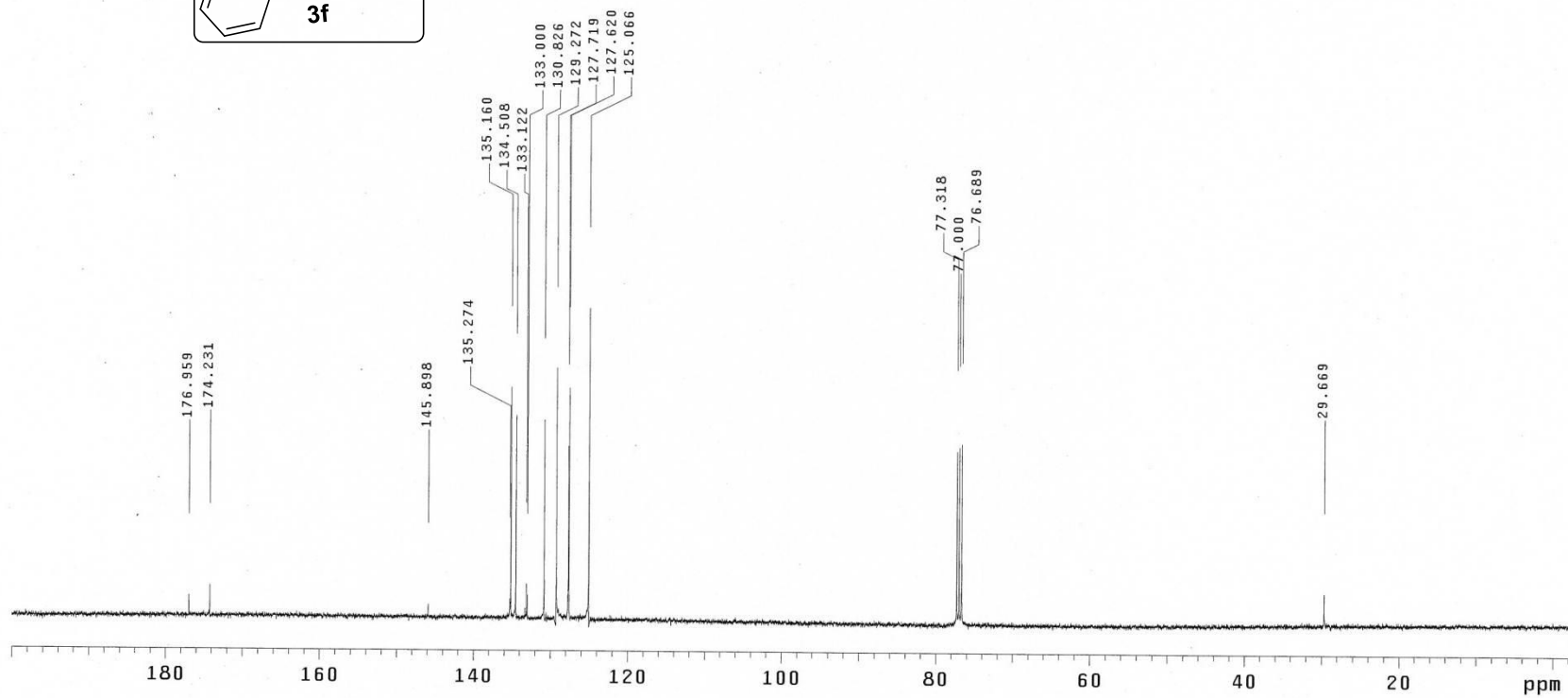
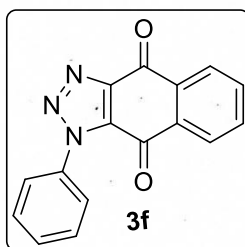
Mercury-400BB "MercuryPlus400"

Date: Mar 26 2014

Solvent: CDCl₃

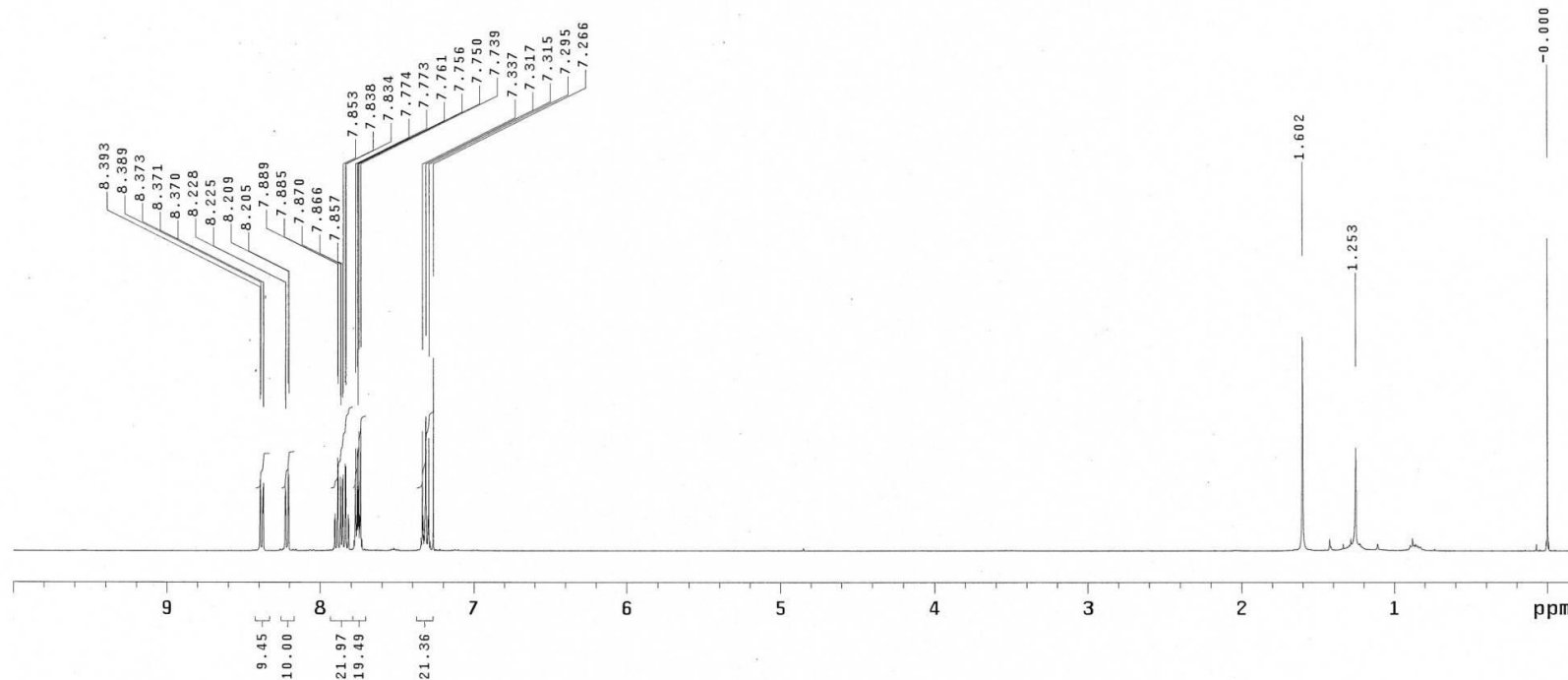
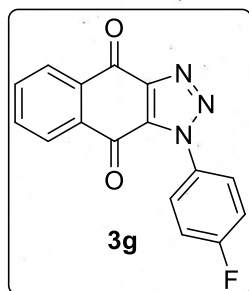
Ambient temperature

Total 7200 repetitions



NP-4F

Pulse Sequence: s2pu1
Mercury-400BB "MercuryPlus400"
Date: Mar 26 2014
Solvent: CDCl3
Ambient temperature
Total 80 repetitions



NP-4C1

Pulse Sequence: s2pu1

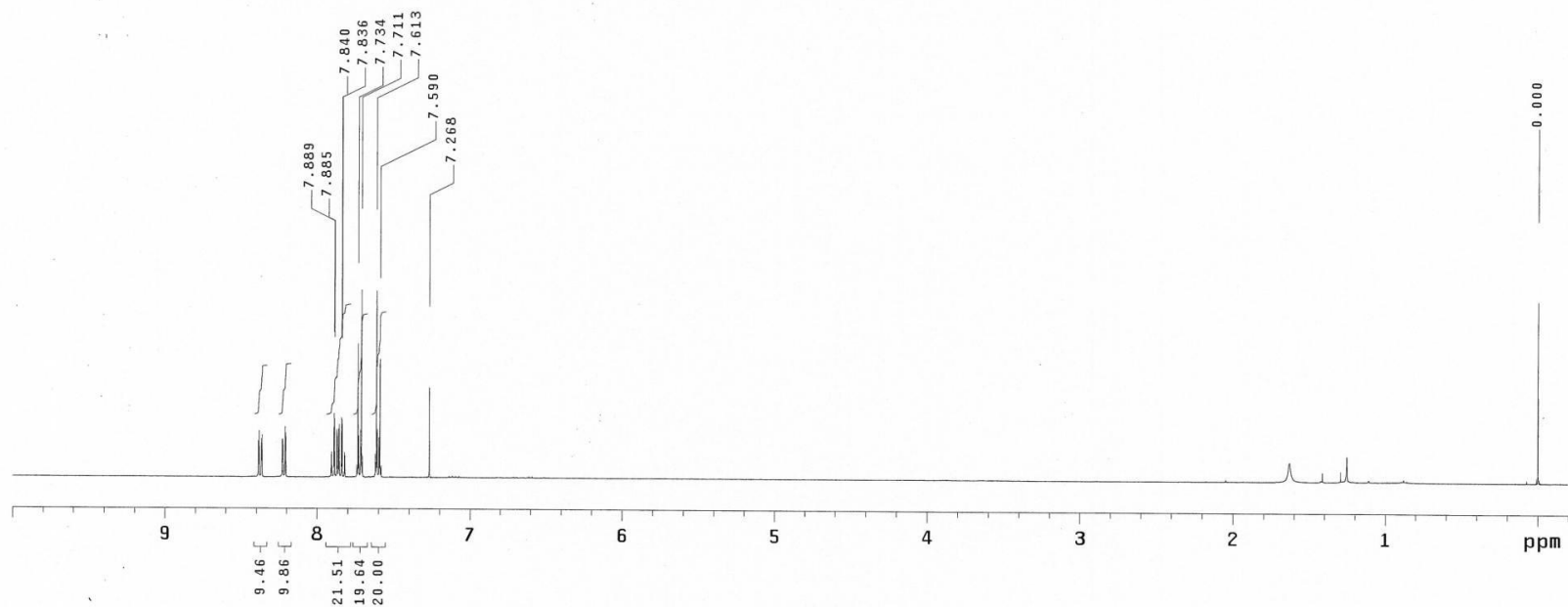
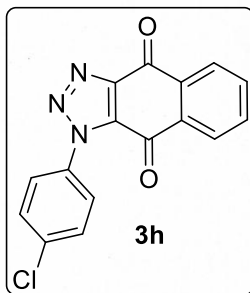
Mercury-400BB "MercuryPlus400"

Date: Mar 13 2014

Solvent: CDCl₃

Ambient temperature

Total 28 repetitions



NP-4C1

Pulse Sequence: s2pu1

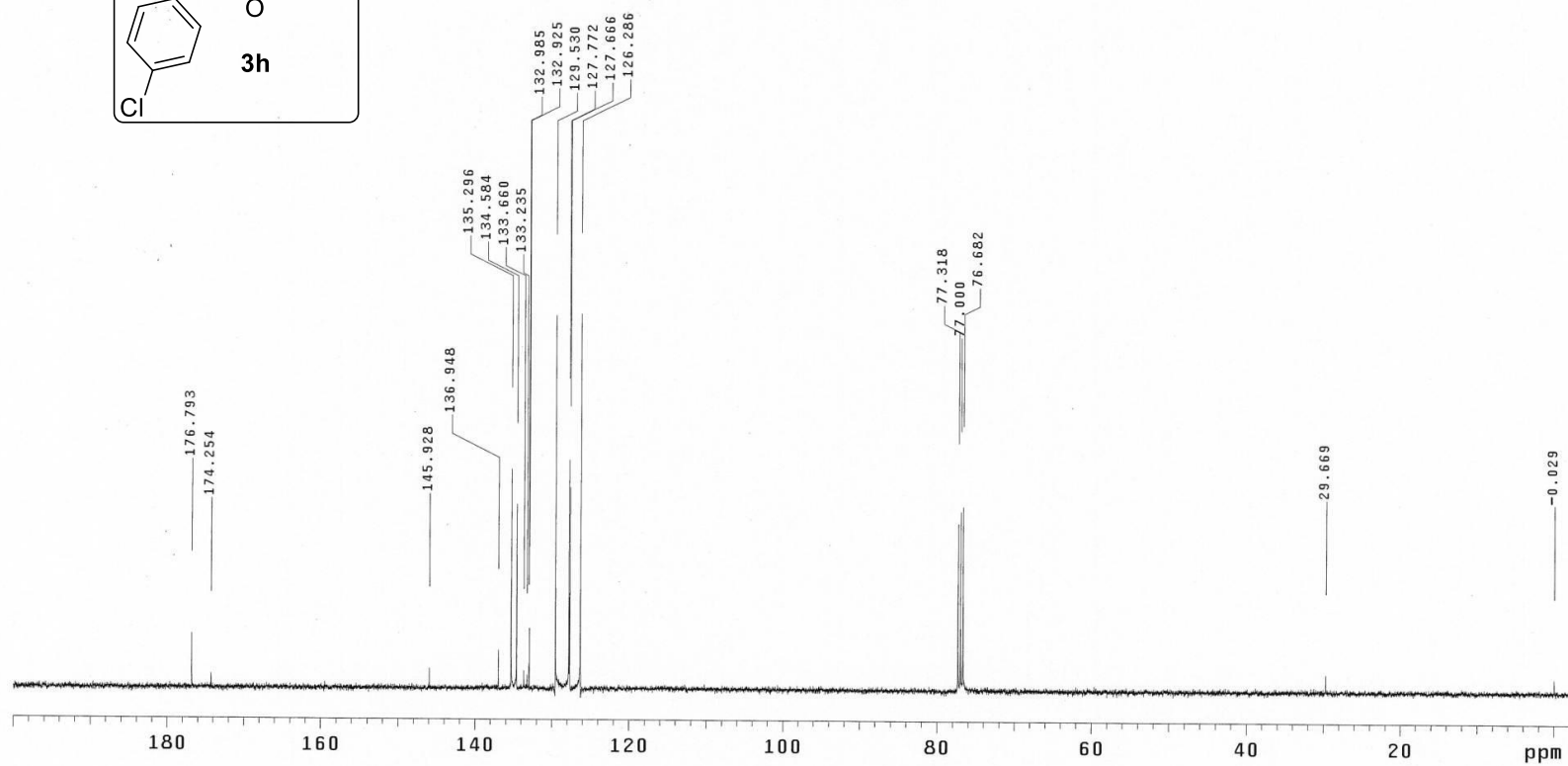
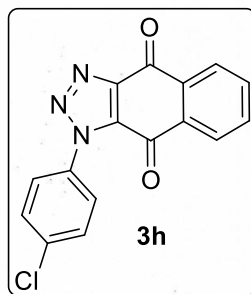
Mercury-400BB "MercuryPlus400"

Date: Mar 13 2014

Solvent: CDCl₃

Ambient temperature

Total 2528 repetitions



NP-3C1

Pulse Sequence: s2pu1

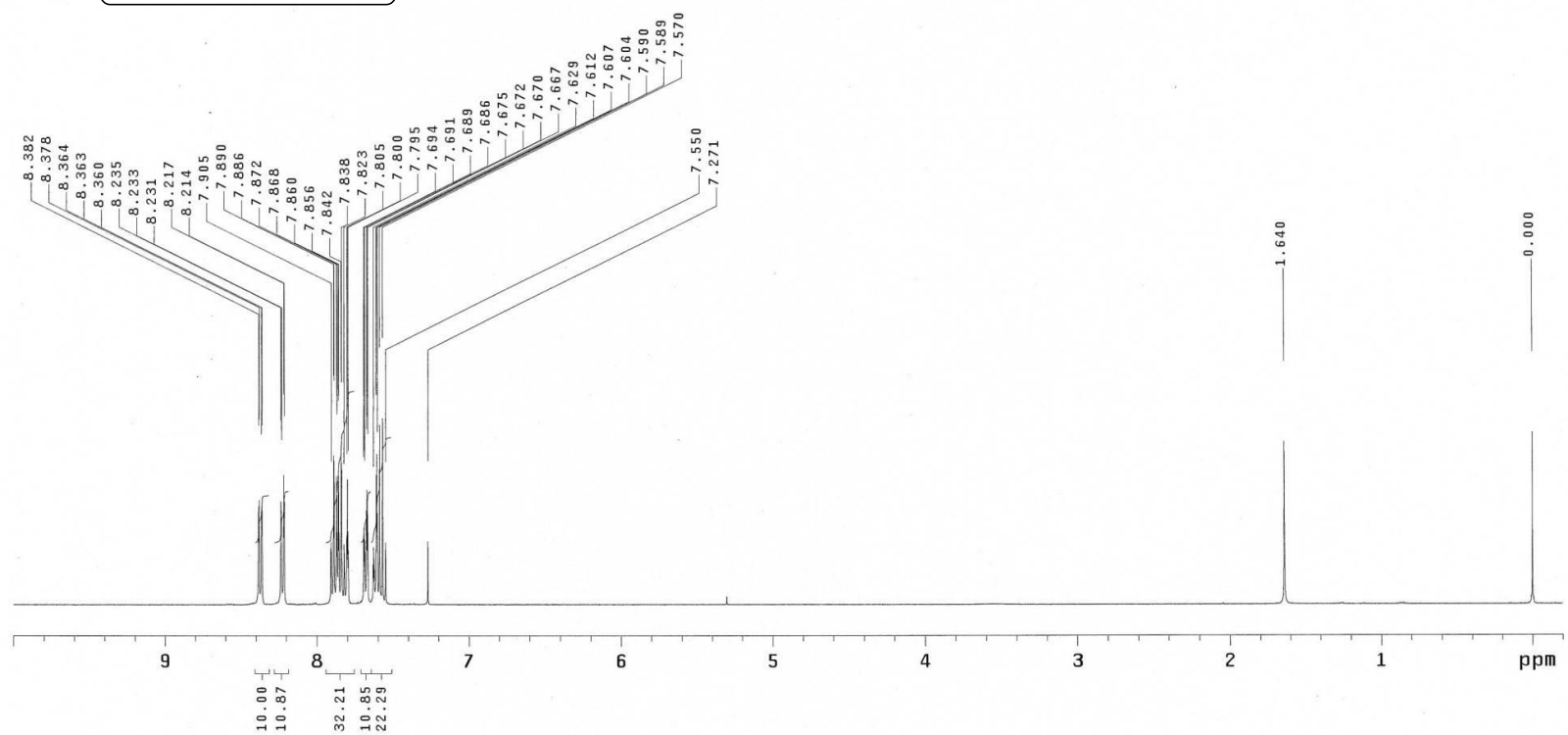
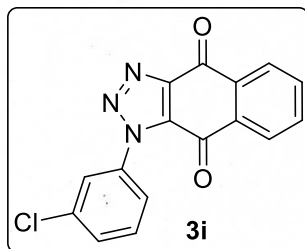
Mercury-400BB "MercuryPlus400"

Date: Mar 27 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



NP-3C1

Pulse Sequence: s2pu1

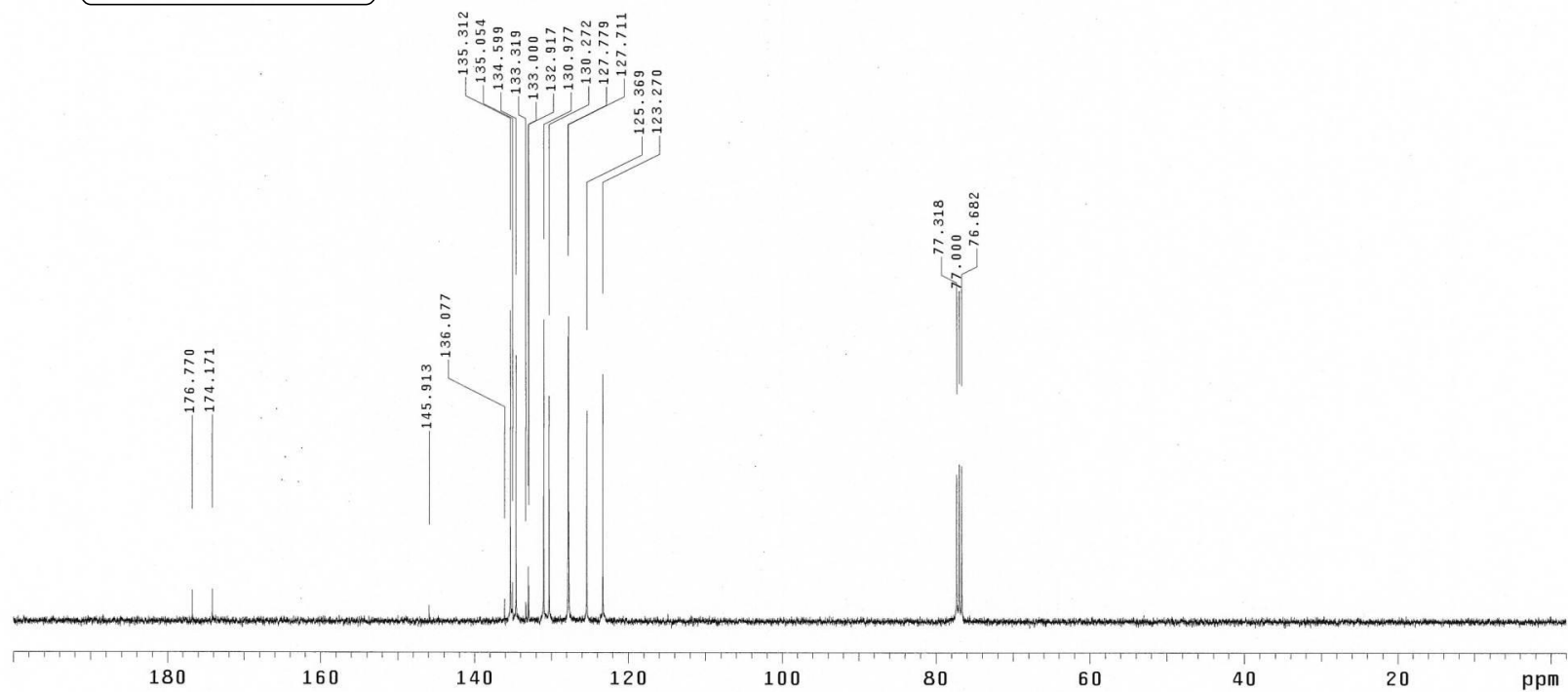
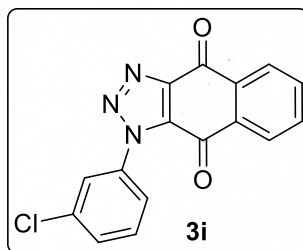
Mercury-400BB "MercuryPlus400"

Date: Mar 27 2014

Solvent: CDCl₃

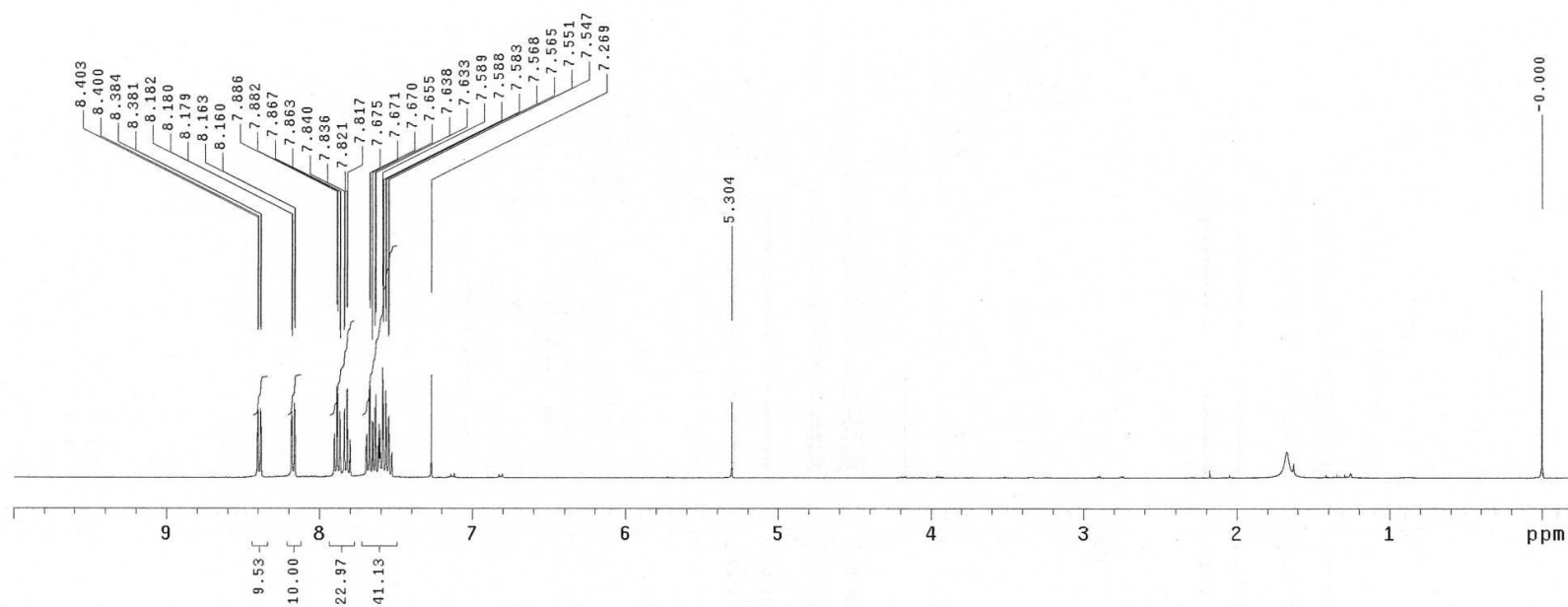
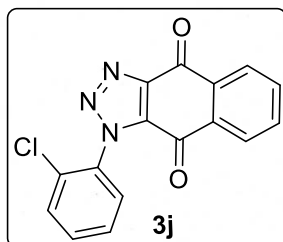
Ambient temperature

Total 9776 repetitions



NP-2C1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Apr 21 2014
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



NP-2C1

Pulse Sequence: s2pu1

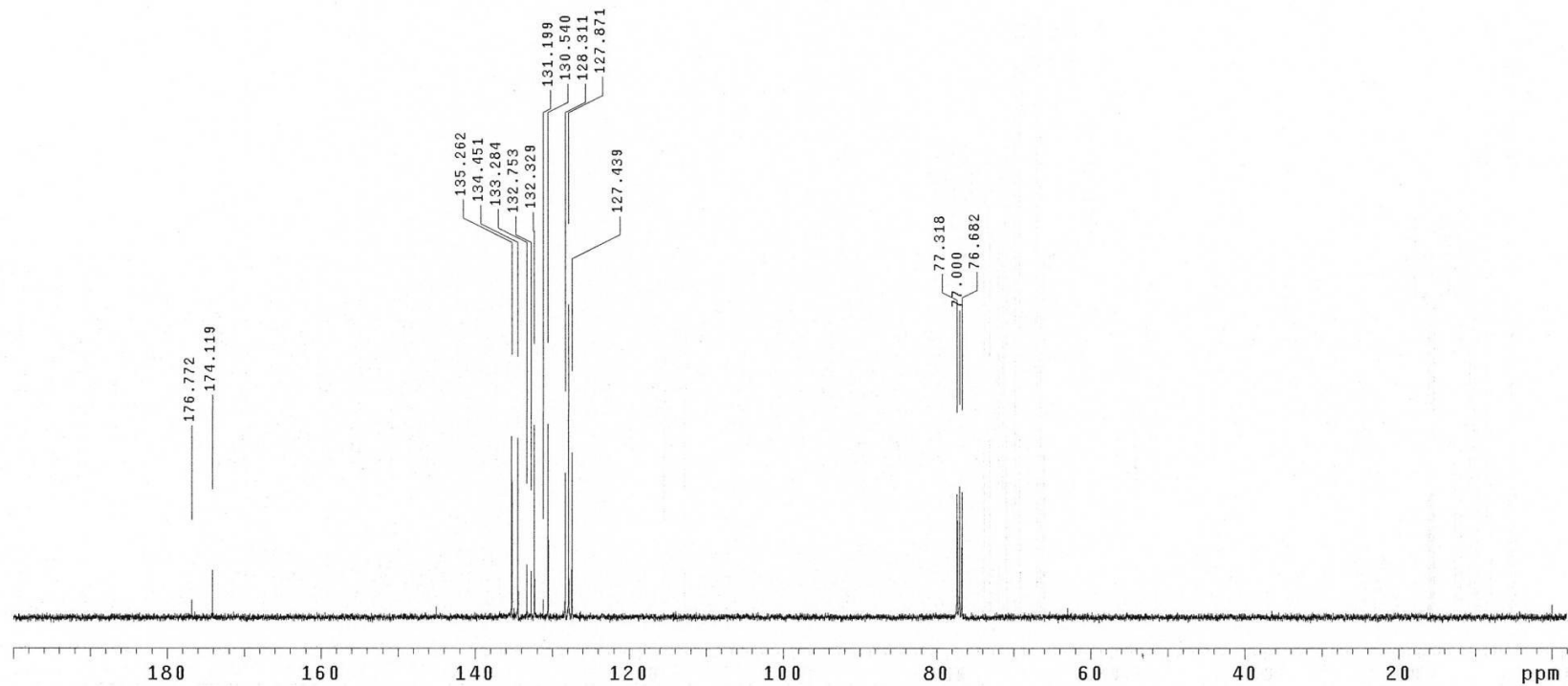
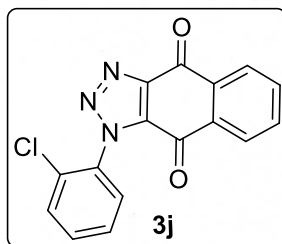
UNITYplus-400 "unity400"

Date: Apr 21 2014

Solvent: CDCl₃

Ambient temperature

Total 4288 repetitions



NP-4Br

Pulse Sequence: s2pu1

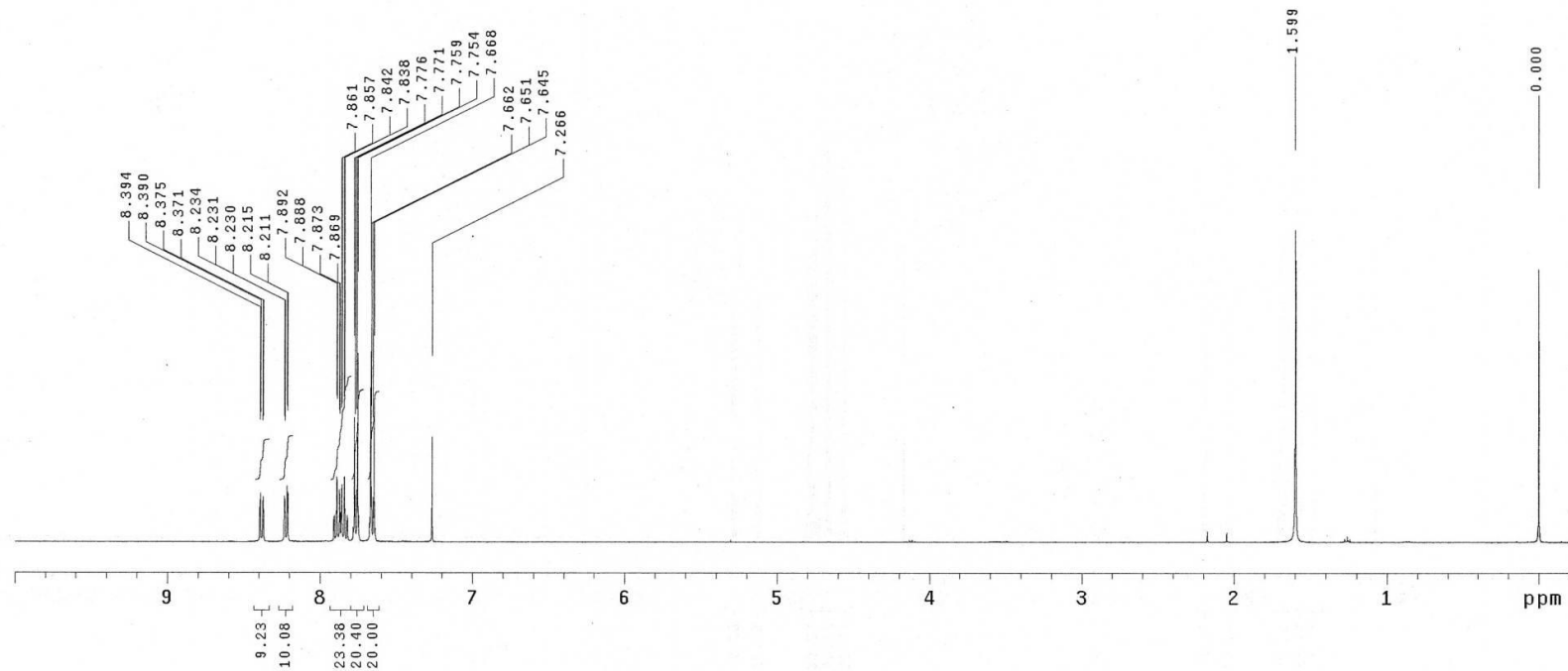
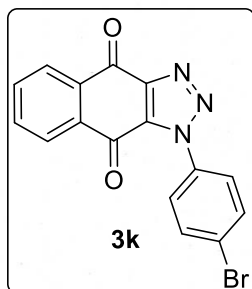
UNITYplus-400 "unity400"

Date: Apr 21 2014

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



NP-4Br

Pulse Sequence: s2pu1

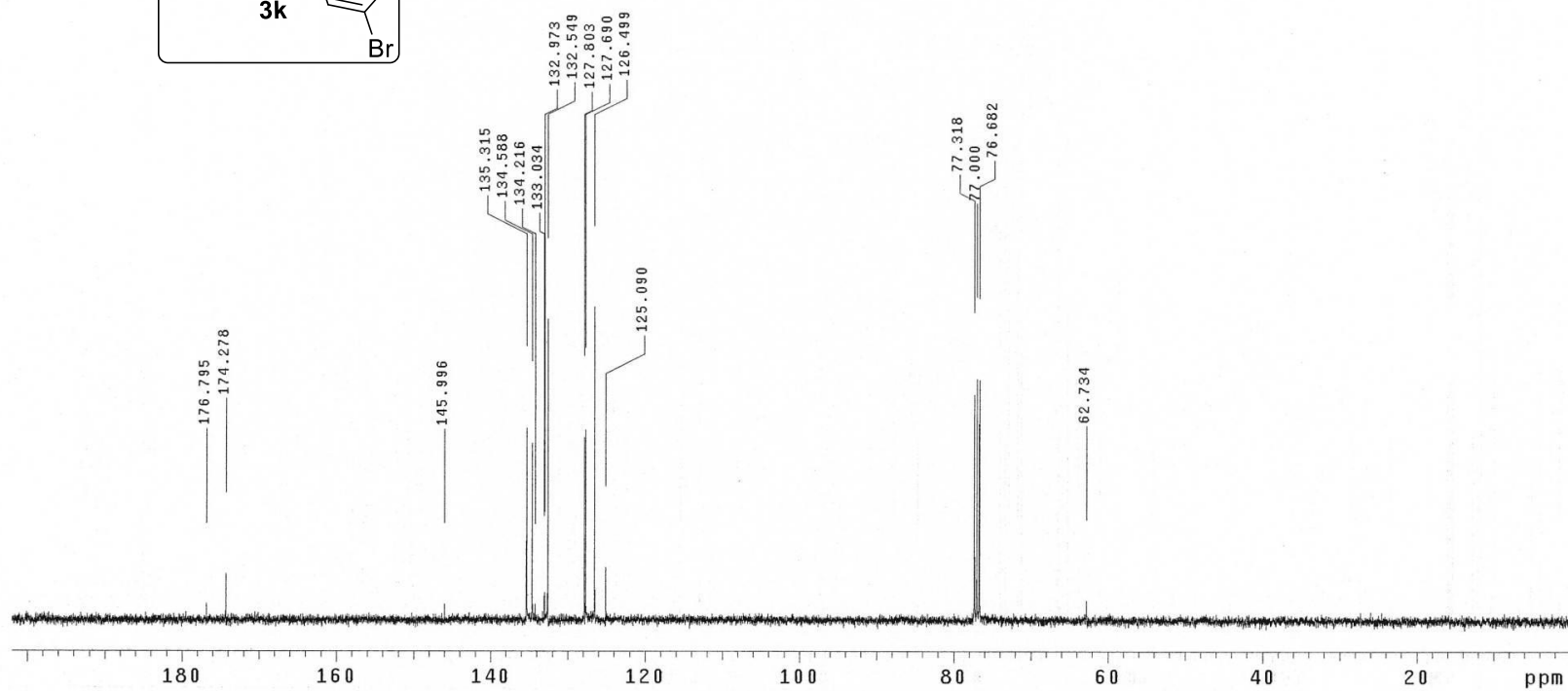
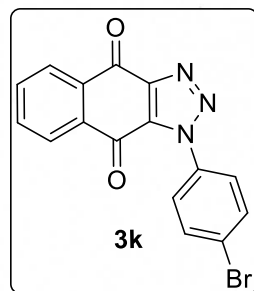
UNITYplus-400 "unity400"

Date: Apr 21 2014

Solvent: CDCl₃

Ambient temperature

Total 10784 repetitions



NP-4I

Pulse Sequence: s2pu1

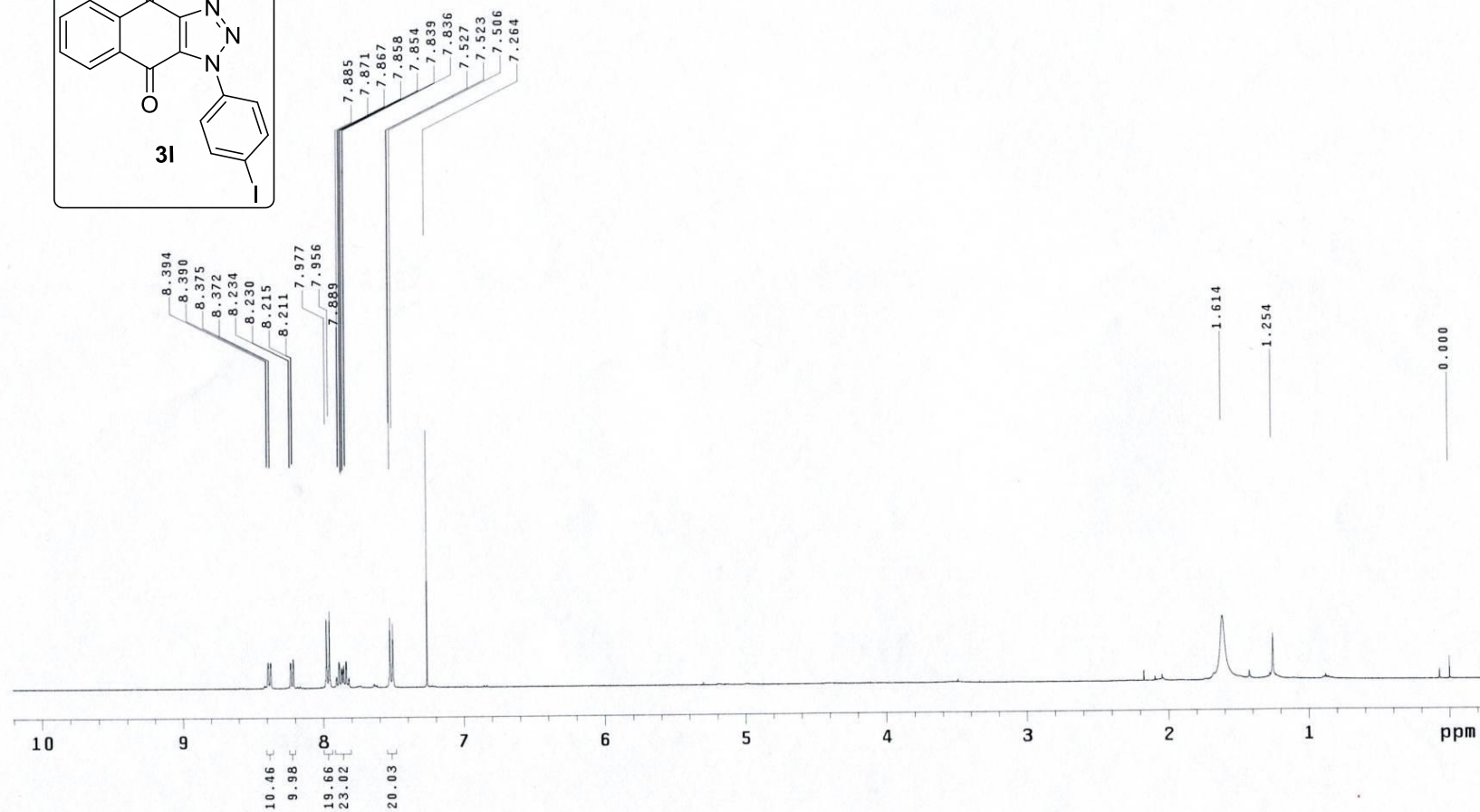
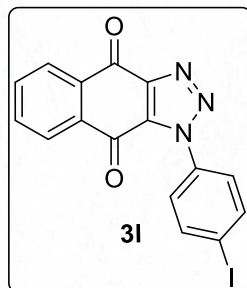
Mercury-400BB "MercuryPlus400"

Date: Aug 7 2014

Solvent: CDCl₃

Ambient temperature

Total 48 repetitions



NP-4I

Pulse Sequence: s2pu1

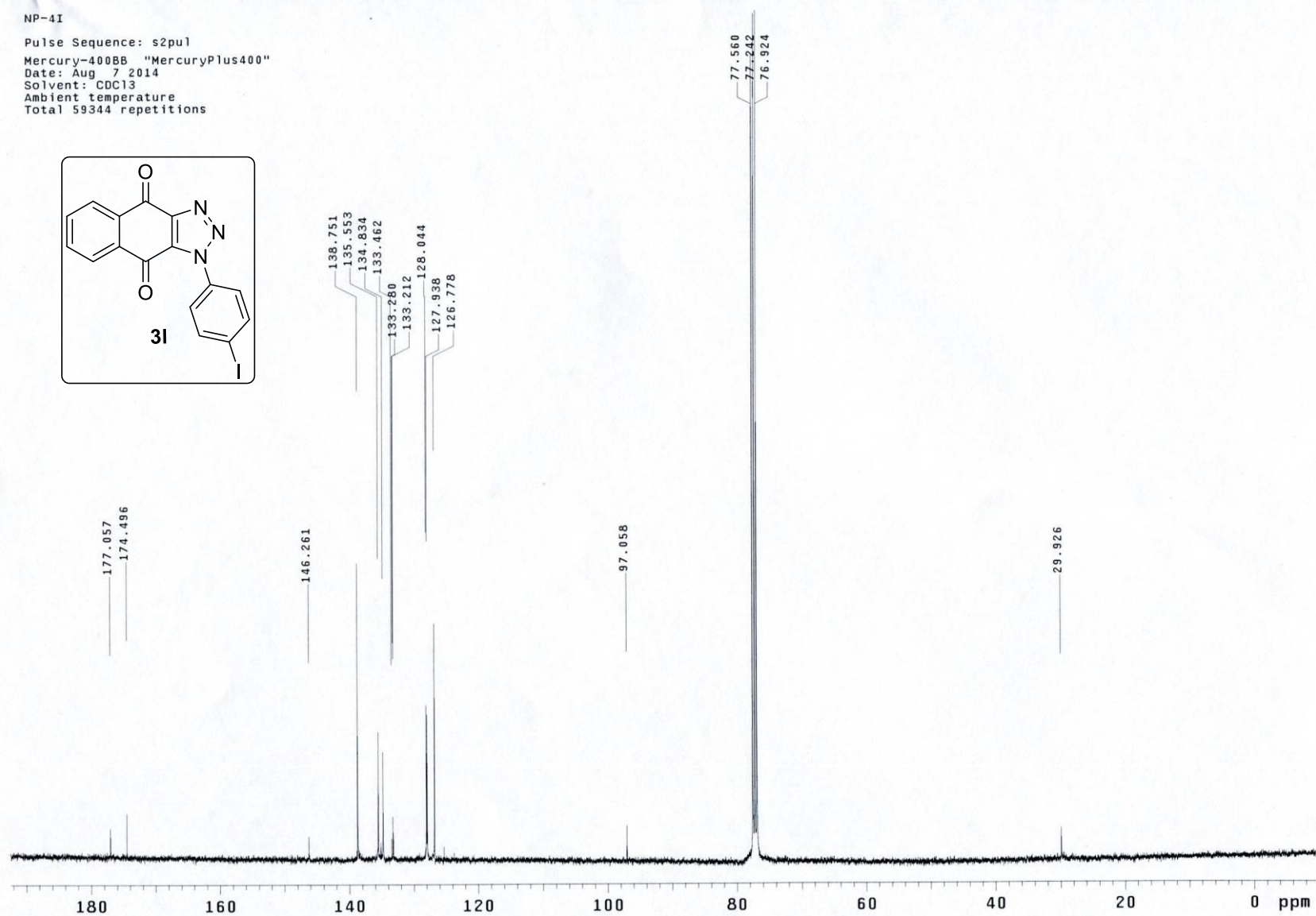
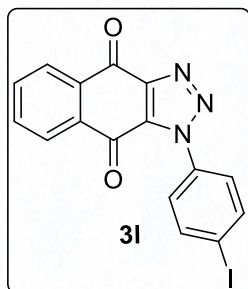
Mercury-400BB "MercuryPlus400"

Date: Aug 7 2014

Solvent: CDCl₃

Ambient temperature

Total 59344 repetitions



NP+5C

Pulse Sequence: s2pu1

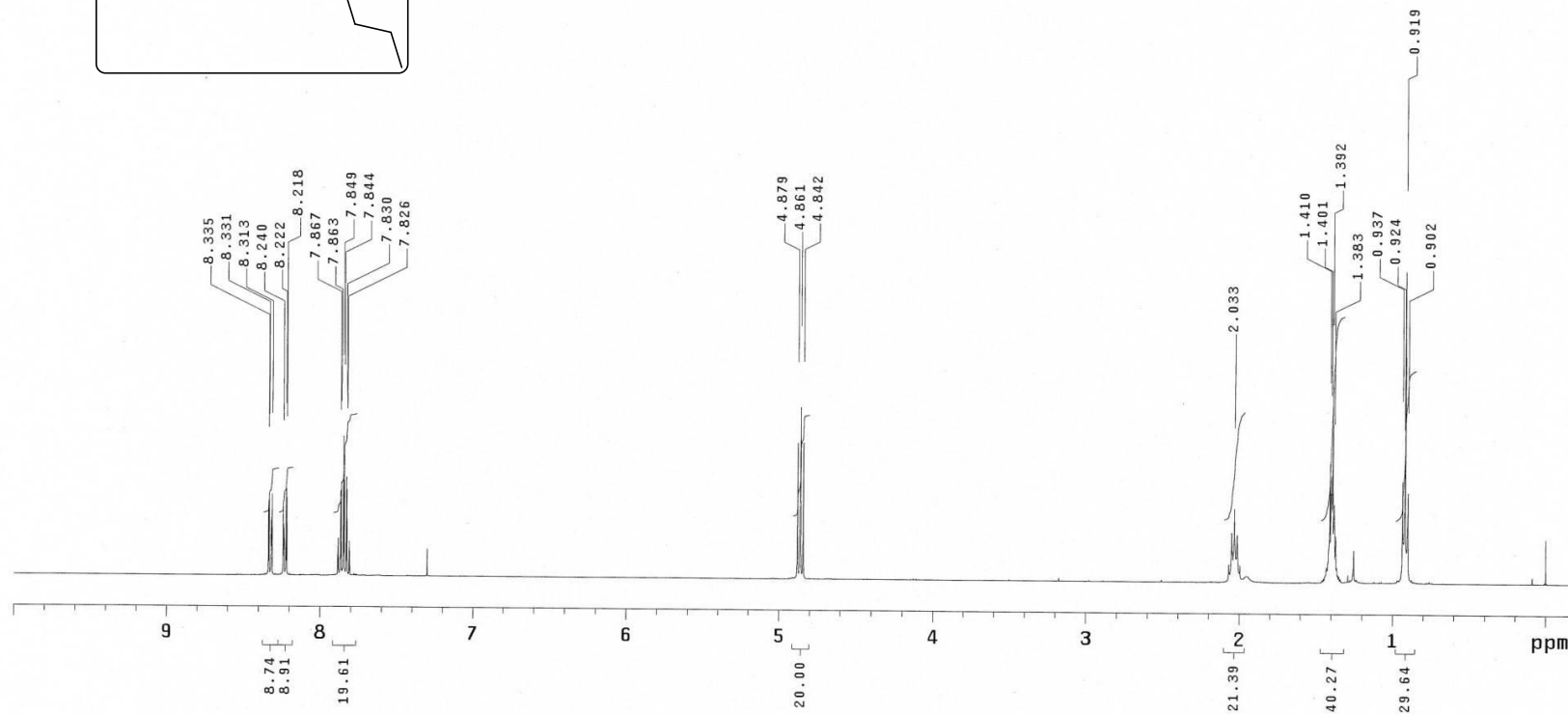
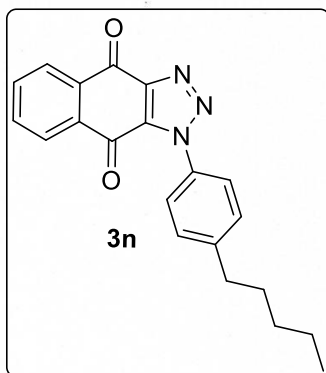
Mercury-400BB "MercuryPlus400"

Date: May 14 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



NP+5C

Pulse Sequence: s2pu1

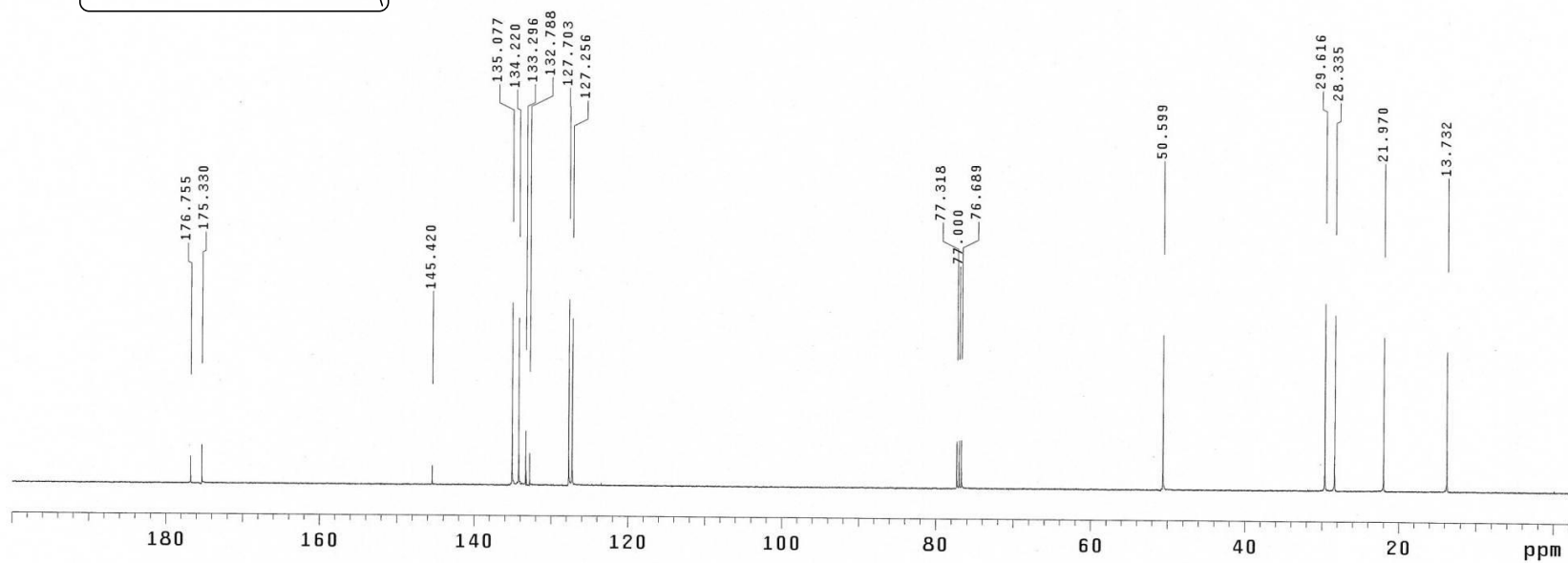
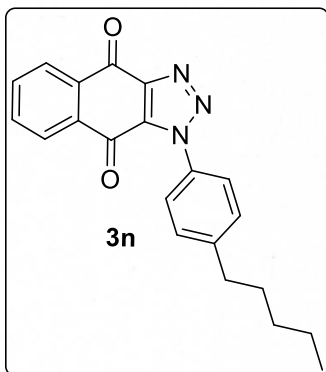
Mercury-400BB "MercuryPlus400"

Date: May 14 2014

Solvent: CDCl₃

Ambient temperature

Total 1840 repetitions



NP-10C

Pulse Sequence: s2pu1

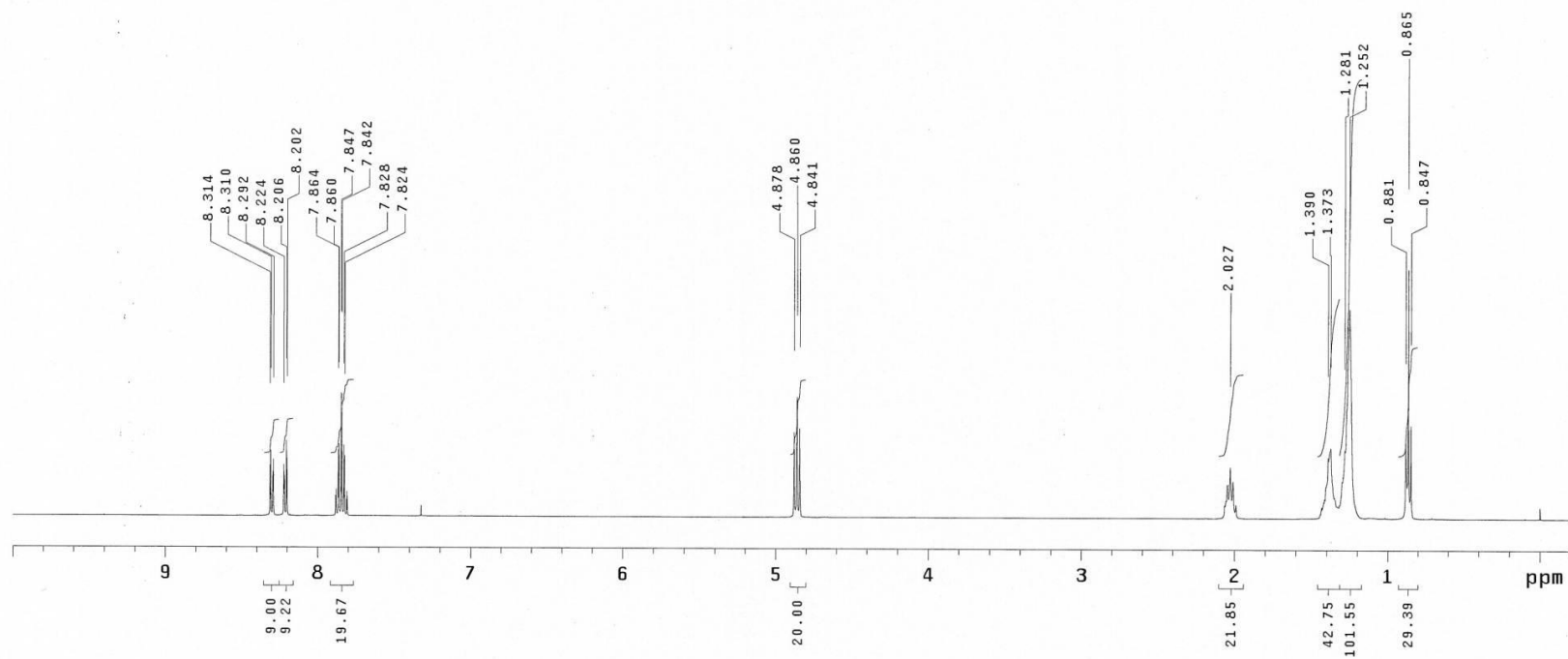
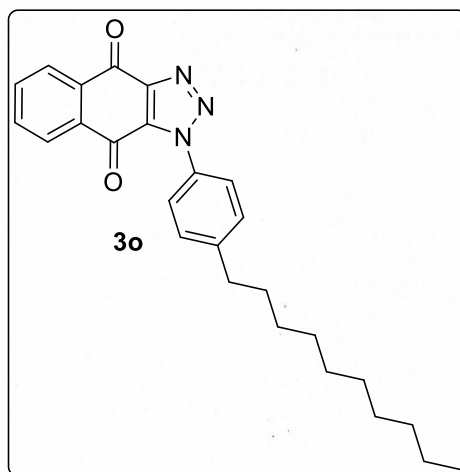
Mercury-400BB "MercuryPlus400"

Date: Mar 13 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



NP-10C

Pulse Sequence: s2pu1

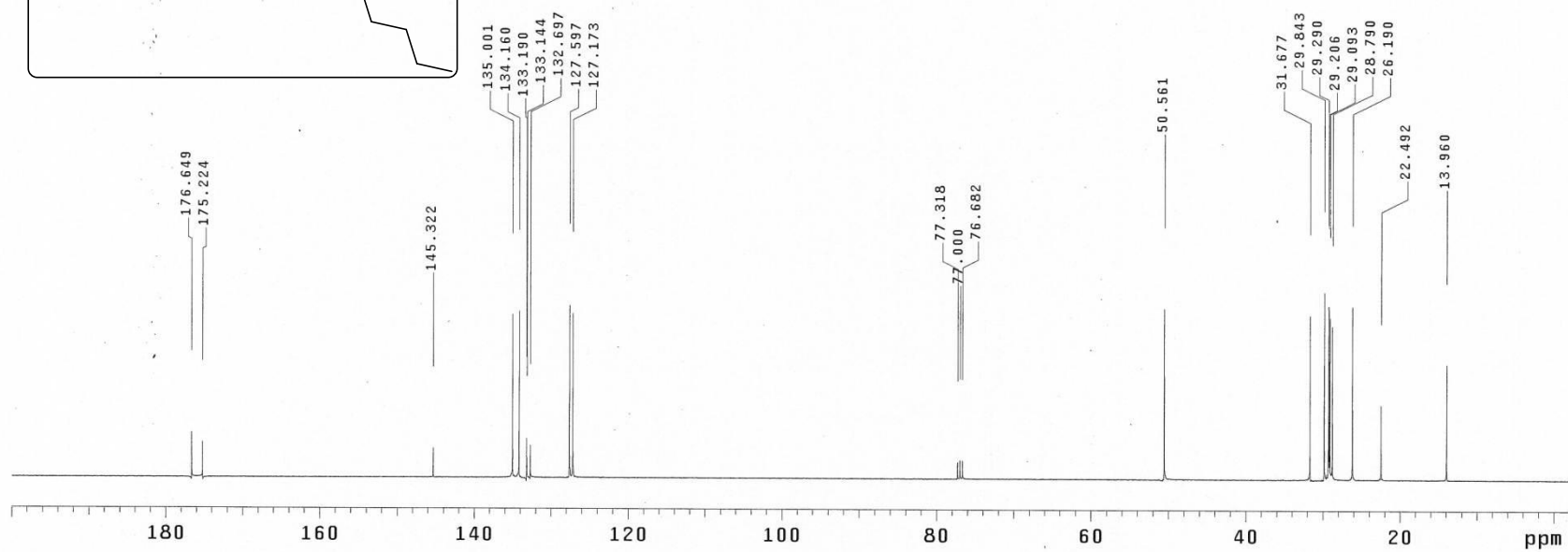
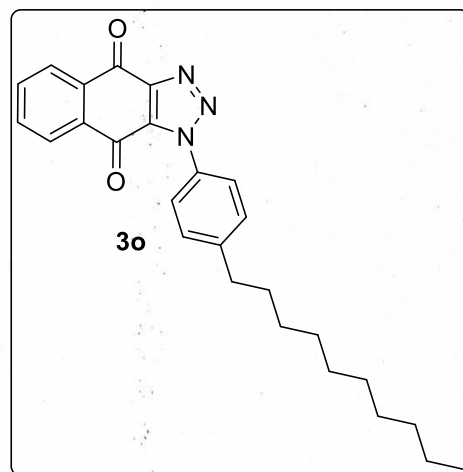
Mercury-400BB : "MercuryPlus400"

Date: Mar 13 2014

Solvent: CDCl₃

Ambient temperature

Total 2240 repetitions



NP-Bn

Pulse Sequence: s2pu1

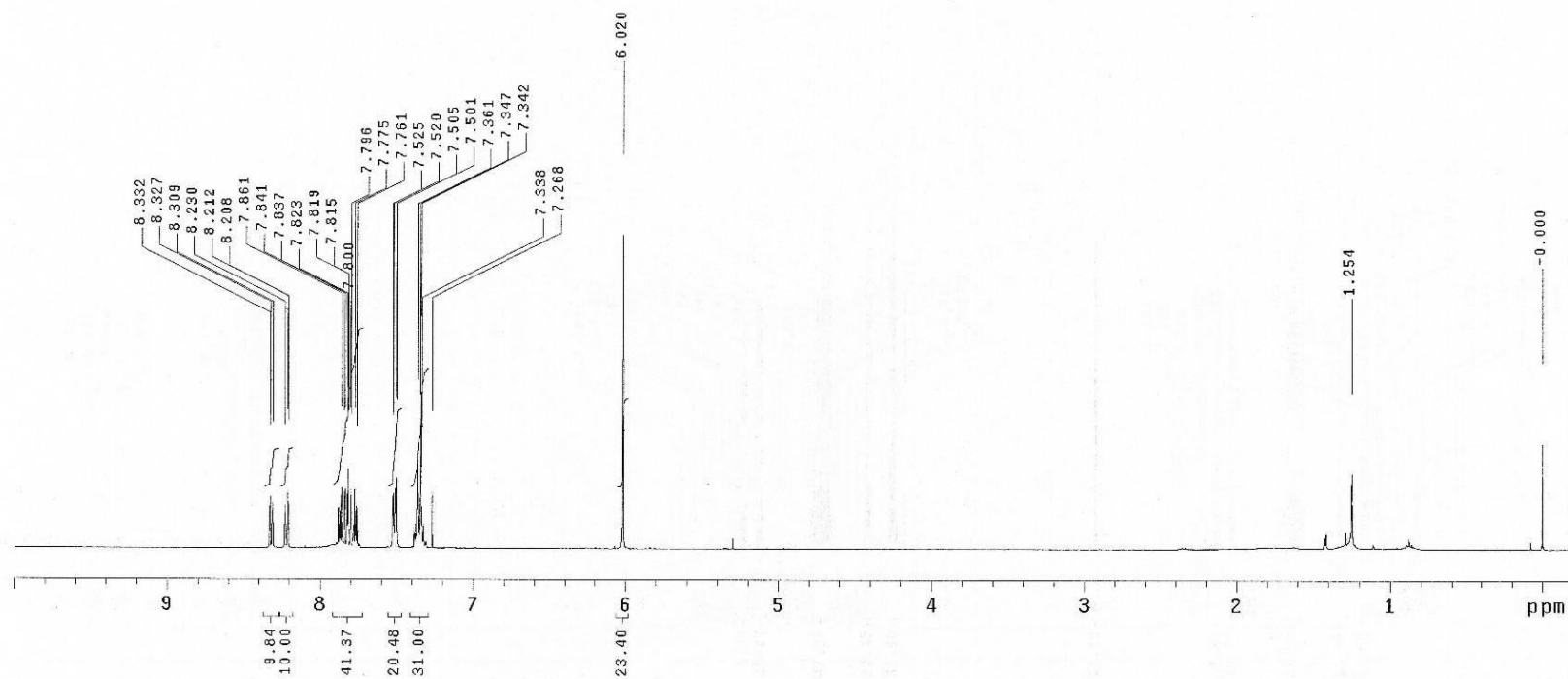
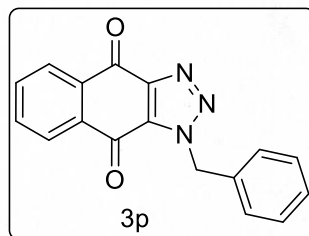
UNITYplus-400 "unity400"

Date: Mar 5 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



NP-Bn

Pulse Sequence: s2pu1

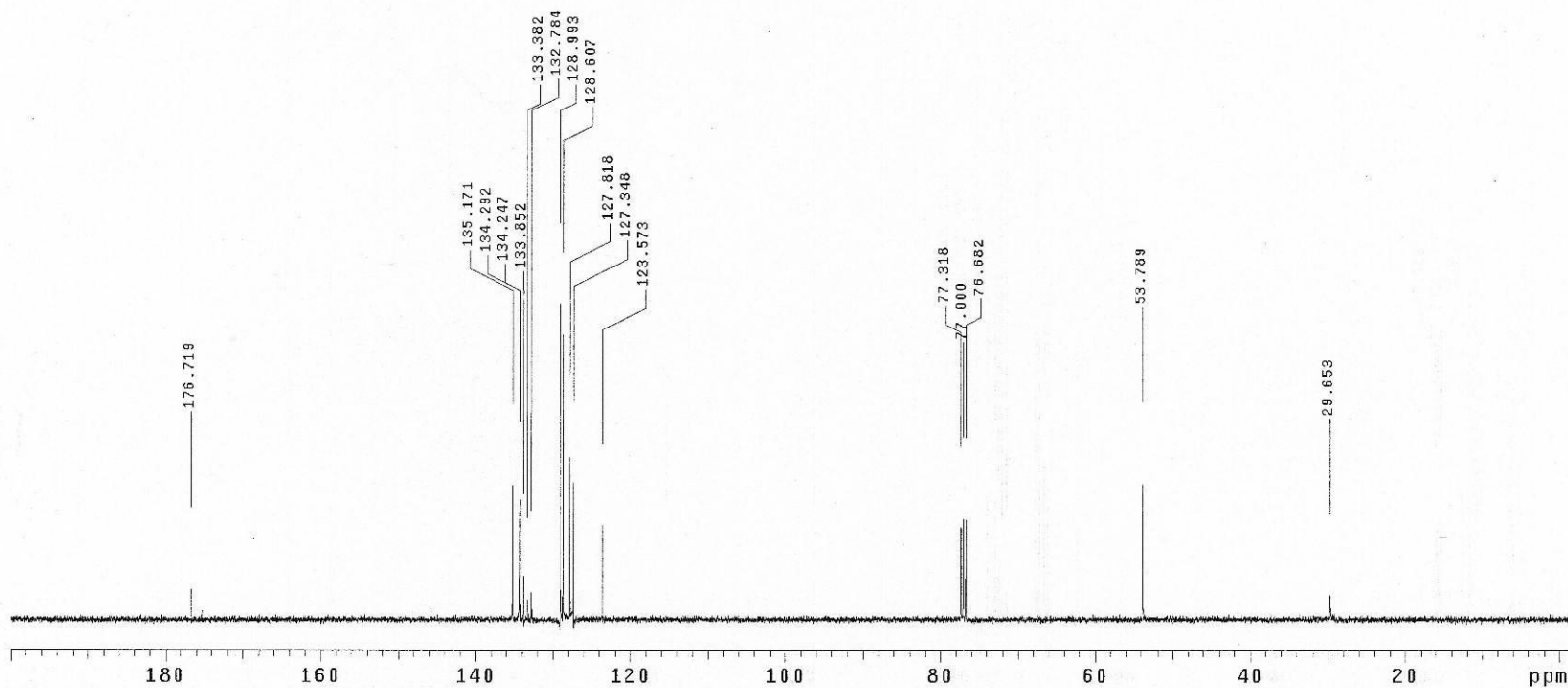
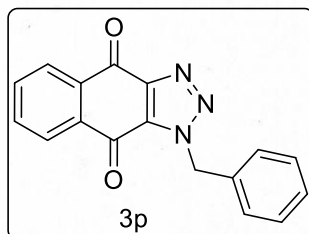
UNITYplus-400 "unity400"

Date: Mar 5 2014

Solvent: CDCl₃

Ambient temperature

Total 3056 repetitions



4N3-NP

Pulse Sequence: s2pu1

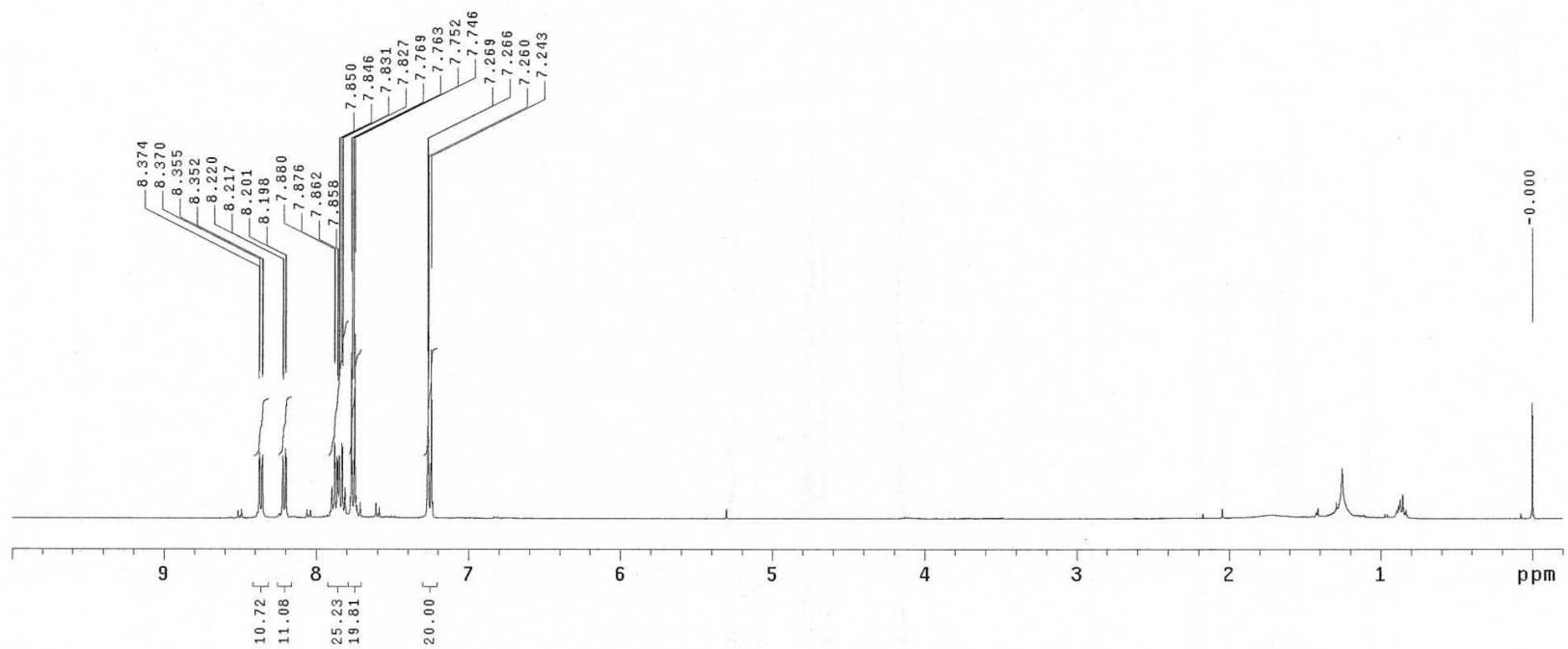
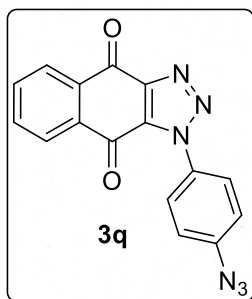
UNITYplus-400 "unity400"

Date: Jun 26 2014

Solvent: CDC13

Ambient temperature

Total 64 repetitions



4N3-NP

Pulse Sequence: s2pu1

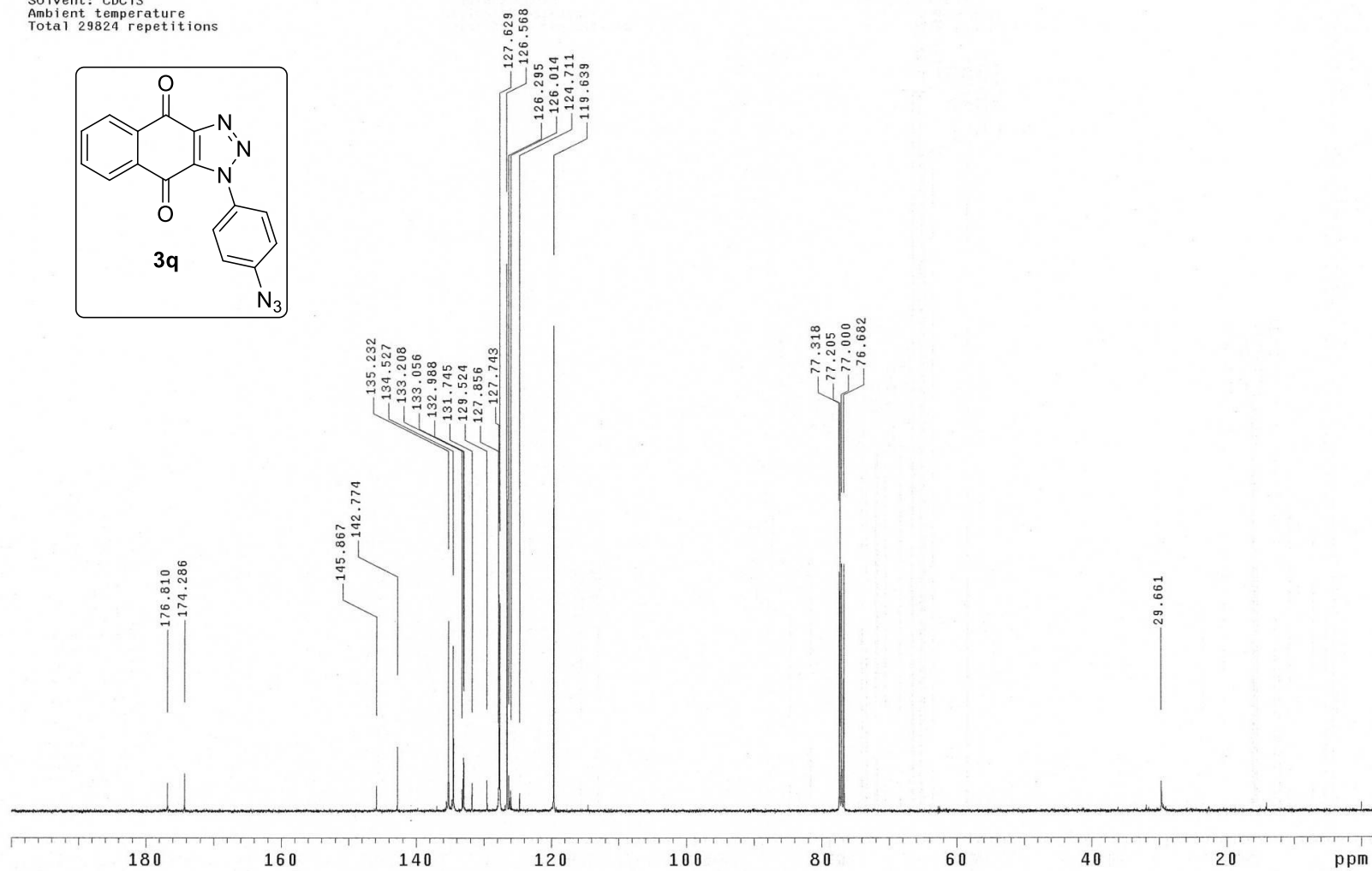
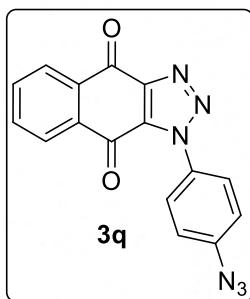
UNITYplus-400 "unity400"

Date: Jun 26 2014

Solvent: CDCl₃

Ambient temperature

Total 29824 repetitions



3N3-NP

Pulse Sequence: s2pu1

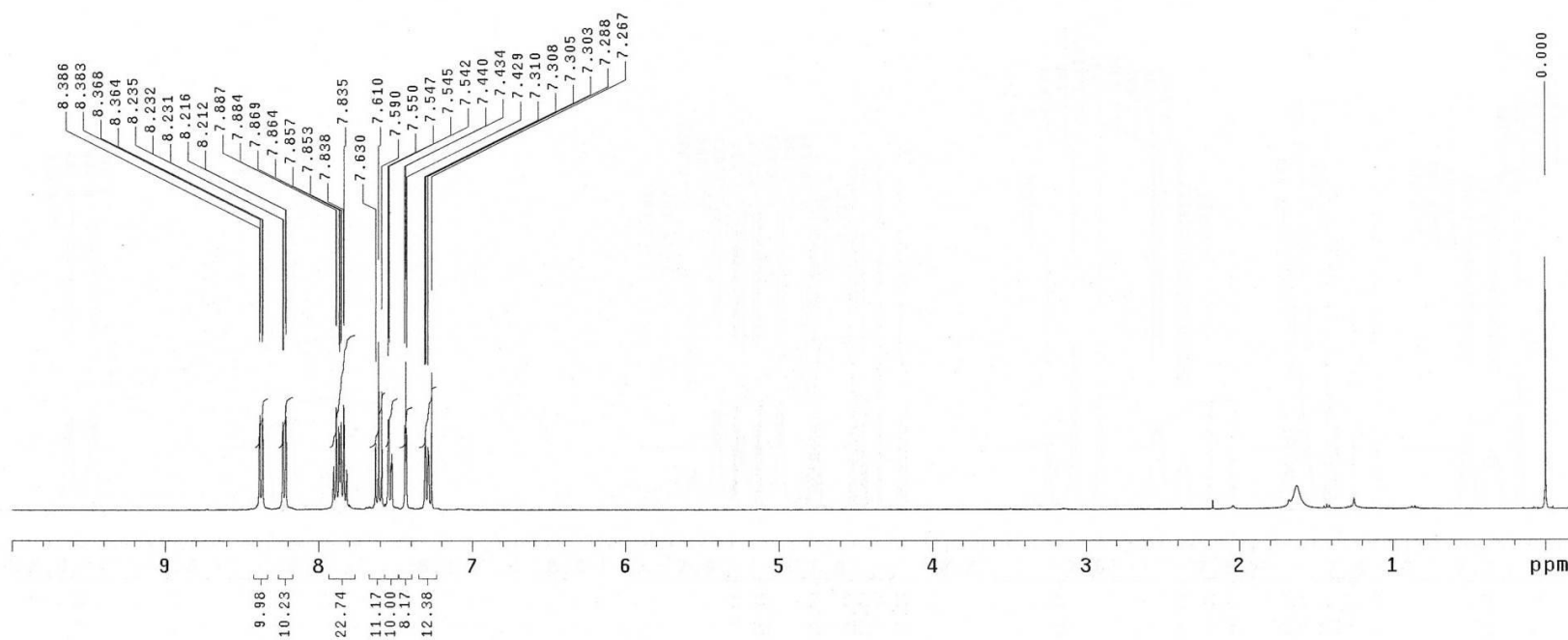
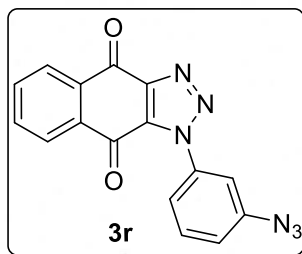
UNITYplus-400 "unity400"

Date: Jun 26 2014

Solvent: CDCl₃

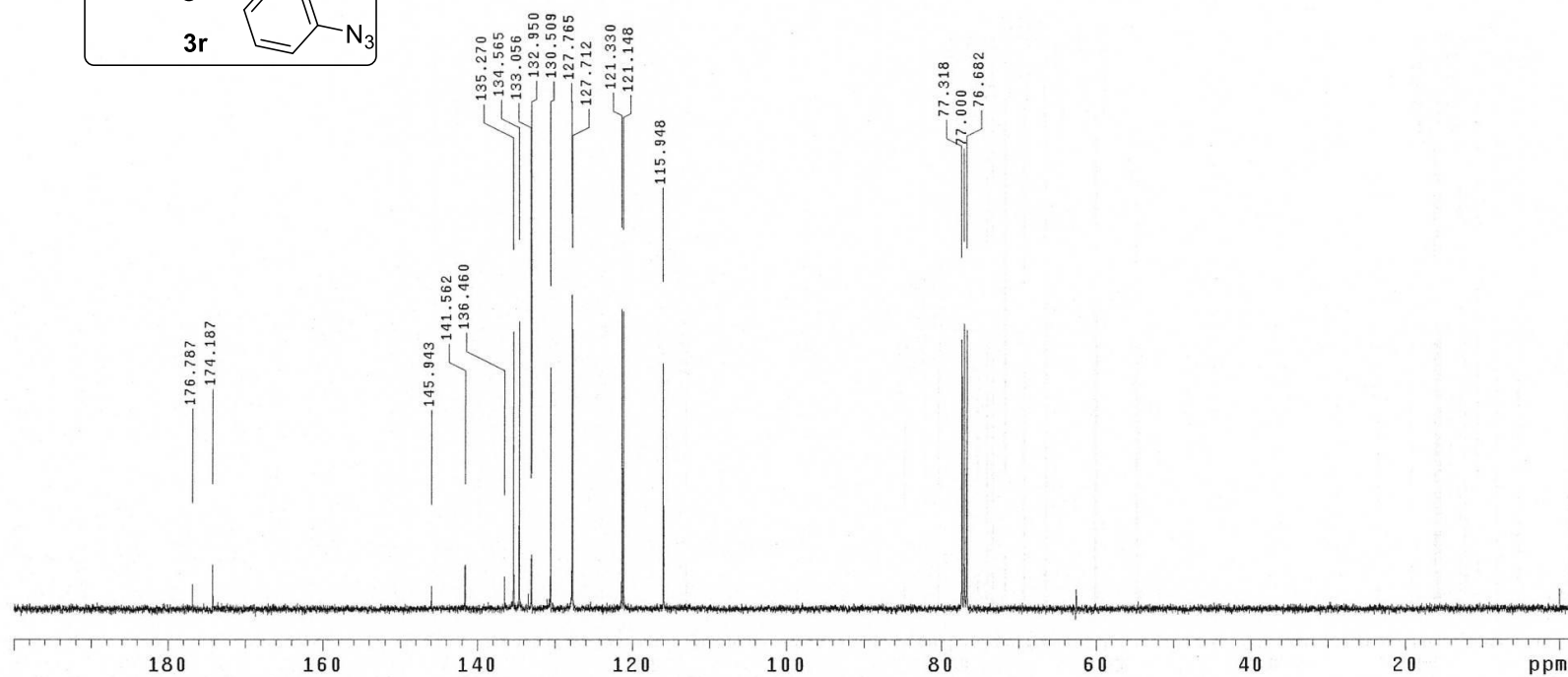
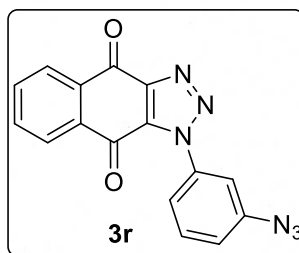
Ambient temperature

Total 64 repetitions



3N3-NP

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jun 26 2014
Solvent: CDCl₃
Ambient temperature
Total 13328 repetitions



BNP-Tome

Pulse Sequence: s2pu1

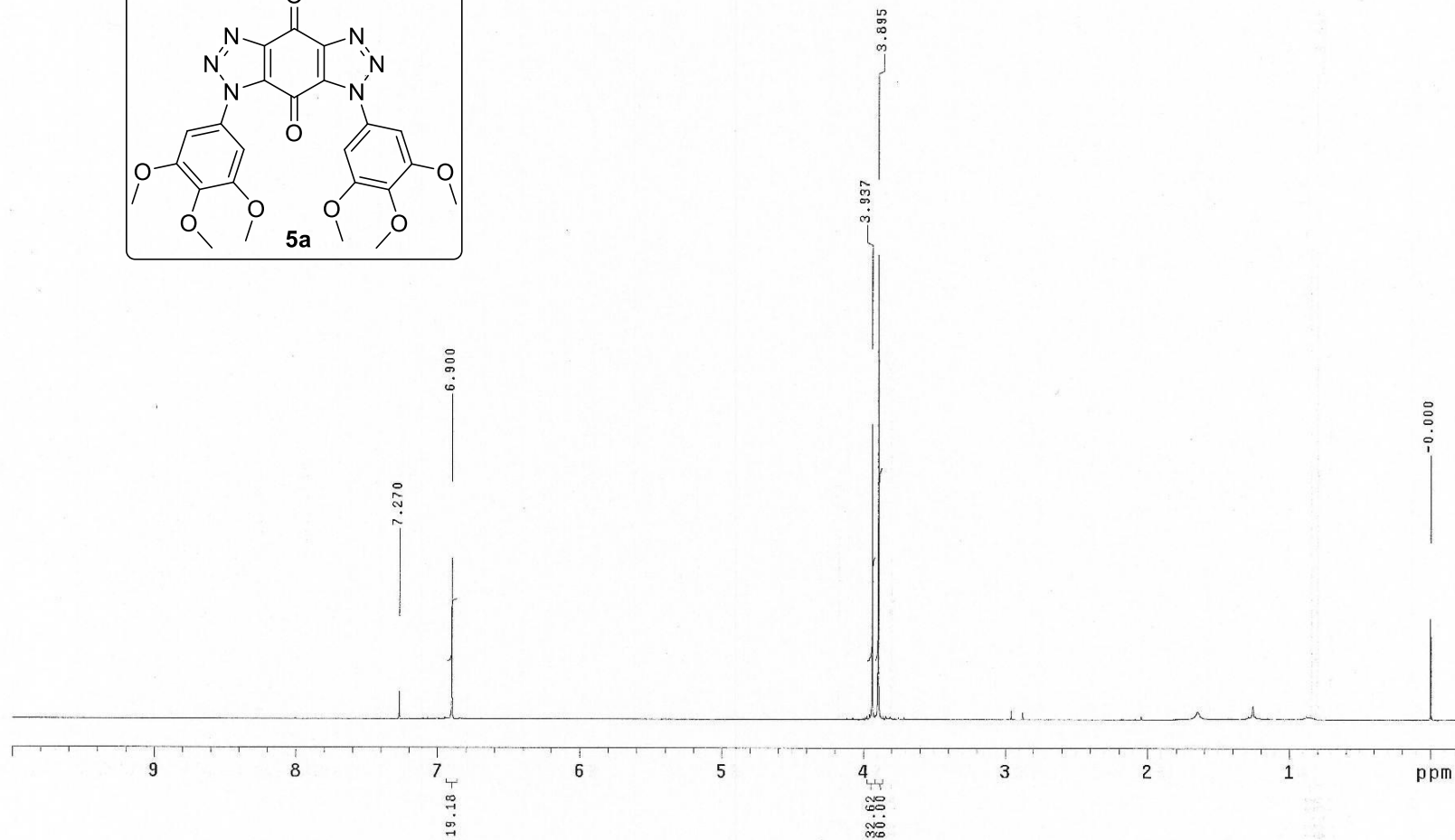
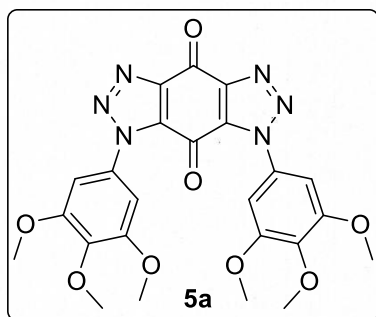
UNITYplus-400 "unity400"

Date: Aug 21 2013

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



BNP-Tome

Pulse Sequence: s2pu1

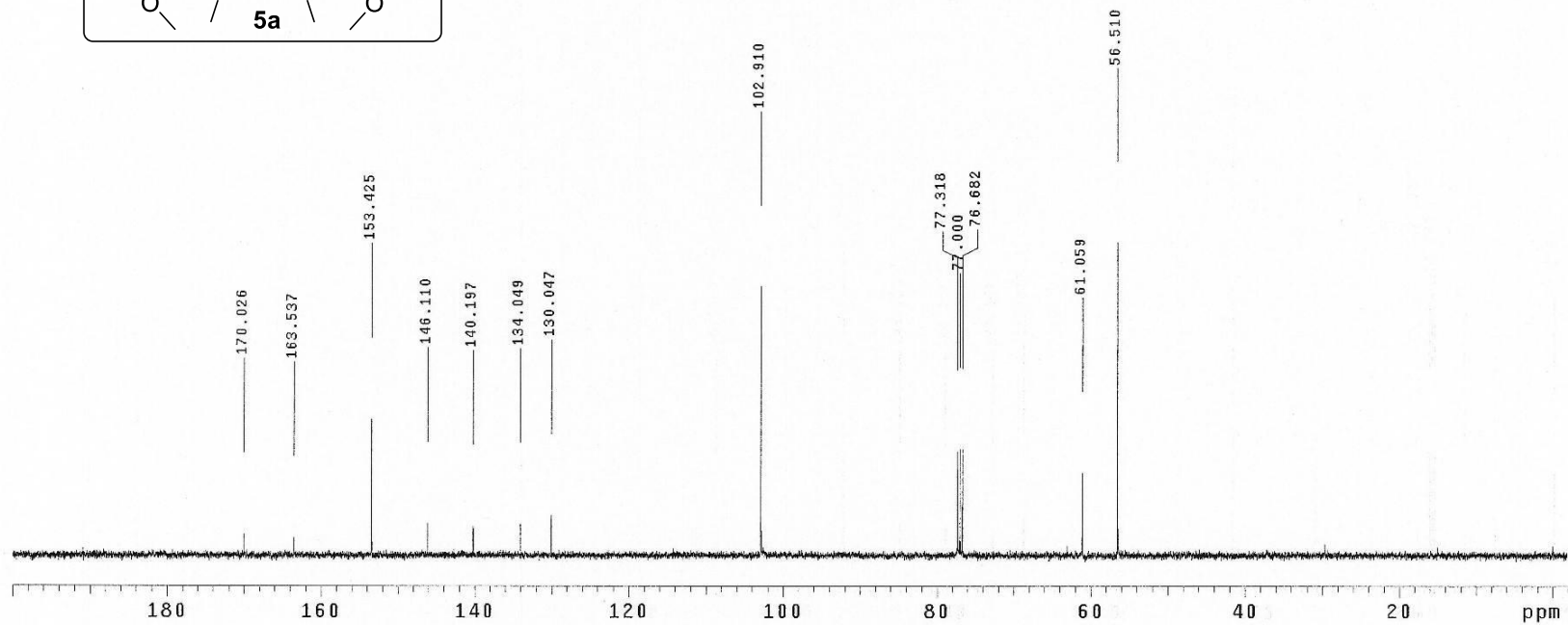
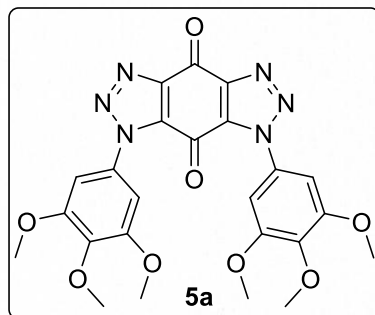
UNITYplus-400 "unity400"

Date: Aug 21 2013

Solvent: CDCl₃

Ambient temperature

Total 2048 repetitions



BN-4OMe

Pulse Sequence: s2pu1

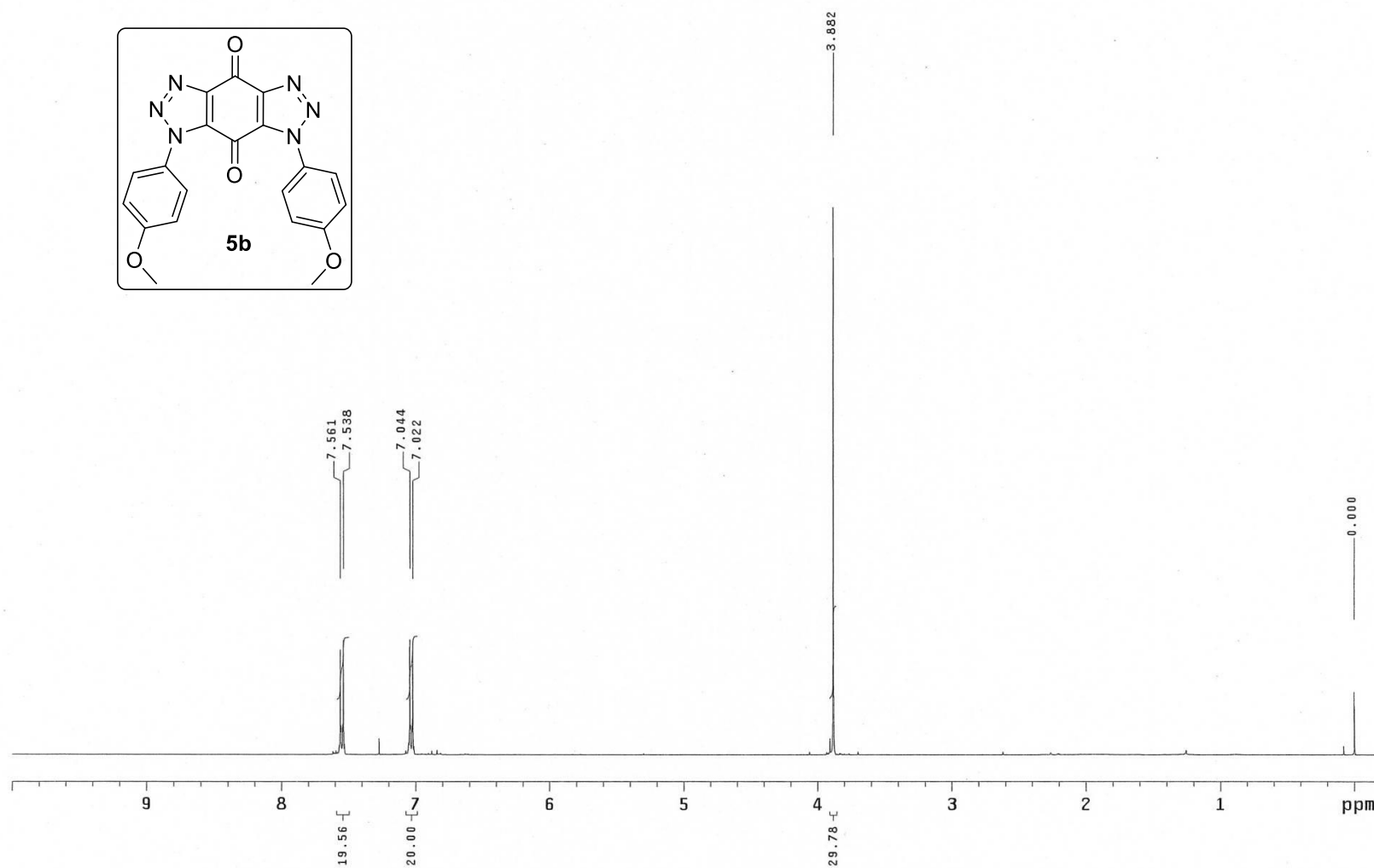
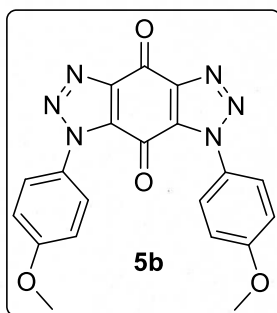
Mercury-400BB "MercuryPlus400"

Date: Apr 28 2014

Solvent: CDCl₃

Ambient temperature

Total 24 repetitions



BN-4OMe

Pulse Sequence: s2pu1

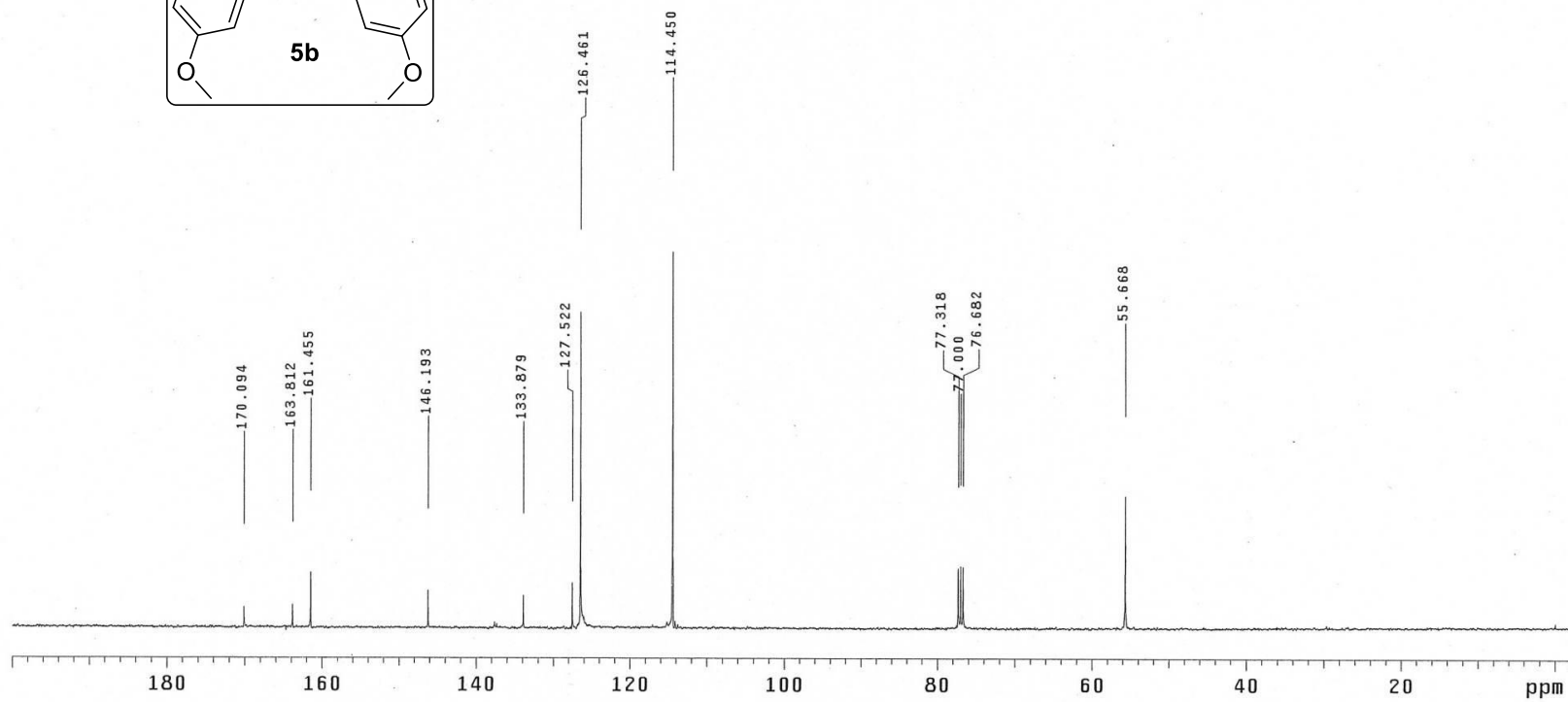
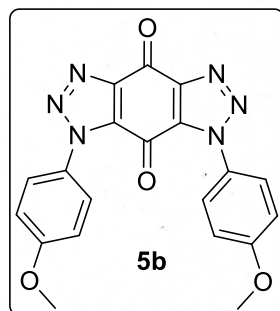
Mercury-400BB "MercuryPlus400"

Date: Apr 28 2014

Solvent: CDCl₃

Ambient temperature

Total 1296 repetitions



BN-2.4Me

Pulse Sequence: s2pu1

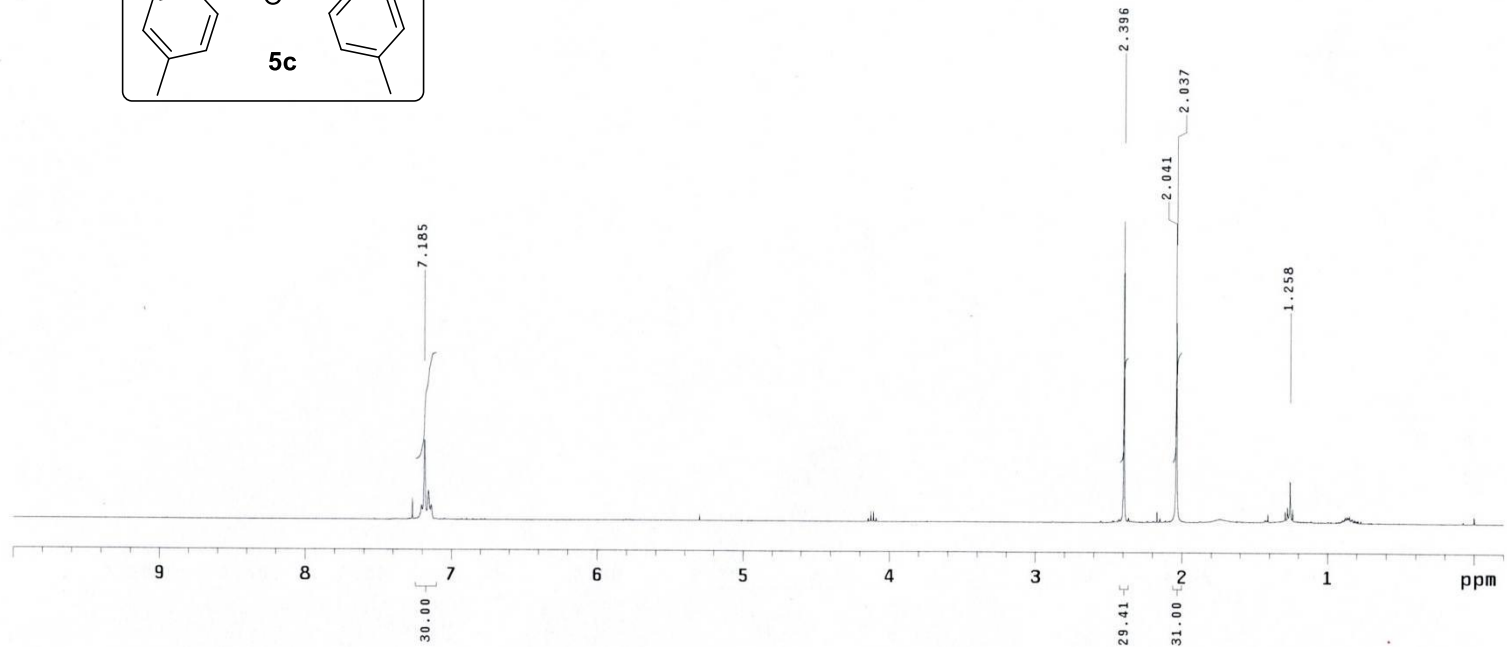
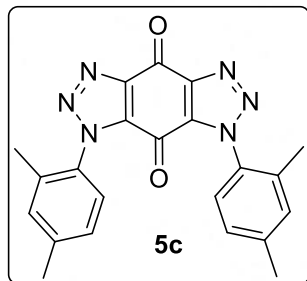
Mercury-400BB "MercuryPlus400"

Date: Aug 26 2014

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



BN-2.4Me

Pulse Sequence: s2pu1

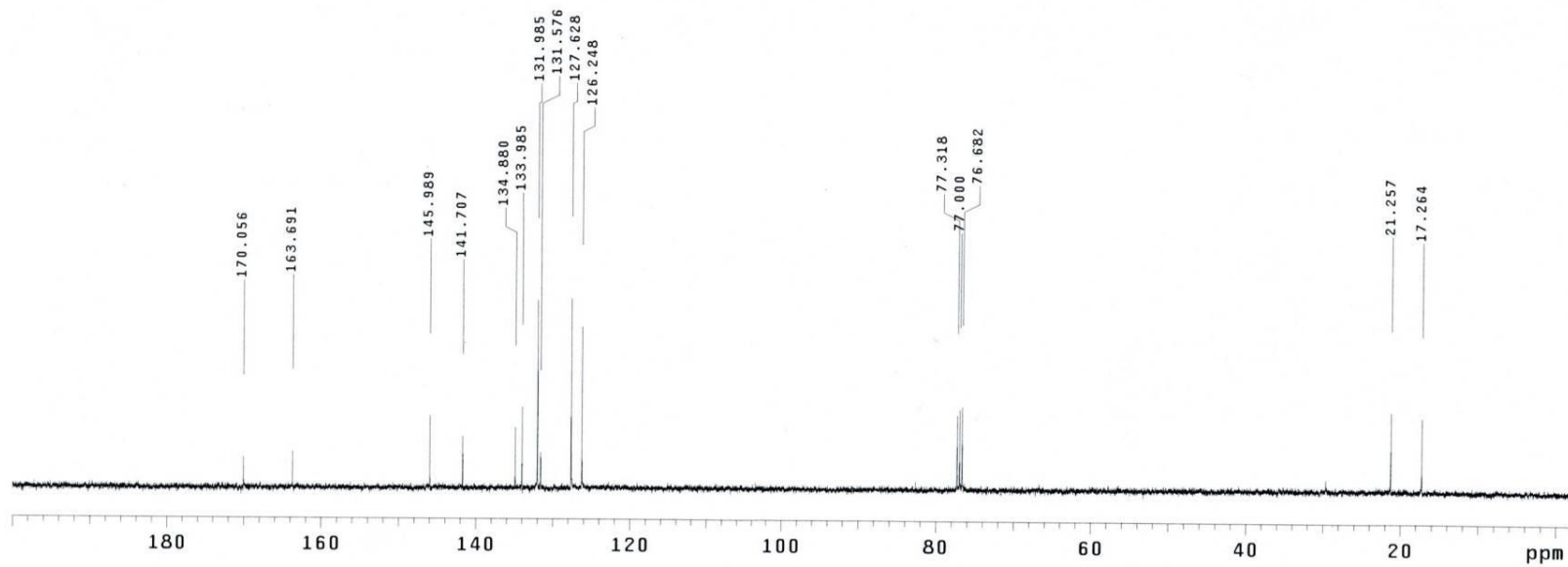
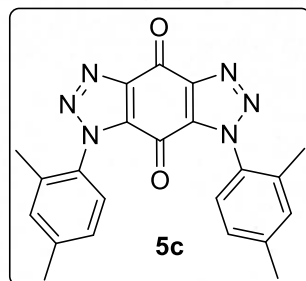
Mercury-400BB "MercuryPlus400"

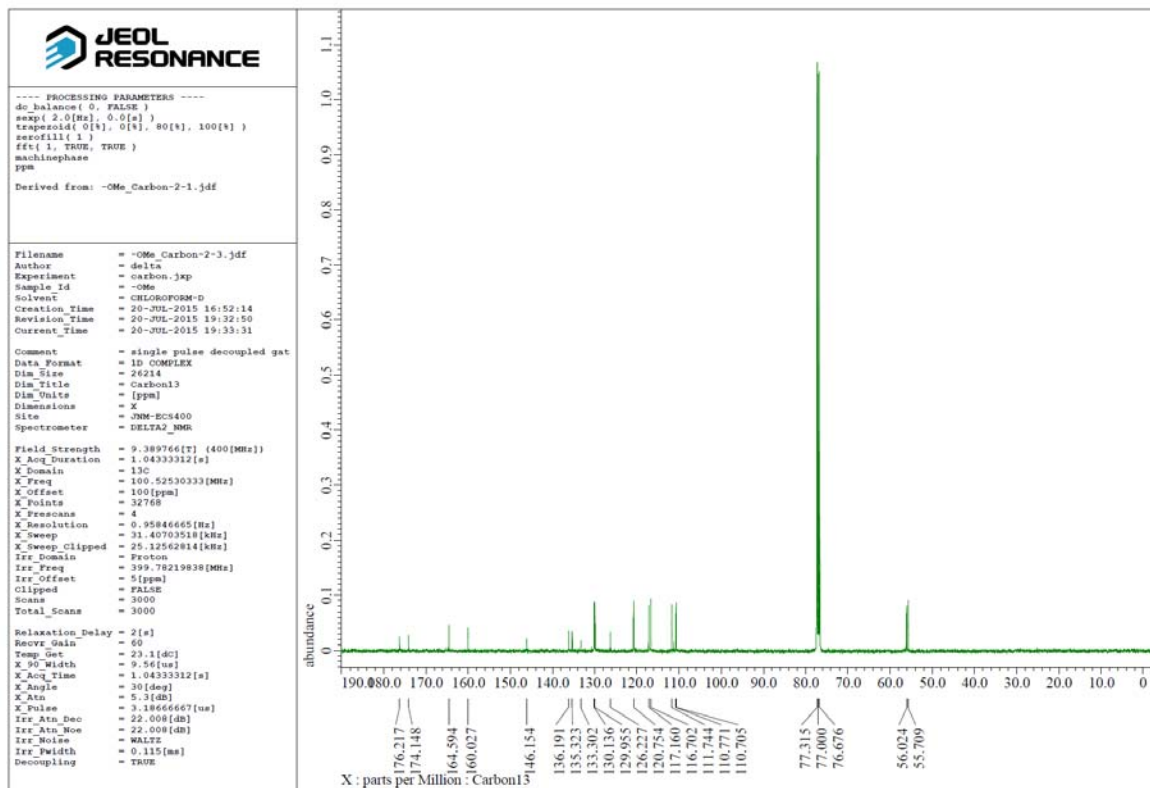
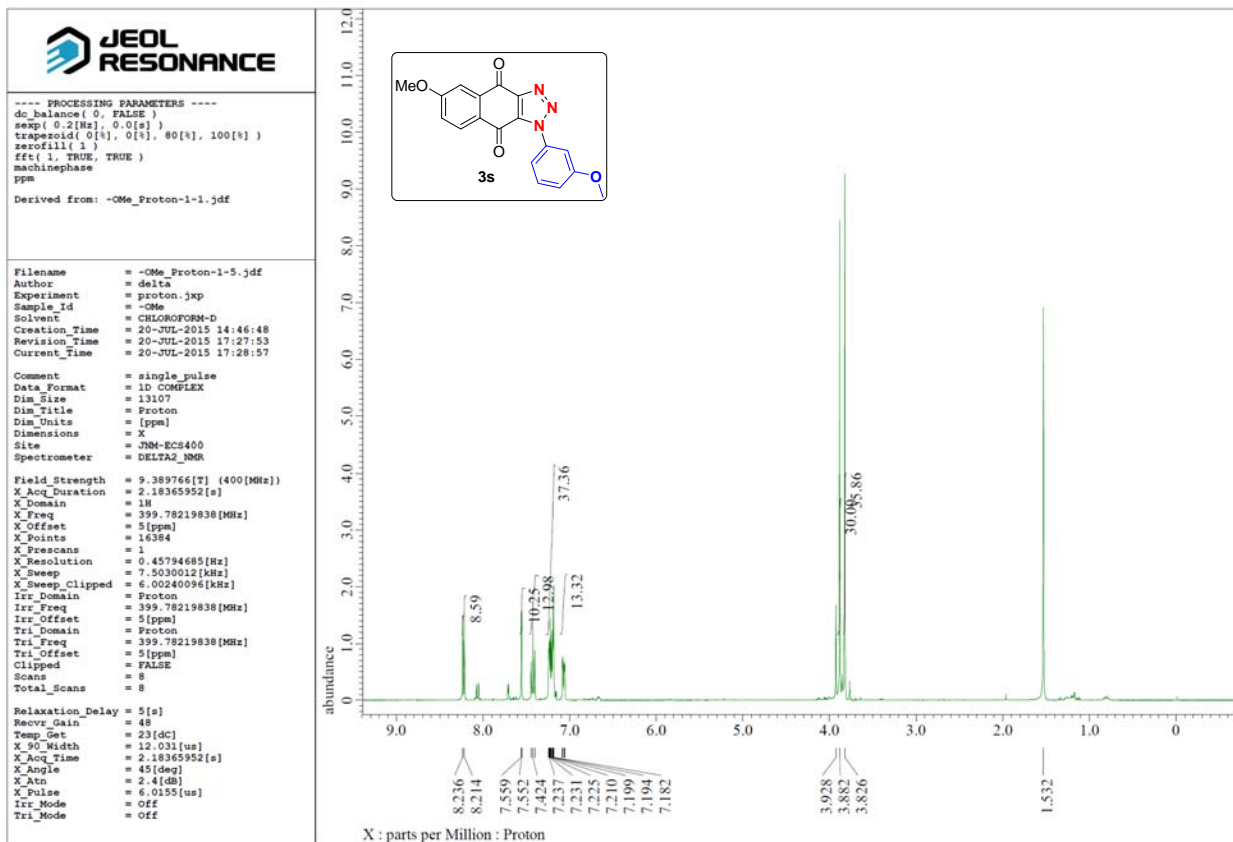
Date: Aug 26 2014

Solvent: CDCl₃

Ambient temperature

Total 320 repetitions







----- PROCESSING PARAMETERS -----

```
de_balance( 0, FALSE )
sext( 0.2[Hz], 0.0[s] )
trapezoid( 0[Hz], 0[Hz], 80[Hz], 100[Hz] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

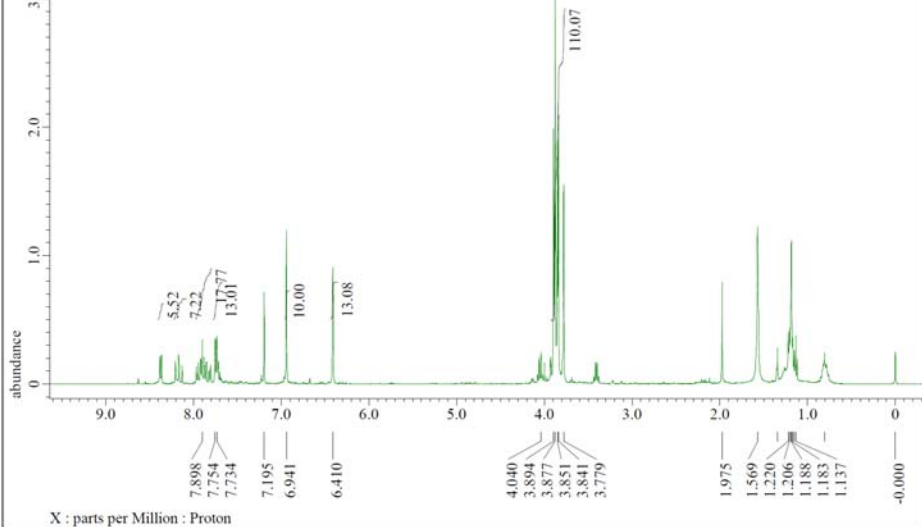
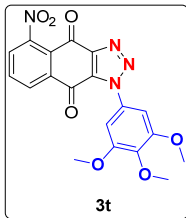
Derived from: 3-NO2-triOMe_Proton-1-1.jdf

Filename = 3-NO2-triOMe_Proton-1-5.jd
Author = delta
Experiment = proton.jxp
Sample_id = 3-NO2-triOMe
Solvent = CHLOROFORM-D
Creation_Time = 20-JUL-2015 12:52:58
Revision_Time = 20-JUL-2015 17:37:53
Current_Time = 20-JUL-2015 17:38:12

Comment = single_pulse
Data_Format = 1D_COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = 1
Site = JNM-ECS400
Spectrometer = DELTA2_MGR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 23.1[degC]
X_90_Width = 12.031[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 2.4[deg]
X_Pulse = 6.0155[us]
Irr_Mode = Off
Tri_Mode = Off



X : parts per Million : Proton