Journal of
Materials Chemistry

Supporting Information

New Role of Graphene Oxide as Active Hydrogen Donor in the Recyclable Palladium Nanoparticles Catalyzed Ullmann Reaction in Environmental Friendly Ionic Liquid/ Supercritical Carbon Dioxide System

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1. Materials and Characterization

1.1 Materials. Graphite powder (99.99995%, 325 mesh), $PdCl_2$ and palladium on activated carbon powder (5%) were purchased from Alfa Aesar. All the aryl chlorides were purchased from J & K. Aluminum was supplied by National Medicine Group, Shanghai, China. The ionic liquids used in this work were kindly provided by Lanzhou Institute of Chemical Physics, CAS. All the solvents and other reagents were purchased from Beijing Chemicals Co. Ltd. as analytical-grade products.

1.2 Samples Characterization. The powder X-ray diffraction (XRD) measurements of the samples were recorded on a Bruker D8- Advance X-ray powder diffractometer using Cu Kα radiation (λ = 1.5406 Å) with scattering angles (2θ) of 8–60°. JEOL JEM 1200EX and JEOL JEM 2010 transition electronic microscopy were used for transmission electron microscopy (TEM) analysis and high-resolution transmission electron microscopy (HRTEM, equipped with energy dispersive X-ray spectroscopy (EDS, Oxford) and selected area electron diffraction (SAED), excited at 120 kV) analysis at an accelerating voltage of 100 kV, respectively. Samples were prepared by placing one drop of an ethanol suspension of the PdNPs/GO hybrid composite onto a copper grid (3 mm, 200 mesh) coated with carbon film. A JSM-7401 scaning electron microscopy (SEM) operated at 20 kV was used to analyze the sample. The Ullmann products were analyzed on a GC-MS Spectrometer in EI mode using Perkin Elmer ASXL/MS Turbomass instrument, the product partition was done on PE-5 capillary column(30 m × 0.25 mm × 0.25 μm), oven temperature programed from 50°C-210 °C at 5 °C /min with an initial hold of 2 min. All ^{1}H NMR and ^{13}C NMR spectra were recorded at 600 MHz using $CDCl_3$ or d_6-DMSO as solvent using JEOL JNM-ECA 600 spectometer (^{1}H NMR at 600 MHz and ^{13}C NMR at 150 MHz). TLC was performed using commercially prepared 100-400 mesh silica gel plates (HF_{254}, Qingdao Haiyang Chemical Co. Ltd.), and visualization was effected at 254 nm. All melting points are uncorrected.

2. Supplementary Data

2.1 Synthesis of Graphene Oxide

Graphene oxide was prepared by modified Hummers method [1]: Graphite powder (1.5 g, 325 mesh) was put into a mixture of 12 ml concentrated H_2SO_4, 2.5 g $K_2S_2O_8$ and 2.5 g P_2O_5. The solution was heated to 80 ^{o}C and kept stirring for 5 h by using oil-bath. In a next step, the mixture was cooled to room temperature and diluted with deionized water (500 ml) overnight. Then, the product was obtained by filtering using 0.2 micron nylon film and dried naturally. The pre-oxidized graphite was then re-oxidized by Hummers method. Pretreated graphite powder was put into 0 °C concentrated H_2SO_4 (120 ml). Then, 15 g $KMnO_4$ was added gradually under stirring and the temperature of the mixture was kept to be below 20 °C by ice-bath. Successively, the mixture was stirred at 35 °C for 4 h, and then diluted with 250 mL deionized water by keeping the temperature under 50 ^{o}C. 700 ml deionized water was then injected into the mixture followed by adding 20 ml 30% H_2O_2 drop by drop. The mixture was filtered and washed with 1 : 10 HCl aqueous solution (1 L) to remove metal ions followed by 1 L of deionized water to remove the acid. The resulting solid was dried in air and diluted to make graphene oxide dispersion (0.5% *w/w*). Finally, it

was purified by dialysis for one week to remove the remaining metal species, finally, the sample of graphite oxide was obtained by filtration and dried in vacuum for 24 h at 60 ^{o}C. Successively, the sample of graphite oxide was re-dispersed in water (0.5 mg/ml) and ultrasoniced for 1 h, graphene oxide can be afforded by filtration, washing and vacuum-dried.

2.2 Typical Procedures for Pd NPs/C Preparation

To obtain the Pd NPs/C composites, 10.5 mg graphite (325 mesh, Alfa Aesar) was dispersed in 48 ml water by ultrasonic treatment for 1 h, and 2 ml 0.02 M $PdCl_2$ was added under stirring. And the pH value of this mixture was adjusted to 10 using 1 M NaOH. Then 280 mg $NaBH_4$ was slowly added to the mixture, with stirring for 48 h under room temperature. Finally, the solid sample with Pd loading was collected after washing extensively with ethanol and deionized water, and the unsupported Pd (II) cation can be removed completely, the sample was vacuum-dried at 40 ^{o}C, giving the catalyst: graphite-supported Pd NPs: Pd NPs/C.

2.3 Supplementary Characterization of the Catalyst

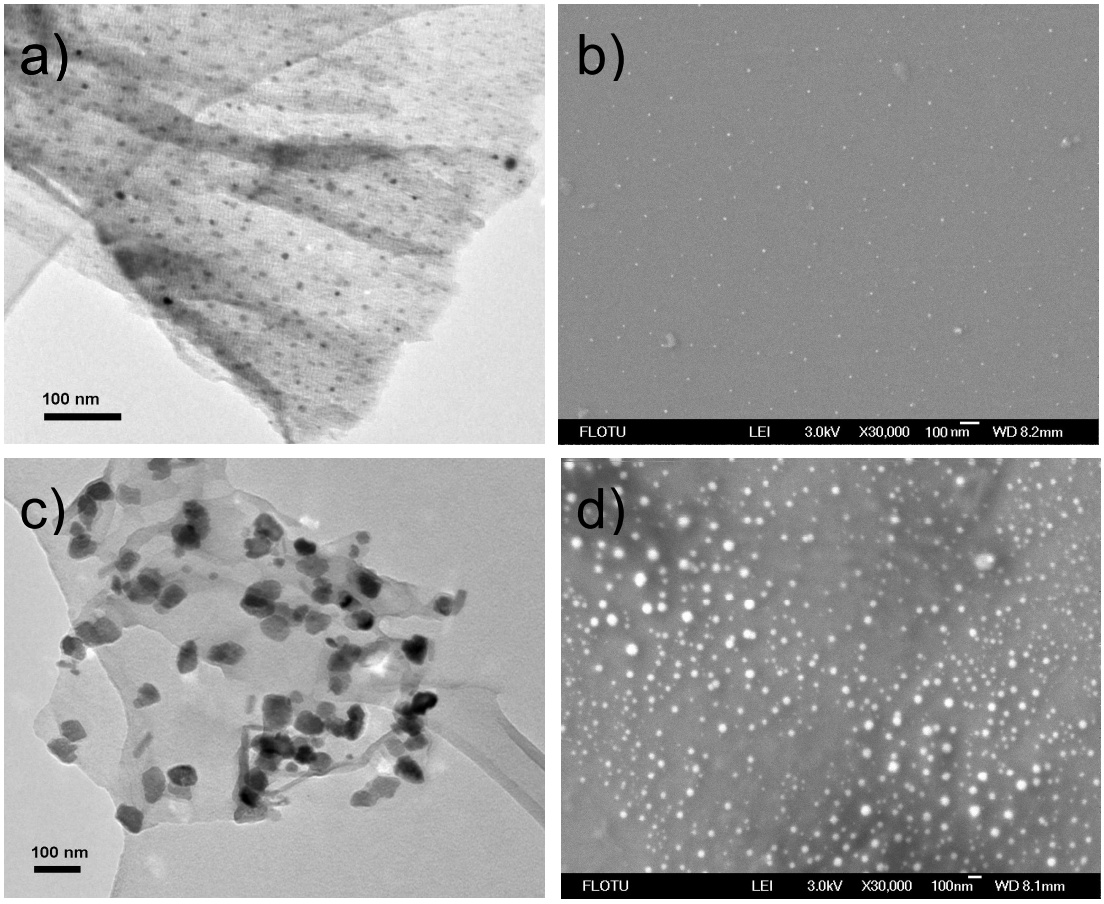


Figure S1. TEM a) and SEM b) images of the recycled catalyst (after 3 run of reaction) in the IL/$ScCO_2$ system; TEM c) and SEM d) images of the recycled catalyst in the H_2O/$ScCO_2$ system (after 3 run of reaction), indicating IL can stabilized Pd NPs.

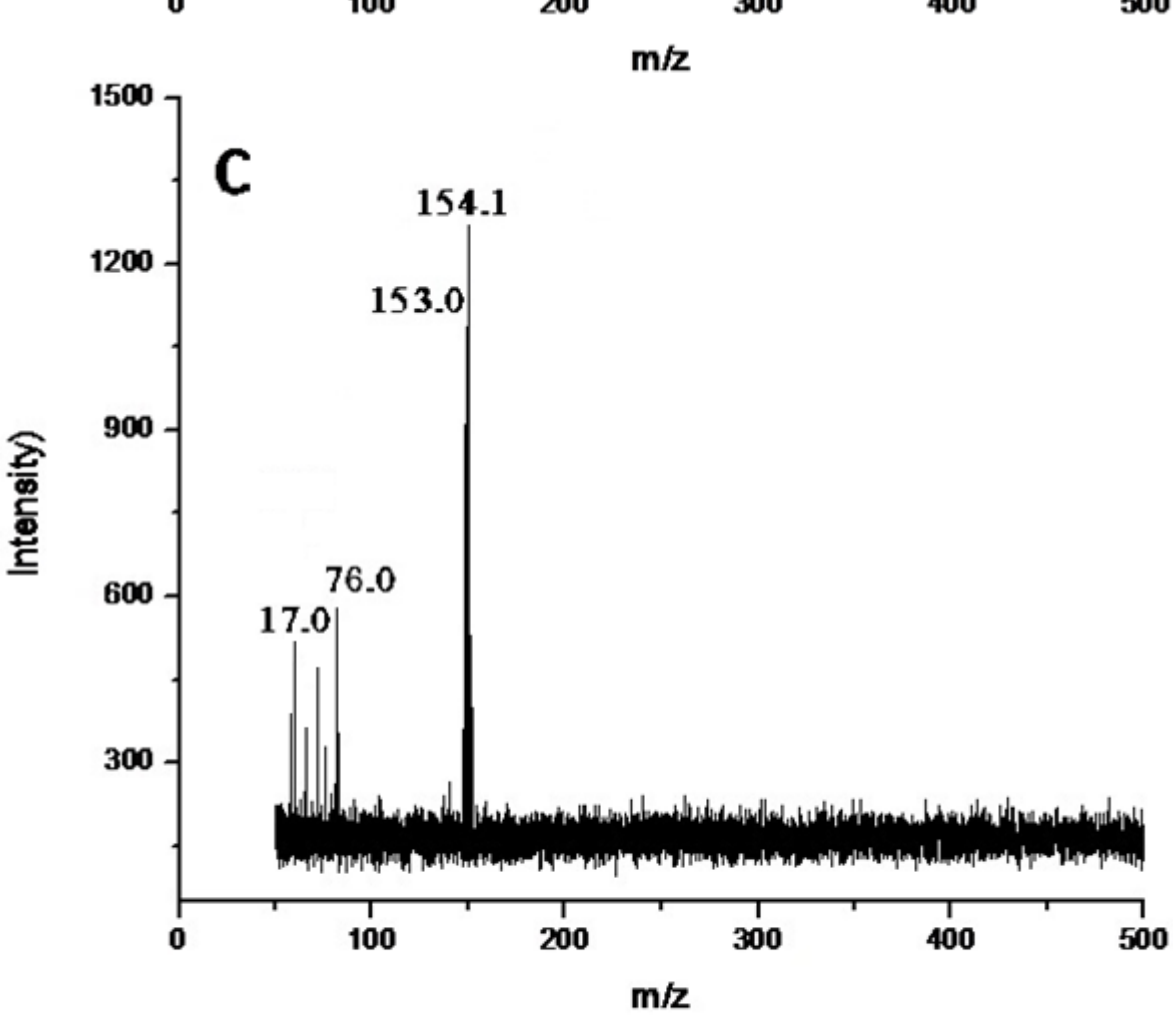


Figure S2. Structure illustrations of the ionic liquids used in this work.

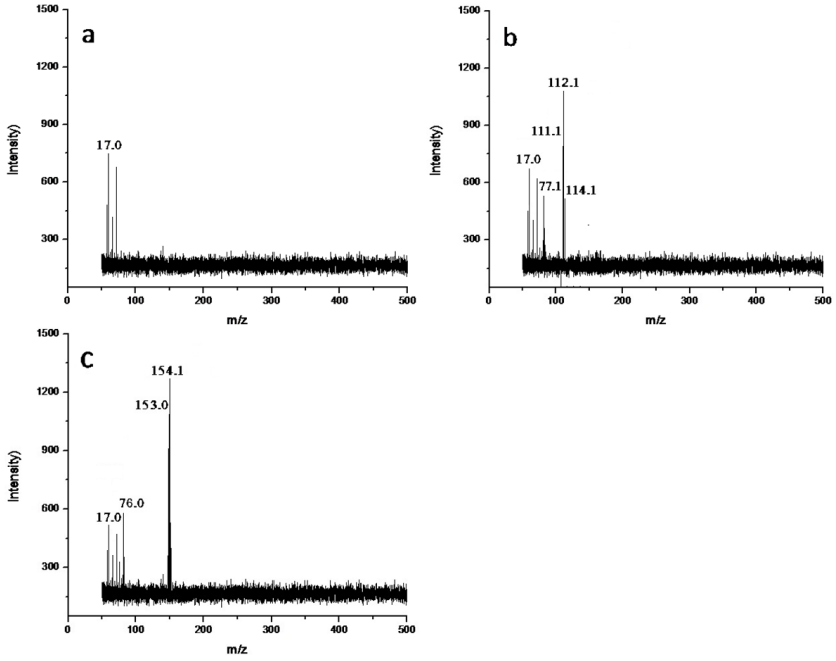
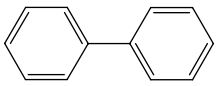


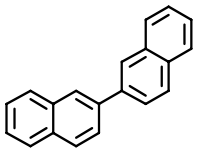
Figure S3. Supplementary MALDI-TOF MS analysis for the SET pathway of the Pd NPs/GO catalyzed Ullmann reaction of benzene chloride: a) intermediate **4** (Pd NPs/GO), b) intermediate **5** and c) intermediate **8**.

2.5 Analysis of the Ullmann Products



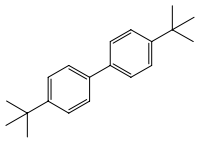
2a

Biphenyl (2a): Solid, m. p. 66-68 °C (Lit. [2] 68-69 °C) , ^{1}H NMR (600 MHz, $CDCl_3$, 27 °C): δ 7.5928-7.6054 (d, 4H), 7.4337-7.4589 (t, 4H); 7.3398-7.3638 (t, 2H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 °C): δ 127.3072, 127.3934, 128.8967, 141.3821, 131.2712, 134.6224, 165.4435; MS *m/z*: 156, 155, 154, 153, 152, 151, 77, 75.



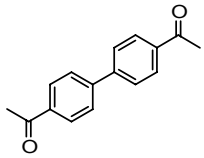
2b

2, 2′-Binaphthyl (2b): white crystalline, m. p. 155-157 °C (Lit. [3] 155-156 °C), ^{1}H NMR (600 MHz, $CDCl_3$, 27 °C): δ 7.4852-7.5367 (d, 4H), 7.8780-7.8918 (m, 4H), 7.9273-7.9650 (q, 4H), 8.1712 (s, 2H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 °C): δ 125.8327, 126.1104, 126.2157, 126.4551, 127.7764, 128.3317, 128.6190, 132.7553, 133.8372, 138.5097; MS *m/z*: 256, 255, 254, 252, 250, 226, 126, 113.



2c

4, 4'-Di-*tert*-butylbiphenyl (2c): White solid, m. p. 127-128 °C (Lit. [4] 127-128 °C), ^{1}H NMR (600 MHz, $CDCl_3$, 27 ℃): 1.3594-1.3628 (d, 18H), 7.4440-7.4611 (m, 4H), 7.5196-7.5367 (m, 4H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 ℃): δ 31.5021, 34.6139, 76.9152, 77.1259, 77.3365, 125.7466, 126.7710, 138.3086, 150.0090; MS *m/z*: 267, 266, 251, 221, 165, 118, 90, 57.



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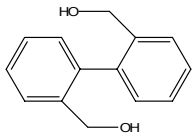
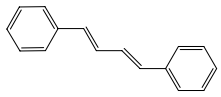
4, 4'-Diacetylbiphenyl (2d): White solid, m. p. 191-192 °C (Lit. [5] 190-191 °C), ^{1}H NMR (600 MHz, $CDCl_3$, 27 °C): δ 2.6581 (s, 6H), 7.7200-7.7337 (d, 2H), 8.0567-8.0704 (d, 2H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 °C): δ 26.7913, 127.5179, 129.0882, 136.6426, 144.3982, 197.6818; MS *m/z*: 239, 238, 223, 165, 152, 151, 43.



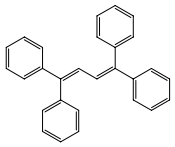
2e

2, 2'-Biphenyldimethanol (2e): Solid, m. p. 111-113 °C (Lit. [6] 110-112 °C) , ^{1}H NMR (600 MHz, $CDCl_3$, 27 °C): δ 2.8104-3.0749 (m, 2H), 4.3198-4.3530 (m, 4H), 7.1396-7.1554 (t, 2H), 7.2573 (s, 1H), 7.3272-3501 (t, 2H), 7.3718-7.4062 (q, 2H), 7.4623-7.4898 (t, 2H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 ^{o}C): δ 127.7477, 128.1785, 129.6339, 129.7392, 138.7108, 140.0608; MS *m/z*: 214, 213, 197, 196, 183, 182, 181, 165, 133, 89, 39.



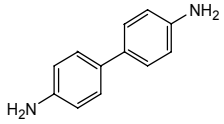
2f

***trans, trans*-1, 4-Diphenyl-1, 3-butadiene (2f):** Solid, m. p. 150.5-152 °C (Lit. [7] 150-151 °C), ^{1}H NMR (600 MHz, $CDCl_3$, 27 ℃): δ 6.6469-6.6973 (q, 2H), 6.9298-6.9802 (q, 2H),7.2184-7.2436 (t, 2H), 7.3168-7.3409- (t, 4H), 7.4325-7.4451 (d, 4H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 °C): δ 126.4838, 127.6711, 128.7626, 129.3371, 132.9180, 137.4373; MS *m/z*: 208, 207, 206, 205, 191, 129, 128, 91, 89, 77.



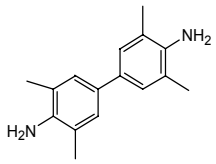
2g

1, 1, 4, 4-Tetraphenyl-1, 3-butadiene (2g): Solid, m. p. 206-209 °C (Lit. [8] 200 °C), ^{1}H NMR (600 MHz, $CDCl_3$, 27 °C): δ 6.7809 (s, 2H), 7.1577-7.1703 (t, 6H), 7.2023-7.2470 (m, 6H), 7.3100-7.3214 (d, 6H), 7.3478-7.3718 (t, 2H), 7.4016-7.4256 (t, 6H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 ^{o}C): δ 126.1104, 127.4604, 127.6041, 127.8147, 128.2360, 128.3413, 130.8020, 139.9842, 142.5886, 144.1301; MS *m/z*: 360, 359, 358, 279, 267, 265, 167, 165, 152, 126.



2h

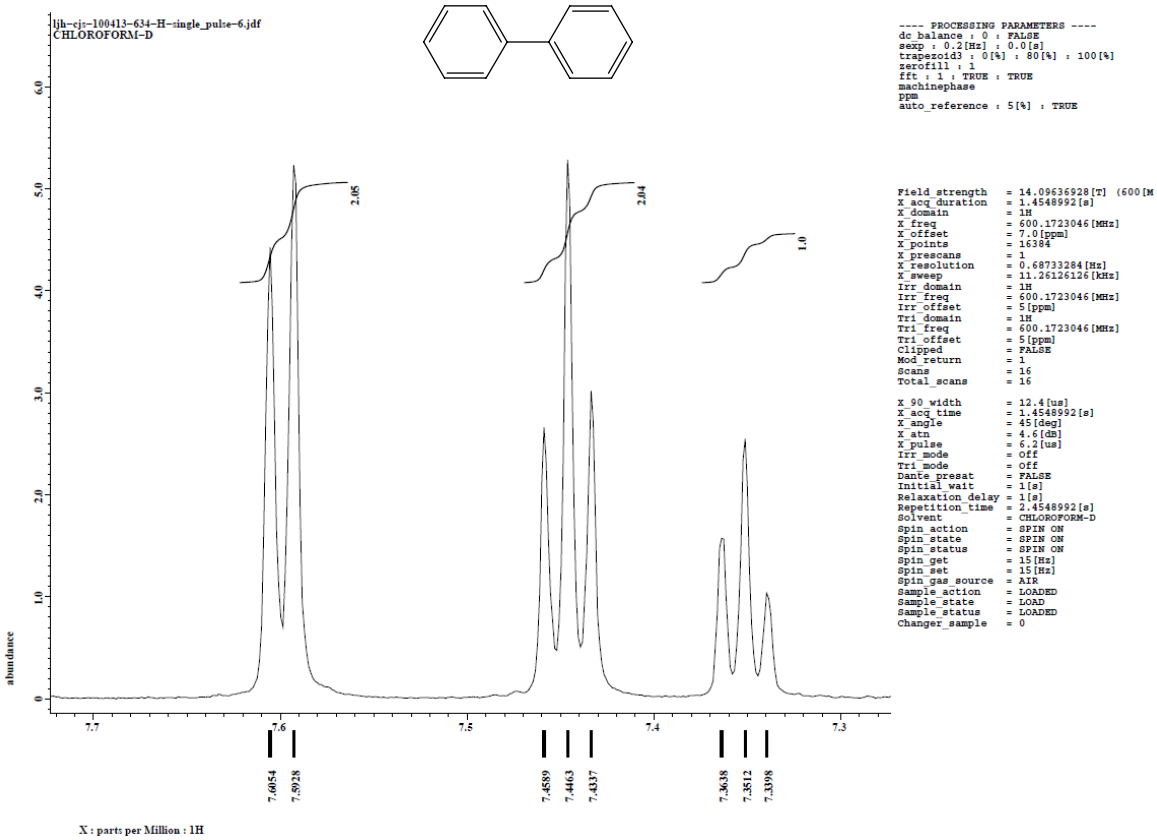
4, 4′-Diaminobiphenyl (2h): Solid, m. p. 128-129 °C (Lit. [9] 128-129 °C), ^{1}H NMR (600 MHz, $CDCl_3$, 27 °C): δ 3.6498 (s, 4H), 6.7110-6.7259 (d, 4H), 7.3294-7.3432 (d, 4H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 ^{o}C): δ 115.5686, 127.3838, 131.9223, 145.0397; MS *m/z*: 253, 252, 222, 221, 193, 103, 75, 59.



2i

4, 4′-Bi-2, 6-xylidine (2i): Solid, m. p. 168-170 °C (Lit. [10] 168-171 °C), ^{1}H NMR (600 MHz, $CDCl_3$, 27 °C): δ 2.2206 (m, 12H), 3.5422 (m, 4H), 7.2023-7.2470 (m, 4H), 7.1267-7.1302 (m, 4H); ^{13}C NMR(150 MHz, $CDCl_3$, 27 ^{o}C): δ 17.9347, 122.0794, 126.5891, 131.7116, 141.3917; MS *m/z*: 253, 252, 222, 221, 193, 103, 75, 59.

2a- ^{1}H NMR



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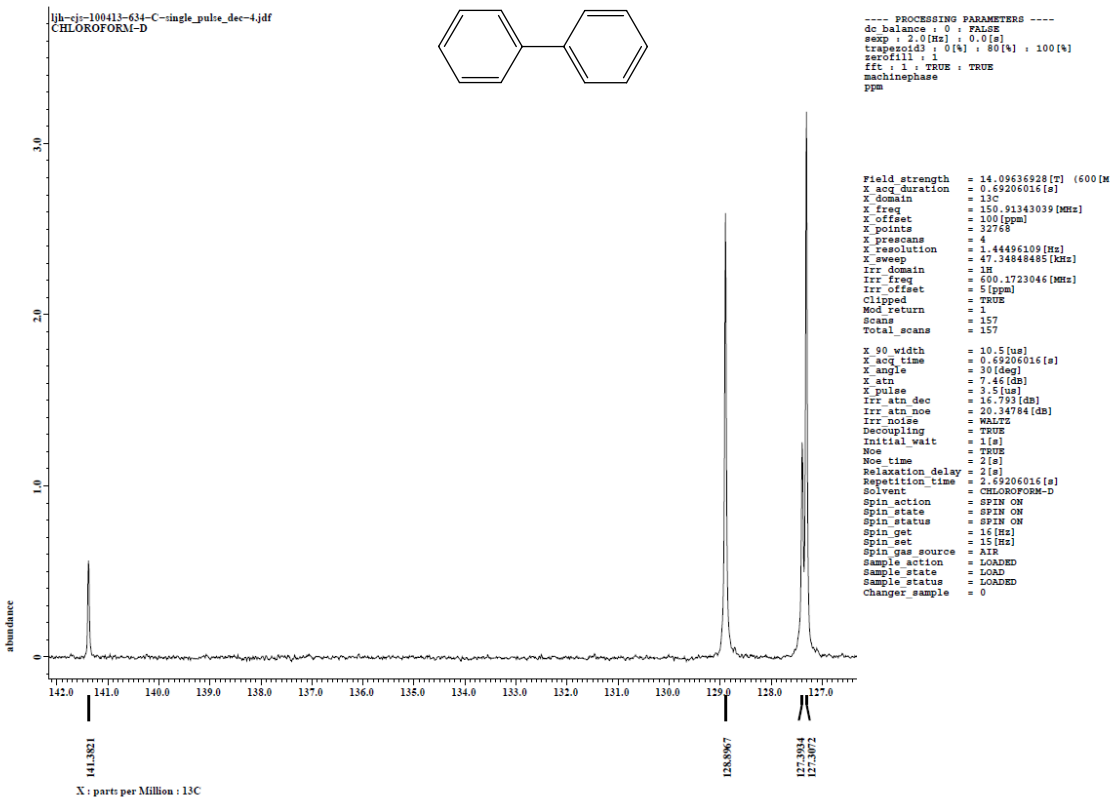
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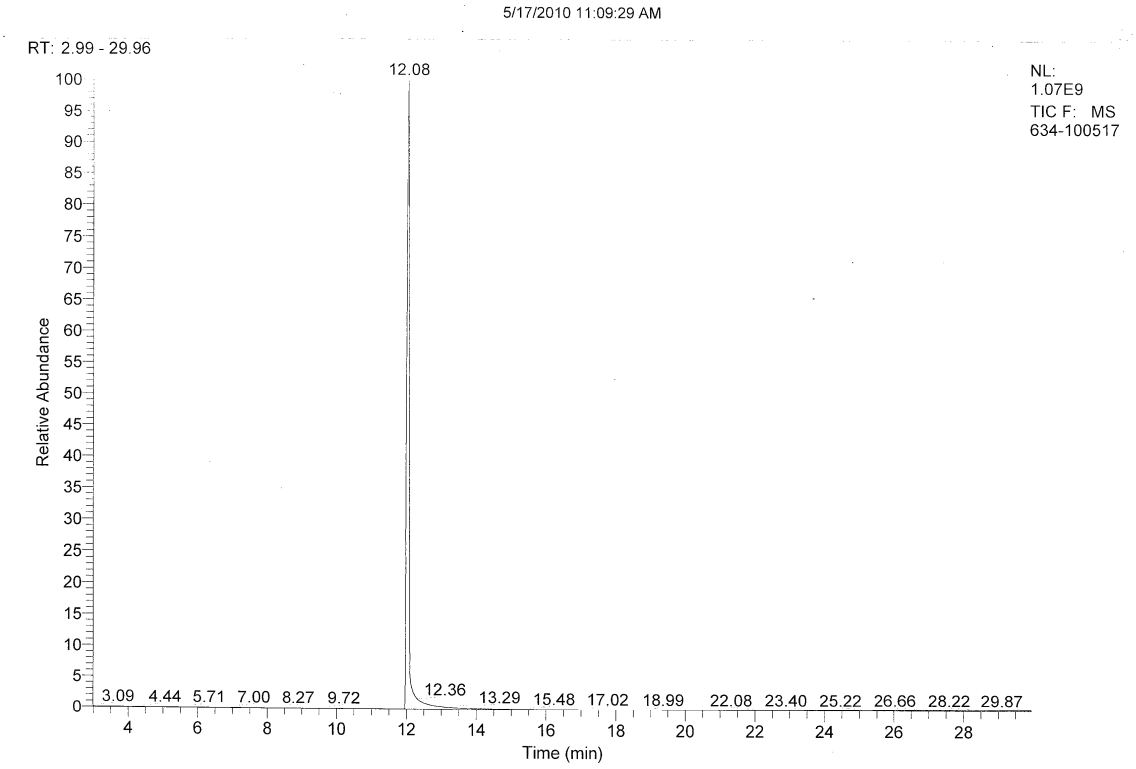
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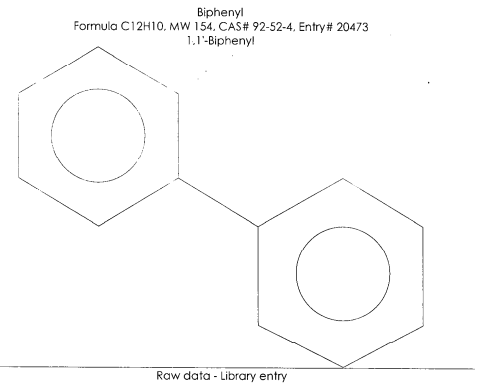

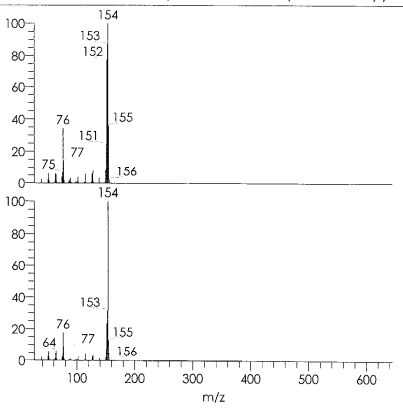

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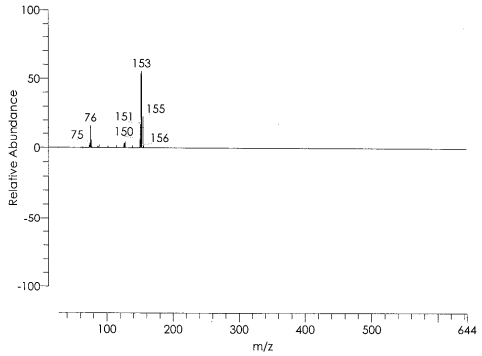
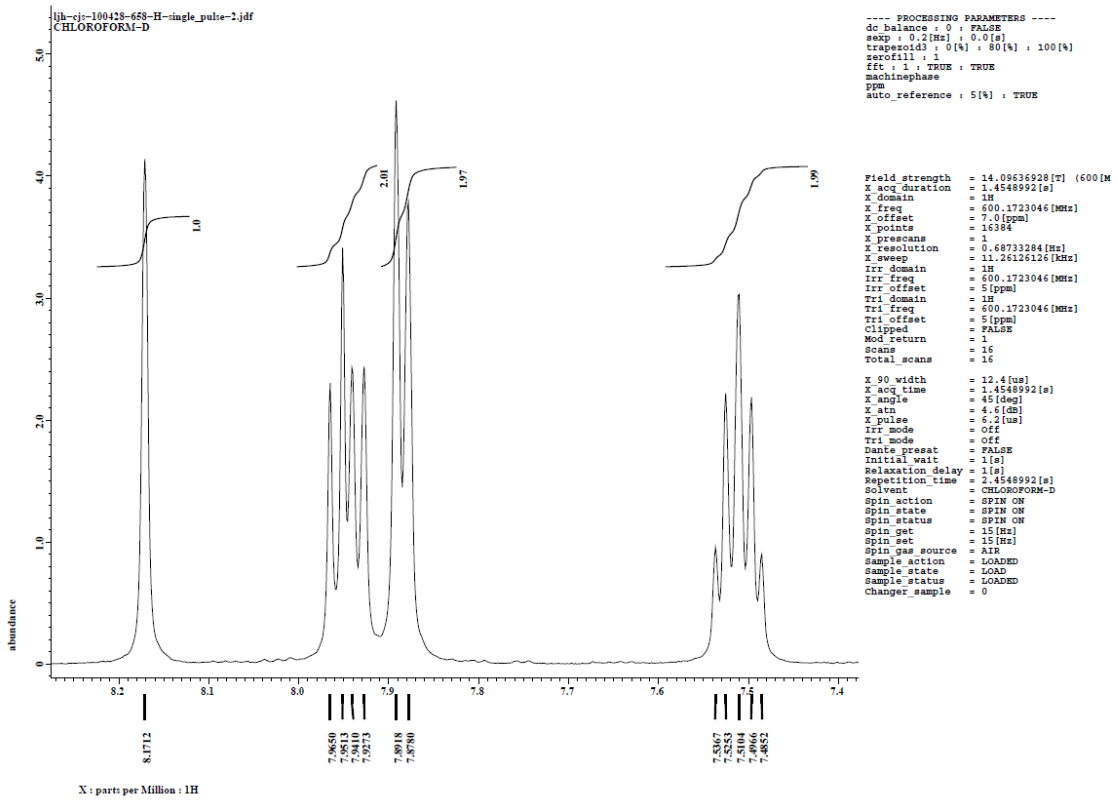


2b- ^{1}H NMR

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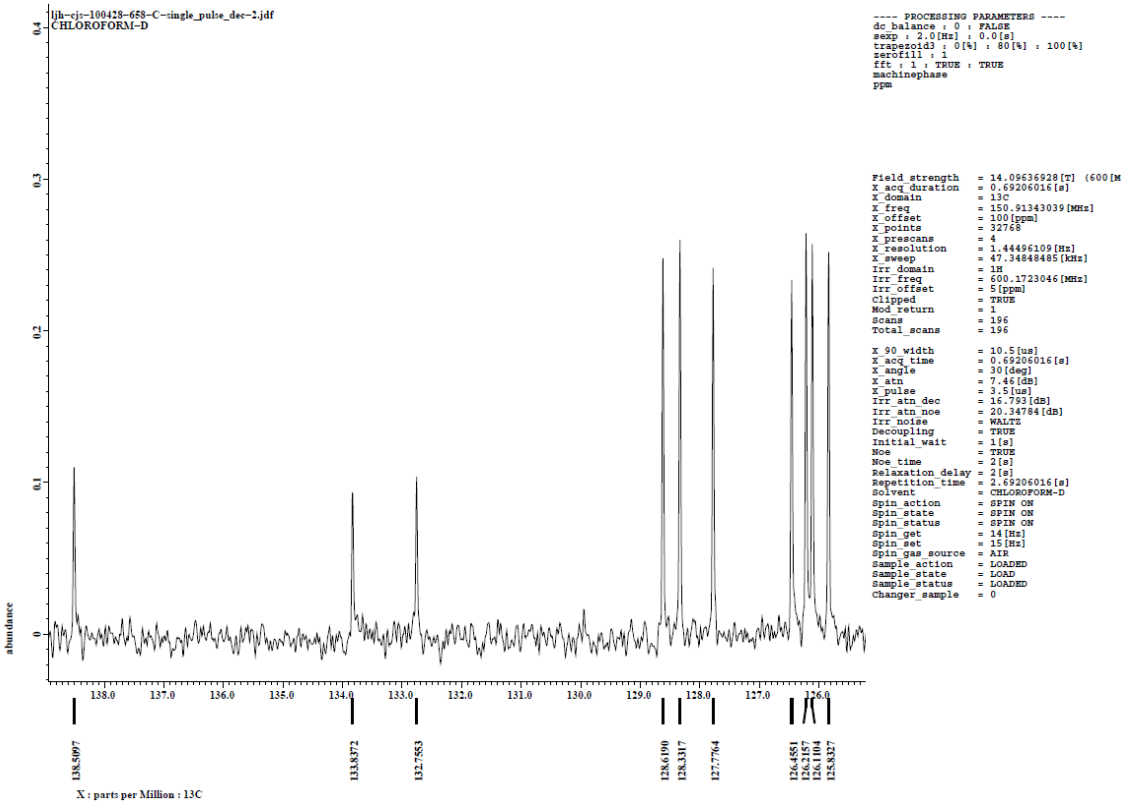
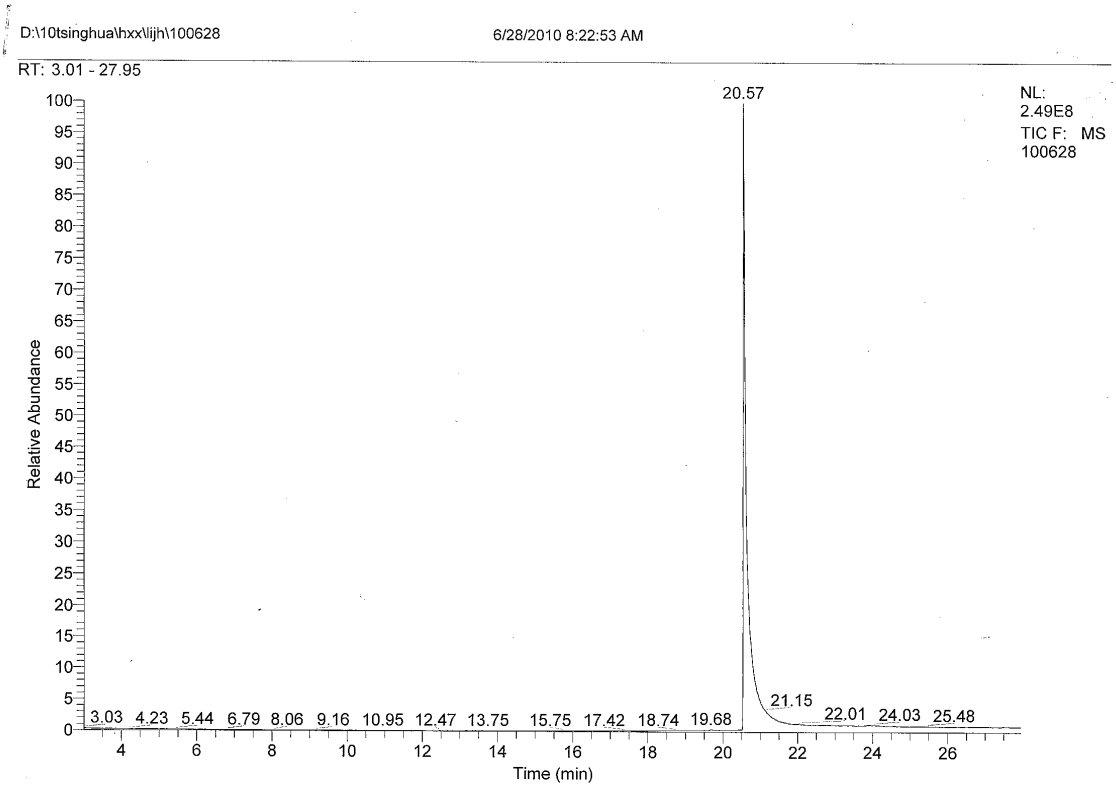
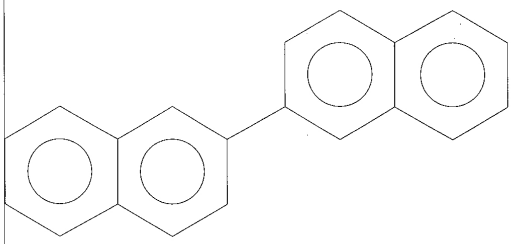

ljh-cjz-100428-658-C-single_pulse_dec-2.jdf
CHLOROFORM-D
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 196
Total_scans = 196
X_90_width = 10.5[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.46[dB]
X_pulse = 3.5[us]
Irr_atn_dec = 16.793[dB]
Irr_atn_noe = 20.34784[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 14[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
X : parts per Million : 13C

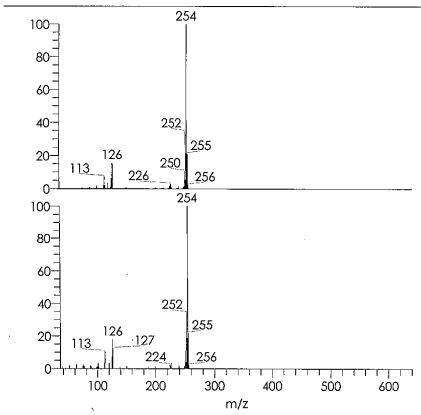
2b-MS


D:\10tsinghua\hxx\lijh\100628
6/28/2010 8:22:53 AM
RT: 3.01 - 27.95
NL:
2.49E8
TIC F: MS
100628
Relative Abundance
Time (min)
20.57
21.15
3.03
4.23
5.44
6.79
8.06
9.16
10.95
12.47
13.75
15.75
17.42
18.74
19.68
22.01
24.03
25.48

Hit	SI	RSI	Prob	Name	Library Name
1	917	940	37.79	2,2'-Binaphthalene	mainlib
2	891	891	11.32	1,2'-Binaphthalene	replib
3	890	890	37.79	2,2'-Binaphthalene	replib
4	890	890	10.88	Anthracene, 9-phenyl-	mainlib
5	889	889	10.46	1,1'-Binaphthalene	replib
6	889	893	10.46	6,6'-Biazulene,	mainlib
7	888	892	11.32	1,2'-Binaphthalene	mainlib
8	885	887	8.83	Phenanthrene, 2-phenyl-	mainlib
9	881	882	10.88	Anthracene, 9-phenyl-	replib
10	881	881	10.46	1,1'-Binaphthalene	mainlib
11	862	862	3.22	9H-Fluorene, 9-(phenylmethylene)-	replib
12	860	891	10.88	Anthracene, 9-phenyl-	replib
13	859	859	2.85	9,10[1',2']-Benzenoanthracene, 9,10-dihydr	mainlib
14	856	876	11.32	1,2'-Binaphthalene	replib
15	852	870	2.18	Benzo[a]pyrene, 4,5-dihydro-	mainlib
16	847	852	10.88	Anthracene, 9-phenyl-	replib
17	845	849	10.46	1,1'-Binaphthalene	replib
18	831	831	0.92	2,6-(Etheno[1,4]benzenoetheno)naphthale	mainlib
19	819	839	2.85	9,10[1',2']-Benzenoanthracene, 9,10-dihydr	replib

2,2'-Binaphthalene
Formula C20H14, MW 254, CAS# 612-78-2, Entry# 127377
2,2'-Binaphthyl

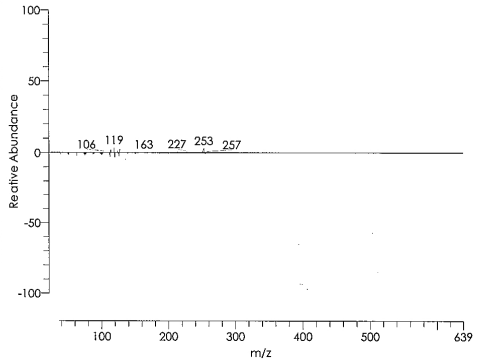




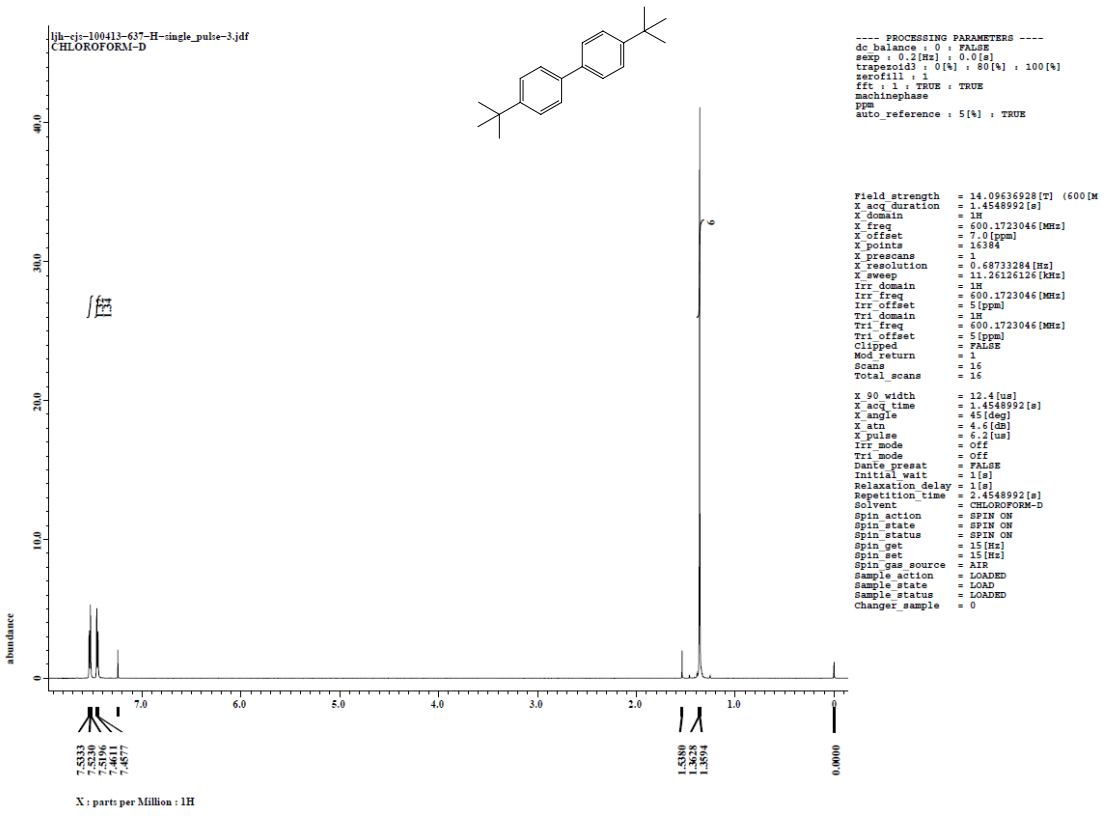
NL: 9.99E2
100628#1655 RT: 20.57
AV: 1 SB: 205 18.75-19.89 , 21.98-23.00 T: + c Full ms [35.00-650.00]

NL: 9.99E2
SI 917, RSI 940, mainlib, Entry# 127377, CAS# 612-78-2, 2,2'-Binaphthalene

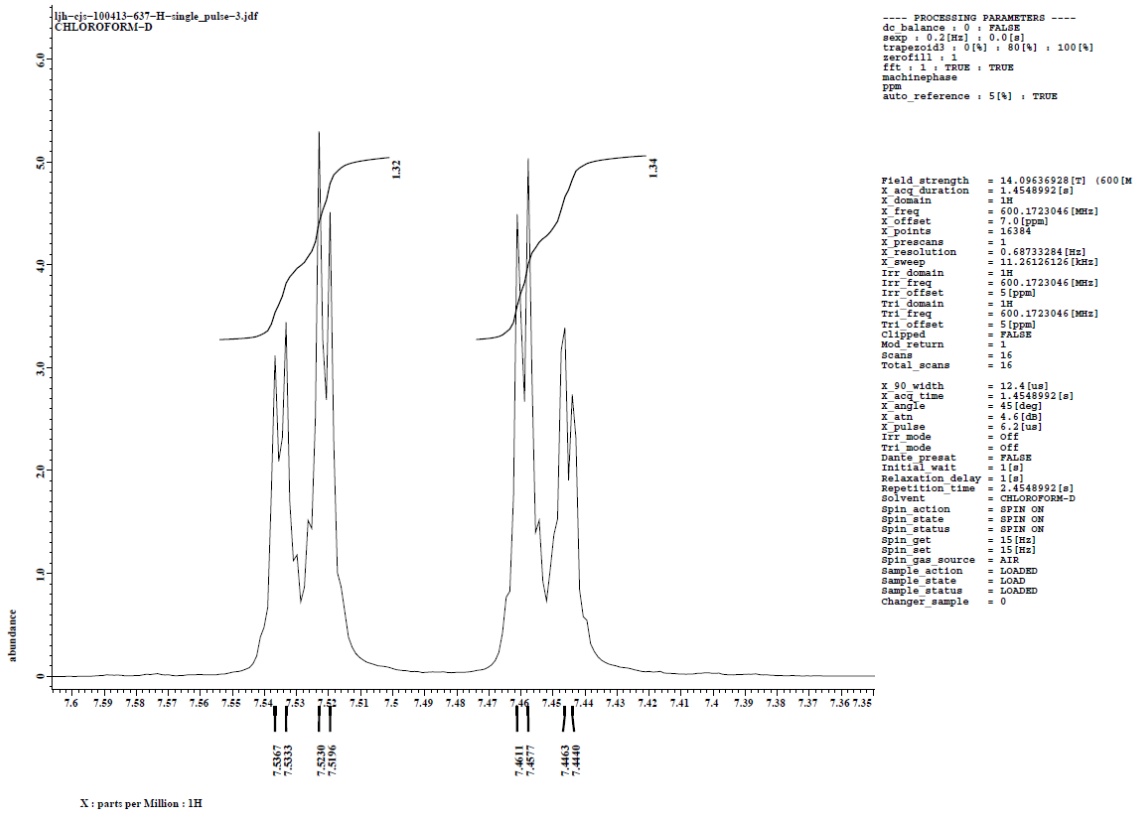
Raw data - Library entry



2c- ^{1}H NMR

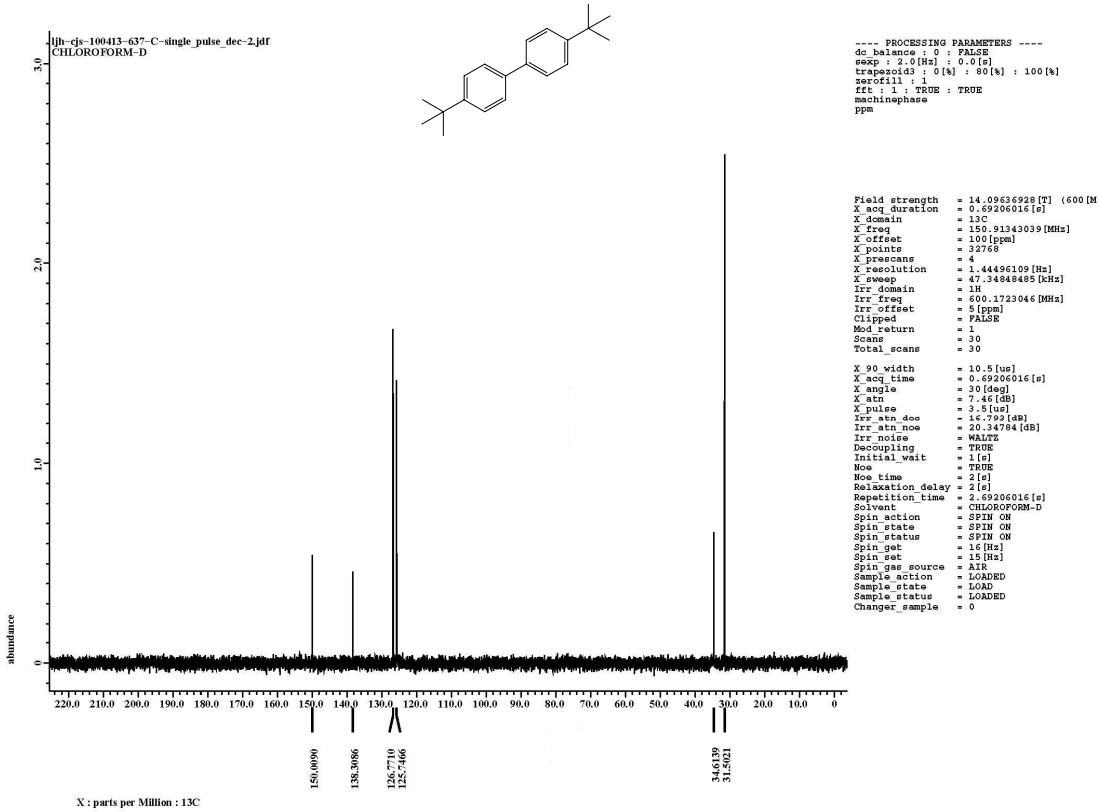



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
auto_reference : 5[%] : TRUE

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 1.4548992[s]
X_domain         = 1H
X_freq           = 600.1723046[MHz]
X_offset         = 7.0[ppm]
X_points         = 16384
X_prescans       = 1
X_resolution     = 0.68733284[Hz]
X_sweep          = 11.26126126[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Tri_domain       = 1H
Tri_freq         = 600.1723046[MHz]
Tri_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 16
Total_scans      = 16

X_90_width       = 12.4[us]
X_acq_time       = 1.4548992[s]
X_angle          = 45[deg]
X_atn            = 4.6[dB]
X_pulse          = 6.2[us]
Irr_mode         = off
Tri_mode         = off
Dante_presat     = FALSE
Initial_wait     = 1[s]
Relaxation_delay = 1[s]
Repetition_time  = 2.4548992[s]
Solvent          = CHLOROFORM-D
Spin_action      = SPIN ON
Spin_state       = SPIN ON
Spin_status      = SPIN ON
Spin_get         = 15[Hz]
Spin_set         = 15[Hz]
Spin_gas_source  = AIR
Sample_action    = LOADED
Sample_state     = LOAD
Sample_status    = LOADED
Changer_sample   = 0
```



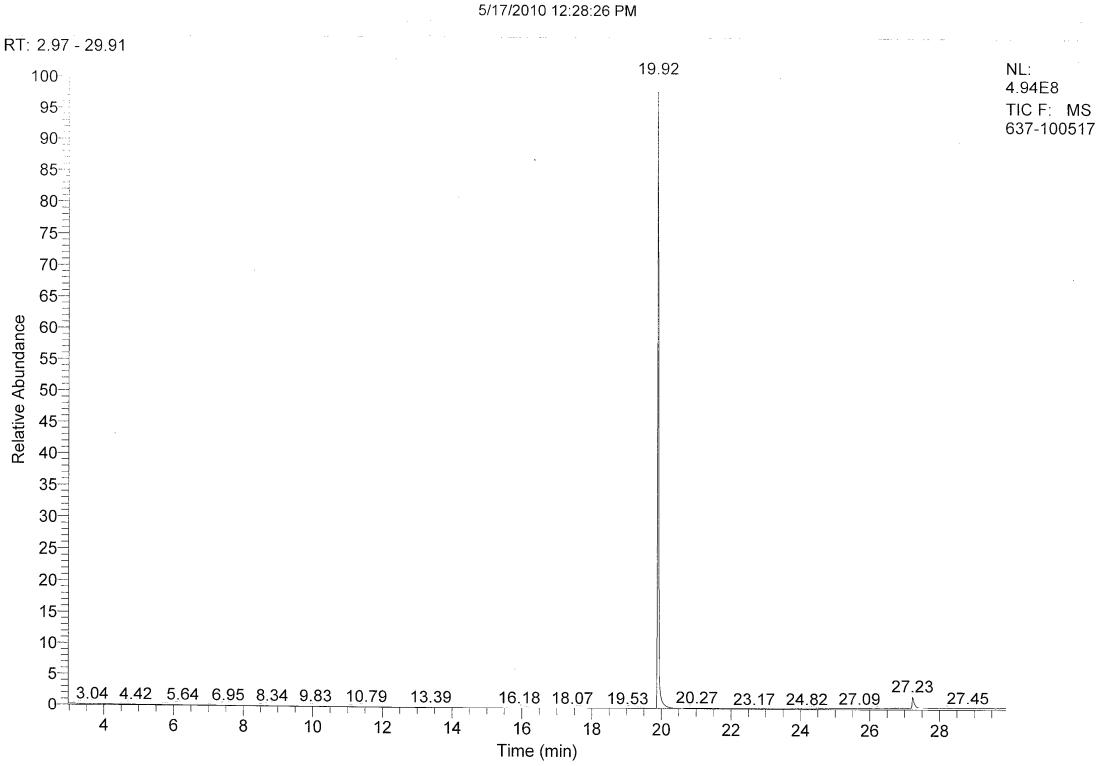

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
auto_reference : 5[%] : TRUE

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 600.1723046[MHz]
X_offset          = 7.0[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 600.1723046[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 12.4[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 4.6[dB]
X_pulse           = 6.2[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Relaxation_delay  = 1[s]
Repetition_time   = 2.4548992[s]
Solvent           = CHLOROFORM-D
Spin_action       = SPIN ON
Spin_state        = SPIN ON
Spin_status       = SPIN ON
Spin_get          = 15[Hz]
Spin_set          = 15[Hz]
Spin_gas_source   = AIR
Sample_action     = LOADED
Sample_state      = LOAD
Sample_status     = LOADED
Changer_sample    = 0
```

2c- ^{13}C NMR

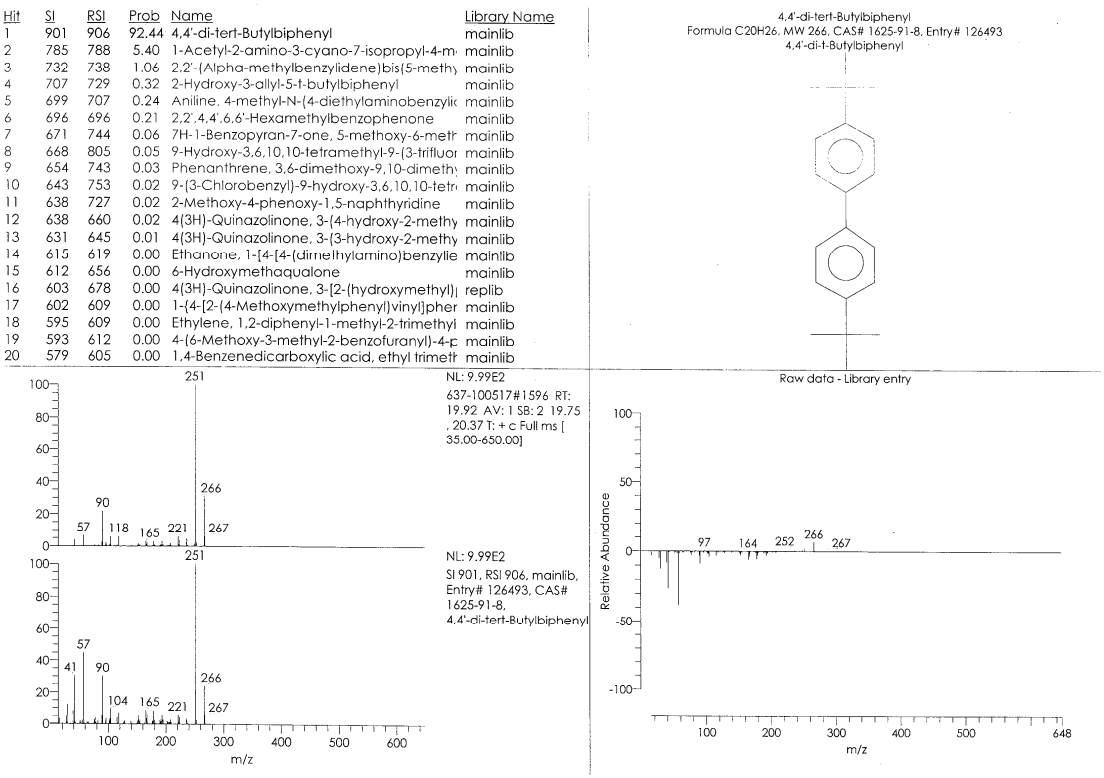



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 0.69206016[s]
X_domain          = 13C
X_freq            = 150.91343039[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.44496109[Hz]
X_sweep           = 47.34848485[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 30
Total_scans       = 30

X_90_width        = 10.5[us]
X_acq_time        = 0.69206016[s]
X_angle           = 30[deg]
X_atn             = 7.46[dB]
X_pulse           = 3.5[us]
Irr_atn_doo       = 16.793[dB]
Irr_atn_noe       = 20.34784[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Relaxation_delay  = 2[s]
Repetition_time   = 2.69206016[s]
Solvent           = CHLOROFORM-D
Spin_action       = SPIN ON
Spin_state        = SPIN ON
Spin_status       = SPIN ON
Spin_get          = 16[Hz]
Spin_set          = 15[Hz]
Spin_gas_source   = AIR
Sample_action     = LOADED
Sample_state      = LOAD
Sample_status     = LOADED
Changer_sample    = 0
```

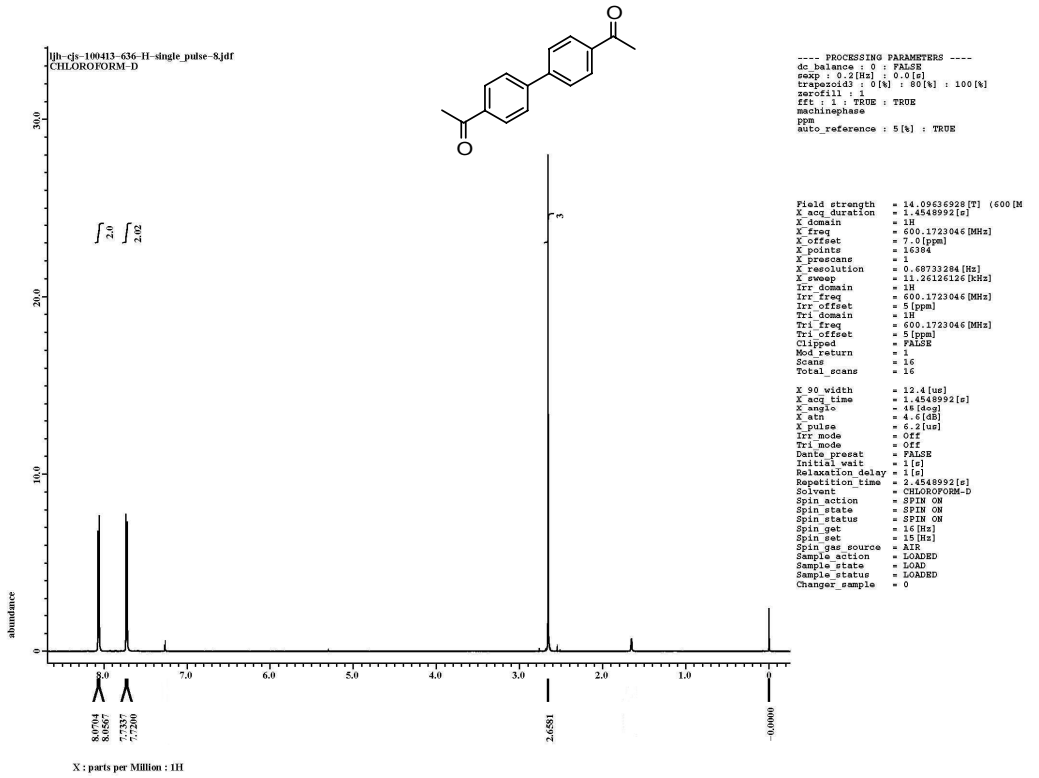
2c-MS



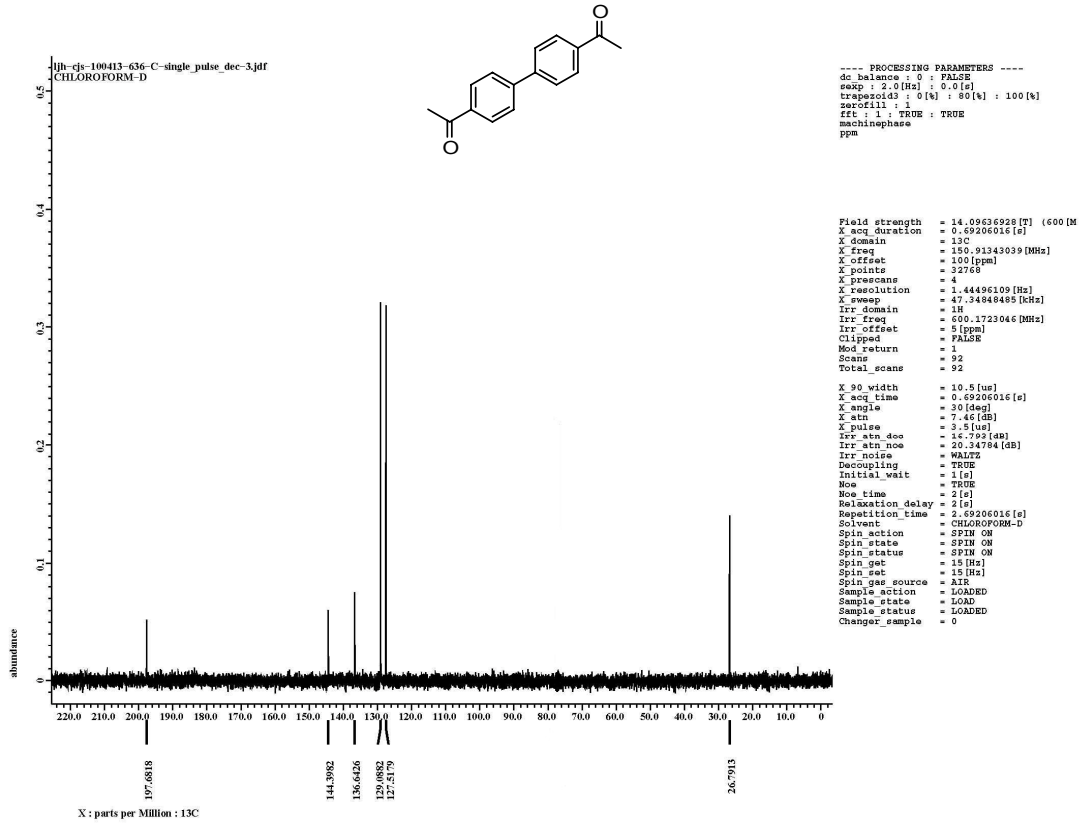
Hit	SI	RSI	Prob	Name	Library Name
1	901	906	92.44	4,4'-di-tert-Butylbiphenyl	mainlib
2	785	788	5.40	1-Acetyl-2-amino-3-cyano-7-isopropyl-4-m	mainlib
3	732	738	1.06	2,2'-(Alpha-methylbenzylidene)bis(5-methy	mainlib
4	707	729	0.32	2-Hydroxy-3-allyl-5-t-butylbiphenyl	mainlib
5	699	707	0.24	Aniline, 4-methyl-N-(4-diethylaminobenzylic	mainlib
6	696	696	0.21	2,2',4,4',6,6'-Hexamethylbenzophenone	mainlib
7	671	744	0.06	7H-1-Benzopyran-7-one, 5-methoxy-6-meth	mainlib
8	668	805	0.05	9-Hydroxy-3,6,10,10-tetramethyl-9-(3-trifluor	mainlib
9	654	743	0.03	Phenanthrene, 3,6-dimethoxy-9,10-dimethy	mainlib
10	643	753	0.02	9-(3-Chlorobenzyl)-9-hydroxy-3,6,10,10-tetr	mainlib
11	638	727	0.02	2-Methoxy-4-phenoxy-1,5-naphthyridine	mainlib
12	638	660	0.02	4(3H)-Quinazolinone, 3-(4-hydroxy-2-methy	mainlib
13	631	645	0.01	4(3H)-Quinazolinone, 3-(3-hydroxy-2-methy	mainlib
14	615	619	0.00	Ethanone, 1-[4-[4-(dimethylamino)benzylie	mainlib
15	612	656	0.00	6-Hydroxymethaqualone	mainlib
16	603	678	0.00	4(3H)-Quinazolinone, 3-[2-(hydroxymethyl)]	replib
17	602	609	0.00	1-(4-[2-(4-Methoxymethylphenyl)vinyl]pher	mainlib
18	595	609	0.00	Ethylene, 1,2-diphenyl-1-methyl-2-trimethyl	mainlib
19	593	612	0.00	4-(6-Methoxy-3-methyl-2-benzofuranyl)-4-p	mainlib
20	579	605	0.00	1,4-Benzenedicarboxylic acid, ethyl trimeth	mainlib



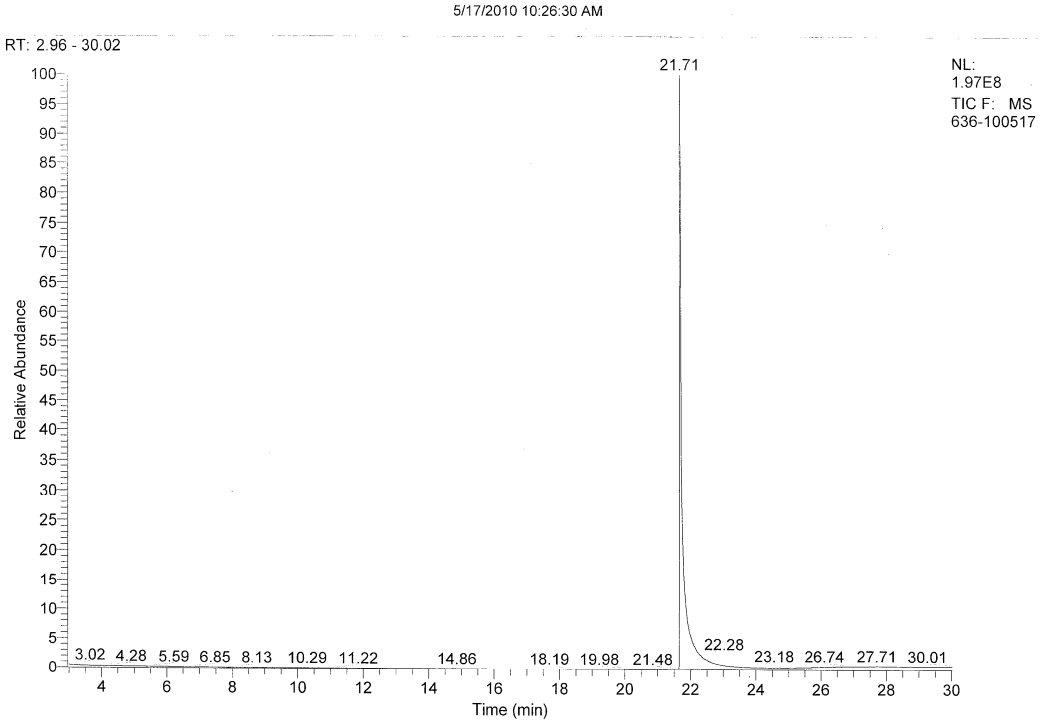
2d- ^{1}H NMR


ljh-cjs-100413-636-H-single_pulse-8.jdf
CHLOROFORM-D
---- 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
auto_reference : 5[%] : TRUE
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 1.4548992[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 7.0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.68733284[Hz]
X_sweep = 11.26126126[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 12.4[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 4.6[dB]
X_pulse = 6.2[us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1[s]
Relaxation_delay = 1[s]
Repetition_time = 2.4548992[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_gat = 16[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
X : parts per Million : 1H

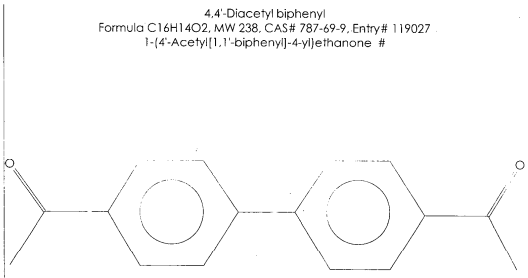
2d- ^{13}C NMR

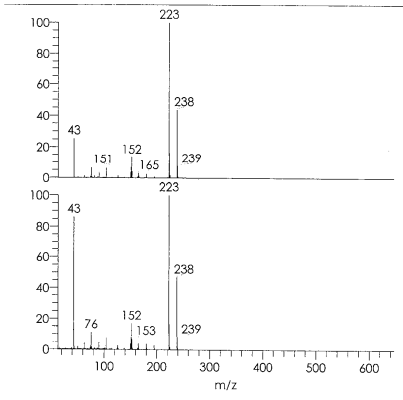

ljh-cjs-100413-636-C-single_pulse_dec-3.jdf
CHLOROFORM-D
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 92
Total_scans = 92
X_90_width = 10.5[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.46[dB]
X_pulse = 3.5[us]
Irr_atn_deo = 16.793[dB]
Irr_atn_noe = 20.34784[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_gat = 15[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
X : parts per Million : 13C

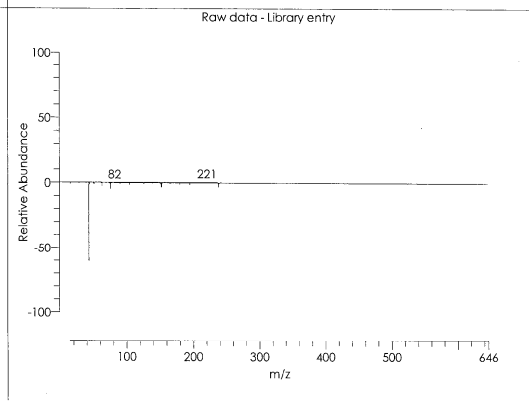
2d-MS



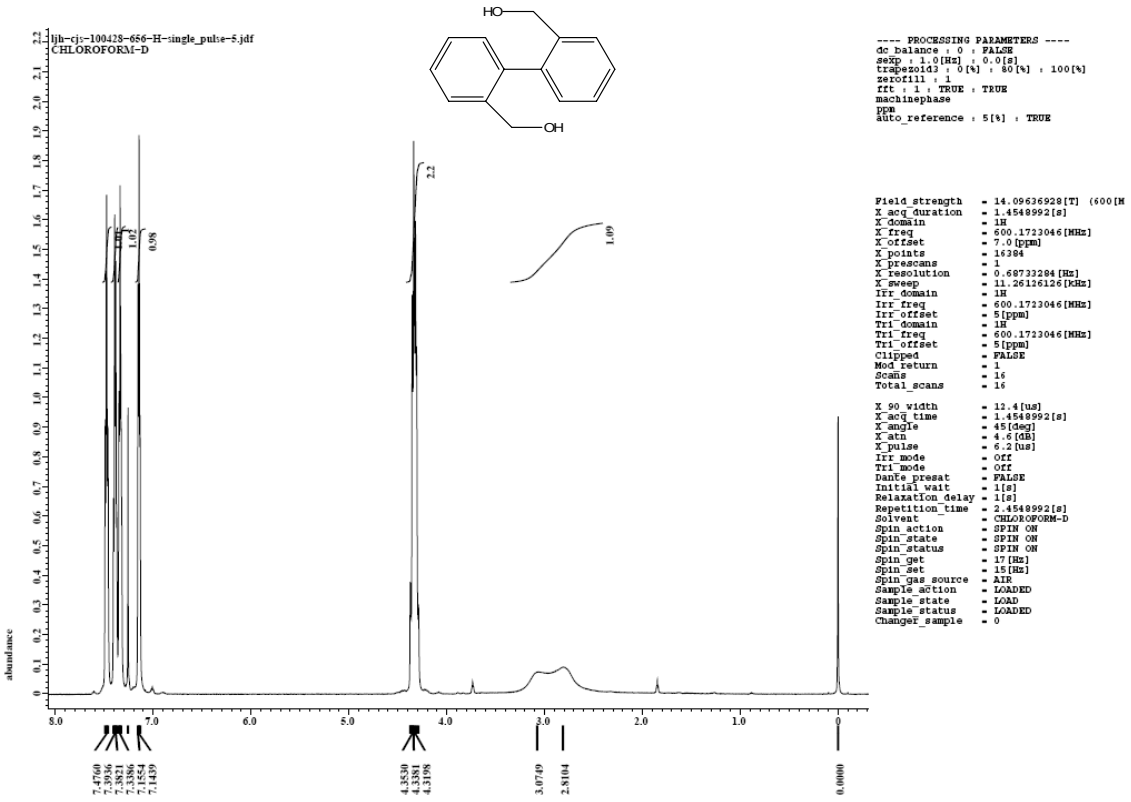
Hit	SI	RSI	Prob	Name	Library Name
1	942	945	80.15	4,4'-Diacetyl biphenyl	mainlib
2	934	939	80.15	4,4'-Diacetyl biphenyl	replib
3	890	891	16.00	3,3'-Diacetylbiphenyl	mainlib
4	825	838	2.57	Anthracene, 9,10-dimethoxy-	replib
5	806	818	2.57	Anthracene, 9,10-dimethoxy-	mainlib
6	788	840	0.62	Benzene, 1,1'-(1,2-ethynediyl)bis[4-methc	mainlib
7	769	772	0.30	4-Isopropylxanthen-9-one	mainlib
8	750	761	0.14	Anthracene, 1,4-dimethoxy-	mainlib
9	745	761	0.14	Anthracene, 1,4-dimethoxy-	replib
10	739	741	0.10	4,4'-Diisopropylbiphenyl	replib
11	715	718	0.03	3,4'-Diisopropylbiphenyl	mainlib
12	681	685	0.10	4,4'-Diisopropylbiphenyl	mainlib
13	679	681	0.00	2-Isopropylxanthen-9-one	mainlib
14	677	685	0.00	3-Methylthio-5,6-di-[p-methoxyphenyl]-1	mainlib
15	673	712	0.00	Phenanthrene, 3,6-dimethoxy-	mainlib
16	656	656	0.00	Benzene, 1,1'-ethylidenebis[4-ethyl-	mainlib
17	653	654	0.00	Benzene, 1,1'-ethylidenebis[3,4-dimethyl-	replib
18	651	657	0.00	4-tert-Butyl-benzophenone	mainlib
19	647	647	0.00	2-Amino-5-isopropyl-3,8-dimethyl-1-azule	mainlib
20	644	645	0.00	Benzene, 1,1'-ethylidenebis[3,4-dimethyl-	mainlib

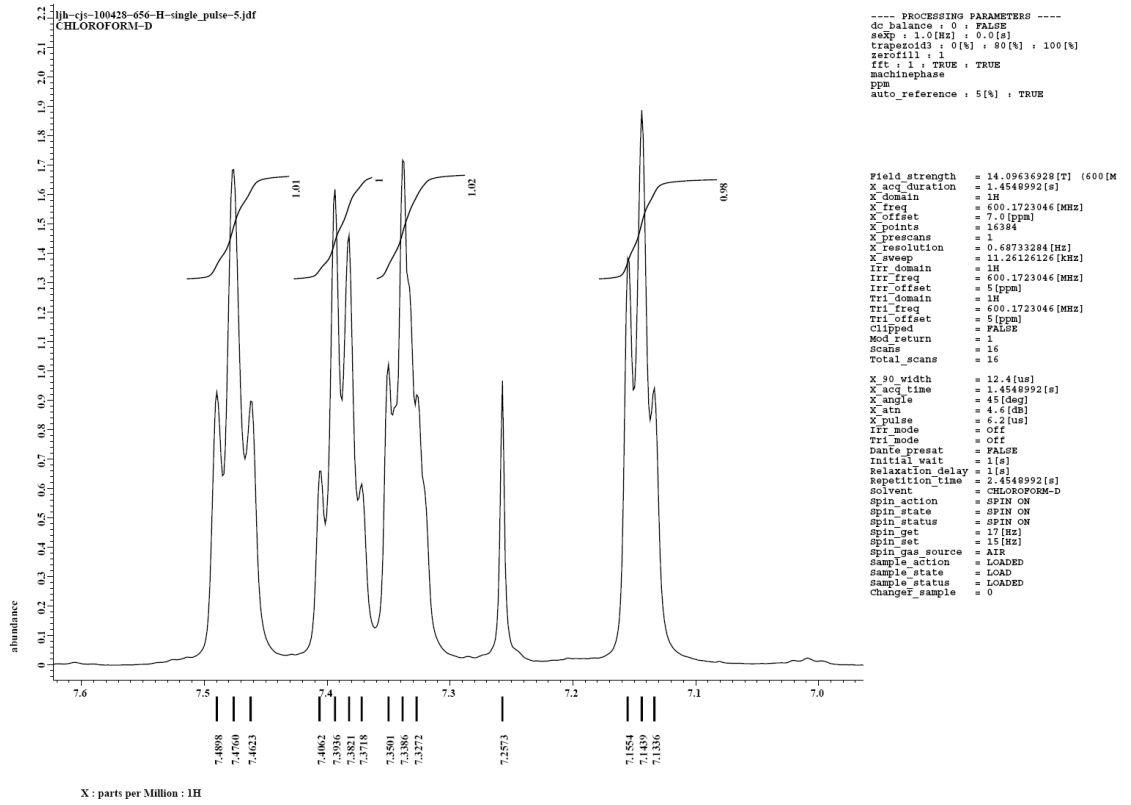




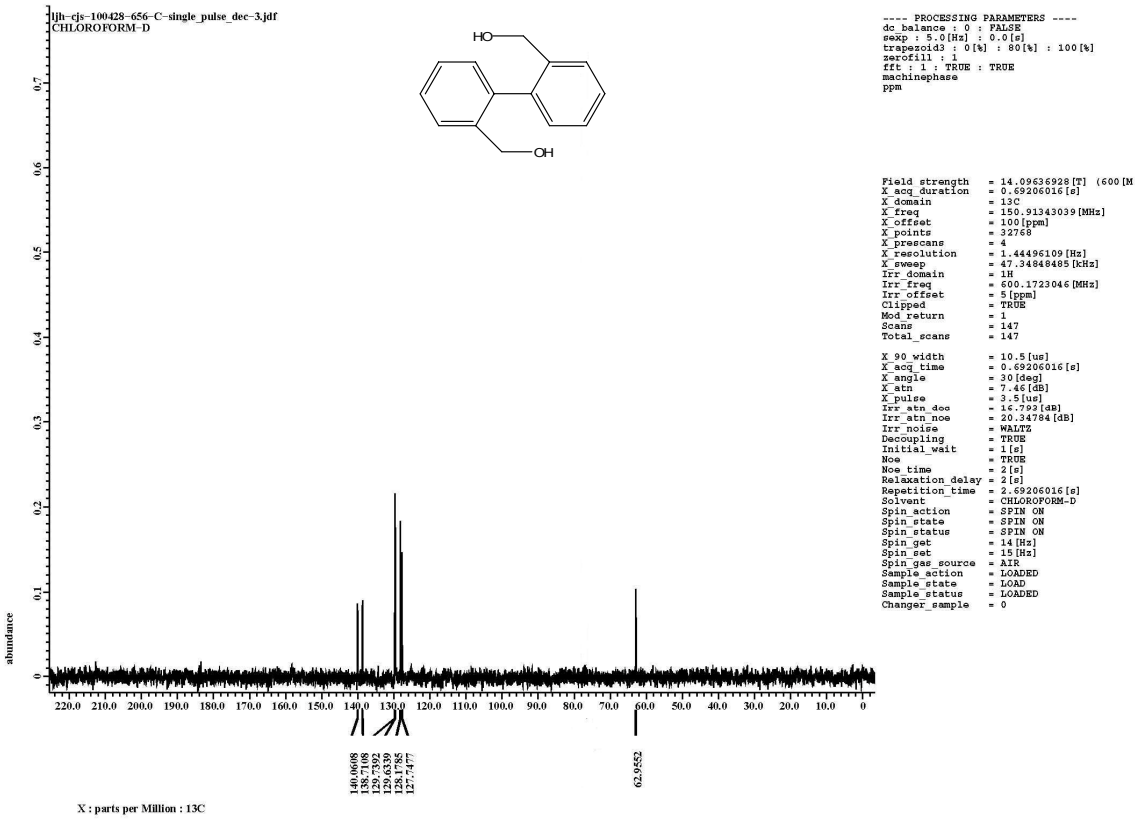


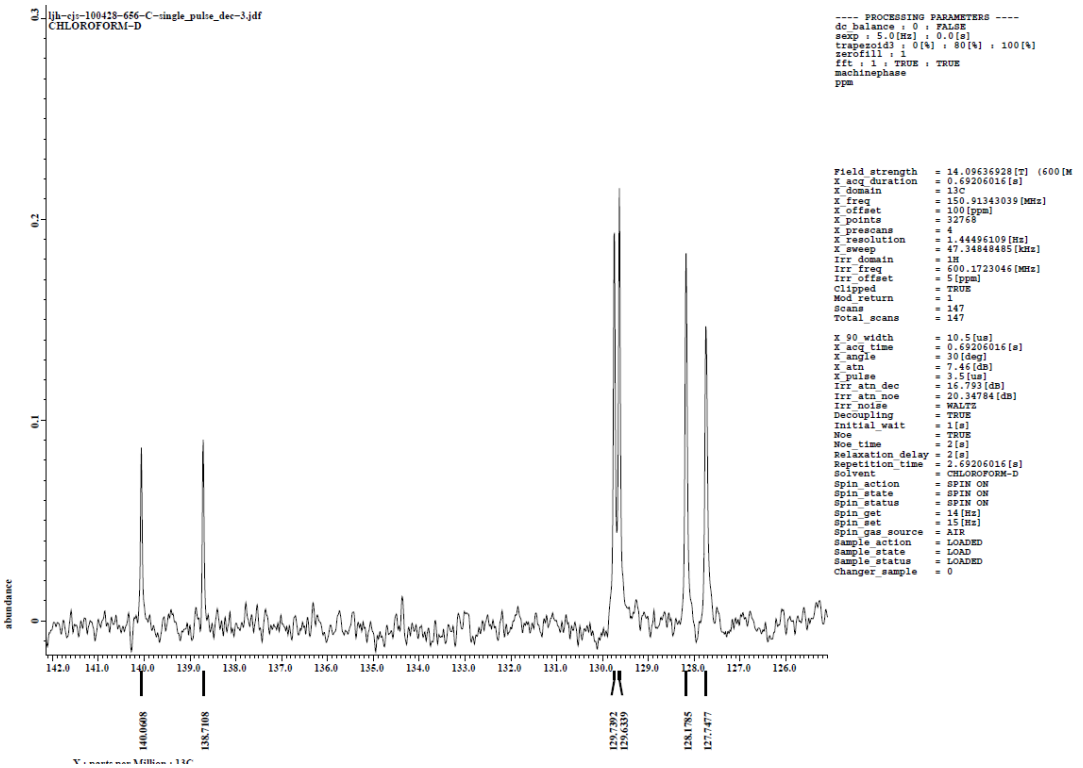
2e- ^{1}H NMR


ljh-cjs-100428-656-H-single_pulse-5.jdf
CHLOROFORM-D
HO
OH
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 1.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
auto_reference : 5[%] : TRUE
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 1.4548992[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 7.0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.68733284[Hz]
X_sweep = 11.26126126[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 12.4[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 4.6[dB]
X_pulse = 6.2[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 1[s]
Repetition_time = 2.4548992[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 17[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
X : parts per Million : 1H

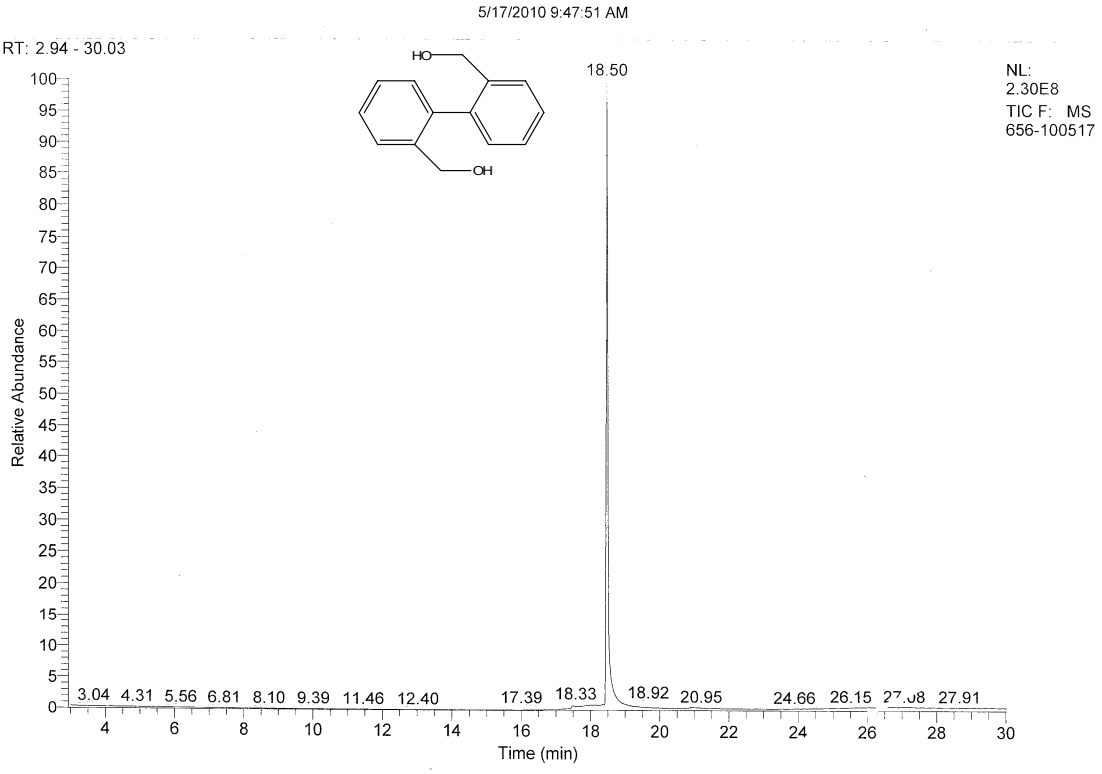

ljh-cjs-100428-656-H-single_pulse-5.jdf
CHLOROFORM-D
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 1.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
auto_reference : 5[%] : TRUE
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 1.4548992[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 7.0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.68733284[Hz]
X_sweep = 11.26126126[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 12.4[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 4.6[dB]
X_pulse = 6.2[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 1[s]
Repetition_time = 2.4548992[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 17[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
X : parts per Million : 1H

2e- ^{13}C NMR

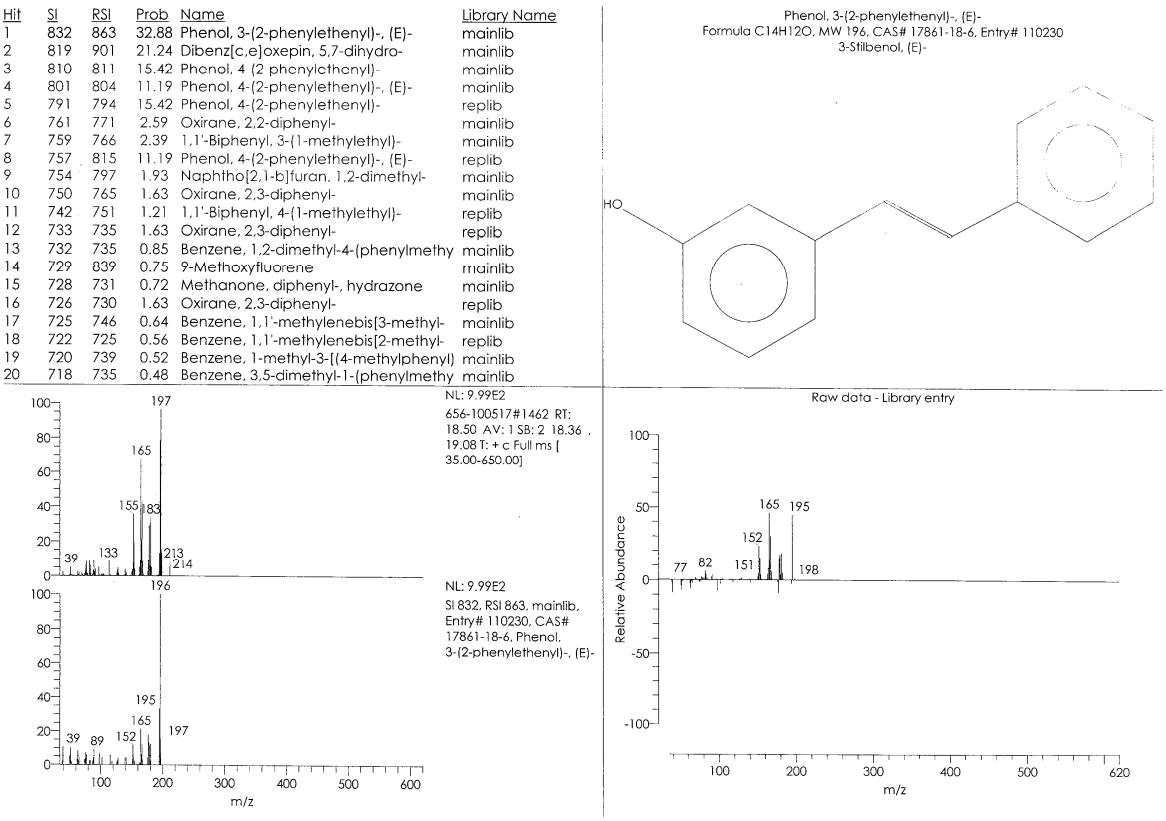

ljh-cjs-100428-656-C-single_pulse_dec-3.jdf
CHLOROFORM-D
HO
OH
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 147
Total_scans = 147
X_90_width = 10.5[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.46[dB]
X_pulse = 3.5[us]
Irr_atn_dec = 16.793[dB]
Irr_atn_noe = 20.34784[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 14[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
140.0608
138.7108
129.7392
129.6339
128.1785
127.7477
62.9552
X : parts per Million : 13C


ljh-cjs-100428-656-C-single_pulse_dec-3.jdf
CHLOROFORM-D
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 5.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 147
Total_scans = 147
X_90_width = 10.5[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.46[dB]
X_pulse = 3.5[us]
Irr_atn_dec = 16.793[dB]
Irr_atn_noe = 20.34784[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 14[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
140.0608
138.7108
129.7392
129.6339
128.1785
127.7477

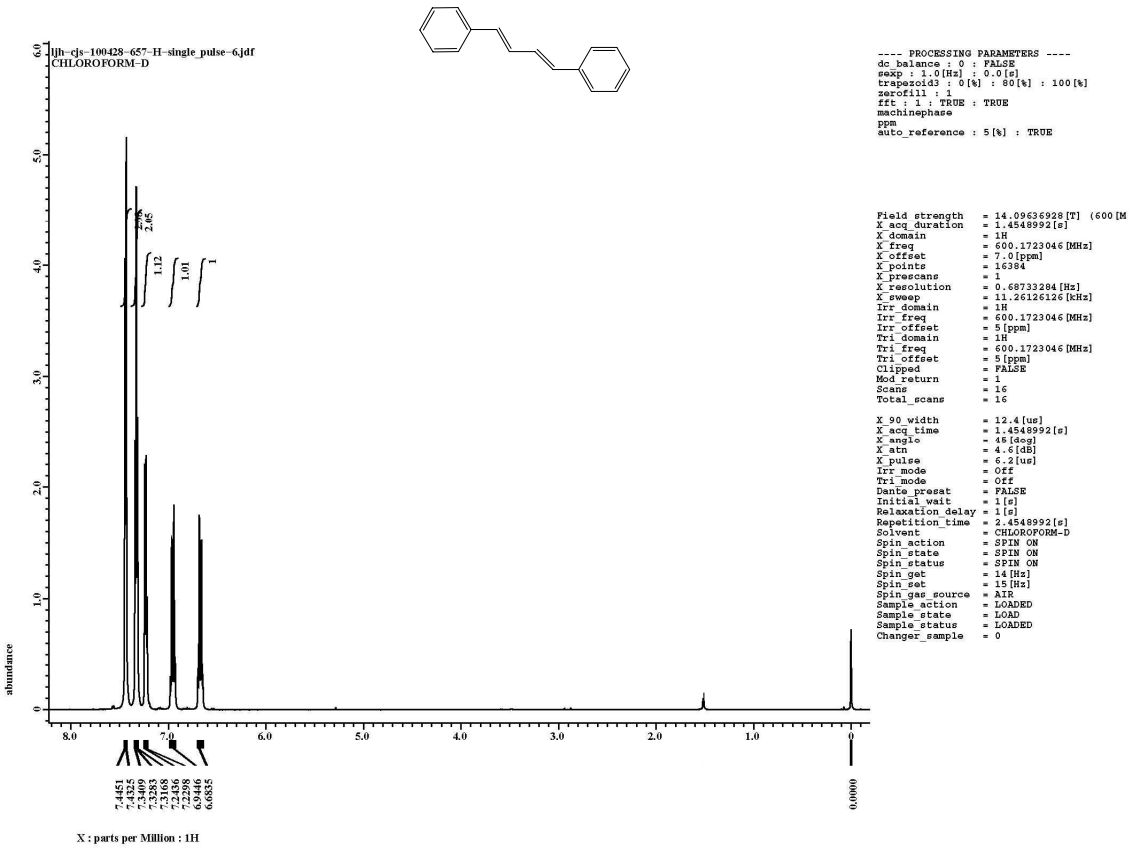
2e-MS



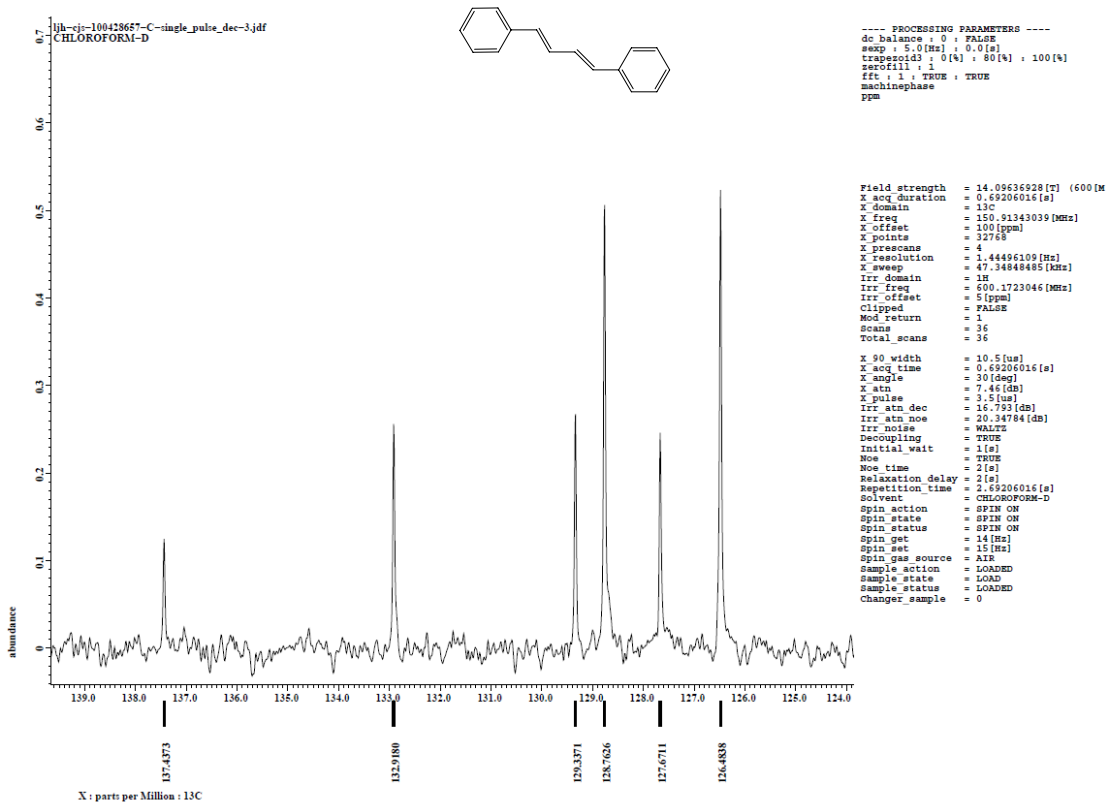
Hit	SI	RSI	Prob	Name	Library Name
1	832	863	32.88	Phenol, 3-(2-phenylethenyl)-, (E)-	mainlib
2	819	901	21.24	Dibenz[c,e]oxepin, 5,7-dihydro-	mainlib
3	810	811	15.42	Phenol, 4 (2 phenylethenyl)-	mainlib
4	801	804	11.19	Phenol, 4-(2-phenylethenyl)-, (E)-	mainlib
5	791	794	15.42	Phenol, 4-(2-phenylethenyl)-	replib
6	761	771	2.59	Oxirane, 2,2-diphenyl-	mainlib
7	759	766	2.39	1,1'-Biphenyl, 3-(1-methylethyl)-	mainlib
8	757	815	11.19	Phenol, 4-(2-phenylethenyl)-, (E)-	replib
9	754	797	1.93	Naphtho[2,1-b]furan, 1,2-dimethyl-	mainlib
10	750	765	1.63	Oxirane, 2,3-diphenyl-	mainlib
11	742	751	1.21	1,1'-Biphenyl, 4-(1-methylethyl)-	replib
12	733	735	1.63	Oxirane, 2,3-diphenyl-	replib
13	732	735	0.85	Benzene, 1,2-dimethyl-4-(phenylmethy	mainlib
14	729	839	0.75	9-Methoxyfluorene	mainlib
15	728	731	0.72	Methanone, diphenyl-, hydrazone	mainlib
16	726	730	1.63	Oxirane, 2,3-diphenyl-	replib
17	725	746	0.64	Benzene, 1,1'-methylenebis[3-methyl-	mainlib
18	722	725	0.56	Benzene, 1,1'-methylenebis[2-methyl-	replib
19	720	739	0.52	Benzene, 1-methyl-3-[(4-methylphenyl)	mainlib
20	718	735	0.48	Benzene, 3,5-dimethyl-1-(phenylmethy	mainlib



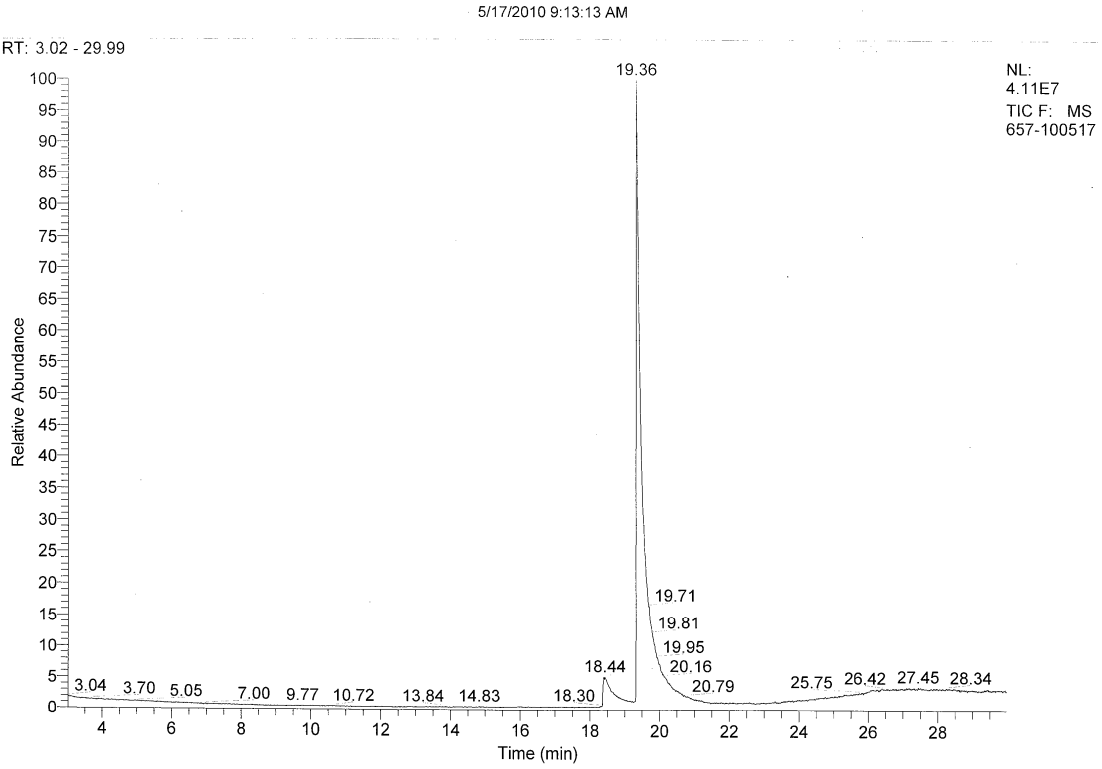
2f- ^{1}H NMR



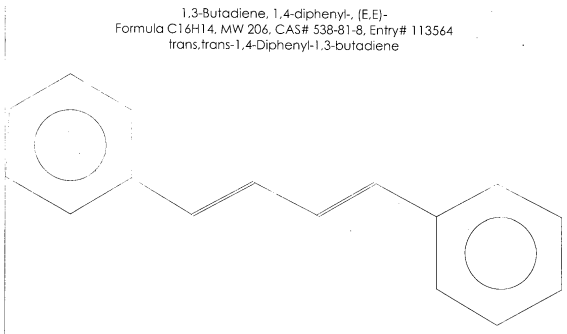
2f- ^{13}C NMR

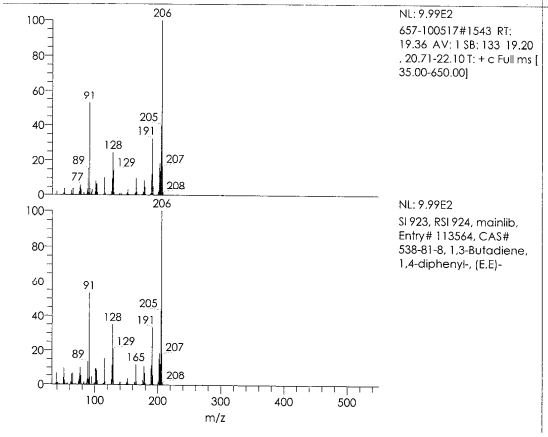


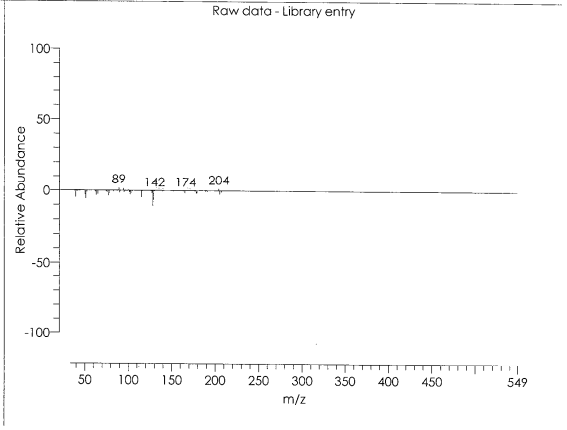
2f-MS



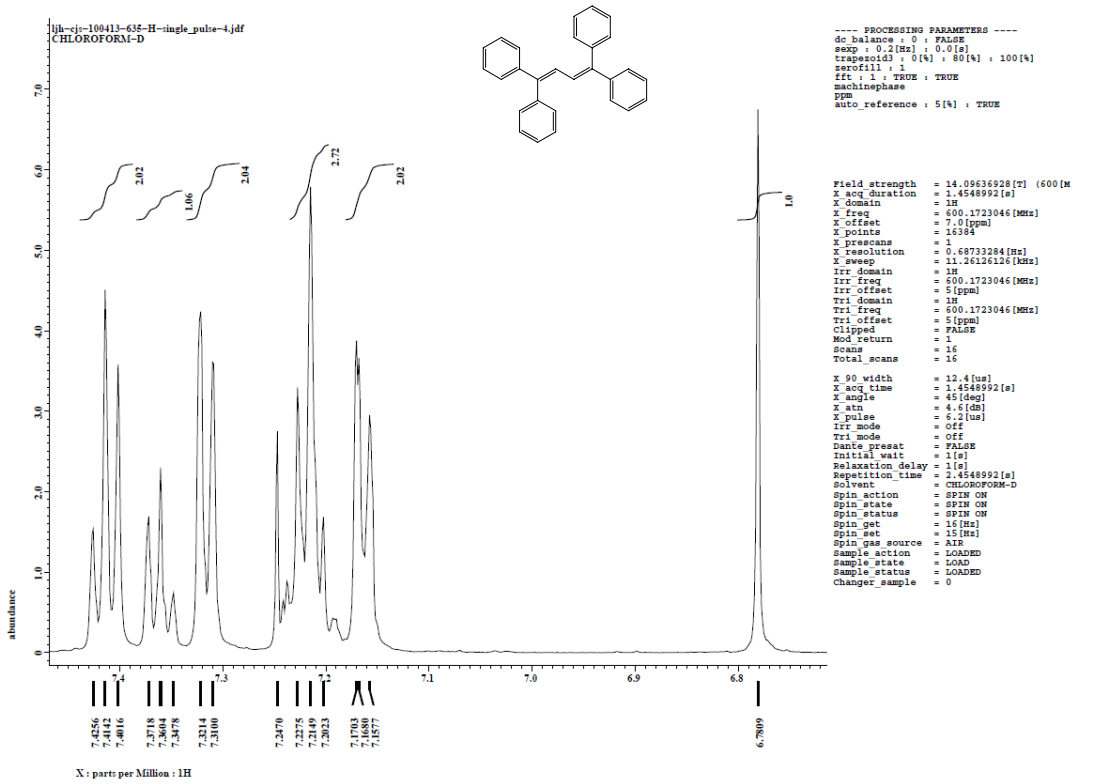
Hit	SI	RSI	Prob	Name	Library Name
1	924	929	18.18	1,4-Diphenyl-1,3-butadiene	replib
2	923	924	17.47	1,3-Butadiene, 1,4-diphenyl-, (E,E)-	mainlib
3	913	914	18.18	1,4 Diphenyl 1,3-butadiene	replib
4	909	910	10.94	Benzene, 1,1'-(1,3-butadienylidene	mainlib
5	907	908	10.09	1,2-Dihydro-3-phenylnaphthalene	mainlib
6	901	902	18.18	1,4-Diphenyl-1,3-butadiene	mainlib
7	897	899	7.12	Benzene, (2-methylene-1-phenylcy	mainlib
8	895	919	6.57	Naphthalene, 1,2-dihydro-1-pheny	mainlib
9	892	898	5.80	Naphthalene, 1,2-dihydro-4-pheny	mainlib
10	889	890	5.80	Naphthalene, 1,2-dihydro-4-pheny	replib
11	884	885	17.47	1,3-Butadiene, 1,4-diphenyl-, (E,E)-	replib
12	883	884	4.21	Benzene, 1,1'-(1-cyclobutene-1,2-c	mainlib
13	875	875	3.14	Indeno[2,1-a]indene, 4b,5,9b,10-te	mainlib
14	875	875	3.14	Indeno[2,1-a]indene, 4b,5,9b,10-te	mainlib
15	872	880	5.80	Naphthalene, 1,2-dihydro-4-pheny	replib
16	864	865	2.15	Benzocyclobutene, 1,1'-bis-	mainlib
17	864	864	2.15	3-Methyl-1-phenyl-1H-indene	mainlib
18	859	859	5.80	Naphthalene, 1,2-dihydro-4-pheny	replib



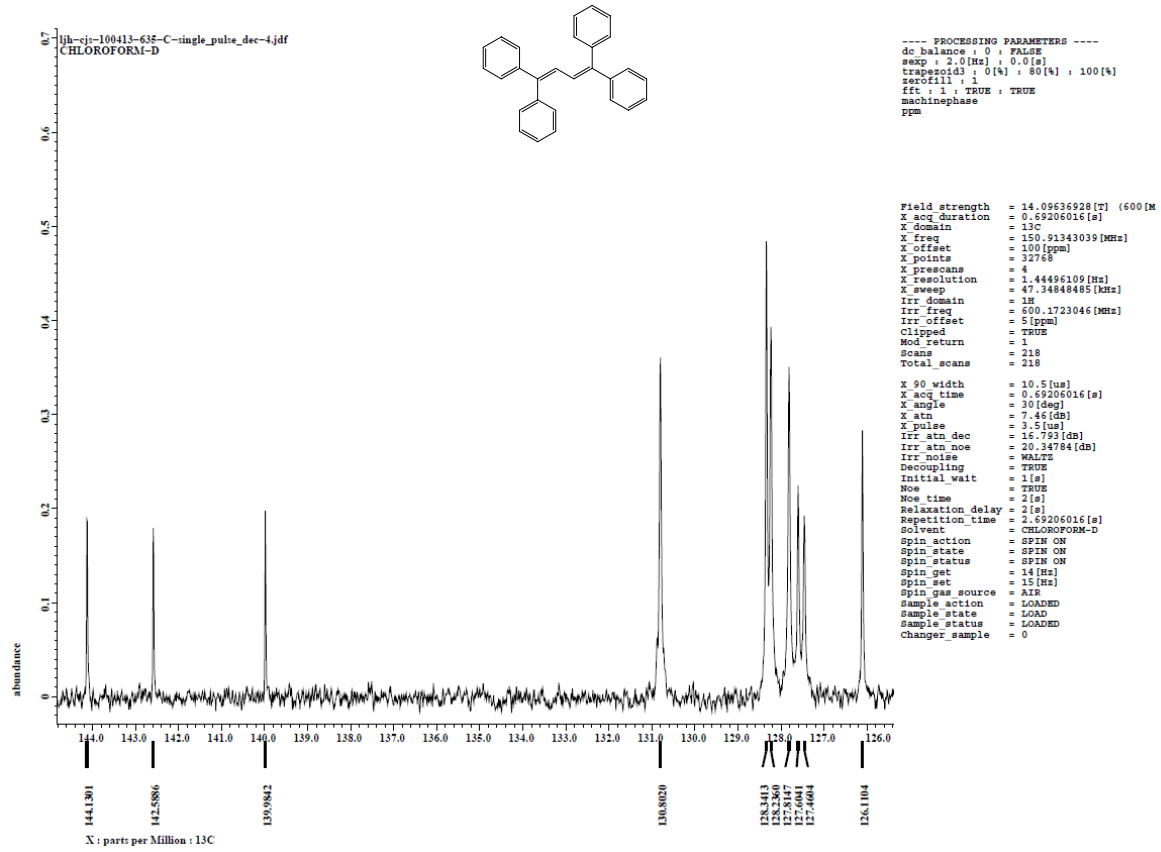




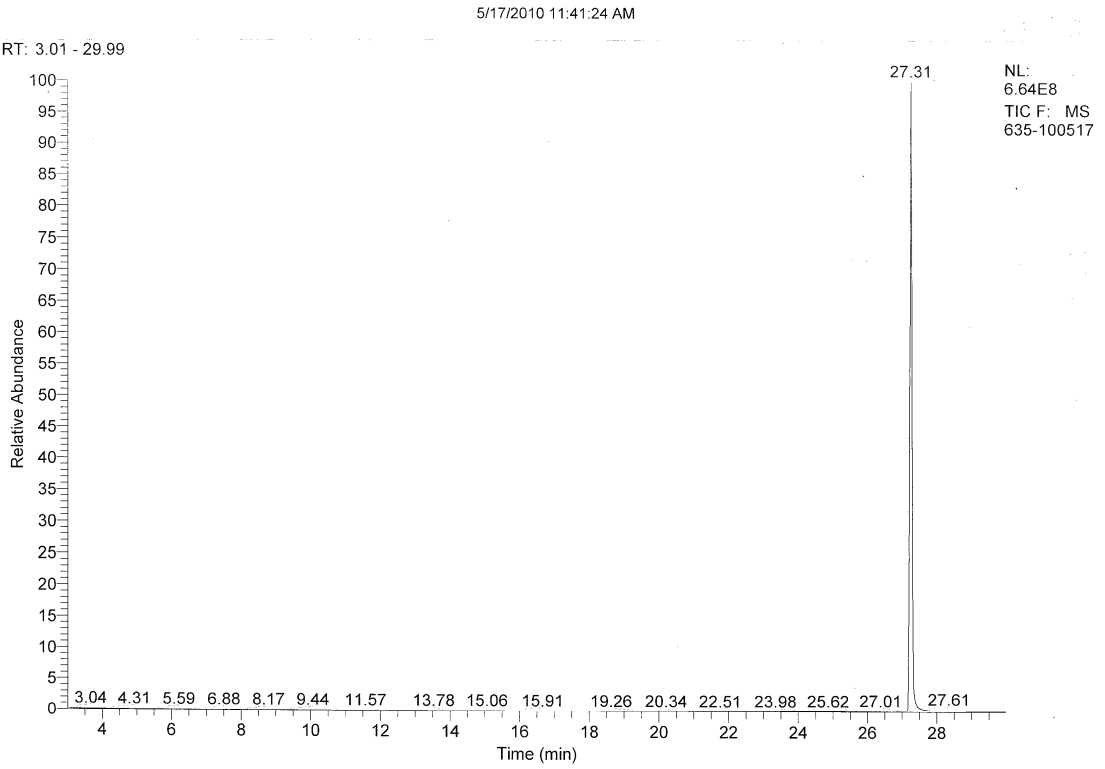
2g- ^{1} H NMR

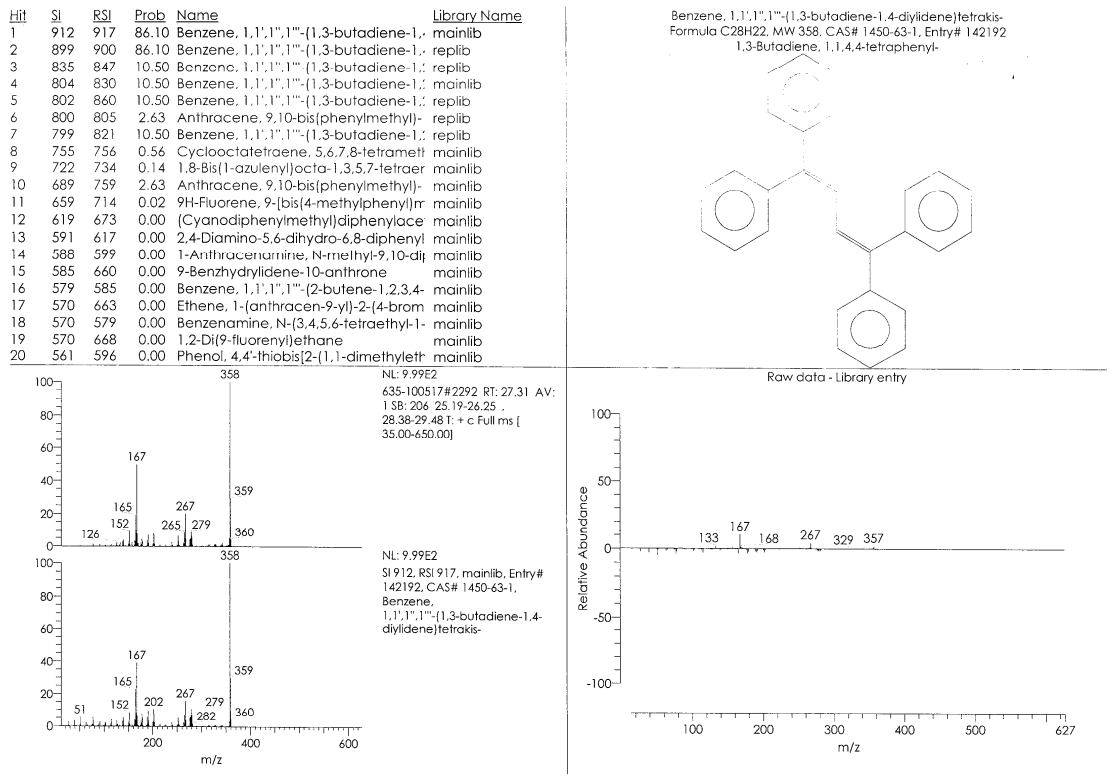

ljh-cjy-100413-635-H-single_pulse-4.jdf
CHLOROFORM-D
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
auto_reference : 5[%] : TRUE
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 1.4548992[s]
X_domain = 1H
X_freq = 600.1723046[MHz]
X_offset = 7.0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.68733284[Hz]
X_sweep = 11.26126126[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 600.1723046[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16
Total_scans = 16
X_90_width = 12.4[us]
X_acq_time = 1.4548992[s]
X_angle = 45[deg]
X_atn = 4.6[dB]
X_pulse = 6.2[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 1[s]
Repetition_time = 2.4548992[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 16[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0

2g- ^{13}C NMR

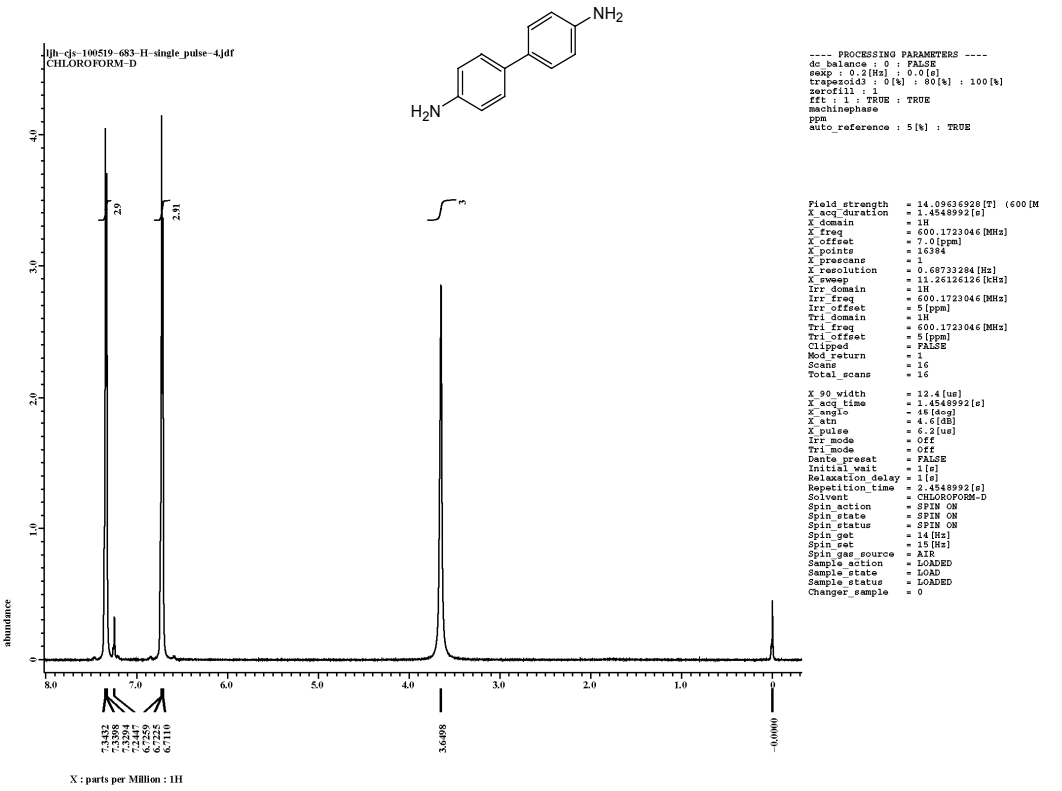

ljh-cjy-100413-635-C-single_pulse_dec-4.jdf
CHLOROFORM-D
abundance
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Field_strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 218
Total_scans = 218
X_90_width = 10.5[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.46[dB]
X_pulse = 3.5[us]
Irr_atn_dec = 16.793[dB]
Irr_atn_noe = 20.34784[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 14[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0

2g-MS

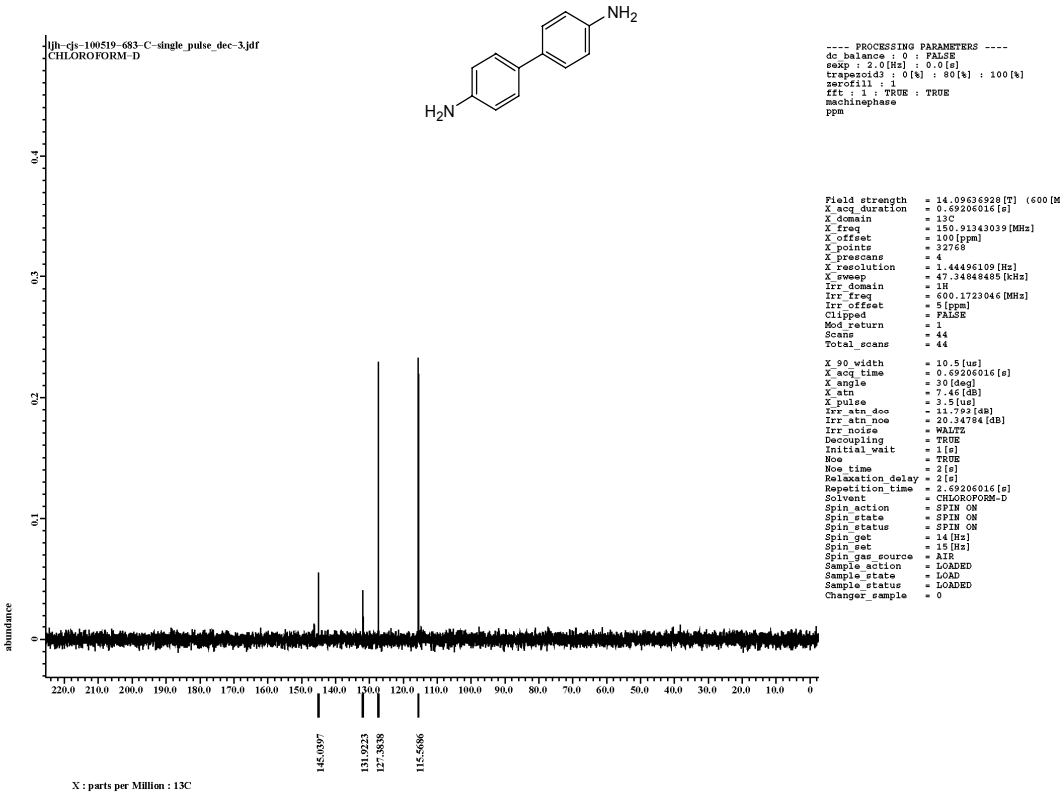




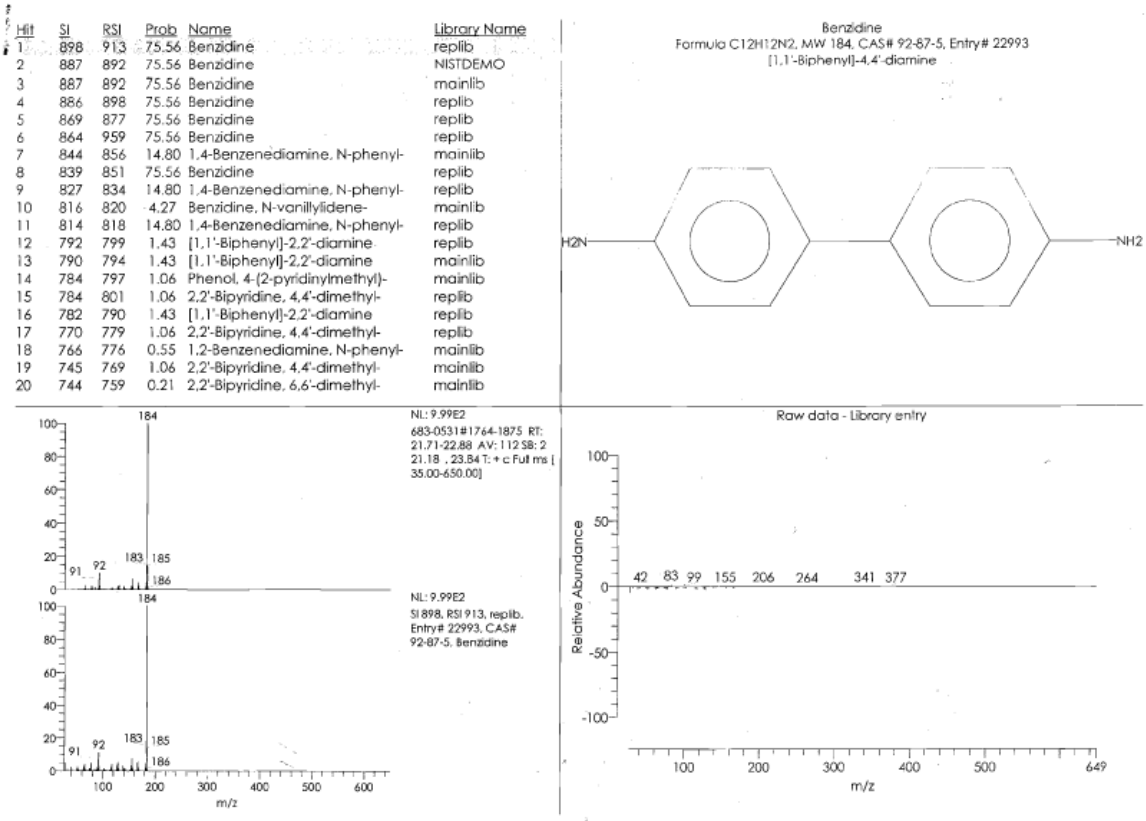
2h- ^{1}H NMR



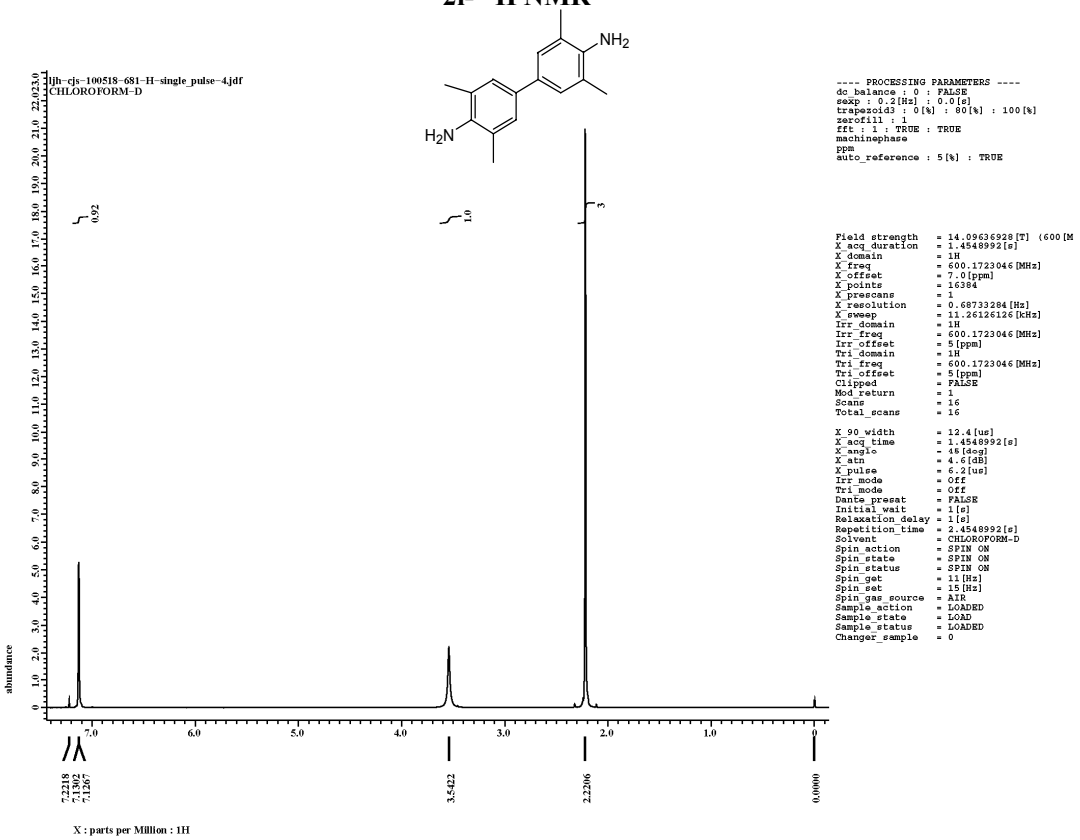
2h- ^{13}C NMR



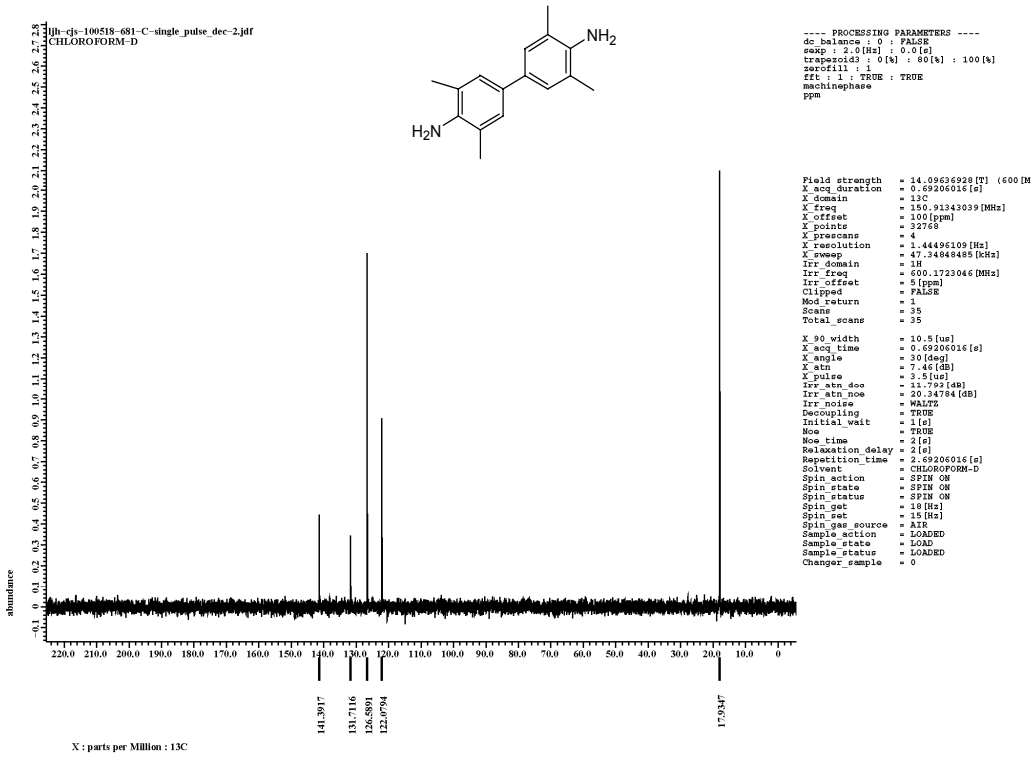
2h-MS



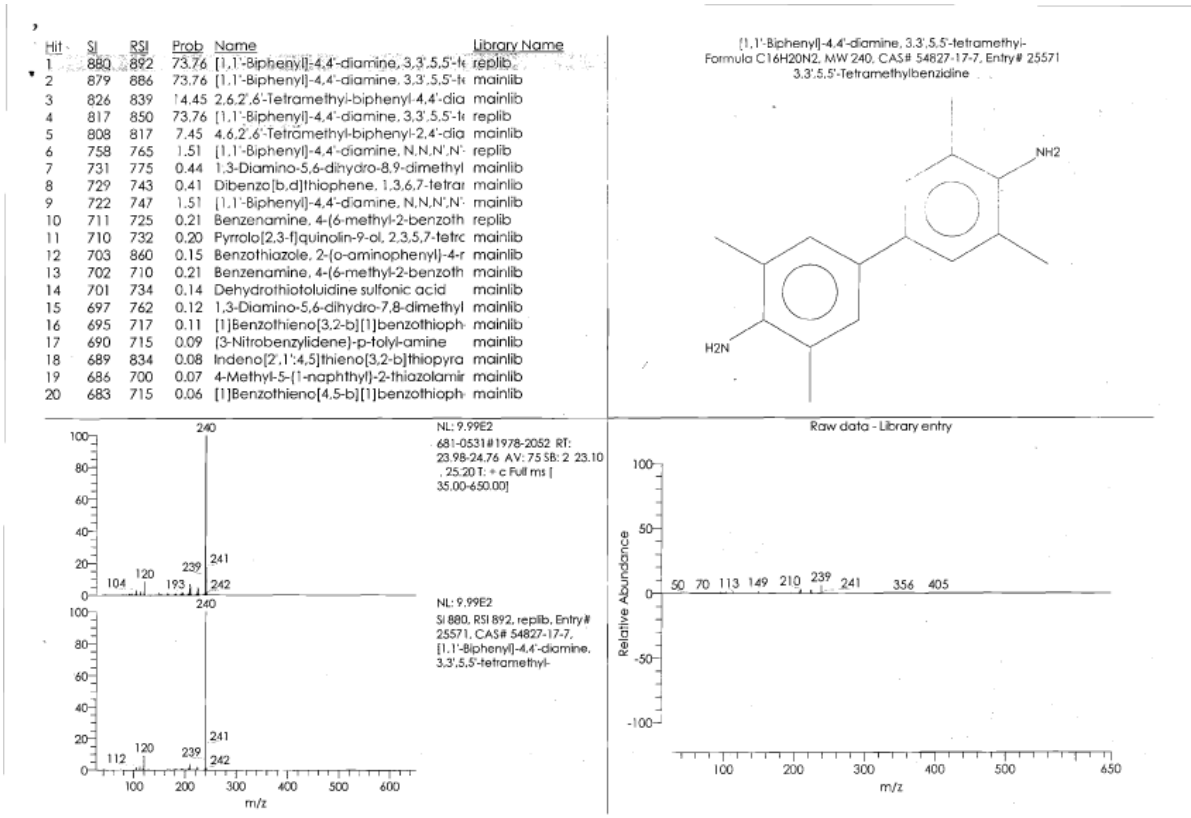
2i- ^{1}H NMR



2i- ^{13}C NMR


ljh-cjs-100518-681-C-single_pulse_dec-2.jdf
CHLOROFORM-D
NH2
H2N
---- 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
Field strength = 14.09636928[T] (600[M
X_acq_duration = 0.69206016[s]
X_domain = 13C
X_freq = 150.91343039[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 1H
Irr_freq = 600.1723046[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 35
Total_scans = 35
X_90_width = 10.5[us]
X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.46[dB]
X_pulse = 3.5[us]
Irr_atn_dec = 11.79[dB]
Irr_atn_noe = 20.34784[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Solvent = CHLOROFORM-D
Spin_action = SPIN ON
Spin_state = SPIN ON
Spin_status = SPIN ON
Spin_get = 18[Hz]
Spin_set = 15[Hz]
Spin_gas_source = AIR
Sample_action = LOADED
Sample_state = LOAD
Sample_status = LOADED
Changer_sample = 0
abundance
141.3917
131.7116
126.5891
122.0794
17.9347
X : parts per Million : 13C

2i-MS


Hit Si RSI Prob Name Library Name
1 880 892 73.76 [1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-t replib
2 879 886 73.76 [1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-t mainlib
3 826 839 14.45 2,6,2',6'-Tetramethyl-biphenyl-4,4'-dia mainlib
4 817 850 73.76 [1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-t replib
5 808 817 7.45 4,6,2',6'-Tetramethyl-biphenyl-2,4'-dia mainlib
6 758 765 1.51 [1,1'-Biphenyl]-4,4'-diamine, N,N,N',N'- replib
7 731 775 0.44 1,3-Diamino-5,6-dihydro-8,9-dimethyl mainlib
8 729 743 0.41 Dibenzo[b,d]thiophene, 1,3,6,7-tetra mainlib
9 722 747 1.51 [1,1'-Biphenyl]-4,4'-diamine, N,N,N',N'- mainlib
10 711 725 0.21 Benzenamine, 4-(6-methyl-2-benzoth replib
11 710 732 0.20 Pyrrolo[2,3-f]quinolin-9-ol, 2,3,5,7-tetra mainlib
12 703 860 0.15 Benzothiazole, 2-(o-aminophenyl)-4-r mainlib
13 702 710 0.21 Benzenamine, 4-(6-methyl-2-benzoth mainlib
14 701 734 0.14 Dehydrothiotoluidine sulfonic acid mainlib
15 697 762 0.12 1,3-Diamino-5,6-dihydro-7,8-dimethyl mainlib
16 695 717 0.11 [1]Benzothieno[3,2-b][1]benzothioph mainlib
17 690 715 0.09 (3-Nitrobenzylidene)-p-tolyl-amine mainlib
18 689 834 0.08 Indeno[2',1':4,5]thieno[3,2-b]thiopyra mainlib
19 686 700 0.07 4-Methyl-5-(1-naphthyl)-2-thiazolamir mainlib
20 683 715 0.06 [1]Benzothieno[4,5-b][1]benzothioph mainlib
[1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-tetramethyl-
Formula C16H20N2, MW 240, CAS# 54827-17-7, Entry# 25571
3,3',5,5'-Tetramethylbenzidine
NH2
H2N
NL: 9.99E2
681-0531#1978-2052 RT: 23.98-24.76 AV: 75 SB: 2 23.10 , 25.20 T: + c Full ms [35.00-650.00]
NL: 9.99E2
Si 880, RSI 892, replib, Entry# 25571, CAS# 54827-17-7, [1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-tetramethyl-
m/z
Raw data - Library entry
Relative Abundance
m/z

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