Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis of *anti*- 2, 3-dihydro-1, 2, 3-trisubstituted-1*H*-naphth [1, 2-e][1, 3] oxazine derivatives via multicomponent approach

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Supporting Information

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(1) Single Crystal XRD Data of 6b and 6c

Single crystal X-ray data[1] were collected on a block shaped crystal which solved and refined in the triclinic space group *P-1* with one molecule in the asymmetric unit ($Z' = 1$) for compound 1 and two molecules for compound 2 ($Z' = 2$). Reflections were collected at 298 K on Bruker SMART APEX II CCD equipped with a graphite monochromator and Mo-Kα fine-focus sealed tube (λ = 0.71073 Å)[1]. Data integration was done using SAINT [2]. Intensities for absorption were corrected using SADABS. Structure solution and refinement were carried out using Bruker SHELXTL 2008[1]. The hydrogen atoms were refined isotropically and the heavy atoms were refined anisotropically. N–H and O–H hydrogens were located from difference electron density maps and C–H hydrogens were fixed using HFIX command in SHELXTL. Crystallographic data are summarized in the table below.

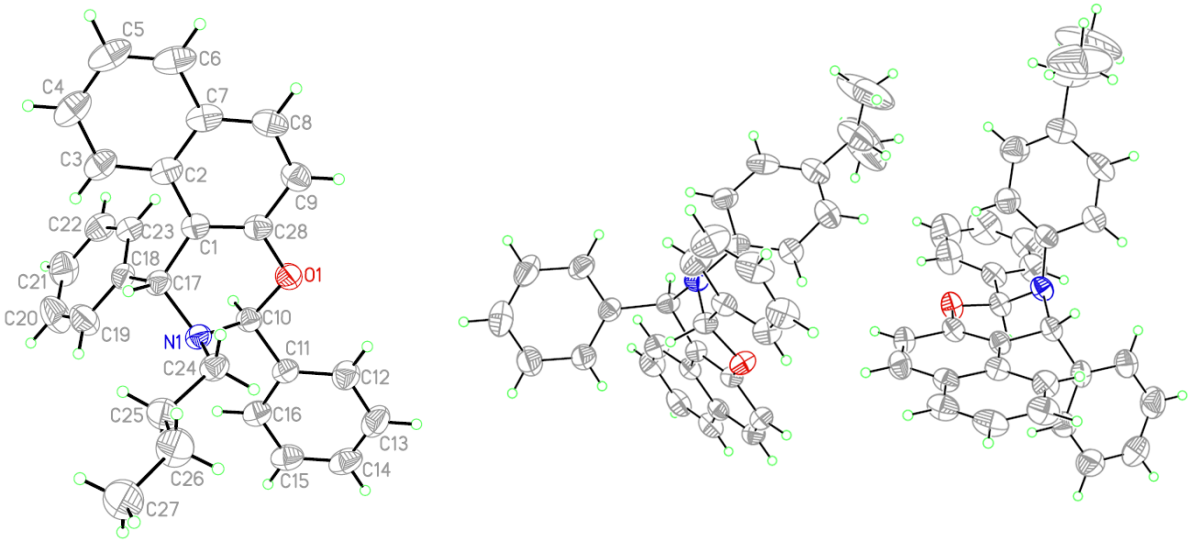
Crystal Data

Table S1: Single crystal data of **6b** and **6c**

	6c[2] [ROFSIP]	**6c**[$] [This article]	**6b**
Chemical formula	$C_{28}H_{27}NO$	$C_{28}H_{27}NO$	$C_{33}H_{29}NO$
Formula weight	393.51	393.51	455.57
Crystal system	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1
T (K)	293	296	296
a/Å	8.8959(15)	8.8634 (4)	8.5795 (2)
b/Å	10.7589(16)	10.7499 (5)	15.1441 (4)
c/Å	11.8401(18)	11.8110 (6)	20.1757 (5)
α/°	96.219(1)	96.088(3)	86.416(2)
β/°	98.366(2)	98.252(3)	85.757(2)
γ/°	97.274(2)	97.358(3)	80.379(2)
V/Å^3	1102.82	1095.62(9)	2574.10(11)
D_{calc}/g cm^{-3}	1.185	1.193	1.176
μ/mm^{-1}	-	0.071	0.070

Z	2	2	4
R_1 [$I > 2\ \sigma(I)$]	0.0721	0.0478	0.0758
wR_2	-	0.1377	0.1951
GOF	-	1.064	0.964
Diffractometer	-	BRUKER-APEX-II CCD	BRUKER-APEX-II CCD

Figure S1 ORTEP of redetermined structure of compound **6c** and newly collected compound **6b** with 35% probability ellipsoid for non-hydrogen atoms.



(a) ORTEP of **6c** (b) ORTEP of **6b**

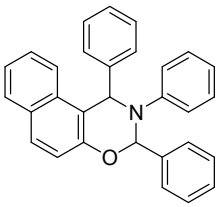
Reference

[1] (a) *SAINT Plus* ,Bruker AXS Inc.: Madison, WI, **2008**; (b)BRUKER AXS (v 6.14): Madison, WI, **2008**; (c) Spek, A. L . *PLATON, A Multipurpose Crystallographic Tool;* Utrecht University: Utrecht, Netherland, **2002**;(d) Spek, A. L. *J Appl. Crystallogr.***2003**, *36*, 7. (3) Bruker SHELXTL v2008/4 (Bruker, 2008)

[2] Li, Y. H.; Zhao, M. M.; Zhang, Y .*Acta. Cryst* , **2008**, *E64*, 01972.

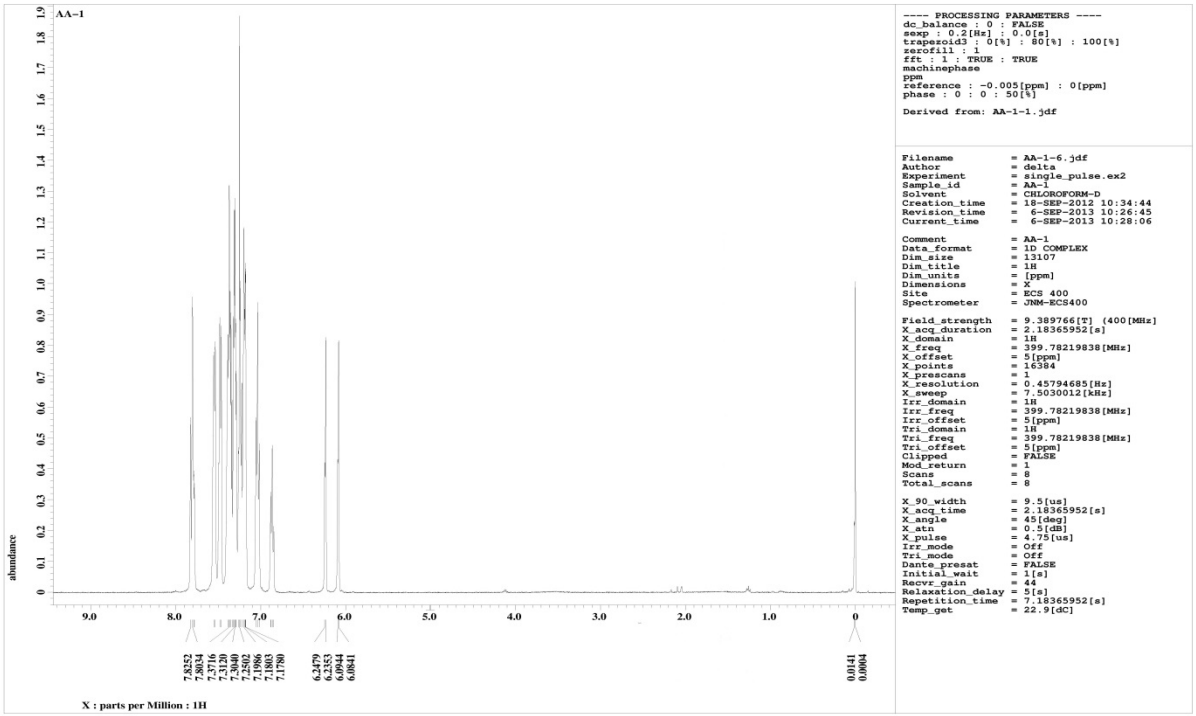
NMR Spectra for Oxazine Product6

[1] 6a



2,3-dihydro-1,2,3-triphenyl-1*H*-naphtho[1,2-*e*][1,3]oxazine

1.1 ^{1}H NMR



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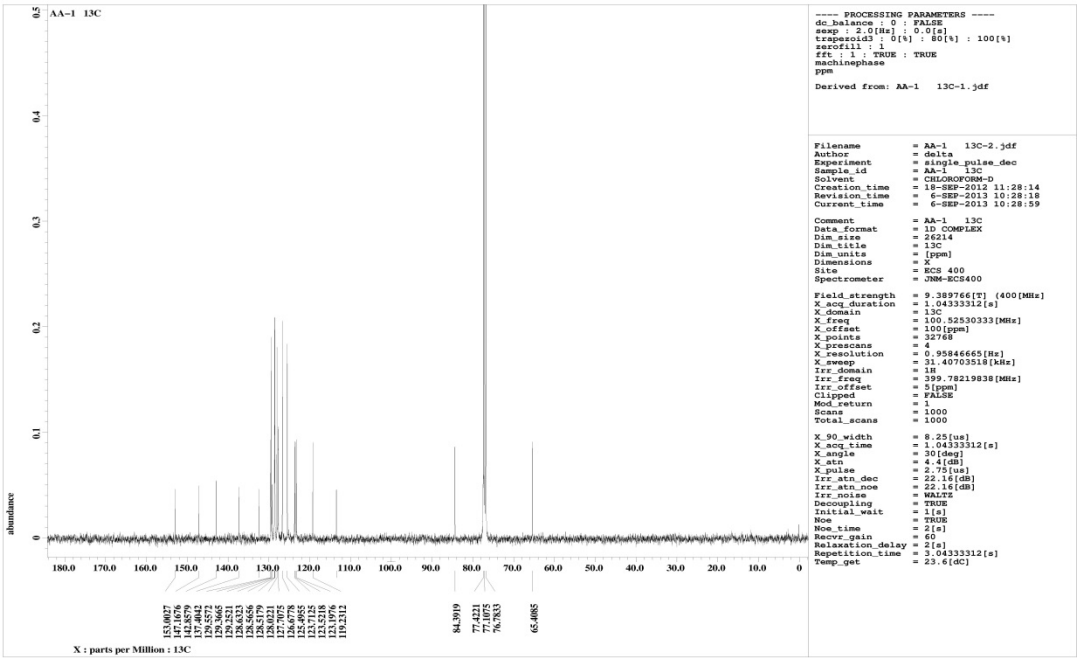

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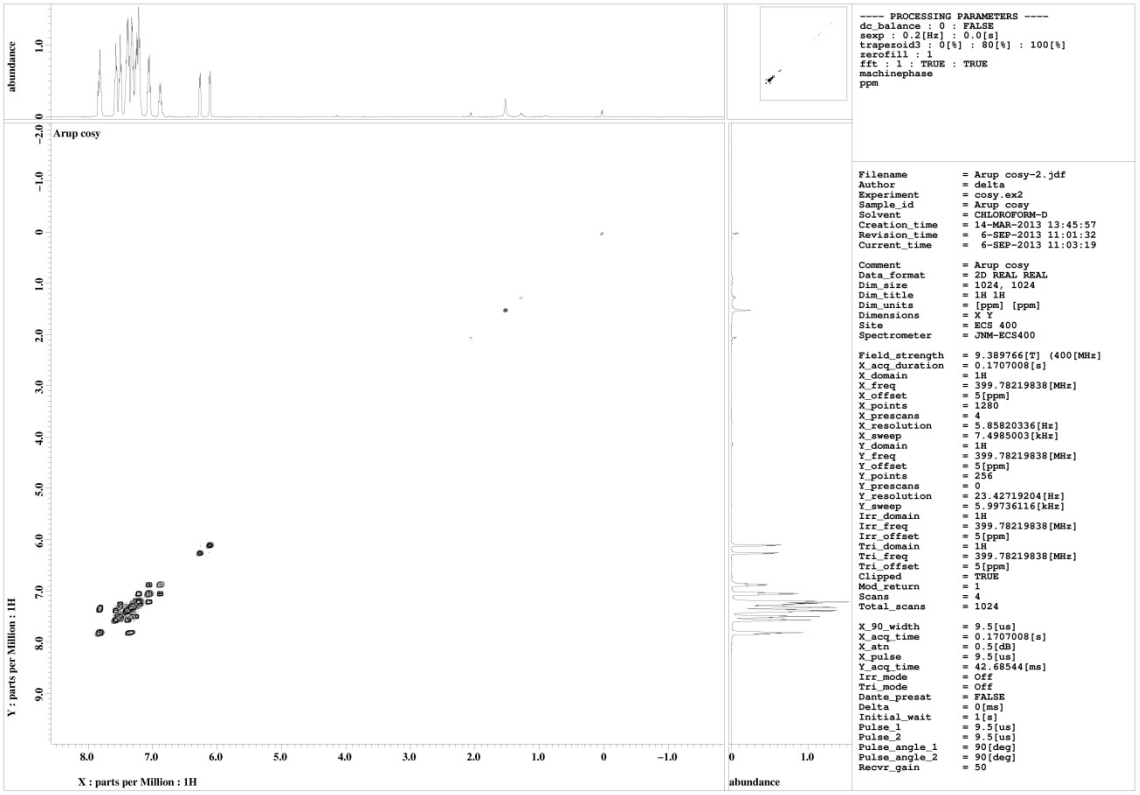

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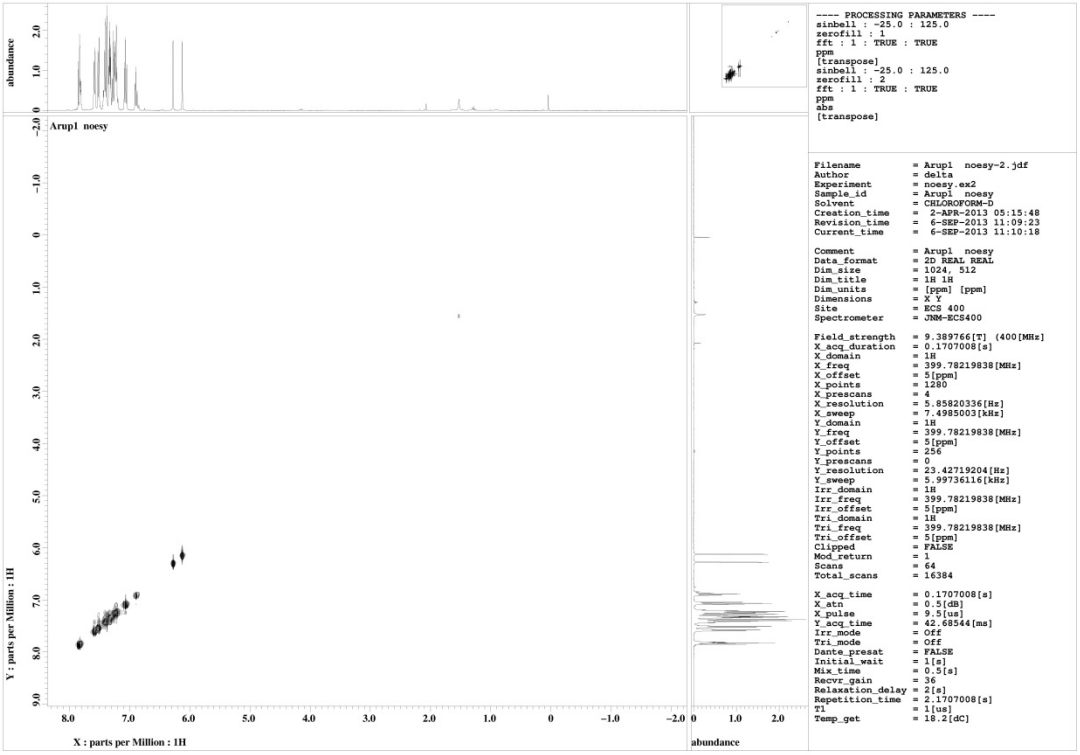

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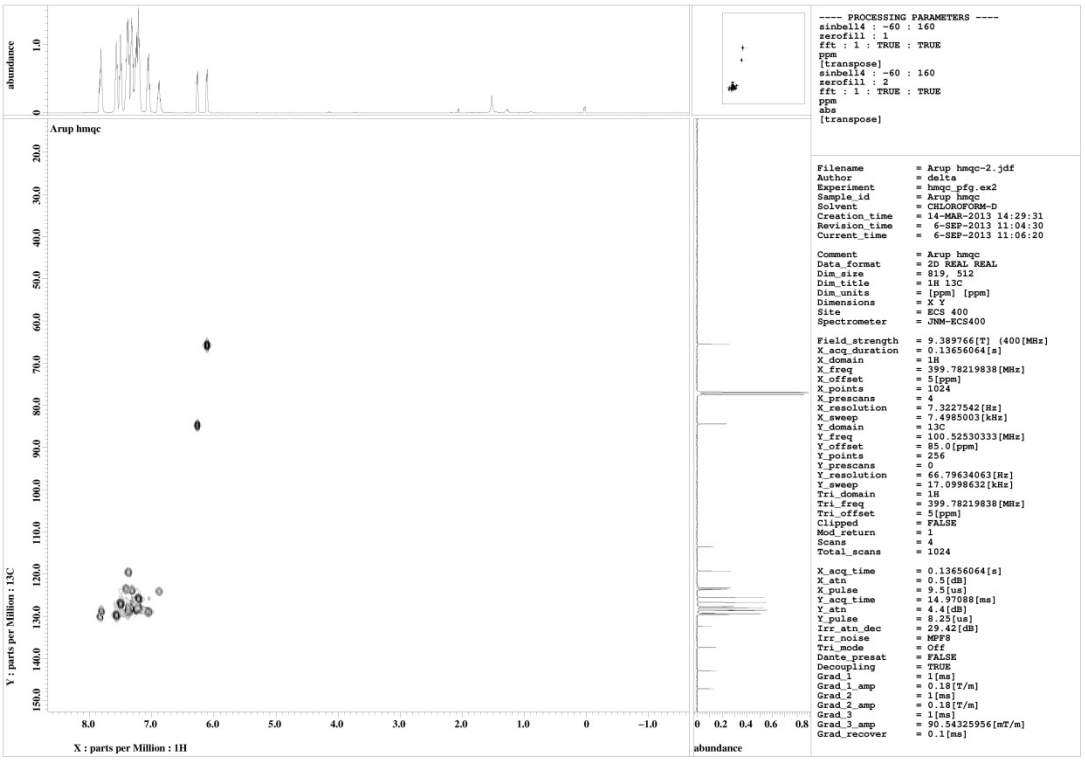
abundance
Arup hmqc
Y : parts per Million : 13C
X : parts per Million : 1H
abundance
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zerofill : 1
fft : 1 : TRUE : TRUE
ppm
[transpose]
sinbell4 : -60 : 160
zerofill : 2
fft : 1 : TRUE : TRUE
ppm
abs
[transpose]
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Y_pulse = 8.25[us]
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Decoupling = TRUE
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Grad_2 = 1[ms]
Grad_2_amp = 0.18[T/m]
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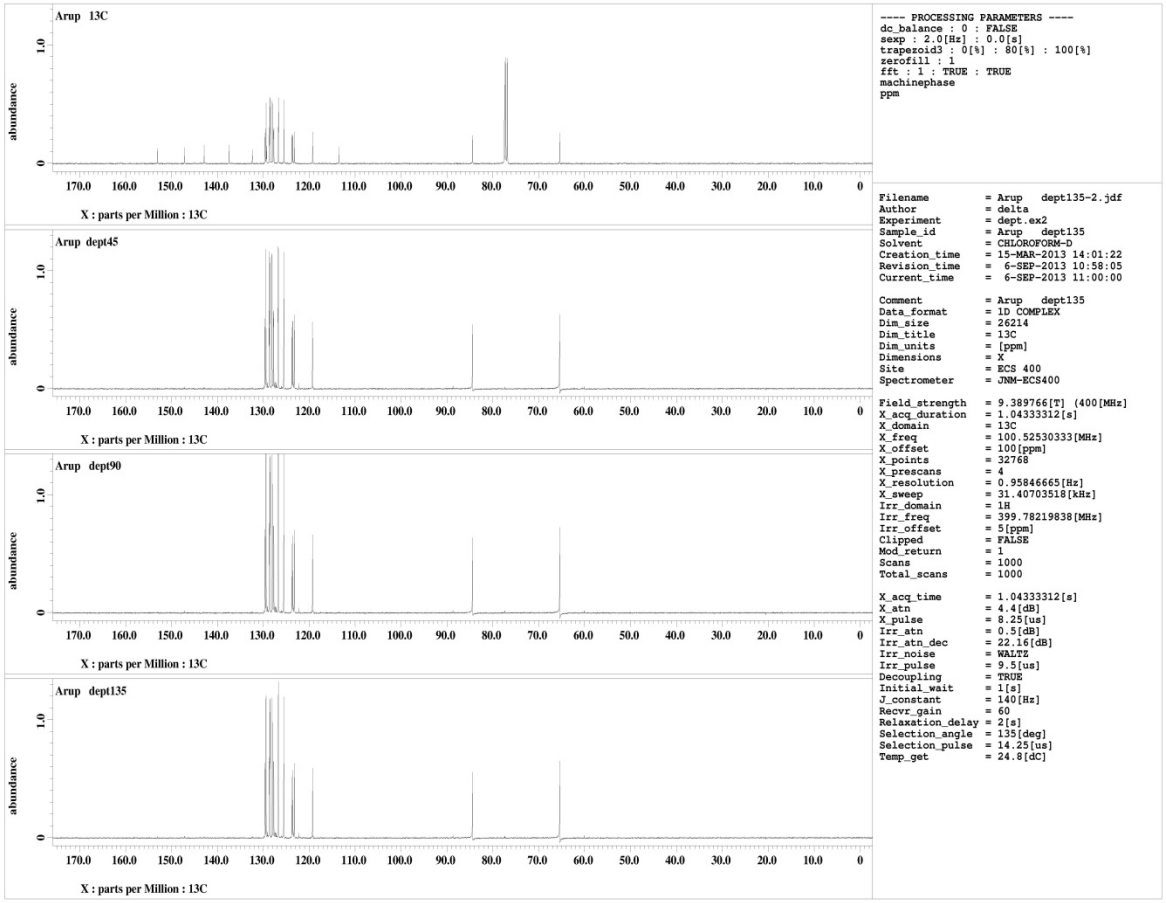
Arup 13C
Arup dept45
Arup dept90
Arup dept135
abundance
1.0
0
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C
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dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
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X_offset = 100[ppm]
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X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_acq_time = 1.04333312[s]
X_atn = 4.4[dB]
X_pulse = 8.25[us]
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Irr_noise = WALTZ
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J_constant = 140[Hz]
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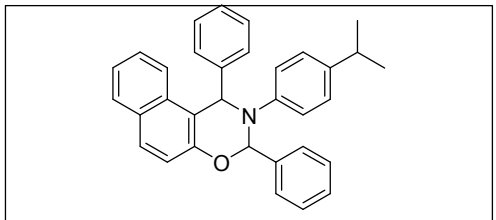
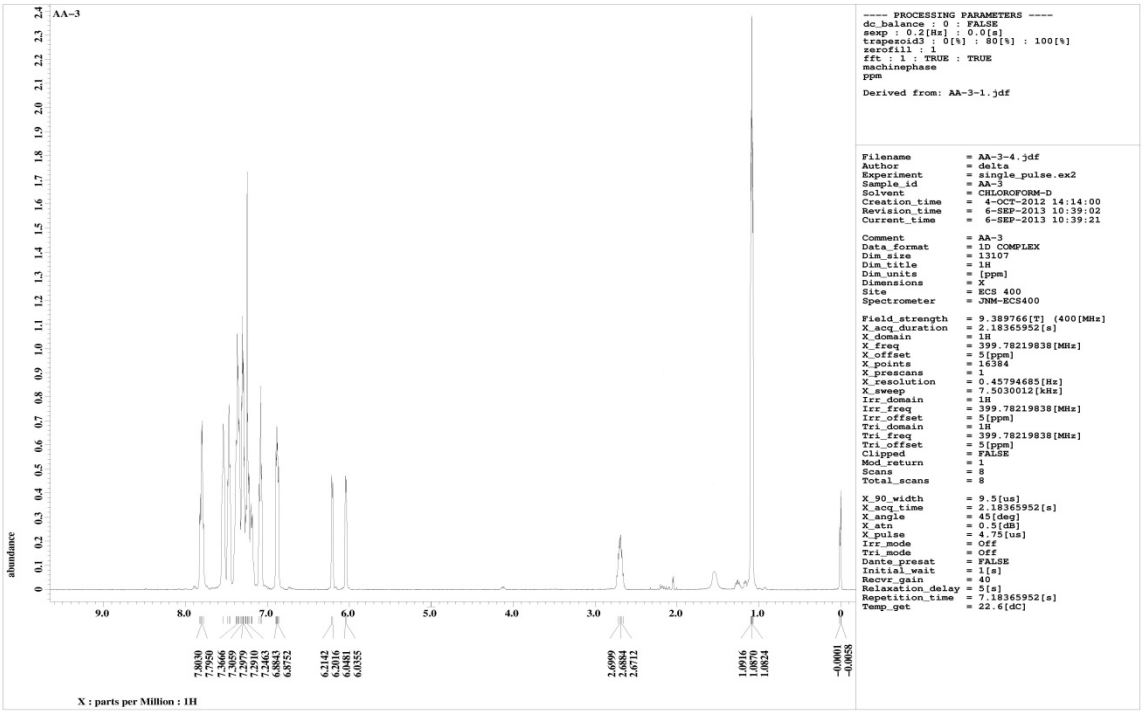
[2] **6b**

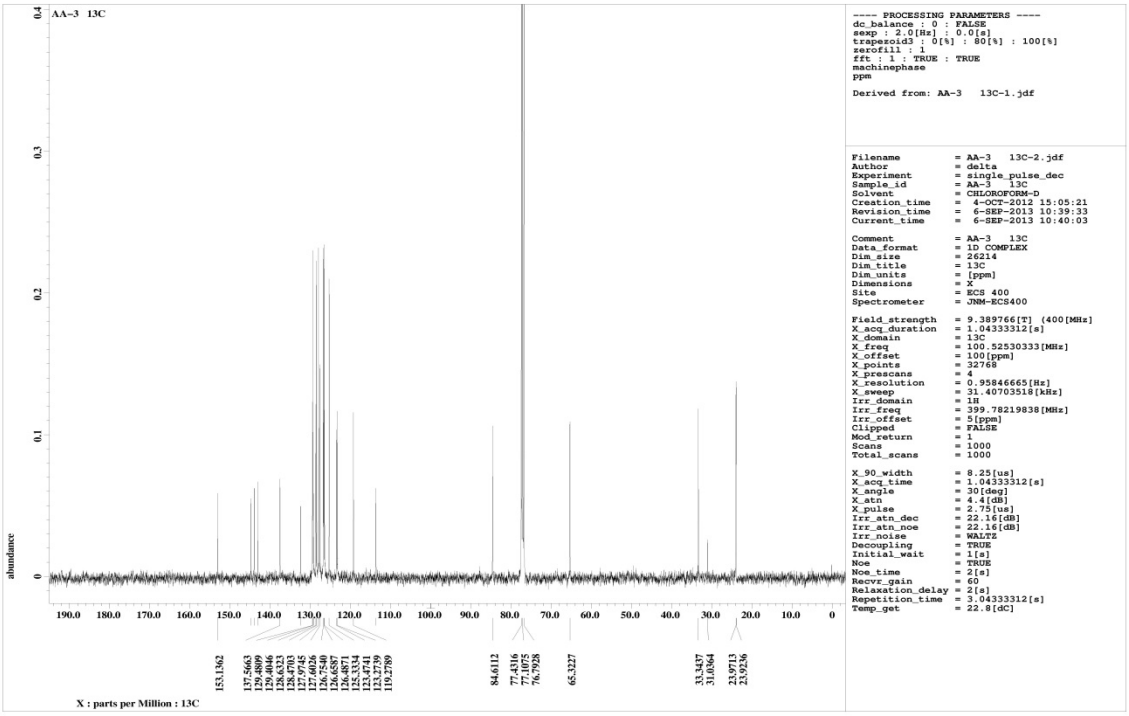


2,3-dihydro-2-(4-isopropylphenyl)-1,3-diphenyl-1*H*-naphtho[1,2-*e*][1,3]oxazine

2.1. ^{1}H NMR



2.1. ^{13}C NMR

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fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: AA-3   13C-1.jdf
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Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
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Spectrometer      = JNM-ECS400

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X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
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Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1000
Total_scans       = 1000

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X_acq_time        = 1.04333312[s]
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Irr_atn_noe       = 22.16[dB]
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Decoupling        = TRUE
Initial_wait      = 1[s]
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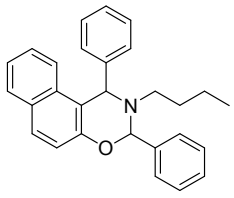
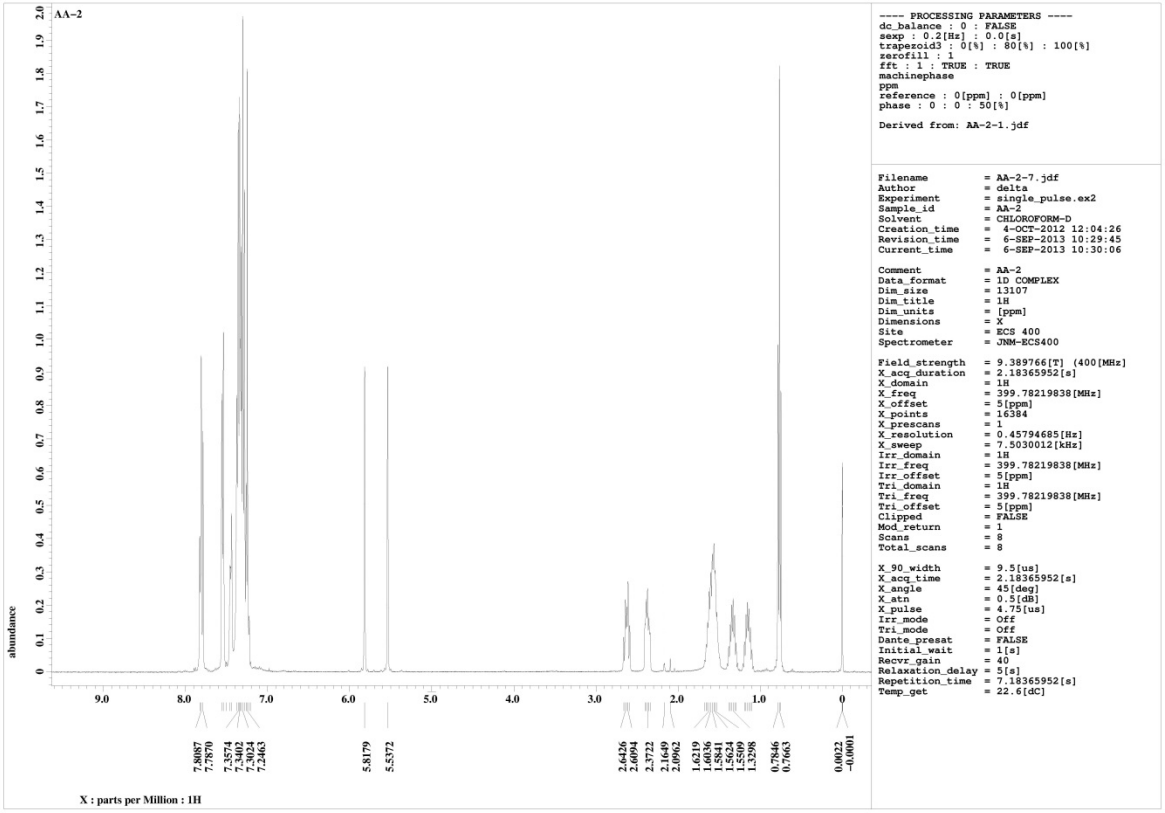
[3] **6c**

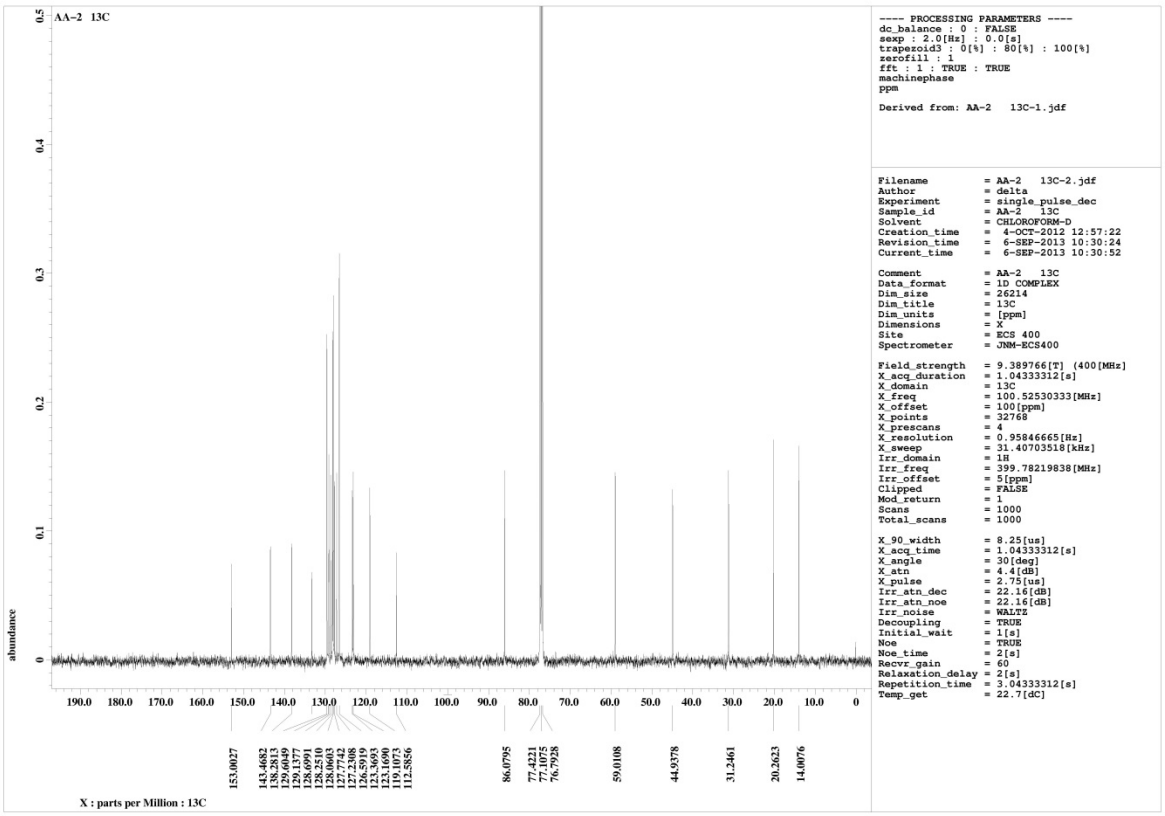


2-butyl-2,3-dihydro-1,3-diphenyl-1*H*-naphtho[1,2-*e*][1,3]oxazine

3.1. ^{1}H NMR



3.2. ^{13}C-NMR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0.4
0.3
0.2
0.1
0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
153.0027
143.4682
138.2851
129.6049
129.1377
128.6991
128.4510
128.1605
127.7742
127.2308
126.5919
124.3648
123.1690
119.1073
112.5856
86.0795
77.4221
77.1075
76.7928
59.0108
44.9378
31.2461
20.2623
14.0076
X : parts per Million : 13C
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ppm
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X_prescans = 4
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X_sweep = 31.40703518[kHz]
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Irr_freq = 399.78219838[MHz]
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Total_scans = 1000
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X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
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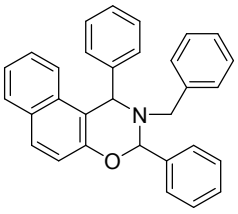
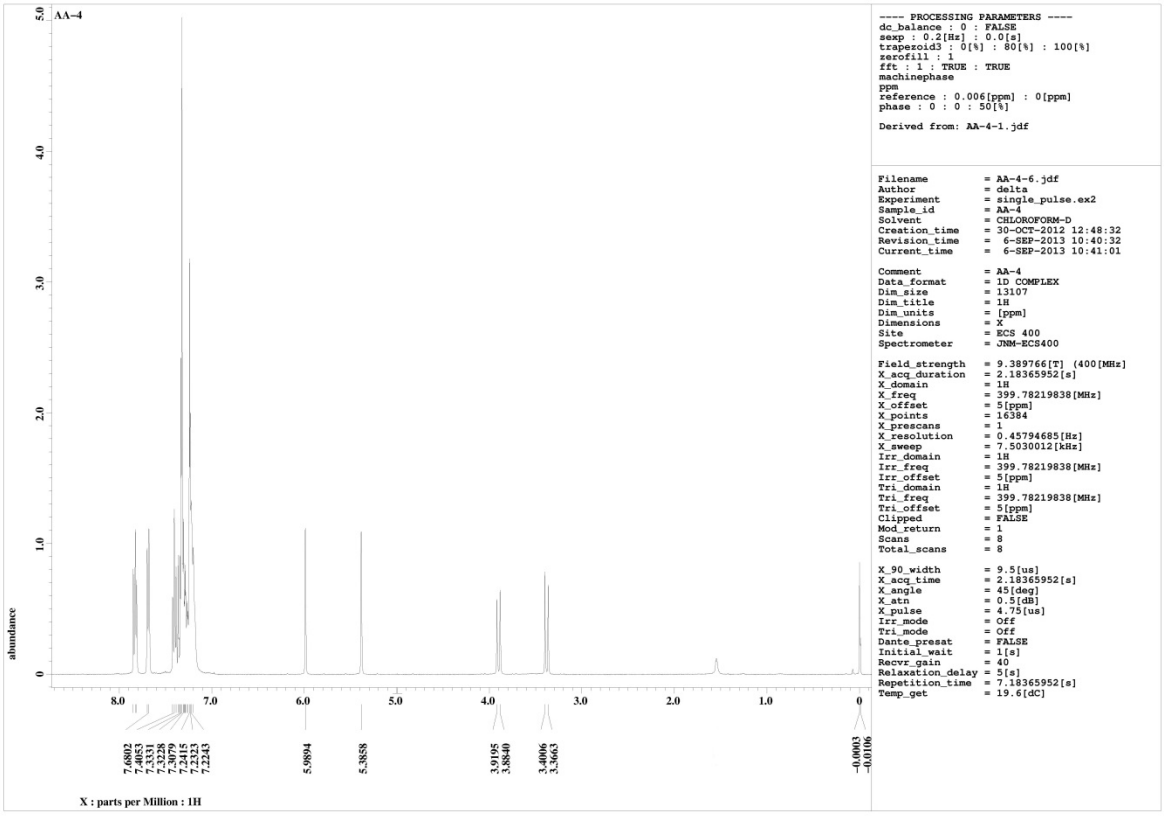
[4] **6d**

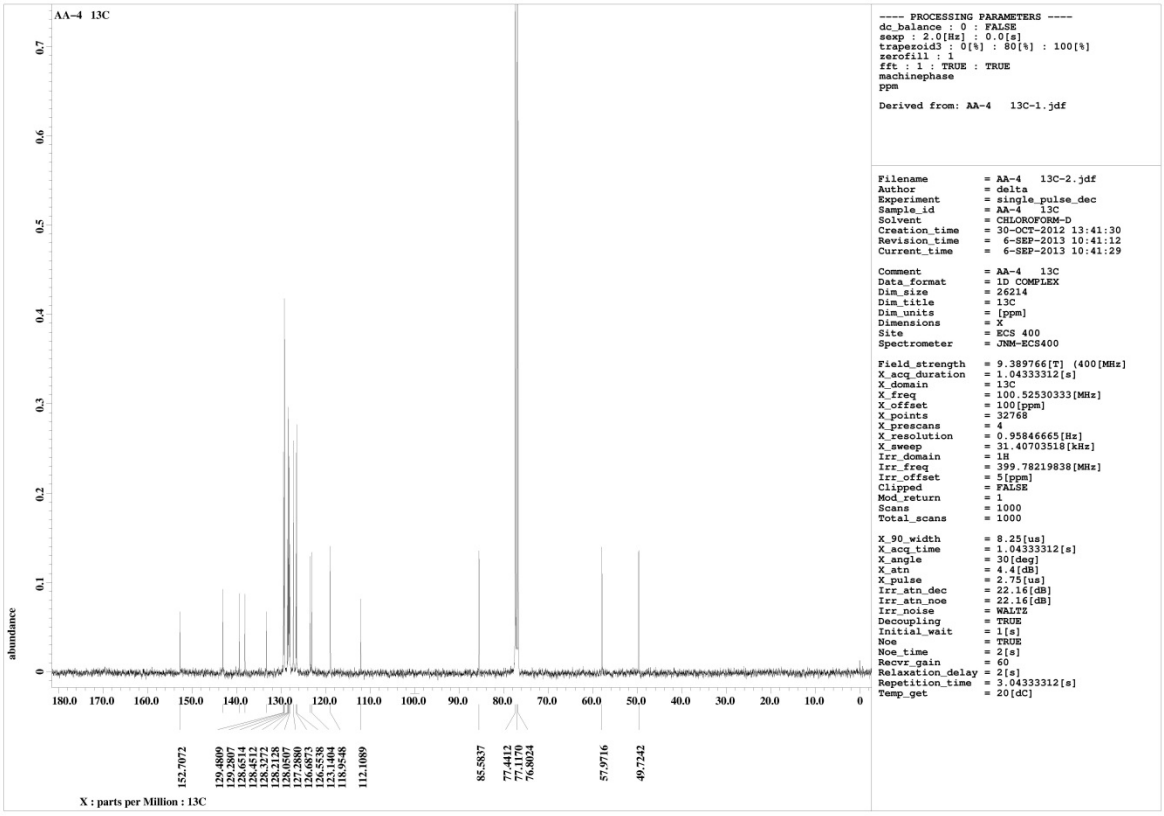


2-benzyl-2,3-dihydro-1,3-diphenyl-1*H*-naphtho[1,2-*e*][1,3]oxazine

4.1. ^{1}H NMR



4.2. ^{13}C-NMR


AA-4 13C
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0.2
0.3
0.4
0.5
0.6
0.7
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
152.7072
129.4809
129.2807
128.6514
128.4512
128.3272
128.2128
128.0587
127.7980
126.6873
126.5538
123.1404
118.9548
112.1089
85.5837
77.4412
77.1170
76.8024
57.9716
49.7342
X : parts per Million : 13C
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X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
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Noe = TRUE
Noe_time = 2[s]
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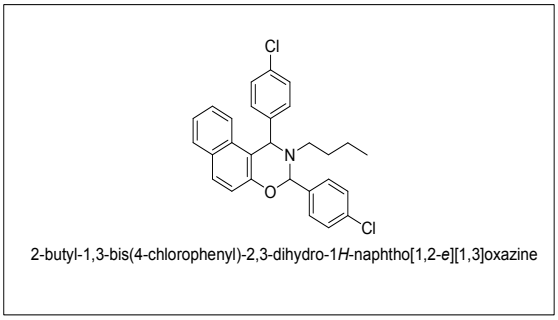
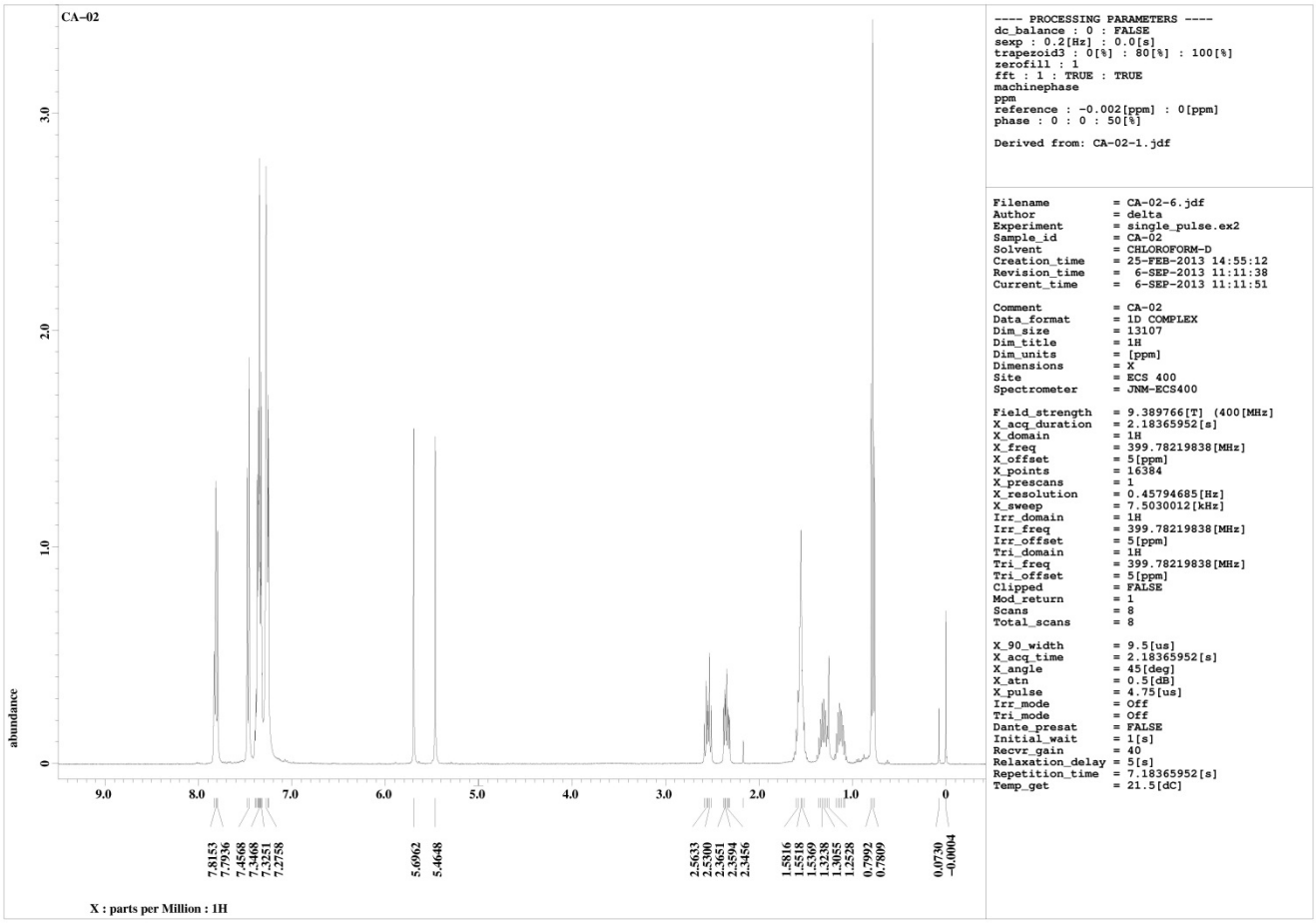
[5] **6f**

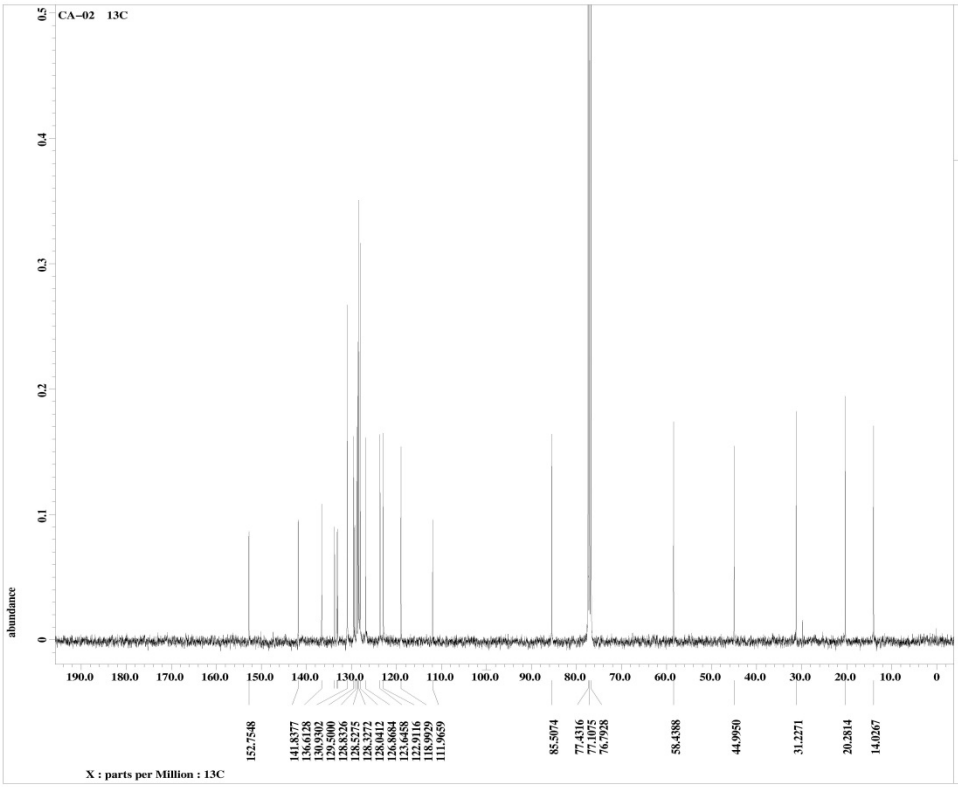


2-butyl-1,3-bis(4-chlorophenyl)-2,3-dihydro-1*H*-naphtho[1,2-e][1,3]oxazine

5.1.^{1}H NMR



5.2. ^{13}C-NMR

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zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: CA-02    13C-1.jdf
```

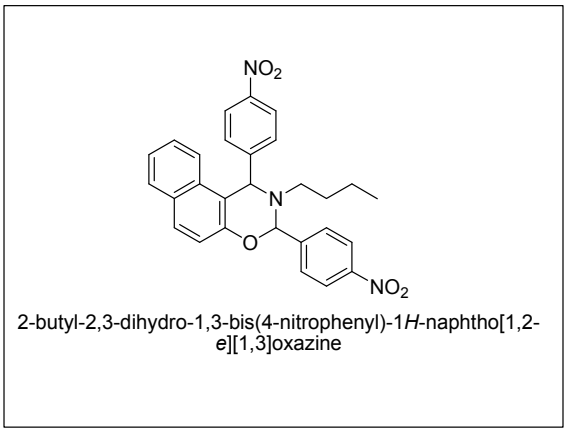
```
Filename          = CA-02    13C-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = CA-02    13C
Solvent           = CHLOROFORM-D
Creation_time     = 25-FEB-2013 15:46:28
Revision_time     =  6-SEP-2013 11:12:03
Current_time      =  6-SEP-2013 11:12:16

Comment           = CA-02    13C
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1000
Total_scans       = 1000

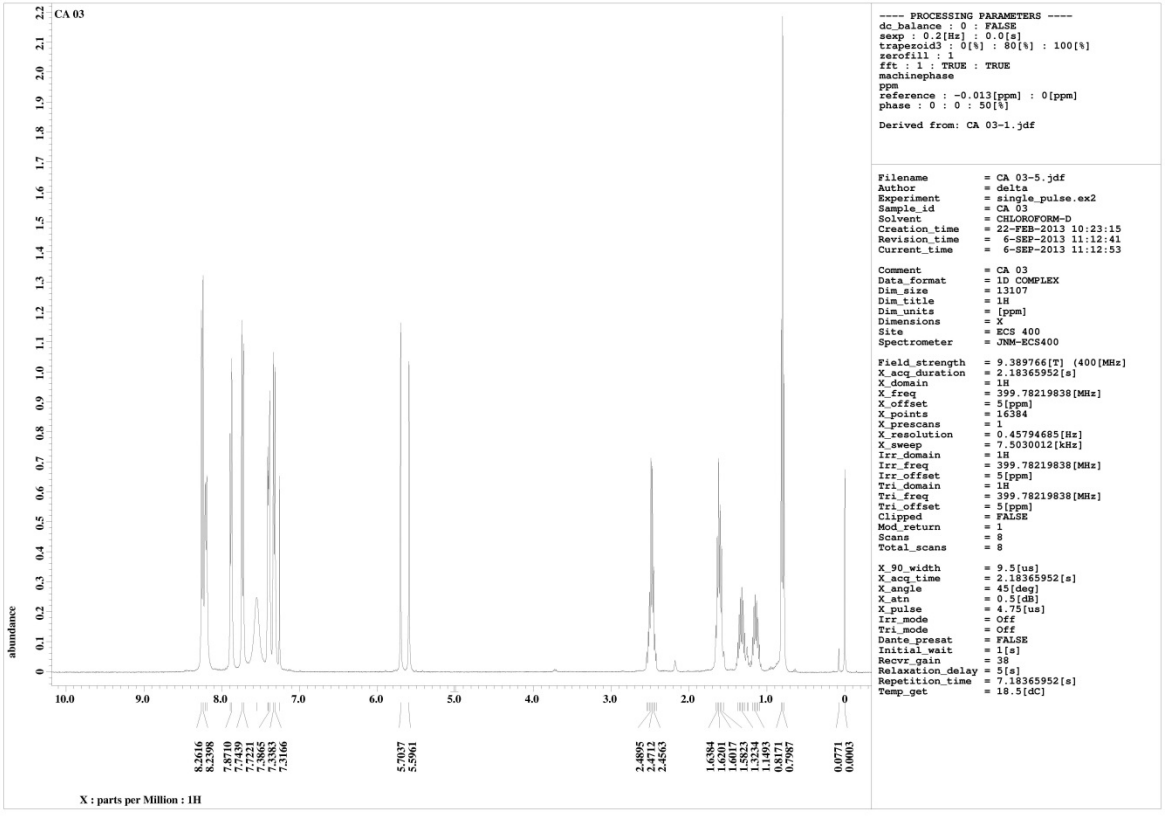
X_90_width        = 8.25[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 4.4[dB]
X_pulse           = 2.75[us]
Irr_atn_dec       = 22.16[dB]
Irr_atn_noe       = 22.16[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 21.1[dC]
```

[6] **6h**

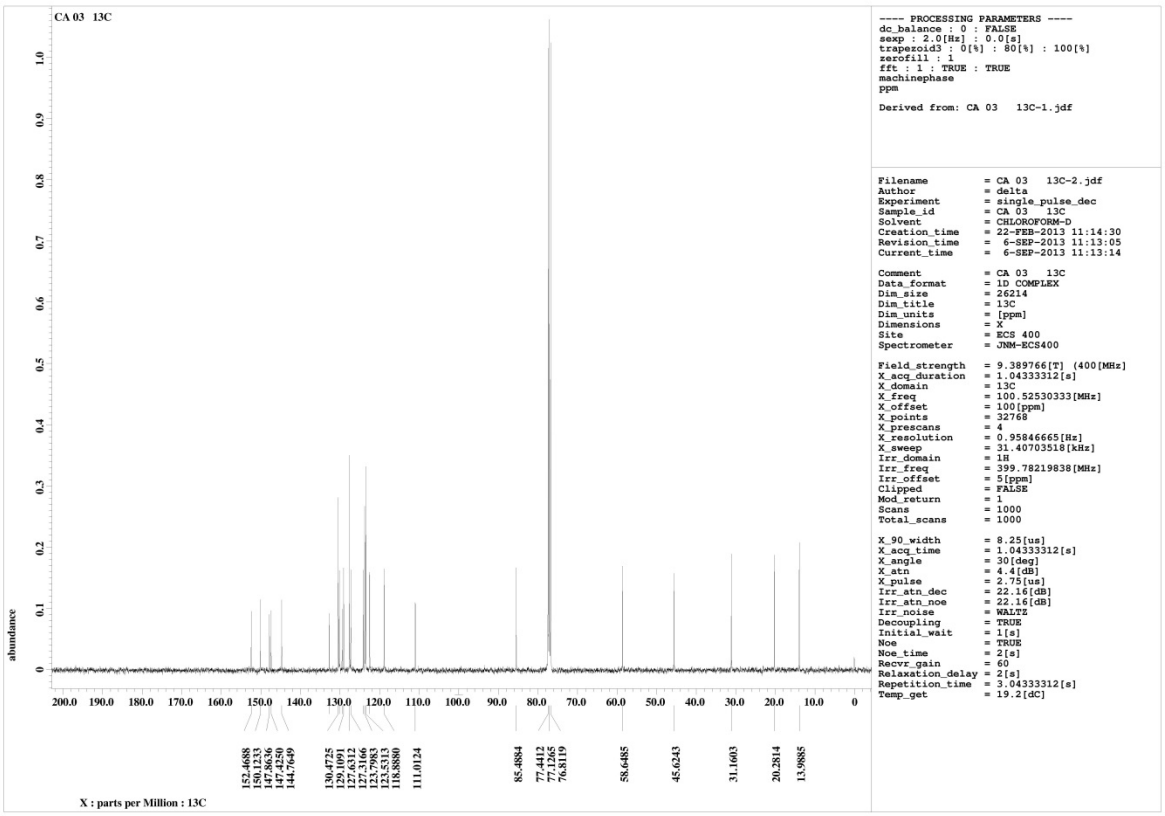


2-butyl-2,3-dihydro-1,3-bis(4-nitrophenyl)-1*H*-naphtho[1,2-*e*][1,3]oxazine

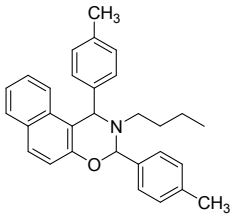
6.1. ^{1}H NMR



6.2. ^{13}C-NMR

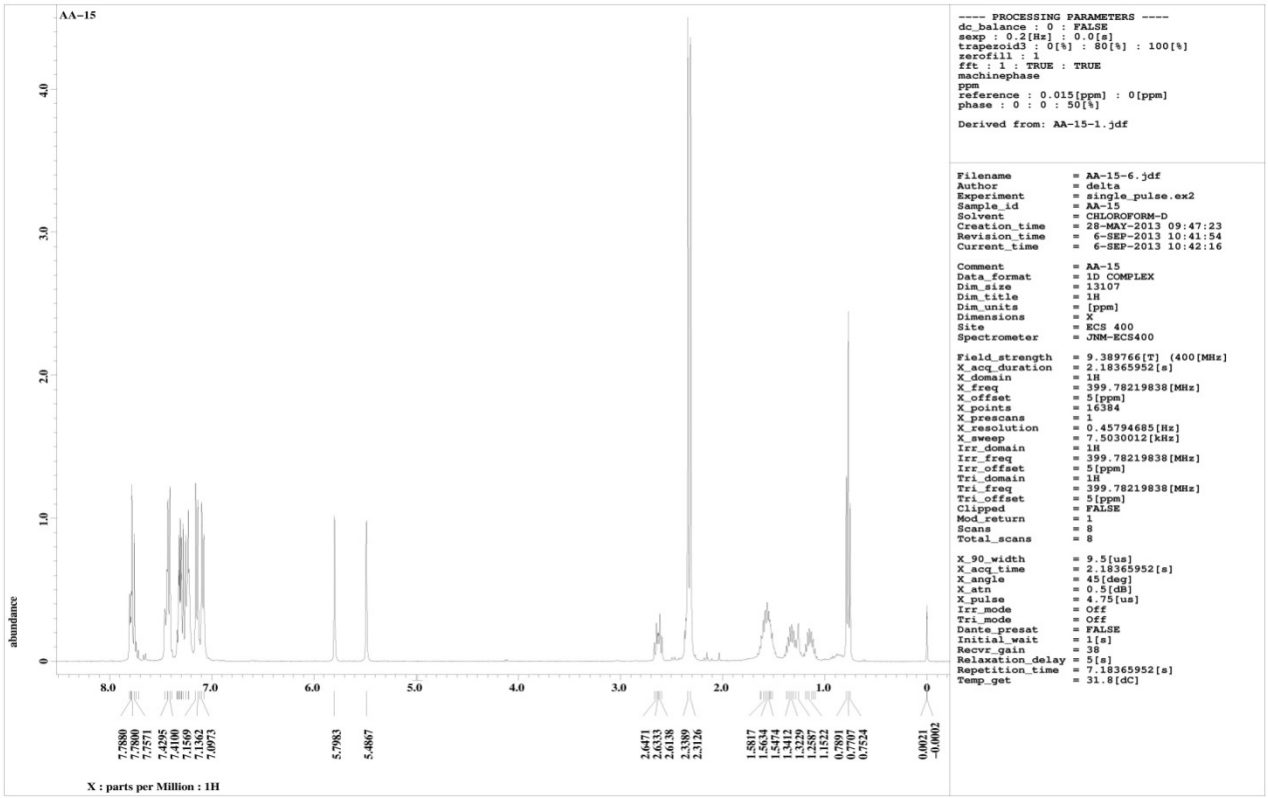

CA 03 13C
abundance
X : parts per Million : 13C
152.4688
150.1233
147.8636
147.4250
144.7649
130.4725
129.1091
127.6312
127.3166
123.7985
123.5313
118.8880
111.0124
85.4884
77.4412
77.1265
76.8119
58.6485
45.6243
31.1603
20.2814
13.9885
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: CA 03 13C-1.jdf
Filename = CA 03 13C-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = CA 03 13C
Solvent = CHLOROFORM-D
Creation_time = 22-FEB-2013 11:14:30
Revision_time = 6-SEP-2013 11:13:05
Current_time = 6-SEP-2013 11:13:14
Comment = CA 03 13C
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 19.2[dC]

[7] **6j**

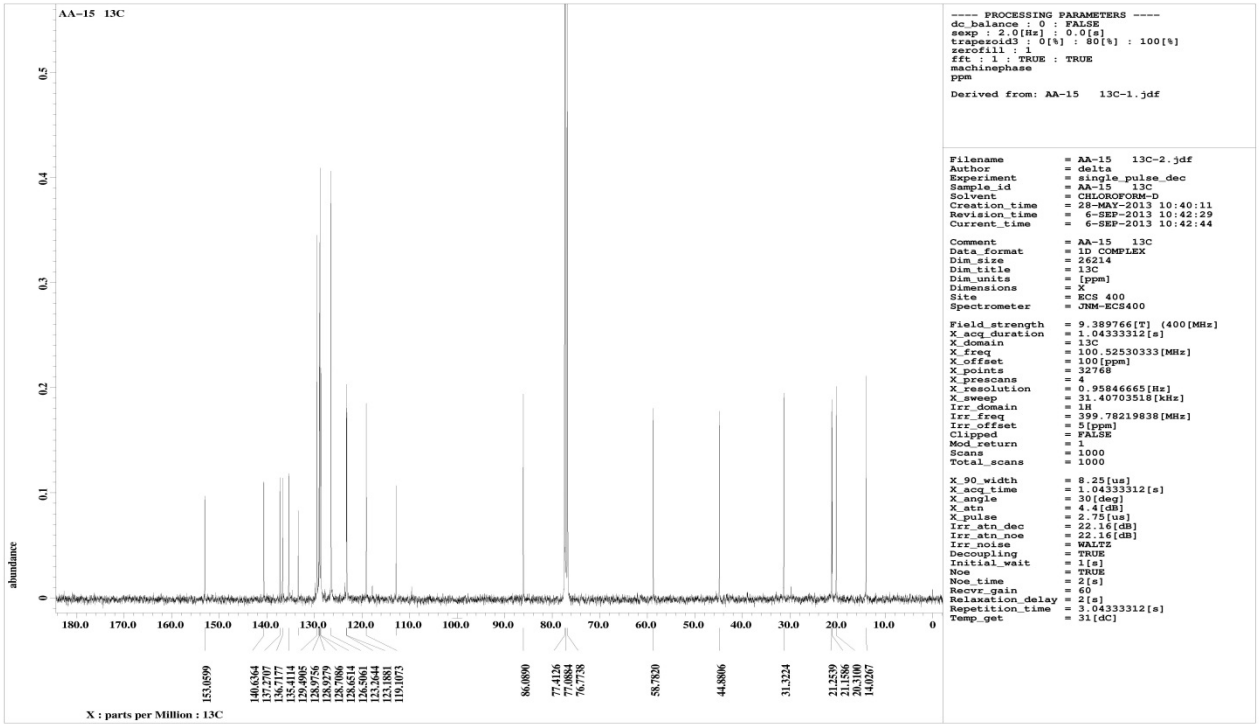


2-butyl-2,3-dihydro-1,3-di*p*-tolyl-1*H*-naphtho[1,2-*e*][1,3]oxazine

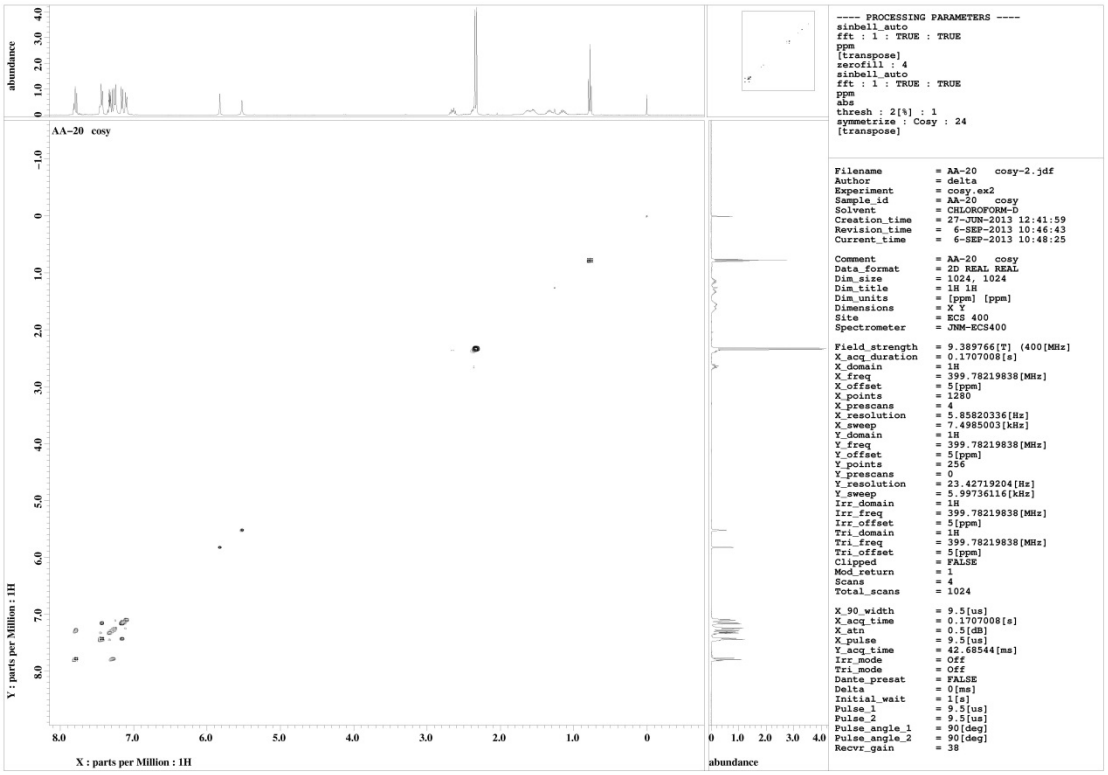
7.1. ^{1}H NMR



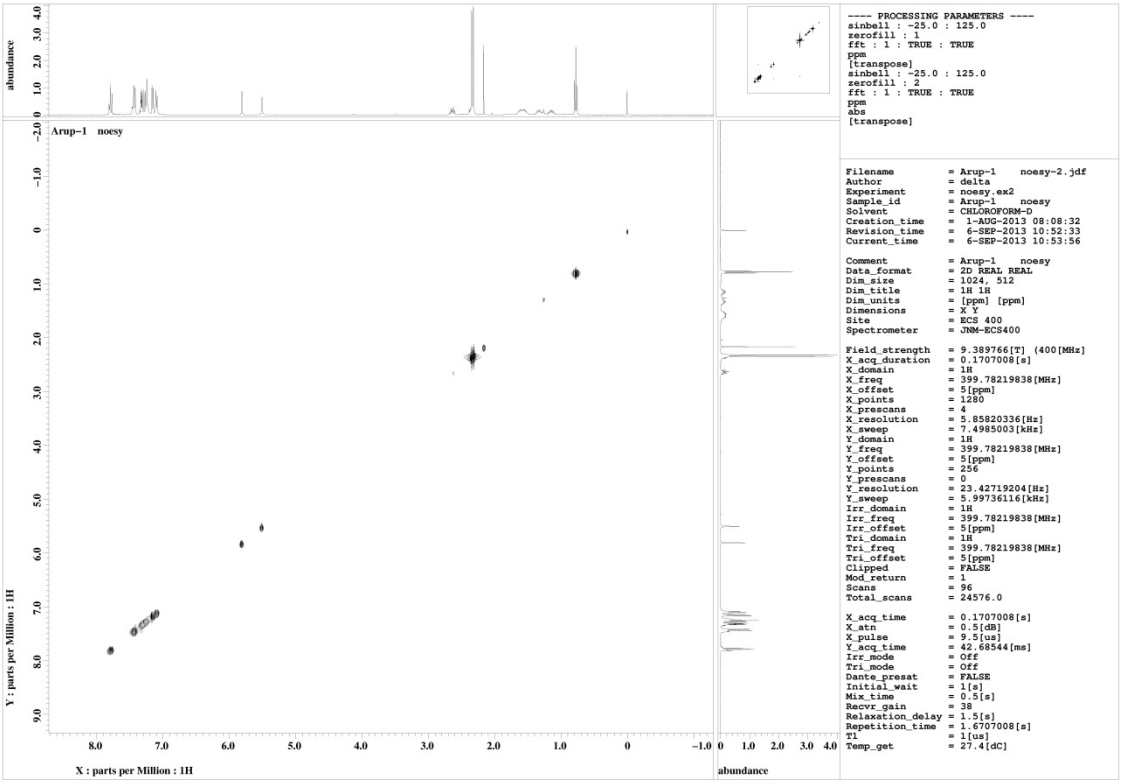
7.2. ^{13}C-NMR



7.3. COSY



7.4. NOESY




```
---- PROCESSING PARAMETERS ----
sinbell : -25.0 : 125.0
zerofill : 1
fft : 1 : TRUE : TRUE
ppm
[transpose]
sinbell : -25.0 : 125.0
zerofill : 2
fft : 1 : TRUE : TRUE
ppm
abs
[transpose]
```

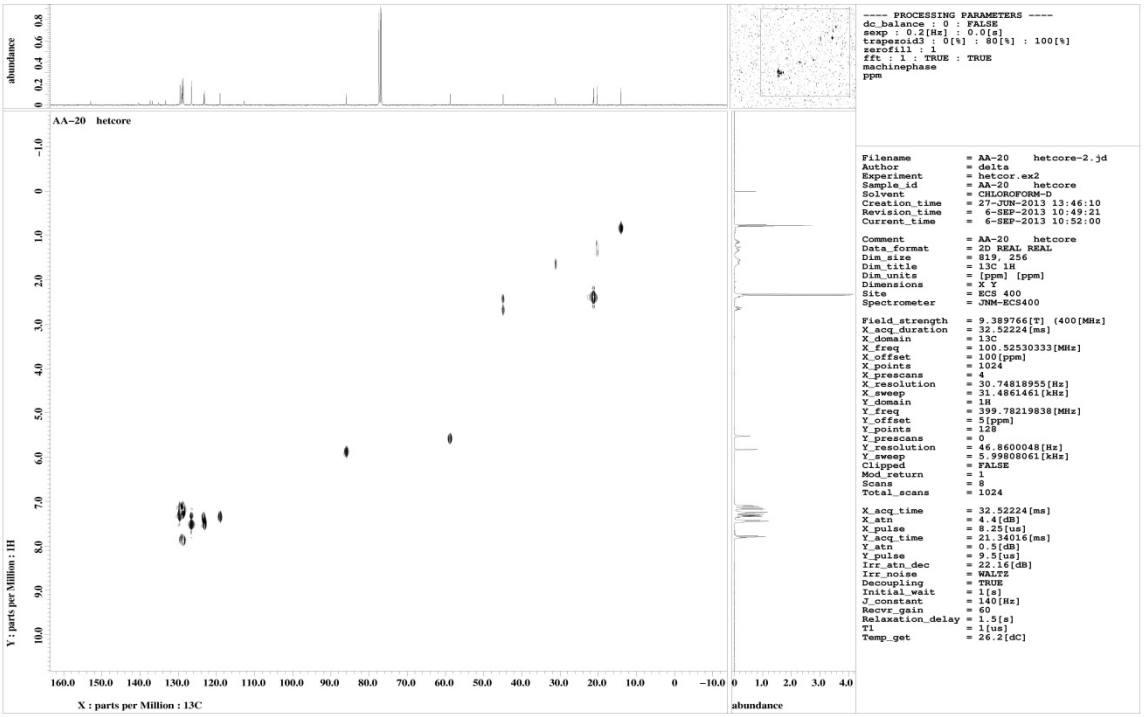
```
Filename          = Arup-1    noesy-2.jdf
Author            = delta
Experiment        = noesy.ex2
Sample_id         = Arup-1    noesy
Solvent           = CHLOROFORM-D
Creation_time     =  1-AUG-2013 08:08:32
Revision_time     =  6-SEP-2013 10:52:33
Current_time      =  6-SEP-2013 10:53:56

Comment           = Arup-1    noesy
Data_format       = 2D REAL REAL
Dim_size          = 1024, 512
Dim_title         = 1H 1H
Dim_units         = [ppm] [ppm]
Dimensions        = X Y
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 0.1707008[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 5[ppm]
X_points          = 1280
X_prescans        = 4
X_resolution      = 5.85820336[Hz]
X_sweep           = 7.4985003[kHz]
Y_domain          = 1H
Y_freq            = 399.78219838[MHz]
Y_offset          = 5[ppm]
Y_points          = 256
Y_prescans        = 0
Y_resolution      = 23.42719204[Hz]
Y_sweep           = 5.99736116[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.78219838[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 96
Total_scans       = 24576.0

X_acq_time        = 0.1707008[s]
X_atn             = 0.5[dB]
X_pulse           = 9.5[us]
Y_acq_time        = 42.68544[ms]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Mix_time          = 0.5[s]
Recvr_gain        = 38
Relaxation_delay  = 1.5[s]
Repetition_time   = 1.6707008[s]
T1                = 1[us]
Temp_get          = 27.4[dC]
```

7.5. HETCOR




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

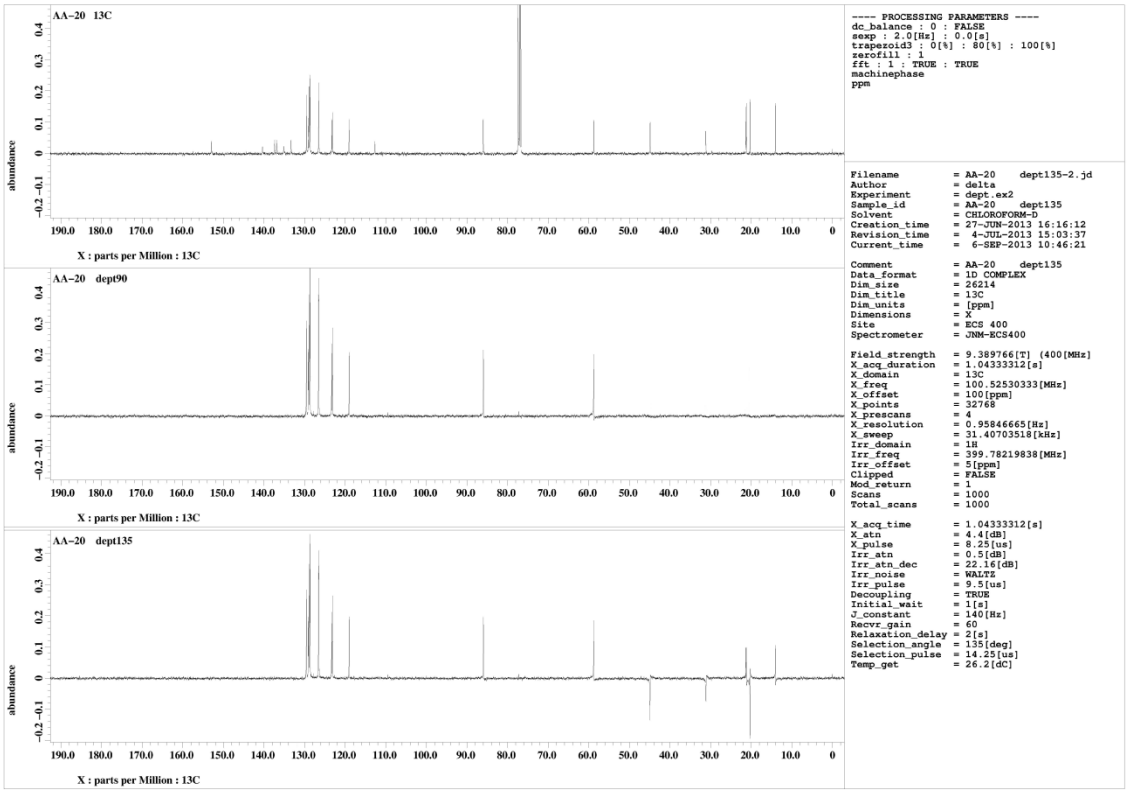
```
Filename          = AA-20     hetcore-2.jd
Author            = delta
Experiment        = hetcor.ex2
Sample_id         = AA-20     hetcore
Solvent           = CHLOROFORM-D
Creation_time     = 27-JUN-2013 13:46:10
Revision_time     =  6-SEP-2013 10:49:21
Current_time      =  6-SEP-2013 10:52:00

Comment           = AA-20     hetcore
Data_format       = 2D REAL REAL
Dim_size          = 819, 256
Dim_title         = 13C 1H
Dim_units         = [ppm] [ppm]
Dimensions        = X Y
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 32.52224[ms]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 1024
X_prescans        = 4
X_resolution      = 30.74818955[Hz]
X_sweep           = 31.4861461[kHz]
Y_domain          = 1H
Y_freq            = 399.78219838[MHz]
Y_offset          = 5[ppm]
Y_points          = 128
Y_prescans        = 0
Y_resolution      = 46.8600048[Hz]
Y_sweep           = 5.99808061[kHz]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 1024

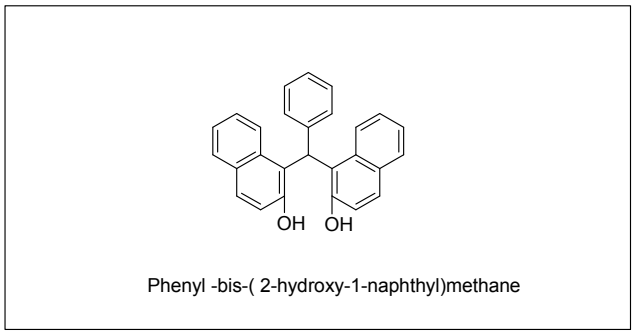
X_acq_time        = 32.52224[ms]
X_atn             = 4.4[dB]
X_pulse           = 8.25[us]
Y_acq_time        = 21.34016[ms]
Y_atn             = 0.5[dB]
Y_pulse           = 9.5[us]
Irr_atn_dec       = 22.16[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
J_constant        = 140[Hz]
Recvr_gain        = 60
Relaxation_delay  = 1.5[s]
T1                = 1[us]
Temp_get          = 26.2[dC]
```

7.6. DEPT


AA-20 13C
abundance
X : parts per Million : 13C
AA-20 dept90
abundance
X : parts per Million : 13C
AA-20 dept135
abundance
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Filename = AA-20 dept135-2.jd
Author = delta
Experiment = dept.ex2
Sample_id = AA-20 dept135
Solvent = CHLOROFORM-D
Creation_time = 27-JUN-2013 16:16:12
Revision_time = 4-JUL-2013 15:03:37
Current_time = 6-SEP-2013 10:46:21
Comment = AA-20 dept135
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_acq_time = 1.04333312[s]
X_atn = 4.4[dB]
X_pulse = 8.25[us]
Irr_atn = 0.5[dB]
Irr_atn_dec = 22.16[dB]
Irr_noise = WALTZ
Irr_pulse = 9.5[us]
Decoupling = TRUE
Initial_wait = 1[s]
J_constant = 140[Hz]
Recvr_gain = 60
Relaxation_delay = 2[s]
Selection_angle = 135[deg]
Selection_pulse = 14.25[us]
Temp_get = 26.2[dC]

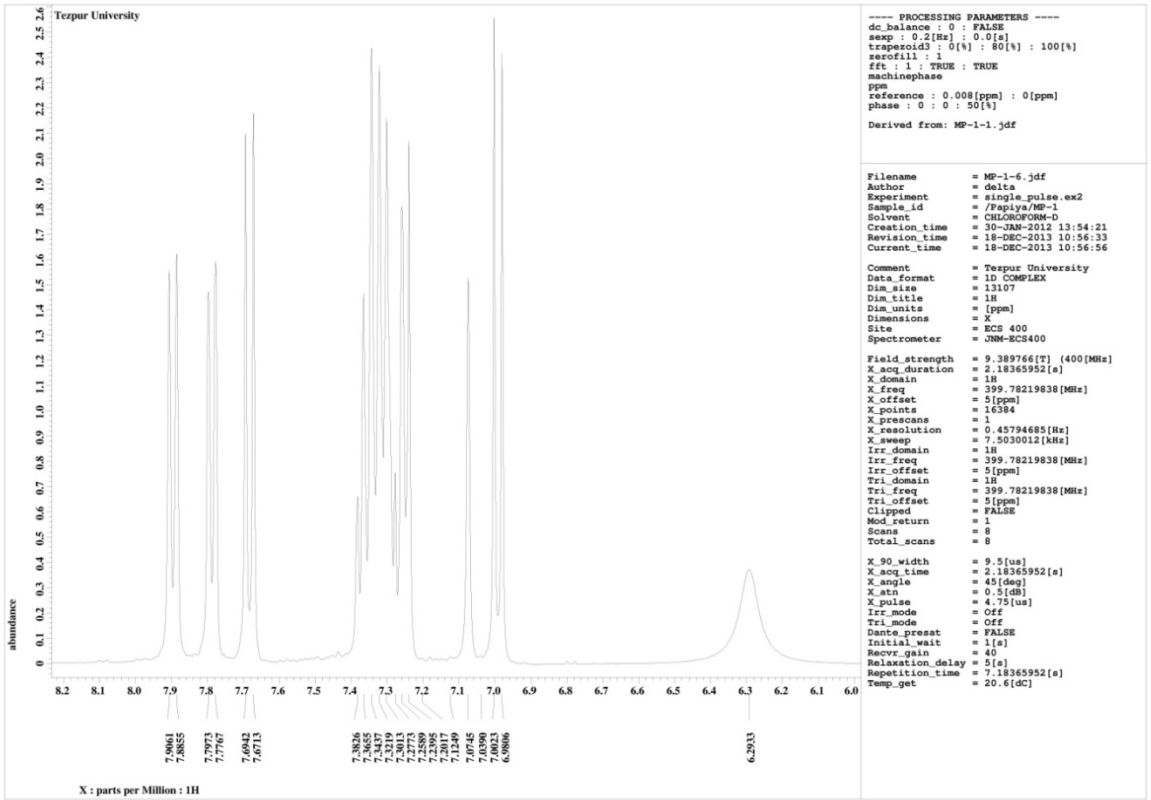
(3) NMR Spectra of <u>23</u> and <u>24</u> Derivatives

[8] Table-3, entry-5, **<u>23</u>**

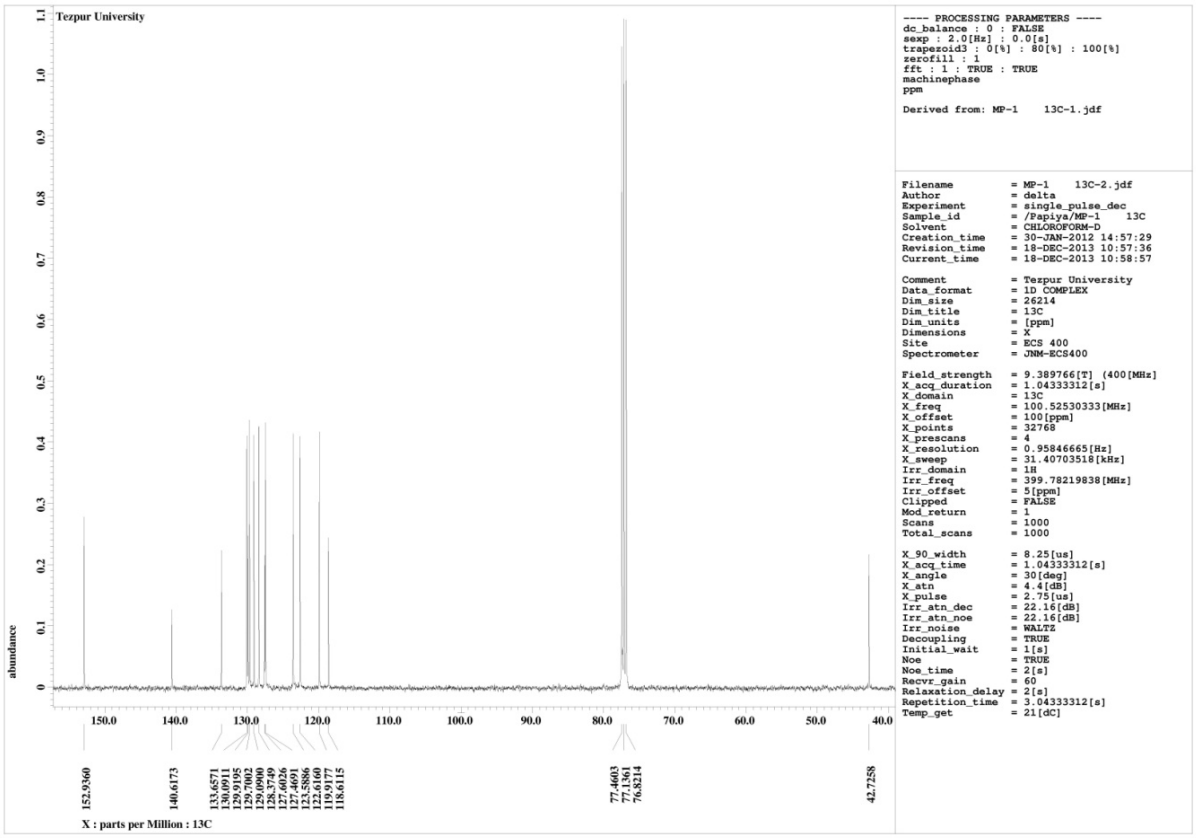


Phenyl -bis-(2-hydroxy-1-naphthyl)methane

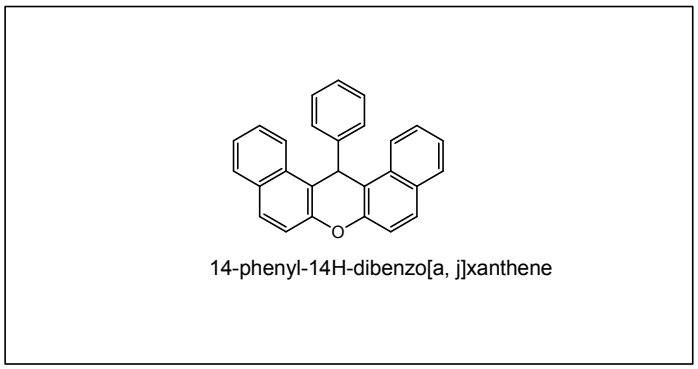
8.1 ^{1}H NMR



8.2 ^{13}C NMR

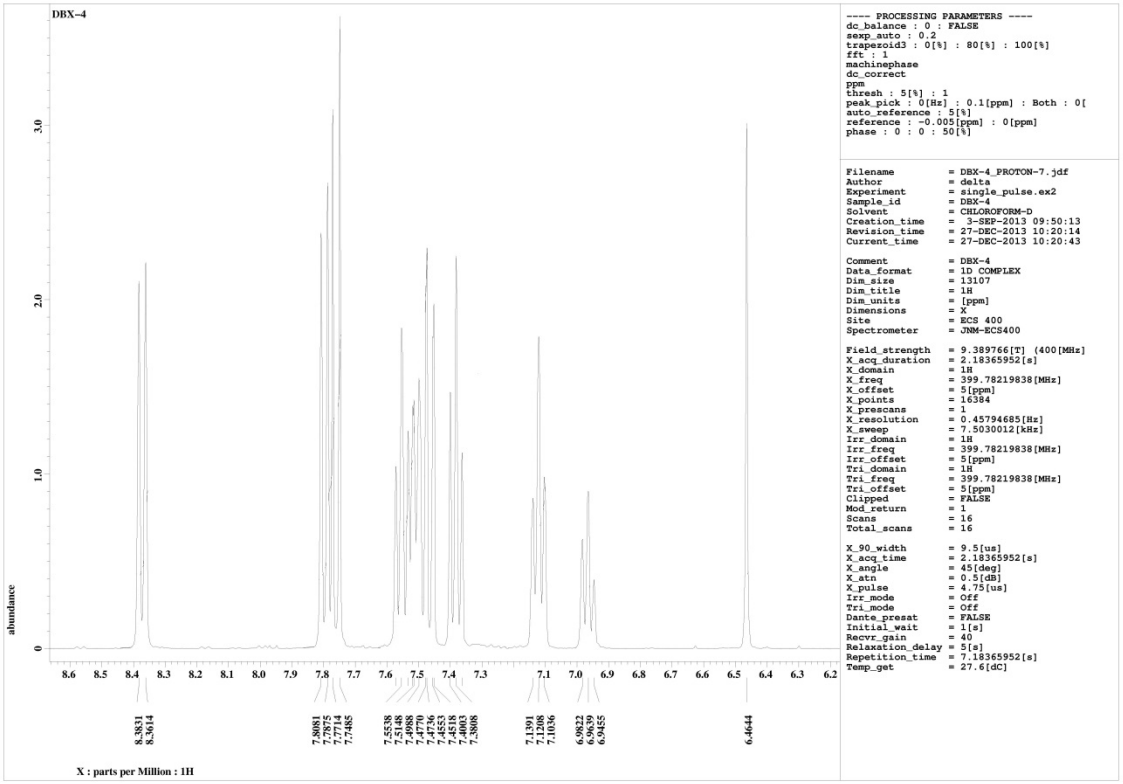

Tezpur University
abundance
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
152.9360
140.6173
133.6571
130.0911
129.9195
129.7002
129.0900
128.7759
127.4026
127.4691
123.5886
122.6160
119.9177
116.6115
77.4603
77.1361
76.8214
42.7258
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: MP-1 13C-1.jdf
Filename = MP-1 13C-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = /Papiya/MP-1 13C
Solvent = CHLOROFORM-D
Creation_time = 30-JAN-2012 14:57:29
Revision_time = 18-DEC-2013 10:57:36
Current_time = 18-DEC-2013 10:58:57
Comment = Tezpur University
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 21[dC]

[9] Table-3, entry-5, **<u>24</u>**

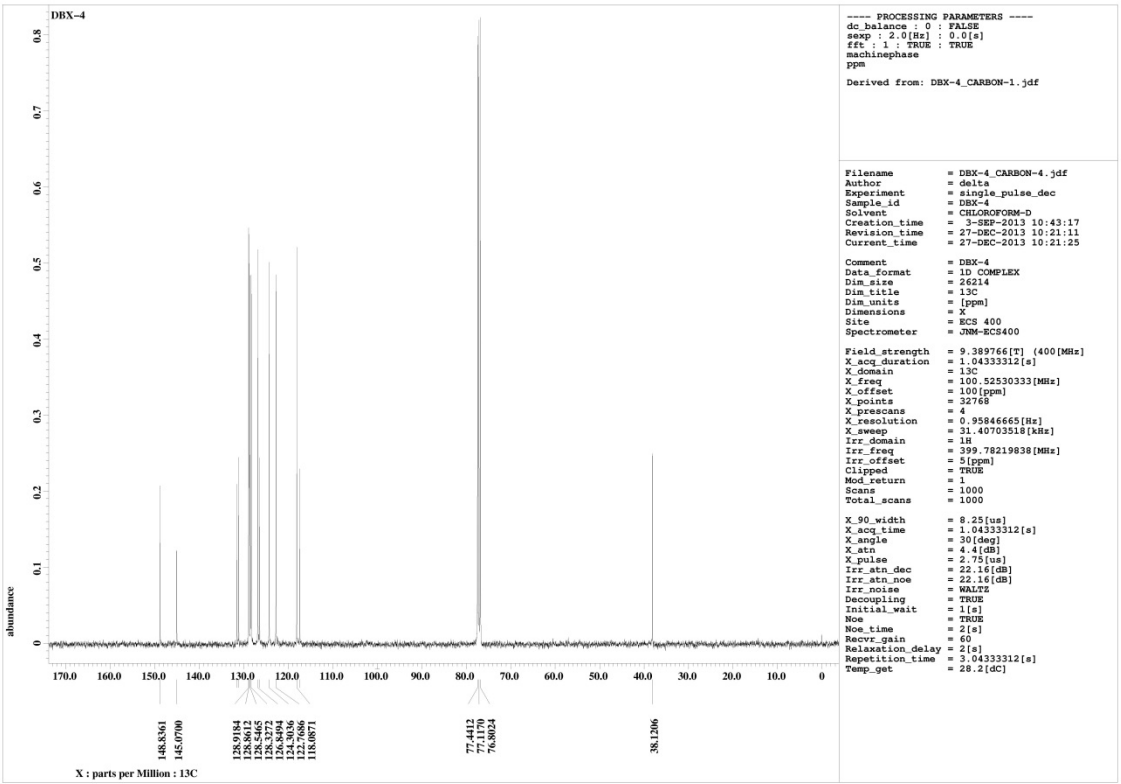


14-phenyl-14H-dibenzo[a, j]xanthene

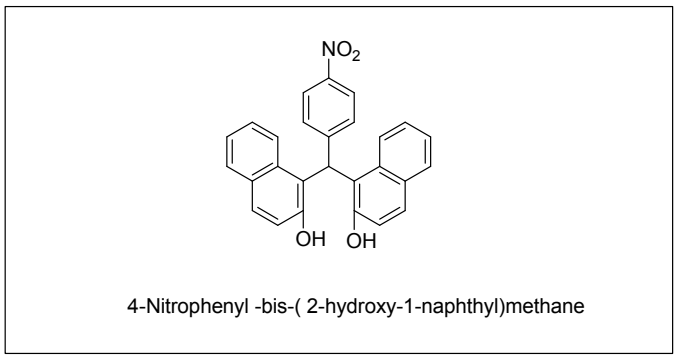
9.2 ^{1}H NMR



9.2 ^{13}C NMR

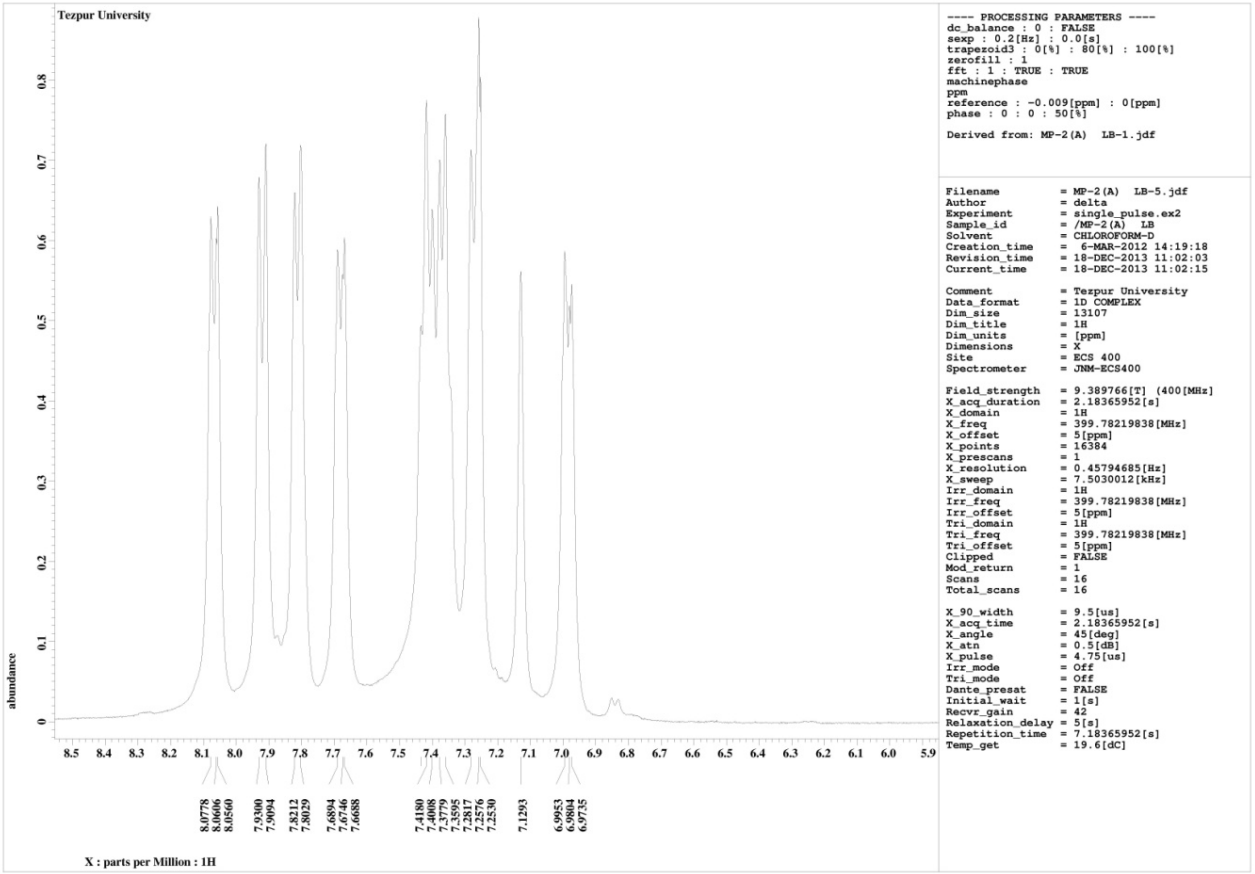

DBX-4
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
148.8361
145.0700
128.9184
128.5612
128.5465
128.3272
126.8494
124.1036
122.7686
118.0871
77.4412
77.1170
76.8024
38.1206
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: DBX-4_CARBON-1.jdf
Filename = DBX-4_CARBON-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = DBX-4
Solvent = CHLOROFORM-D
Creation_time = 3-SEP-2013 10:43:17
Revision_time = 27-DEC-2013 10:21:11
Current_time = 27-DEC-2013 10:21:25
Comment = DBX-4
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 28.2[dC]

[10] Table-3, entry-8, **23**

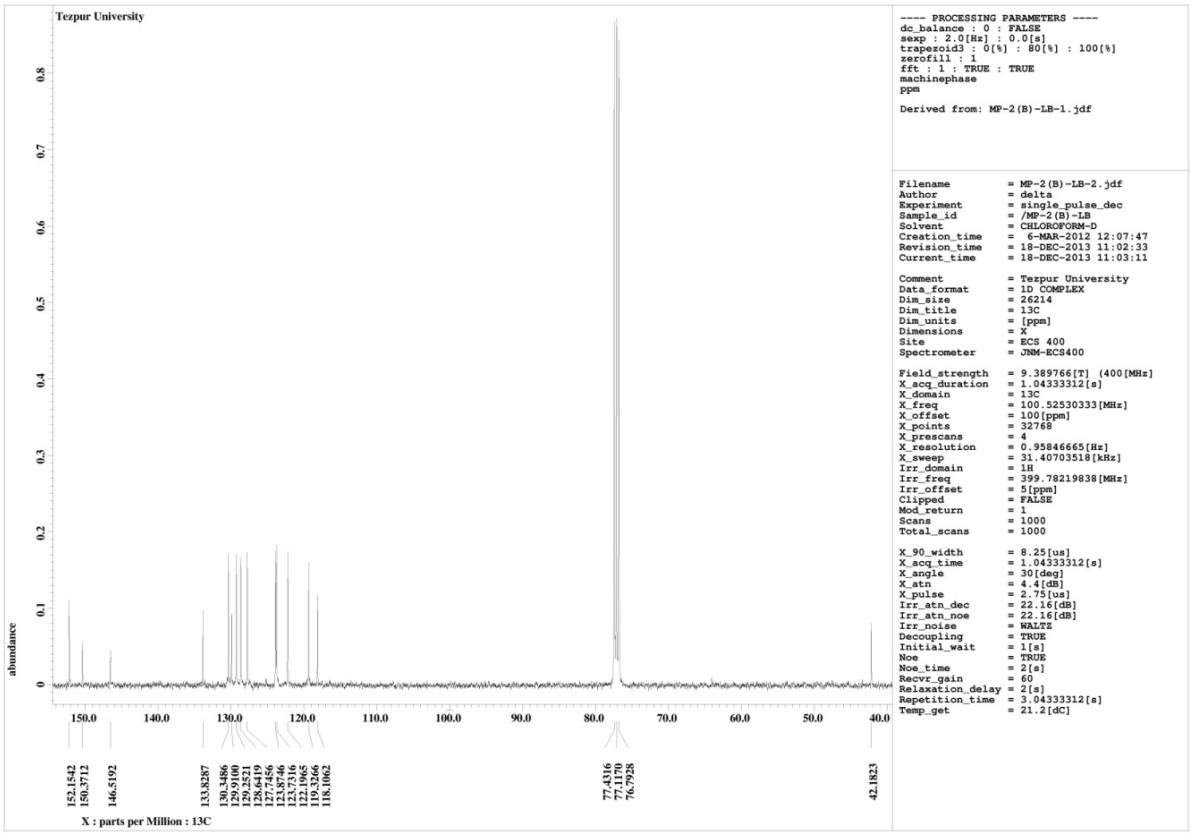


4-Nitrophenyl -bis-(2-hydroxy-1-naphthyl)methane

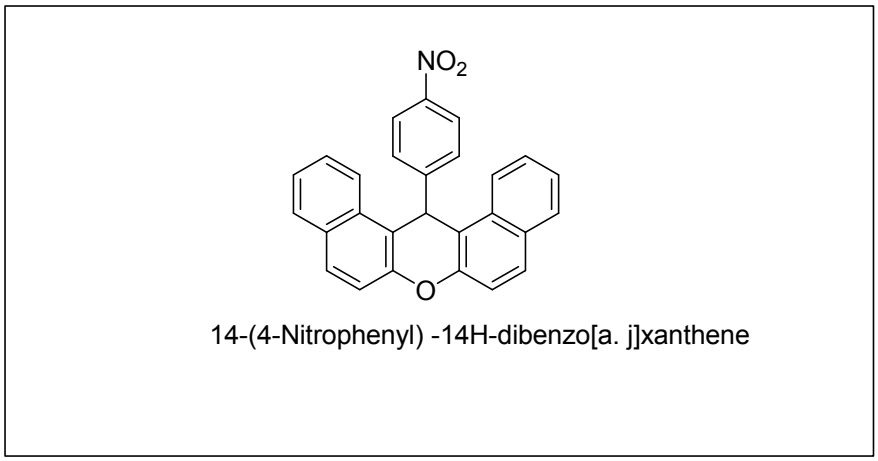
10.1 ^{1}H NMR



10.2.^{13}C NMR

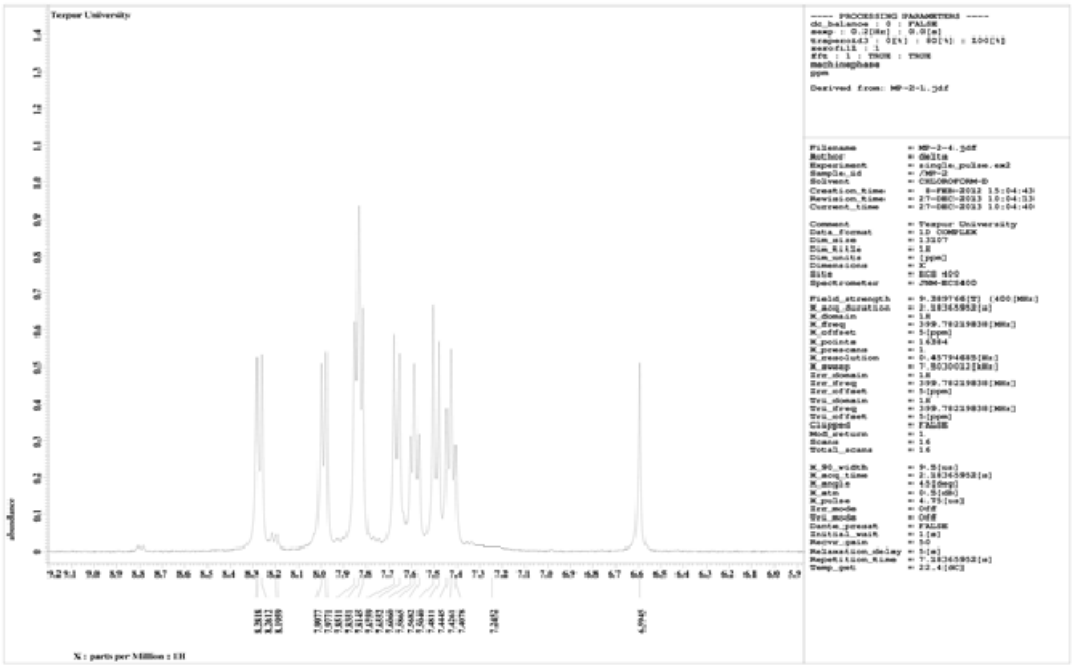

Tezpur University
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
152.1542
150.3712
146.5192
133.8287
130.3486
129.9100
129.2521
128.4419
127.7536
123.8746
123.7316
122.1965
119.3266
118.1062
77.4316
77.1170
76.7928
42.1823
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: MP-2(B)-LB-1.jdf
Filename = MP-2(B)-LB-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = /MP-2(B)-LB
Solvent = CHLOROFORM-D
Creation_time = 6-MAR-2012 12:07:47
Revision_time = 18-DEC-2013 11:02:33
Current_time = 18-DEC-2013 11:03:11
Comment = Tezpur University
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 21.2[dC]

[11] Table 3, entry-8, **24**

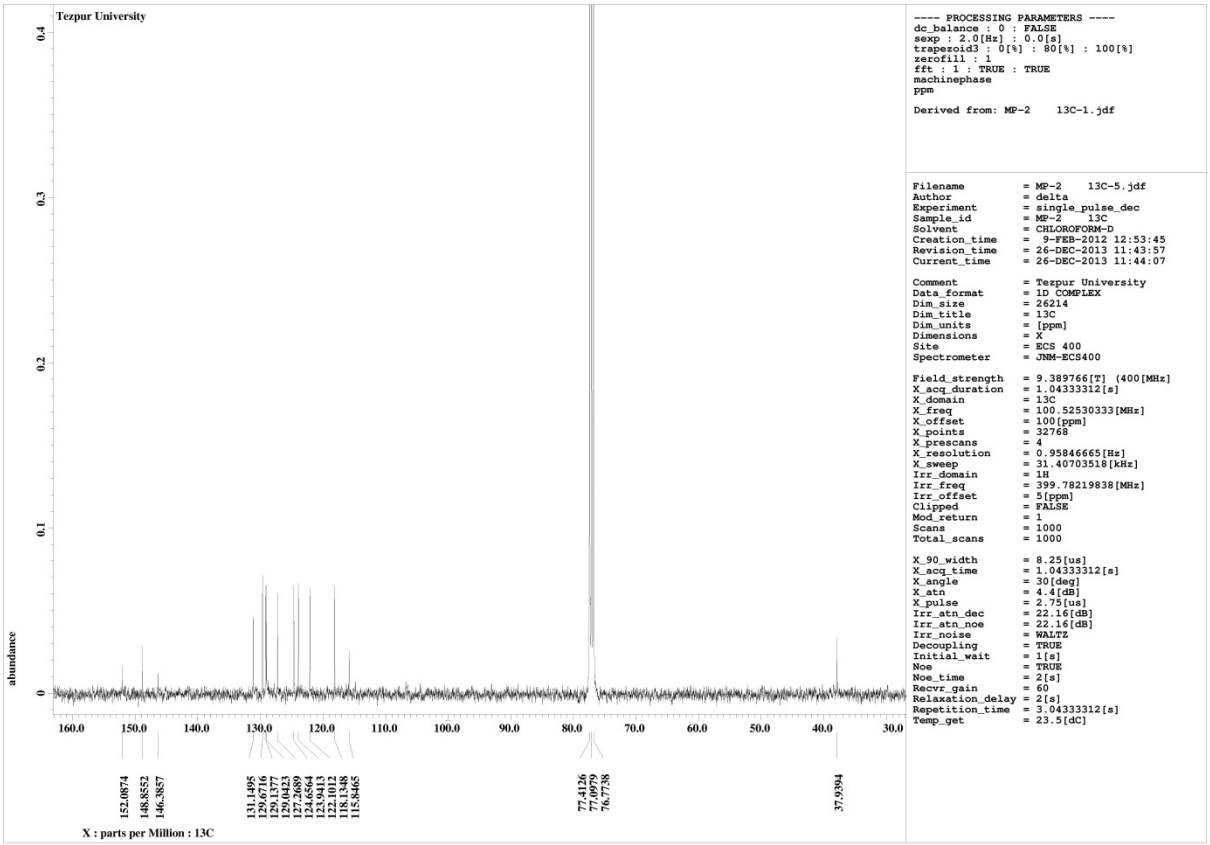


14-(4-Nitrophenyl) -14H-dibenzo[a. j]xanthene

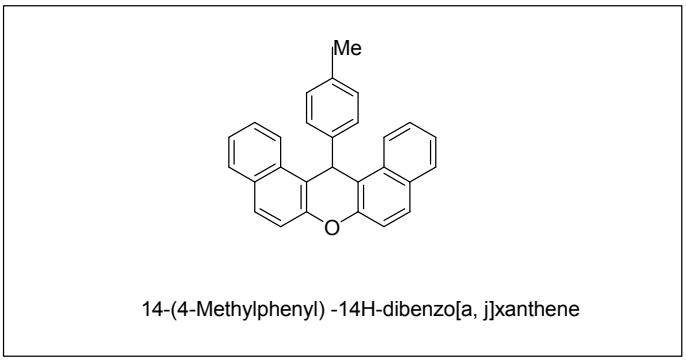
11.1.^{1}H NMR



11.2.^{13}C NMR

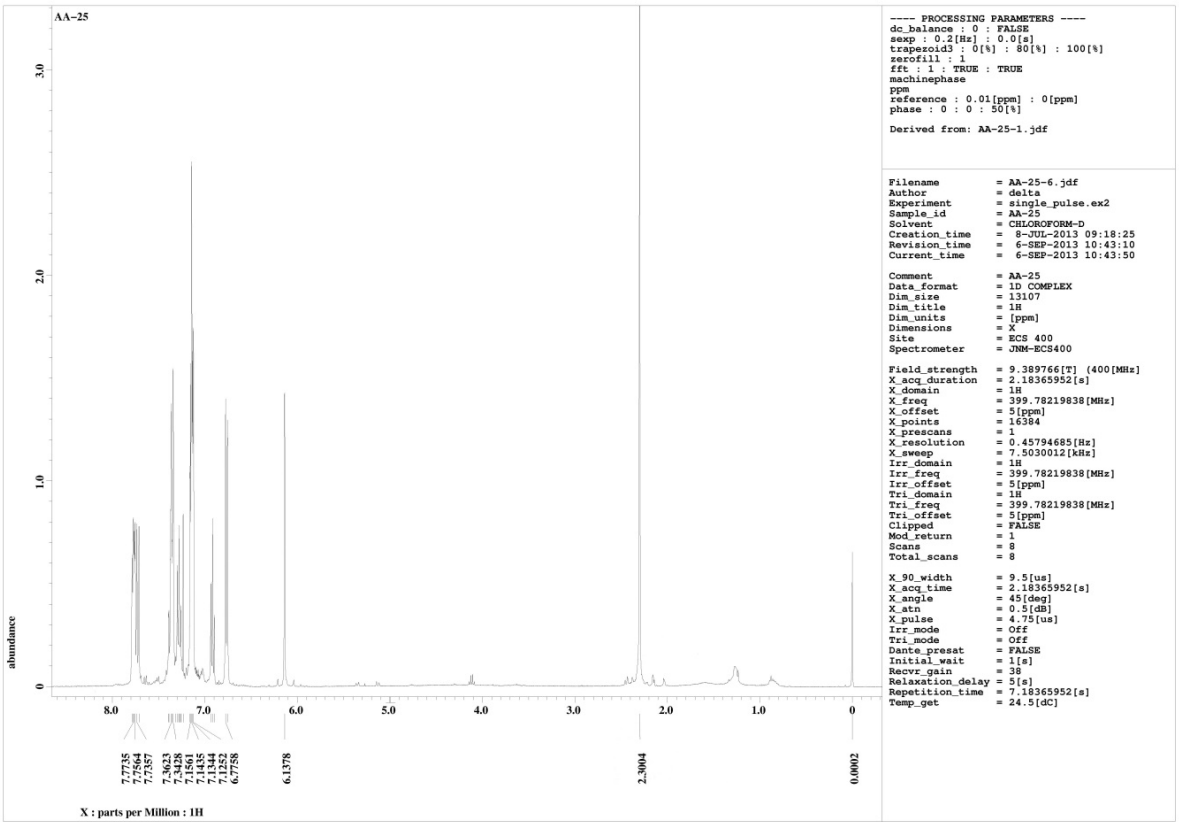

Tezpur University
abundance
0.4
0.3
0.2
0.1
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
152.0874
148.8552
146.3857
131.1495
129.6716
129.1377
129.0423
127.2689
124.6564
123.9413
122.1012
118.1438
115.8468
77.4136
77.0979
76.7738
37.9304
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: MP-2 13C-1.jdf
Filename = MP-2 13C-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = MP-2 13C
Solvent = CHLOROFORM-D
Creation_time = 9-FEB-2012 12:53:45
Revision_time = 26-DEC-2013 11:43:57
Current_time = 26-DEC-2013 11:44:07
Comment = Tezpur University
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 23.5[dC]

[12] Table-3, entry-10, **<u>24</u>**

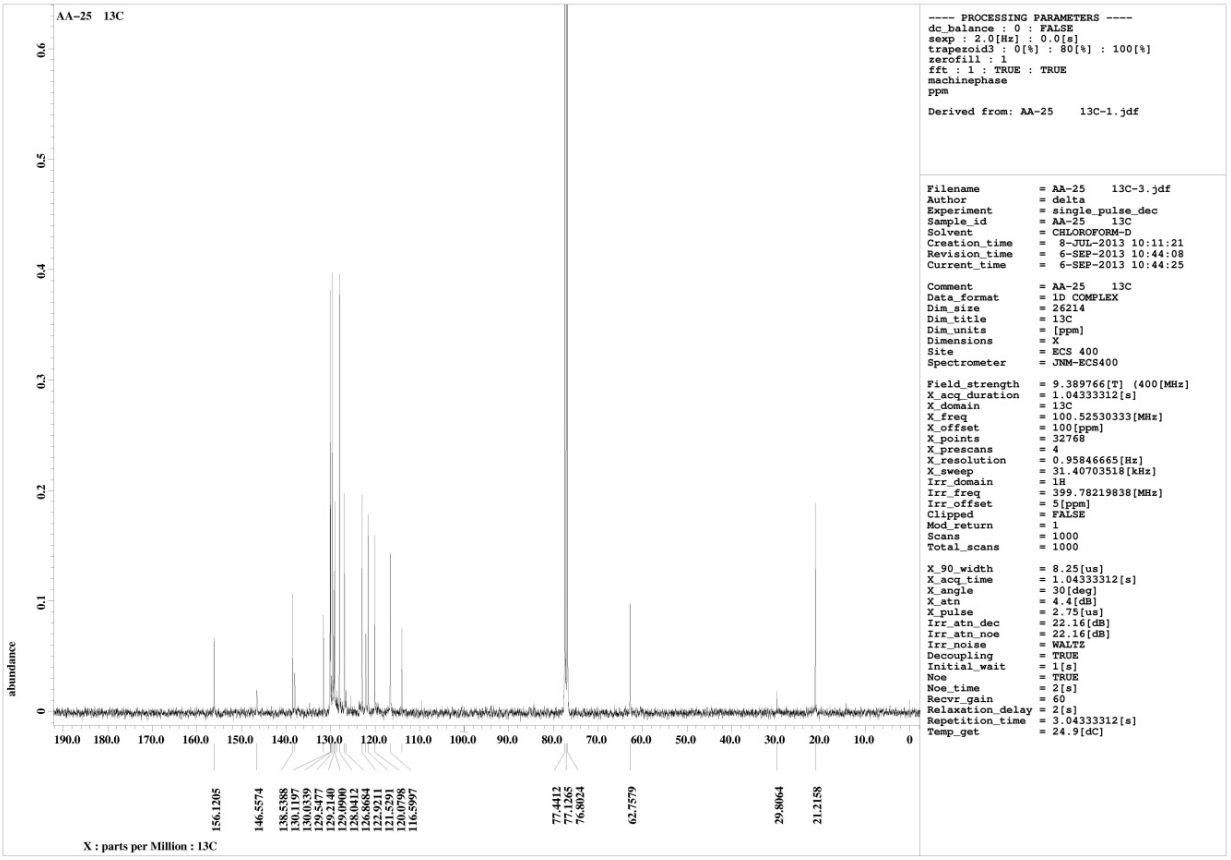


14-(4-Methylphenyl) -14H-dibenzo[a, j]xanthene

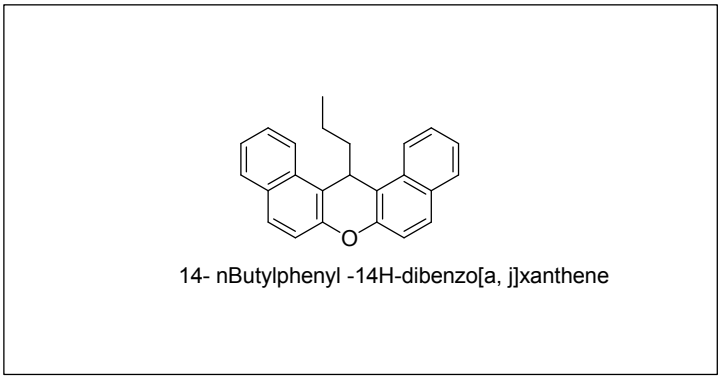
12.1.^{1}H NMR



12.2^{13}C NMR

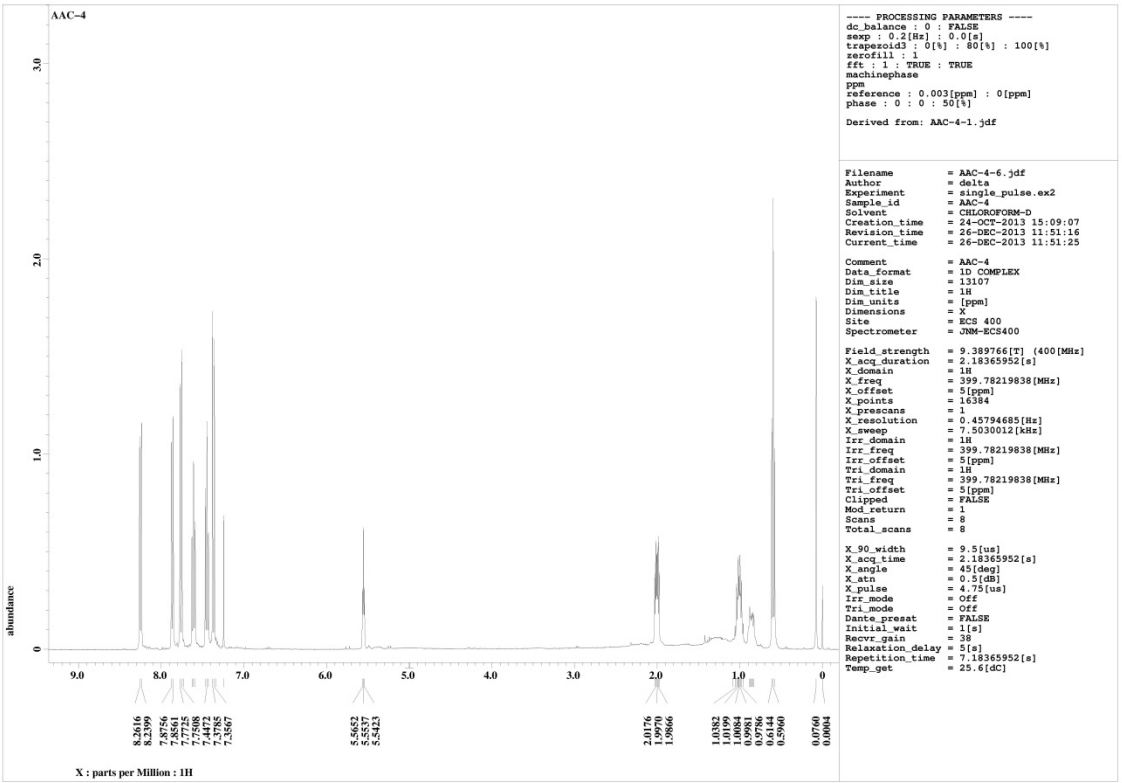

AA-25 13C
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
156.1205
146.5574
138.5388
130.1197
130.0339
129.5477
129.2140
129.0900
128.4412
126.9684
122.9211
121.5291
120.0798
116.5997
77.4412
77.1265
76.8024
62.7579
29.8064
21.2158
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
traperoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: AA-25 13C-1.jdf
Filename = AA-25 13C-3.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = AA-25 13C
Solvent = CHLOROFORM-D
Creation_time = 8-JUL-2013 10:11:21
Revision_time = 6-SEP-2013 10:44:08
Current_time = 6-SEP-2013 10:44:25
Comment = AA-25 13C
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 24.9[dC]

[13] Table-3, entry-12,**24**

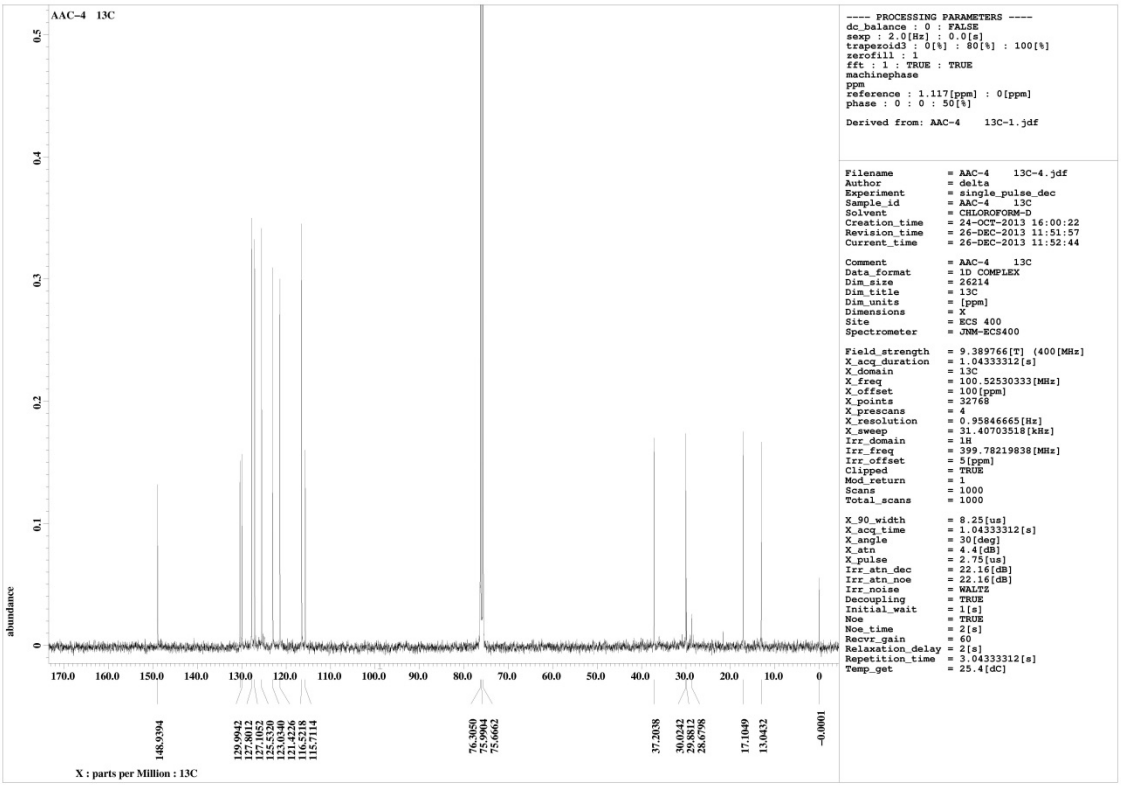


14- nButylphenyl -14H-dibenzo[a, j]xanthene

13.1. ^{1}HNMR



13.2. ^{13}C NMR


AAC-4 13C
abundance
X : parts per Million : 13C
148.9394
129.9942
127.1012
127.1052
125.5320
123.0340
121.4226
116.7258
115.7114
76.3050
75.9904
75.6662
37.2038
30.0242
29.8812
28.6798
17.1049
13.0432
-0.0001
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
reference : 1.117[ppm] : 0[ppm]
phase : 0 : 0 : 50[%]
Derived from: AAC-4 13C-1.jdf
Filename = AAC-4 13C-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = AAC-4 13C
Solvent = CHLOROFORM-D
Creation_time = 24-OCT-2013 16:00:22
Revision_time = 26-DEC-2013 11:51:57
Current_time = 26-DEC-2013 11:52:44
Comment = AAC-4 13C
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 8.25[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 4.4[dB]
X_pulse = 2.75[us]
Irr_atn_dec = 22.16[dB]
Irr_atn_noe = 22.16[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 25.4[dC]