

Copper-Catalyzed Enantioselective Intramolecular Alkene Amination / Intermolecular Heck-type Cascade Coupling

Timothy W. Liwosz, Sherry R. Chemler*

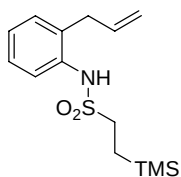
Department of Chemistry, University at Buffalo,
The State University of New York, Buffalo, NY 14260, schemler@buffalo.edu

Supporting Information II

Table of Contents

¹H and ¹³C NMR Spectra

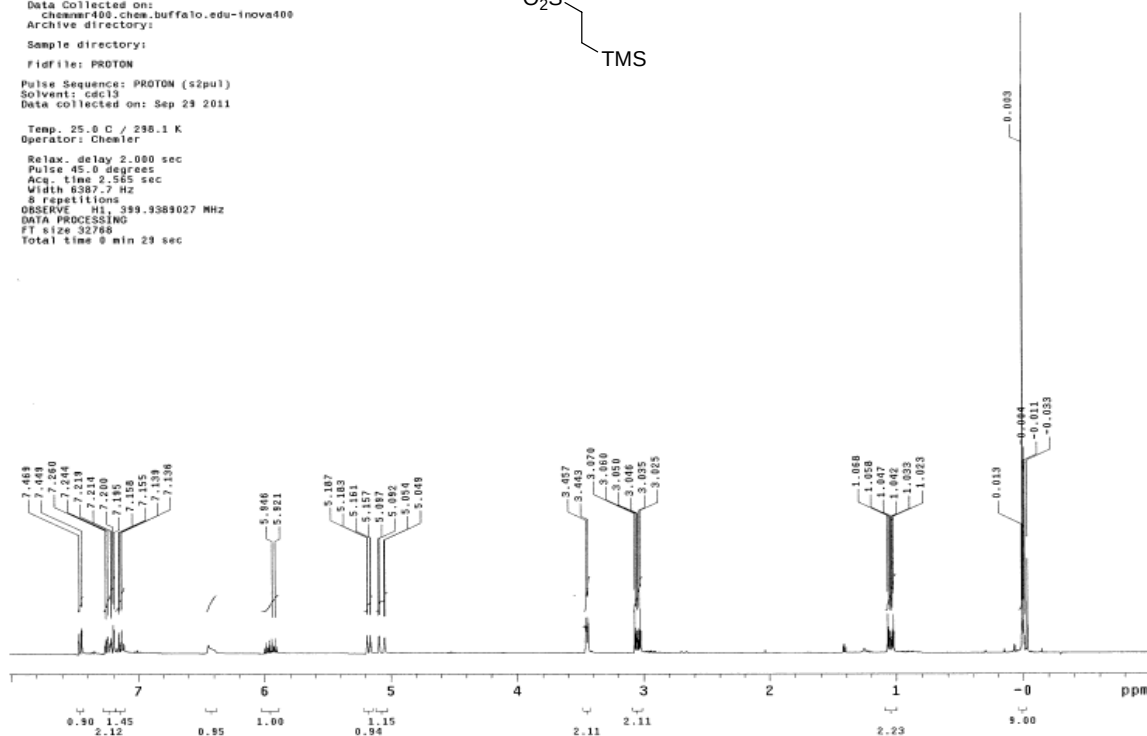
S-2



Sample Name:

Data Collected on:
chemer100.chem.buffalo.edu-inova400
Archive directory:
Sample directory:
Fidfile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 29 2011

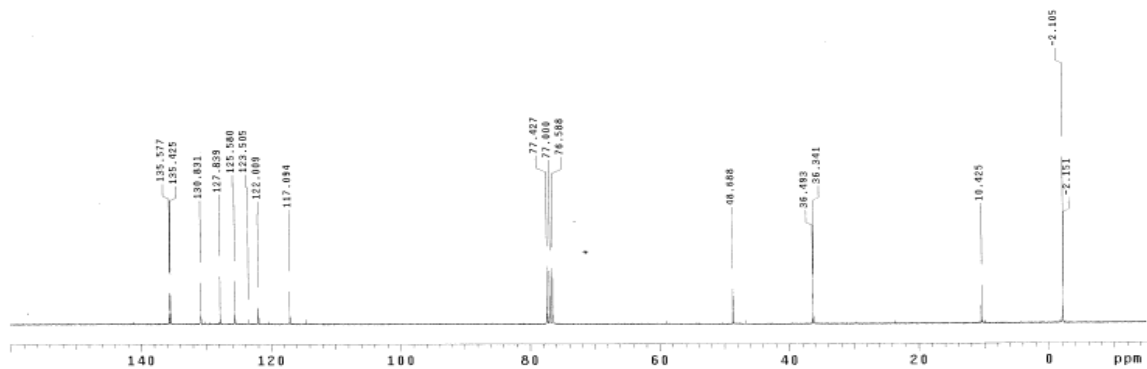
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9389027 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 29 sec



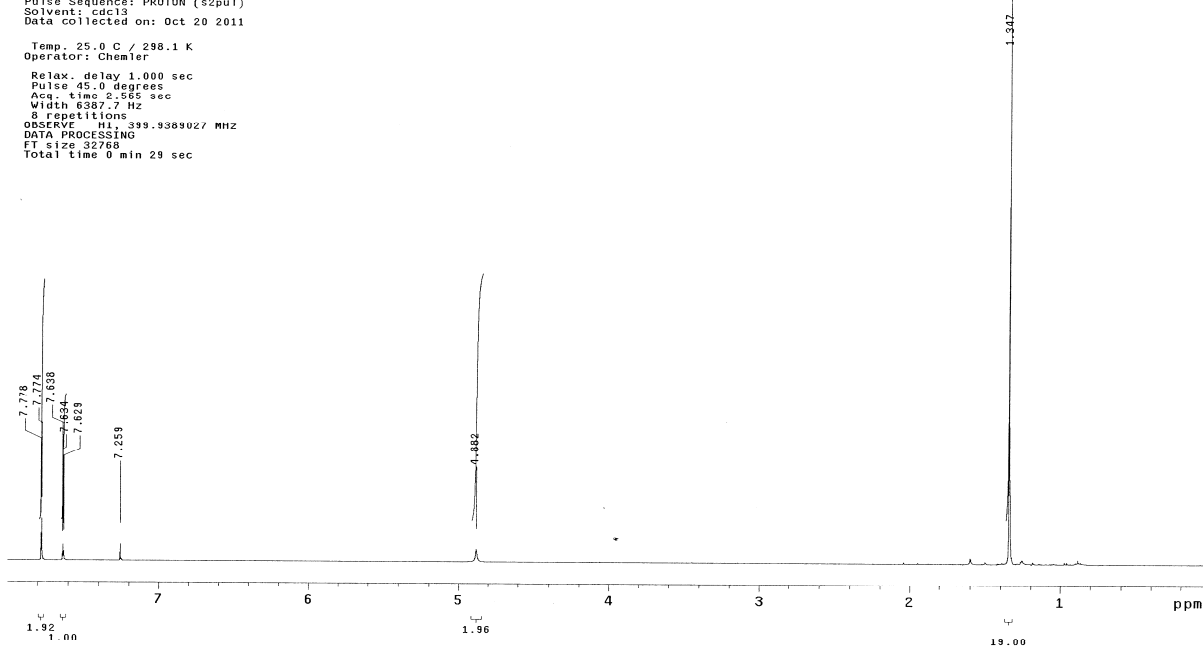
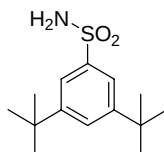
Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
Fidfile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 3 2011

Temp. 22.0 C / 295.1 K
Operator: Sherry
Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.860 sec
Width 18867.9 Hz
1800 repetitions
OBSERVE C13, 75.4536412 MHz
DECOUPLE H1, 300.6754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 41 min

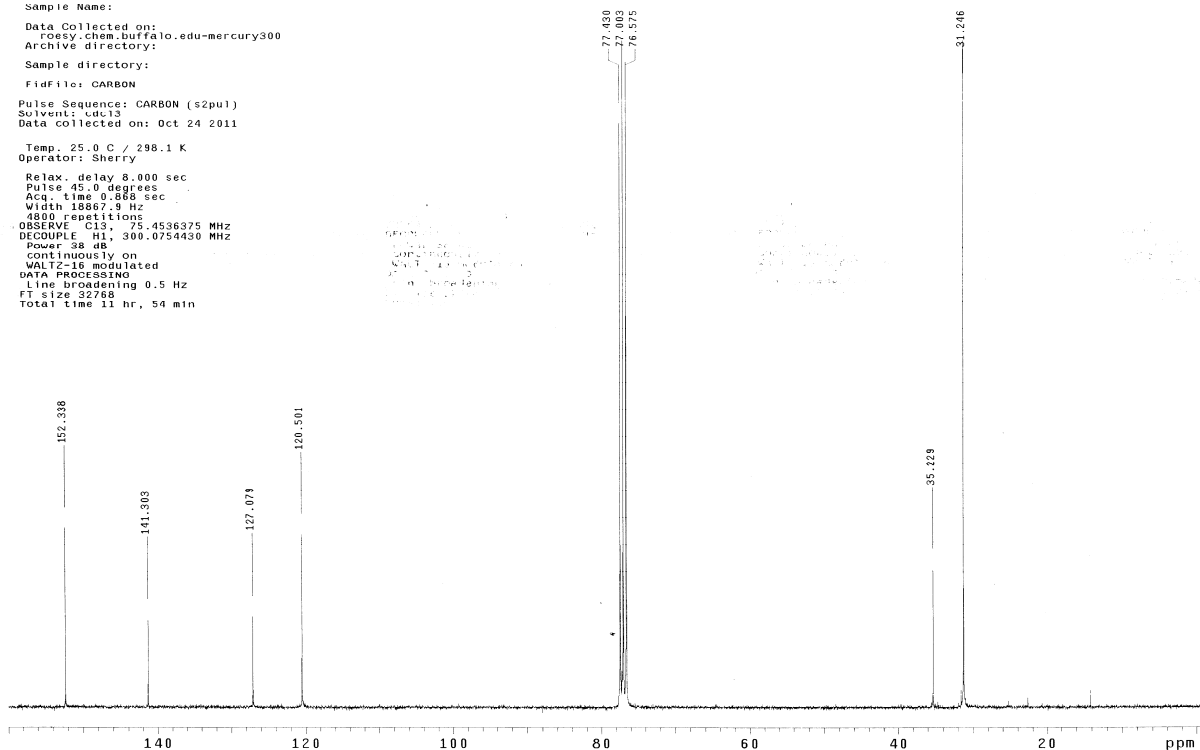


Sample Name:
 Data Collected on:
 chemmm400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pul1)
 Solvent: cdcl3
 Data Collected on: Oct 20 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.565 sec
 Width 6367.7 Hz
 8 repetitions
 OBSERVE H1, 399.9389027 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



STANDARD CARBON PARAMETERS

Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pul1)
 Solvent: cdcl3
 Data Collected on: Oct 24 2011
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 8.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 4800 repetitions
 OBSERVE C13, 75.4536375 MHz
 DECOUPLE H1, 300.0754430 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 11 hr, 54 min



Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)

Pulse Sequence: FROTON (szpul)
Solvent: cdcl3
Data collected on: Oct 21 2011

Data collected on: Oct. 1.

Temp. 25.0 C / 25
Operator: Chemler

Relax. delay 2.000 sec

Relax. delay 2.000
Pulse 45.0 degrees
Acq. time 3.56160 sec

Width 6387.7 Hz

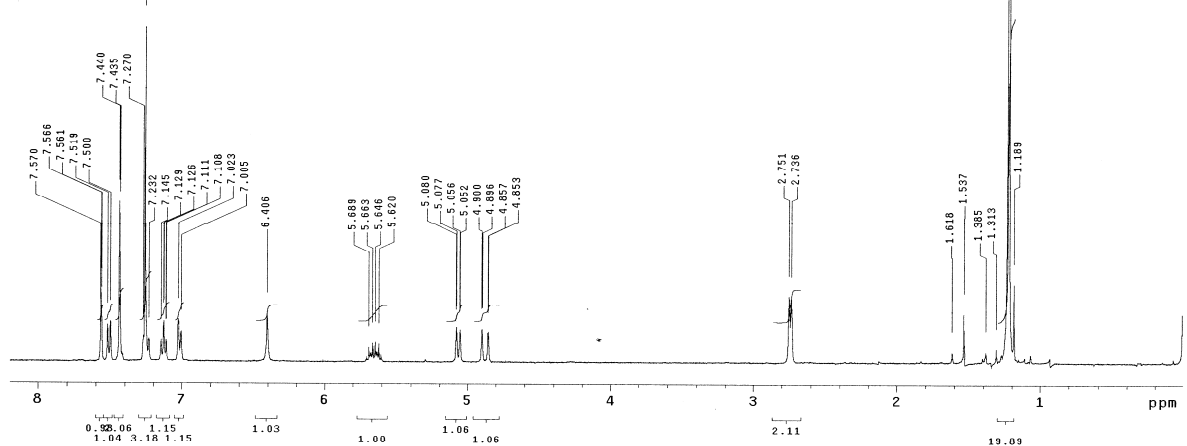
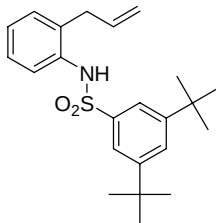
8 repetitions
OBSERVE H1, 399.93

DATA PROCESSING
FT size 32768

Total time 0 mi

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: twl-1-114carbon

Pulse Sequence: CARBON (s2pul)

Pulse Sequence: zgpg30 (zgpg30)
 Solvent: d2o
 Data collected on: Apr 18 2011

data collected on: Apr 3

Temp. 21.0 C / 294.1 K
Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees
Acq. time 0.868 sec

Width 18867.9 Hz
1536 repetitions

```

1536 Repetitions
OBSERVE C13, 75.453640
DECOUPLE H1, 300.076210

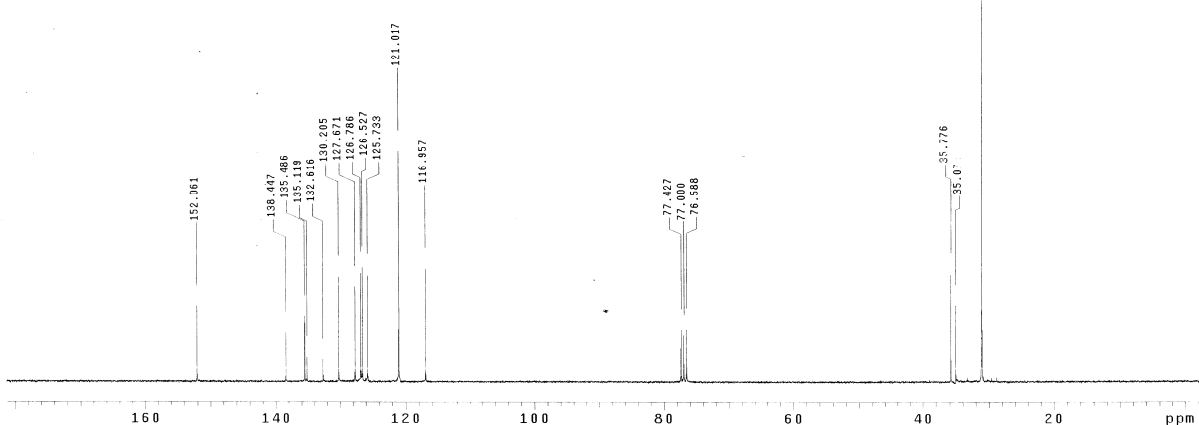
```

Power 38 dB
continuously on

WALTZ-16 modulated
DATA PROCESSING

DATA PROCESSING
Line broadening 0.5 Hz
FT size 20368

FT size 32768
Total time 2 hr, 28 min



tw1-1-239p

Sample Name:

Data Collected on:
chemnar400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Oct 21 2011

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.365 sec

Width 6387.7 Hz

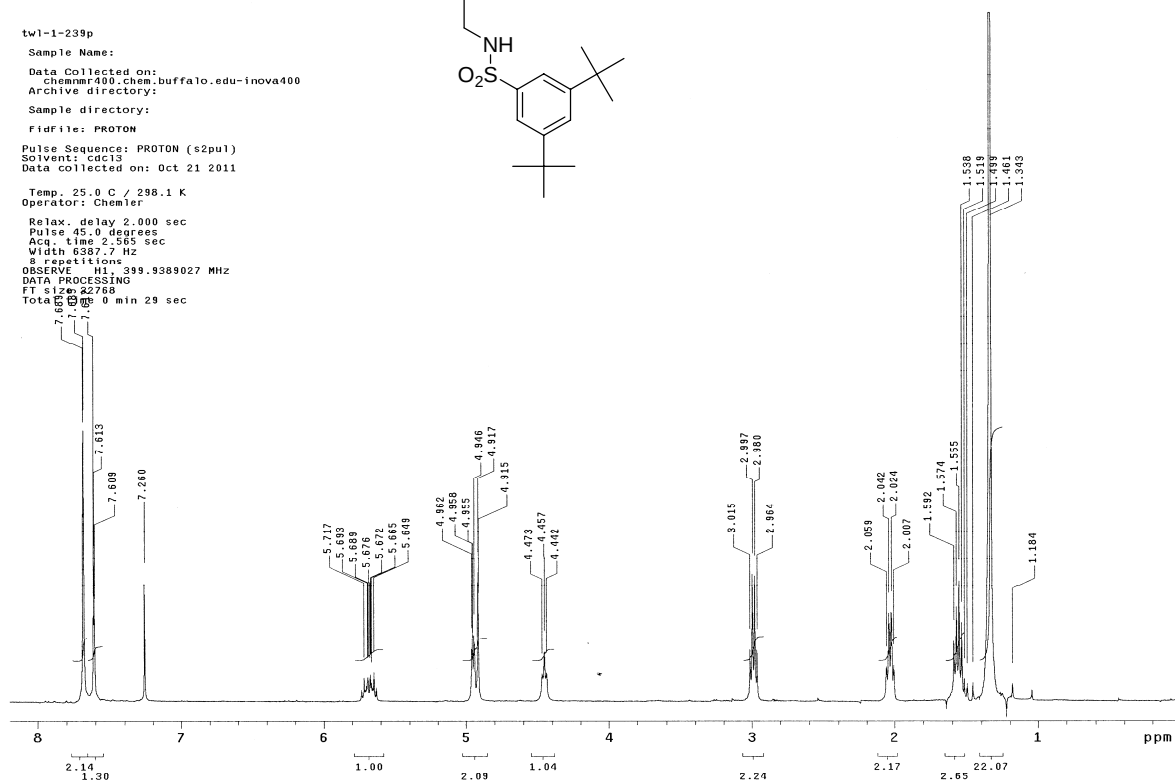
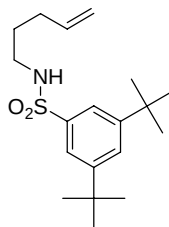
9 repetitions

OBSERVE H1, 399.9389027 MHz

DATA PROCESSING

FT size 82769

Total time 0 min 29 sec



tw1-1-239carbon

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

Fidfile: tw1-1-239carbon

Pulse Sequence: CARBON (s2pul)

Solvent: d2o

Data collected on: Apr 22 2011

Temp. 21.0 C / 294.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.000 sec

Width 18867.9 Hz

792 repetitions

OBSERVE C13, 75.4536405 MHz

DECOUPLE H1, 300.0762142 MHz

Power 38 dB

continuously on

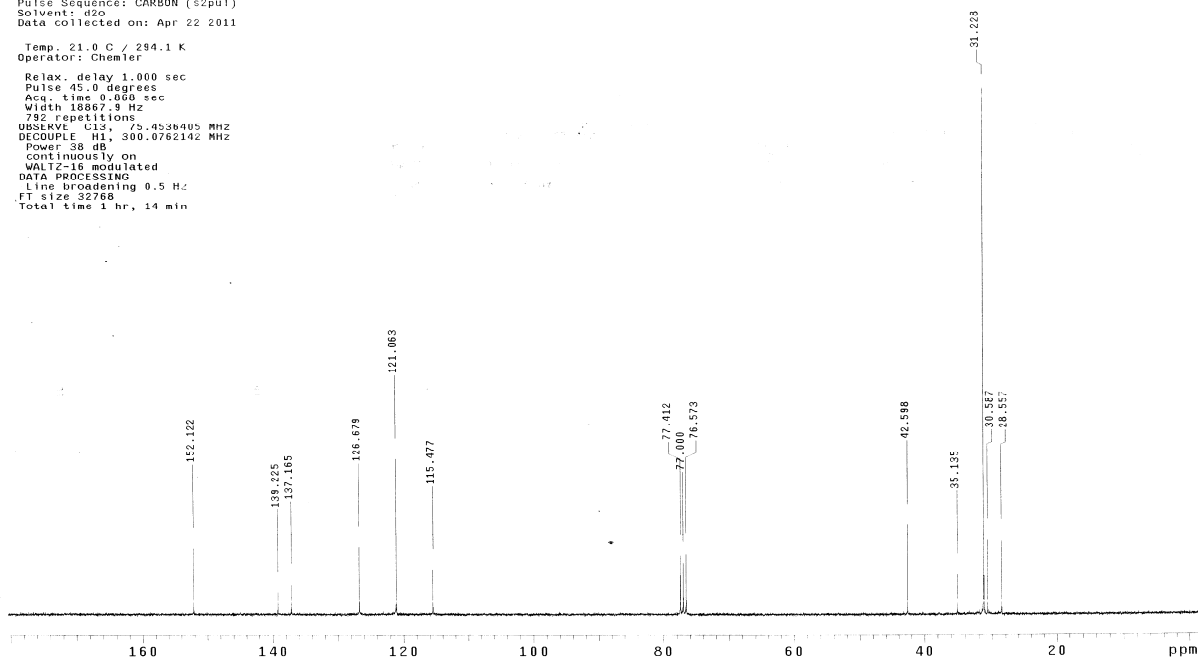
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 1 hr, 14 min



Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

sample directory:

FidFile: twl-1-221a

Bulge Sequence: PROTON (00-03)

Pulse Sequence: PRUGN (szpug)
Solvent: cdcl3
Data collected on: Mar 16 2011

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

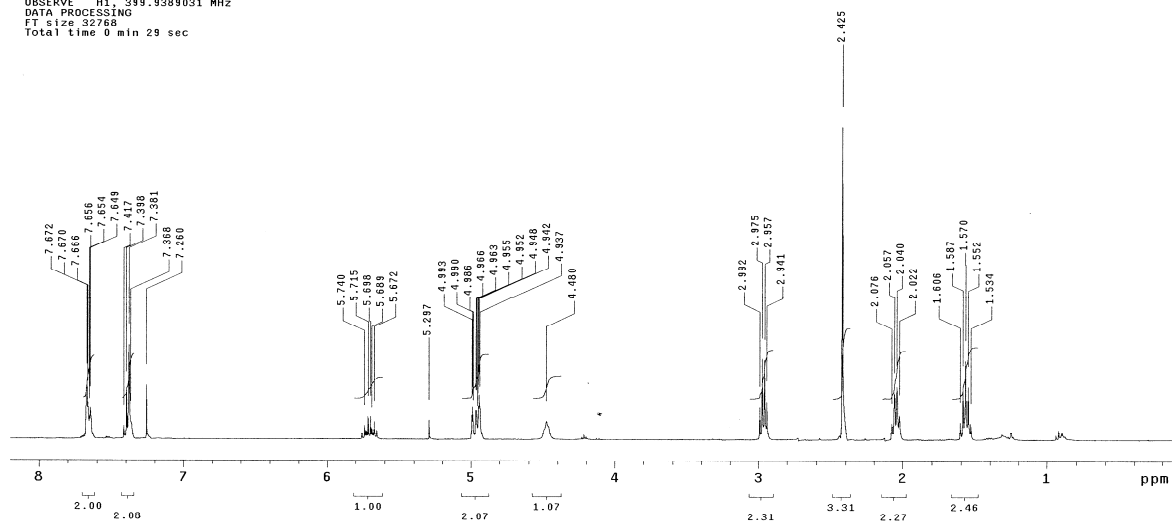
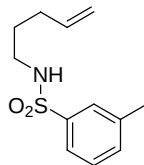
Pulse 45.0 degrees
Acc. time 3.565 sec

Width 6387.7 Hz

```
8 repetitions
OBSERVE      H1, 399.9389031 MHz
```

DATA PROCESSING
ET 2100 20760

Total time 0 min 29 sec



twl-1-221carbon

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

File: tul-1-221carbon

Pulse Sequence: CARRION (c2pul)

Pulse Sequence: CARBON (zgpg3)
Solvent: d2o
Data collected on: Apr 22 2011

data collected on the trip.

Temp. 21.0 C / 2
Operator: Chemler

Relax delay 1.000 sec

Relax. delay 1.000 sec
Pulse 45.0 degrees

Acq. time 0.868 sec
Width 18867.9 Hz

```

848 repetitions
OBSERVE C13 25 45364

```

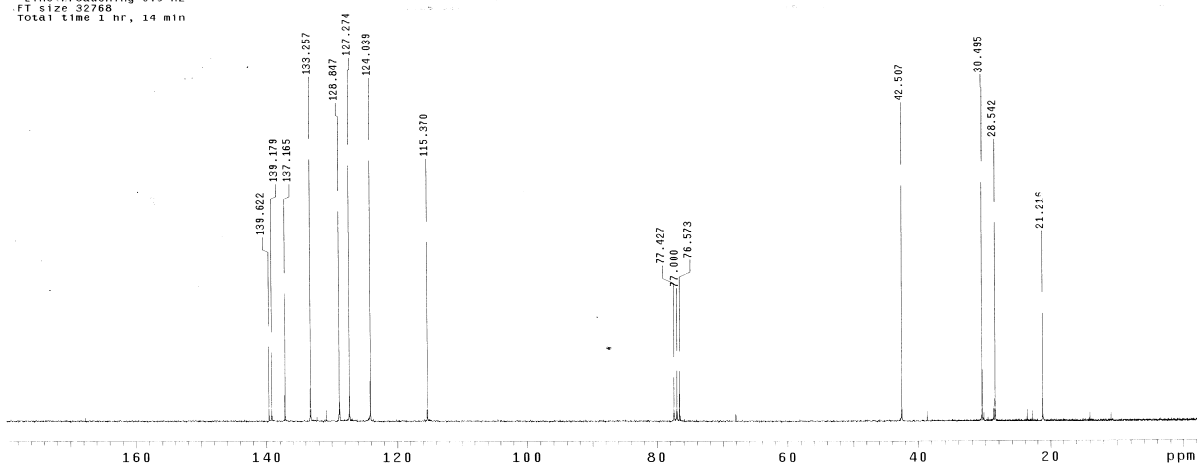
```
DECOUPLE H1, 300.07621
```

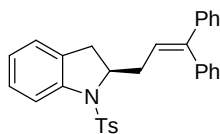
continuously on

WALTZ-16 modulated
DATA PROCESSING

Line 1: roadening 0.5 Hz
FT size 32768

Total time 1 hr, 14 min





tw1-1-036p

Sample Name:

Data Collected on:
Chemmer400-chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Oct 20 2011

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.588 sec

Width 6387.7 Hz

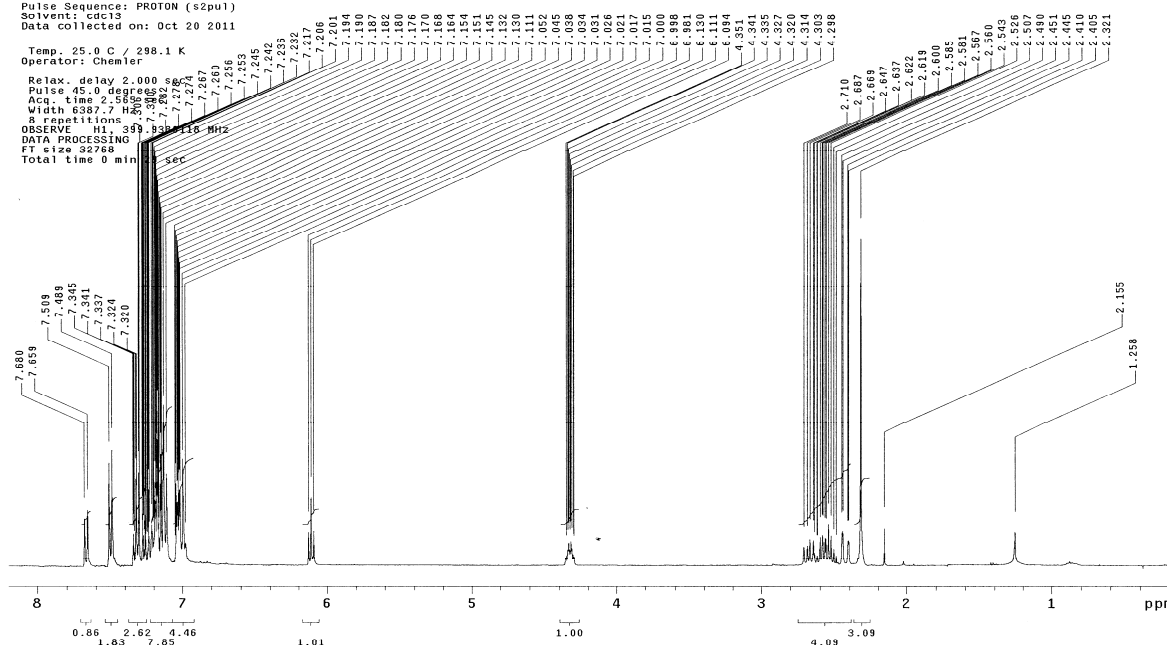
8 repetitions

OBSERVE H1 399.830 MHz

DATA PROCESSING

FT size 32768

Total time 0 min



tw1-1-33carbon

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: tw1-1-033carbon

Pulse Sequence: CARBON (s2pul)

Solvent: d2o

Data collected on: Apr 22 2011

Temp. 21.0 C / 294.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.888 sec

Width 1886.9 Hz

132 repetitions

OBSERVE C13, 75.4536428 MHz

DECOUPLE H1, 500.0762142 MHz

Power 38 dB

continuously on

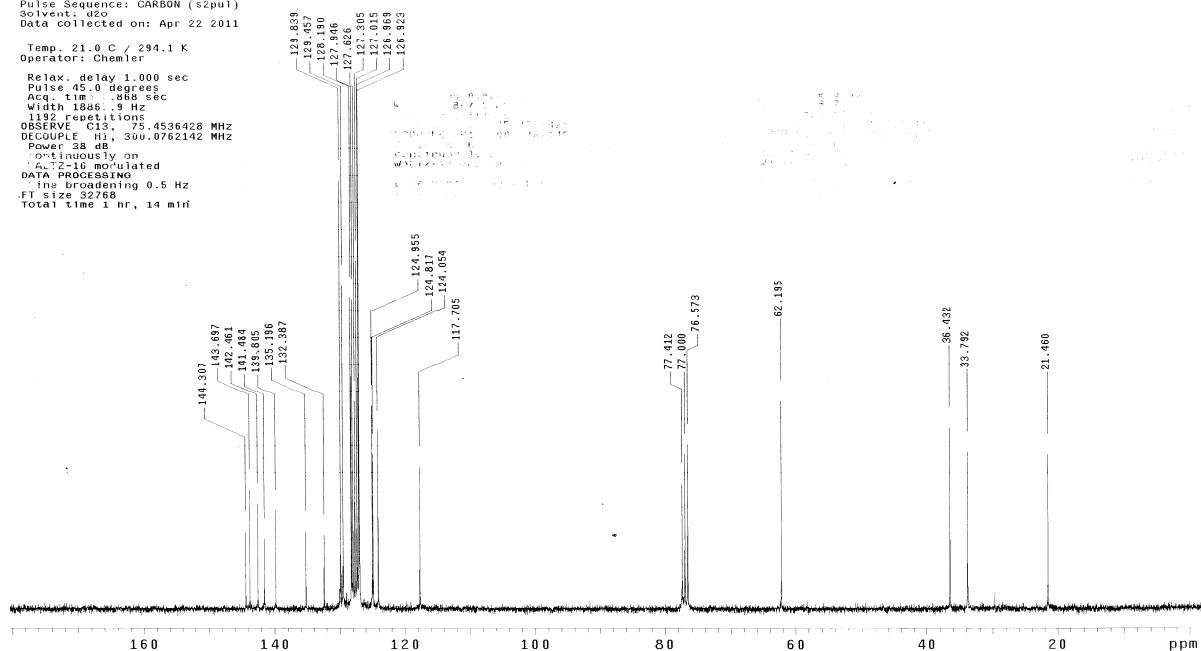
A-Z-16 modulated

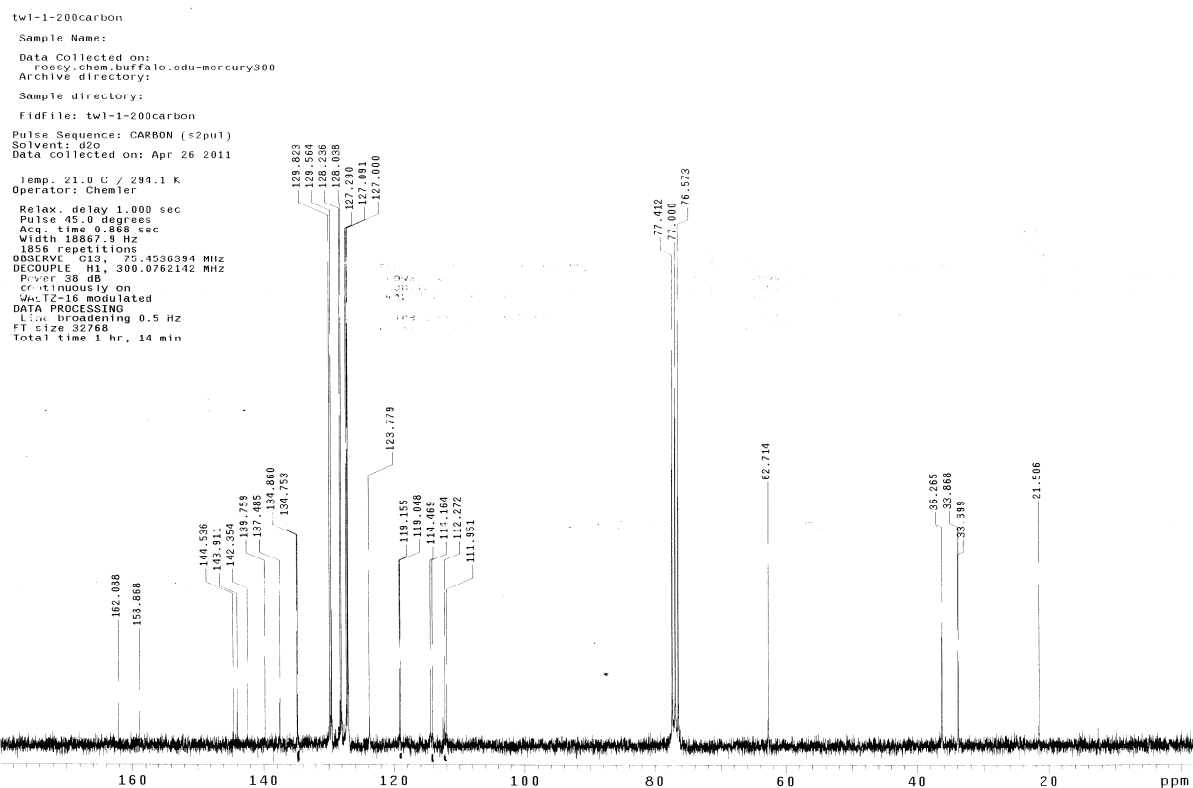
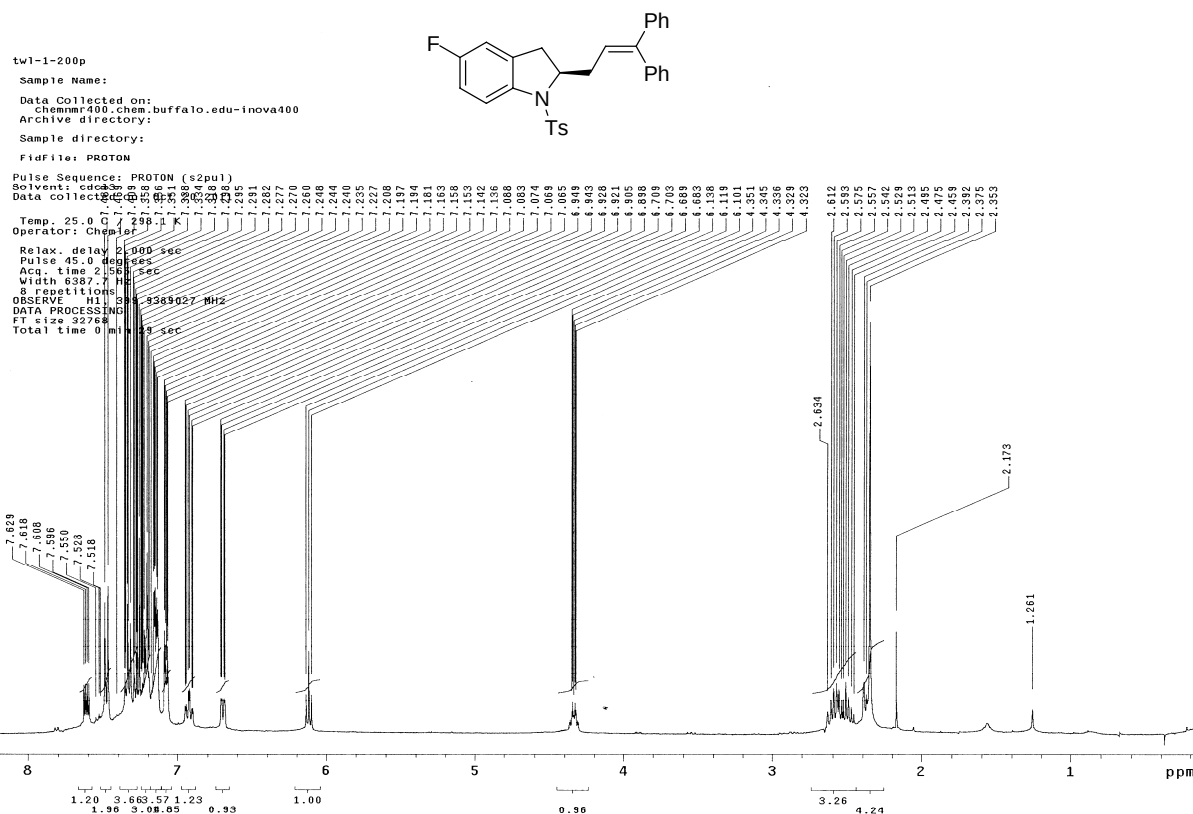
DATA PROCESSING

line broadening 0.5 Hz

FT size 32768

Total time 1 hr, 14 min





tw1-1-252p

Sample Name:

Data Collected on:

chemm1400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Oct 21 2011

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.565400 sec

Width 6387.5 Hz

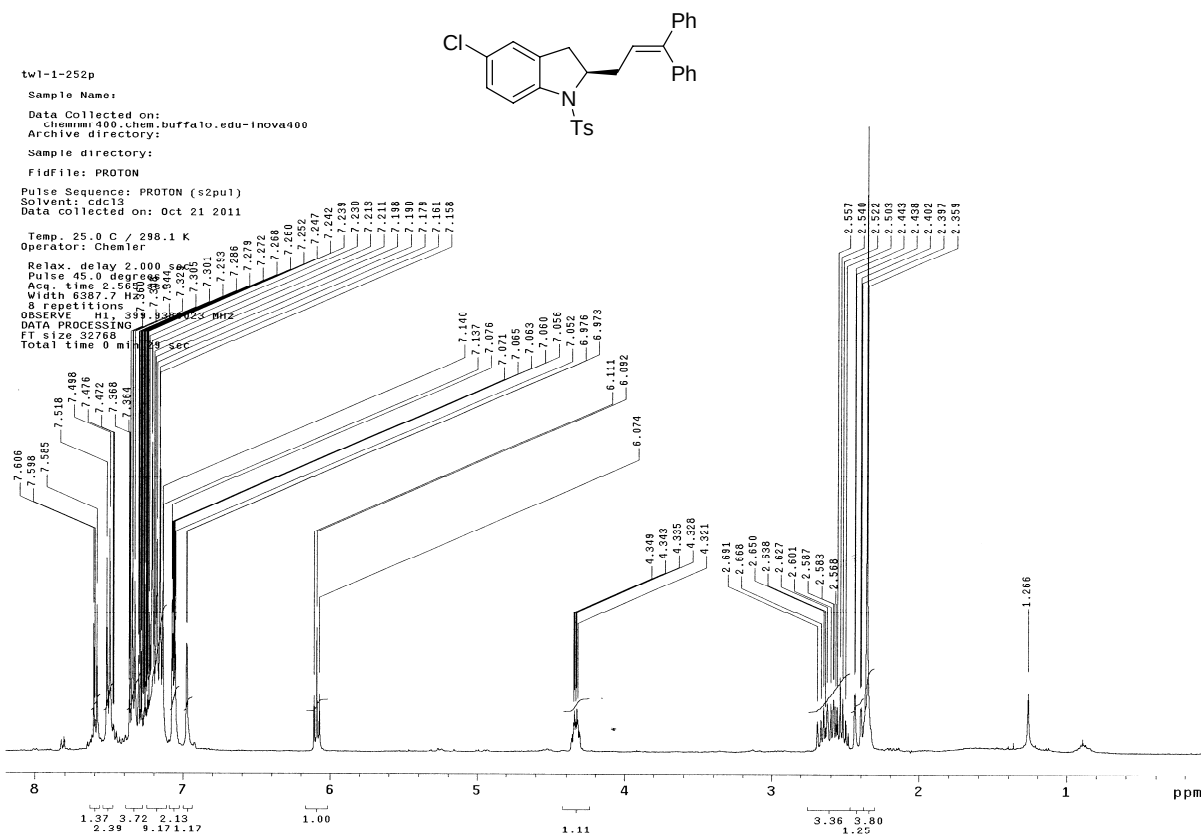
9 repetitions

OBSERVE H1, 399.9340000 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 29 sec



tw1-1-252carbon

Sample Name:

Data Collected on:

roesy.chem.buffalo.edu-mercurys00

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 20 2011

Temp. 26.5 C / 299.6 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.600 sec

Width 18867.9 Hz

1672 repetitions

OBSERVE C13, 75.4536389 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

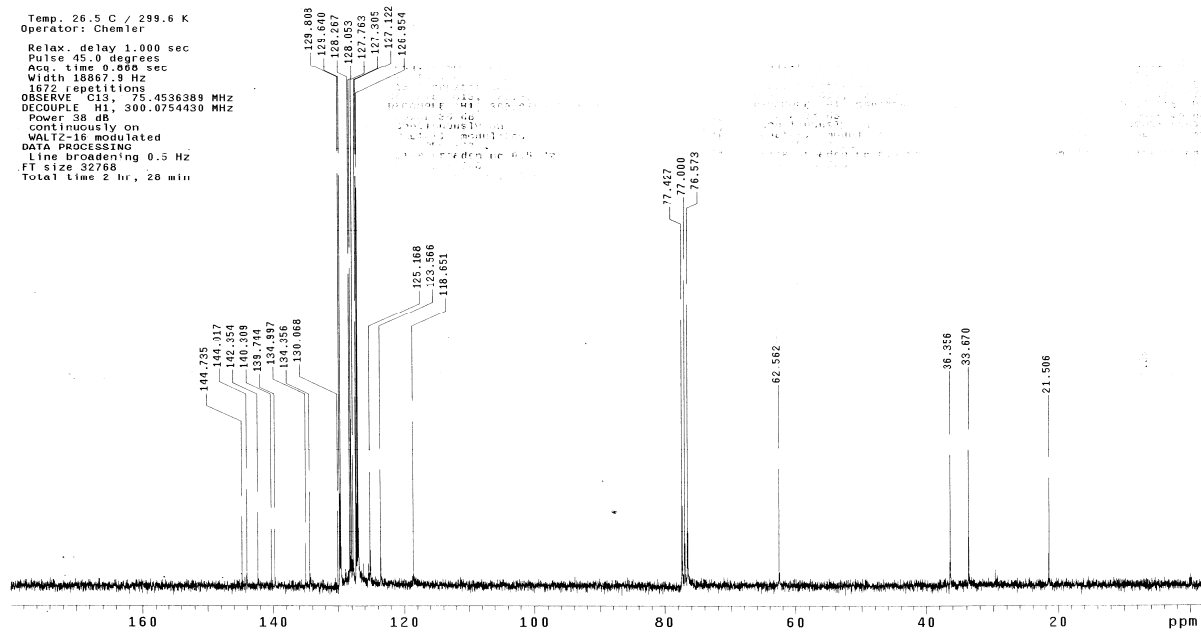
WALTZ-16 modulated

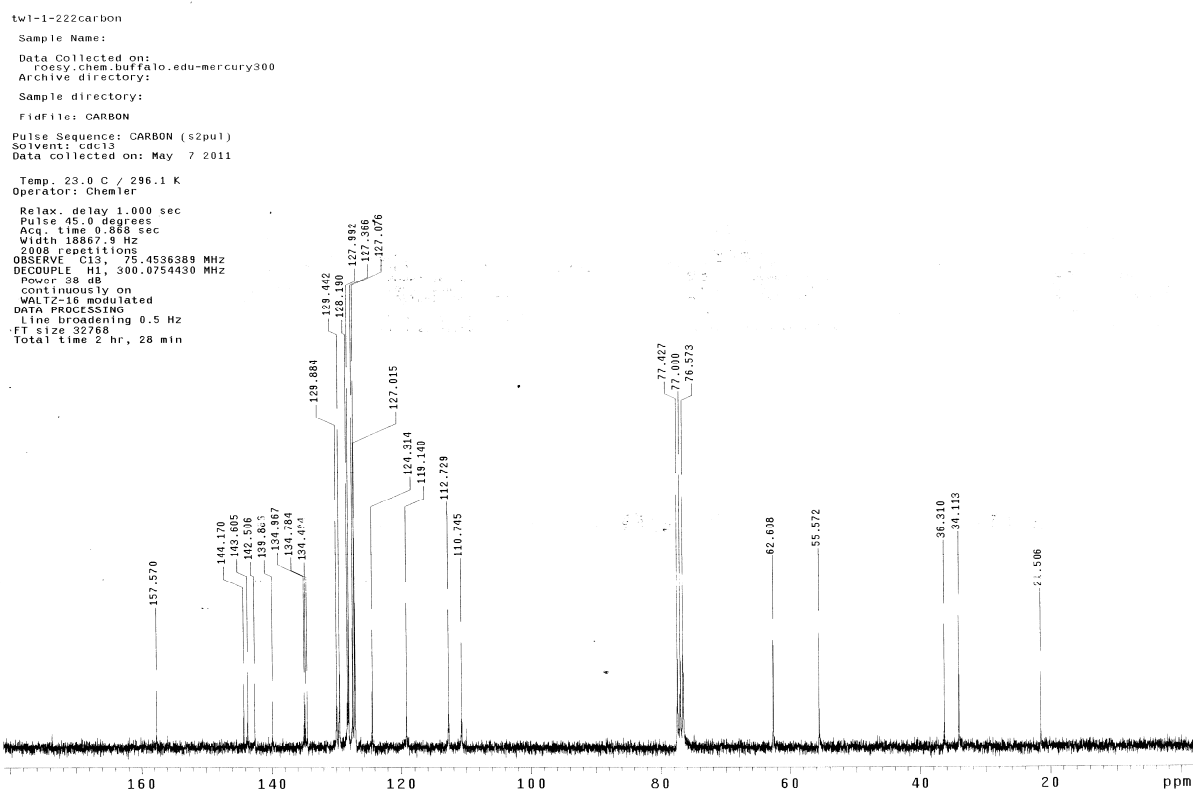
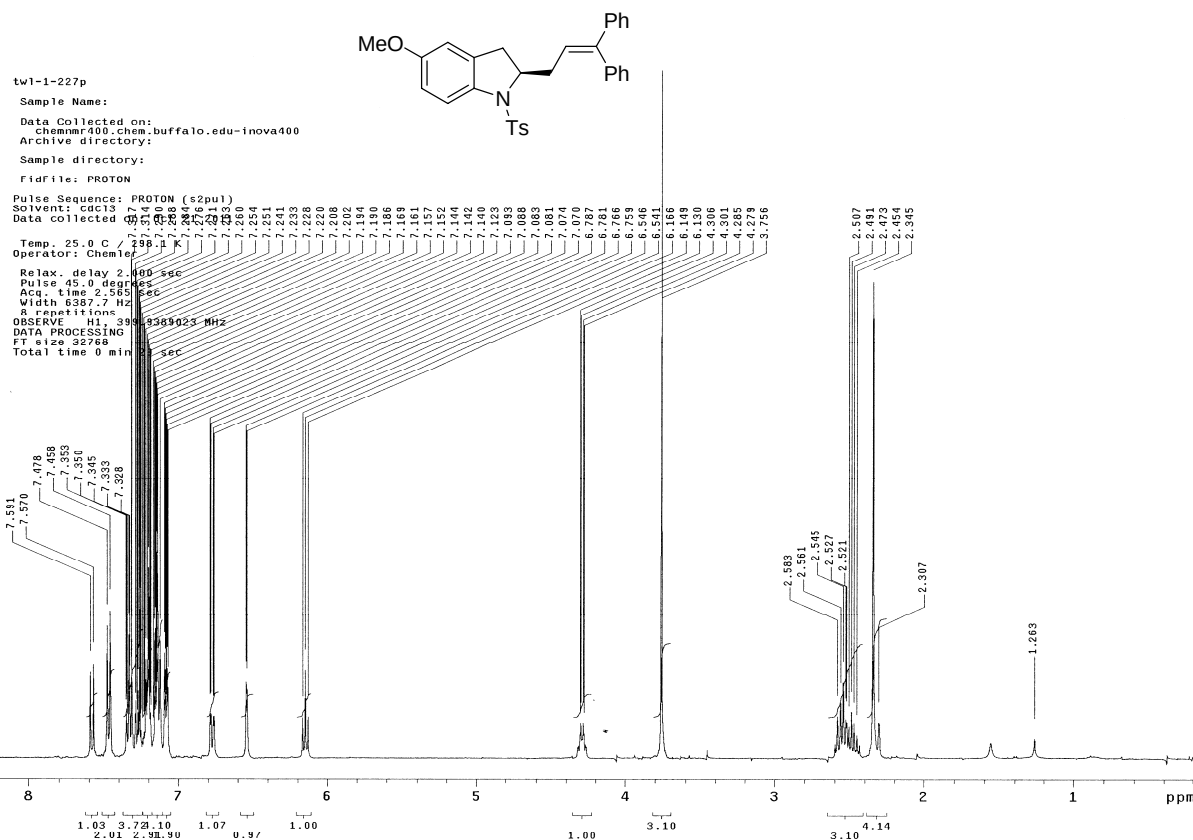
DATA PROCESSING

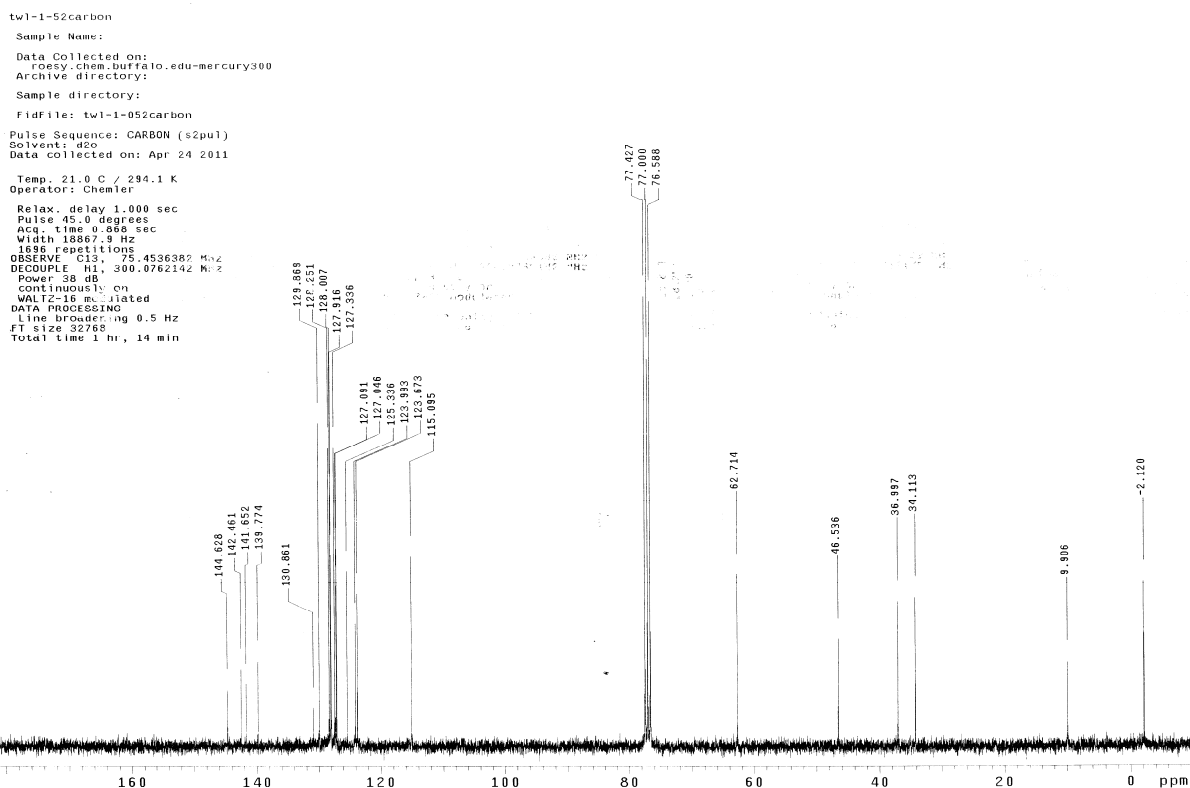
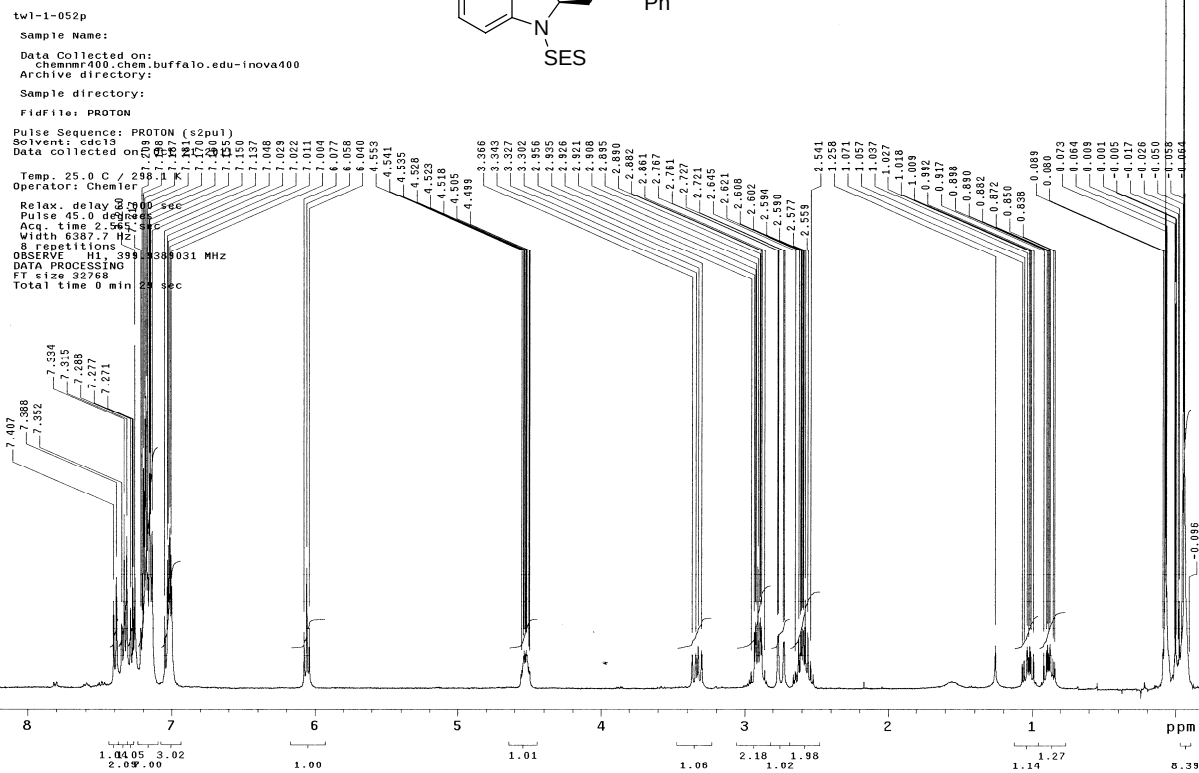
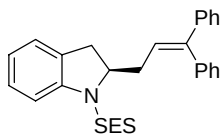
Line broadening 0.5 Hz

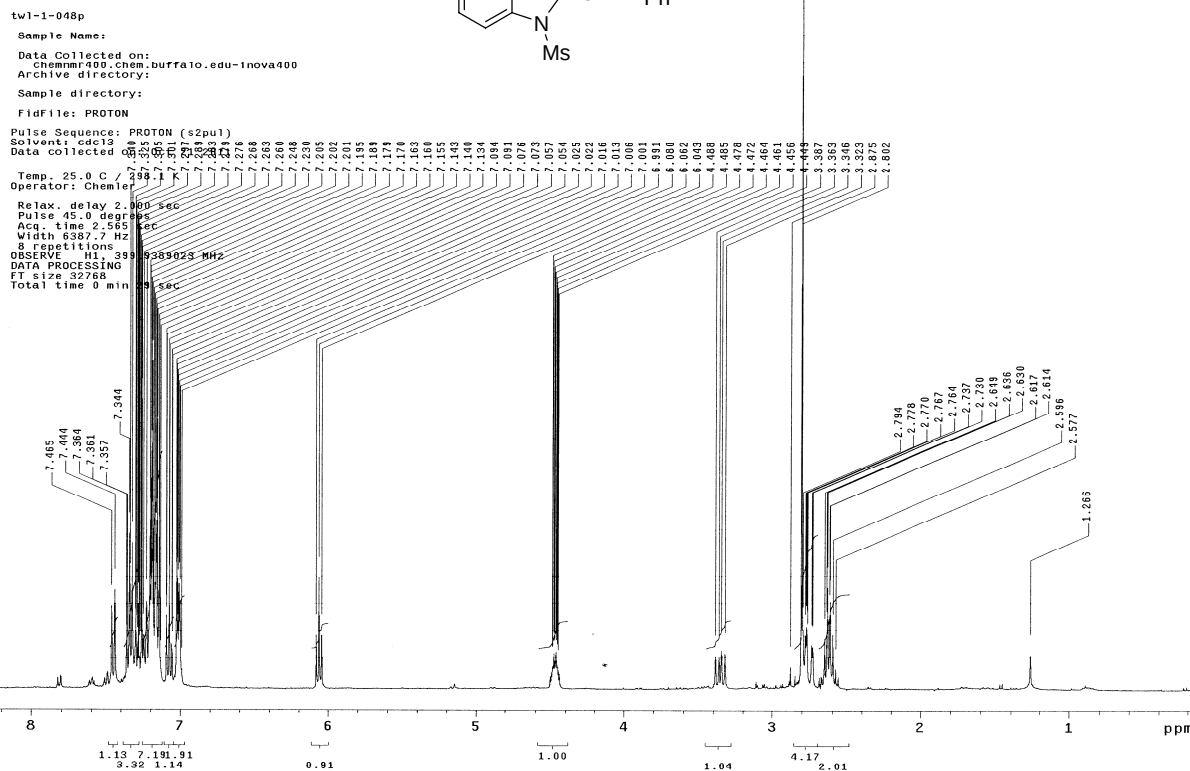
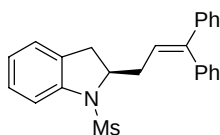
FT size 32768

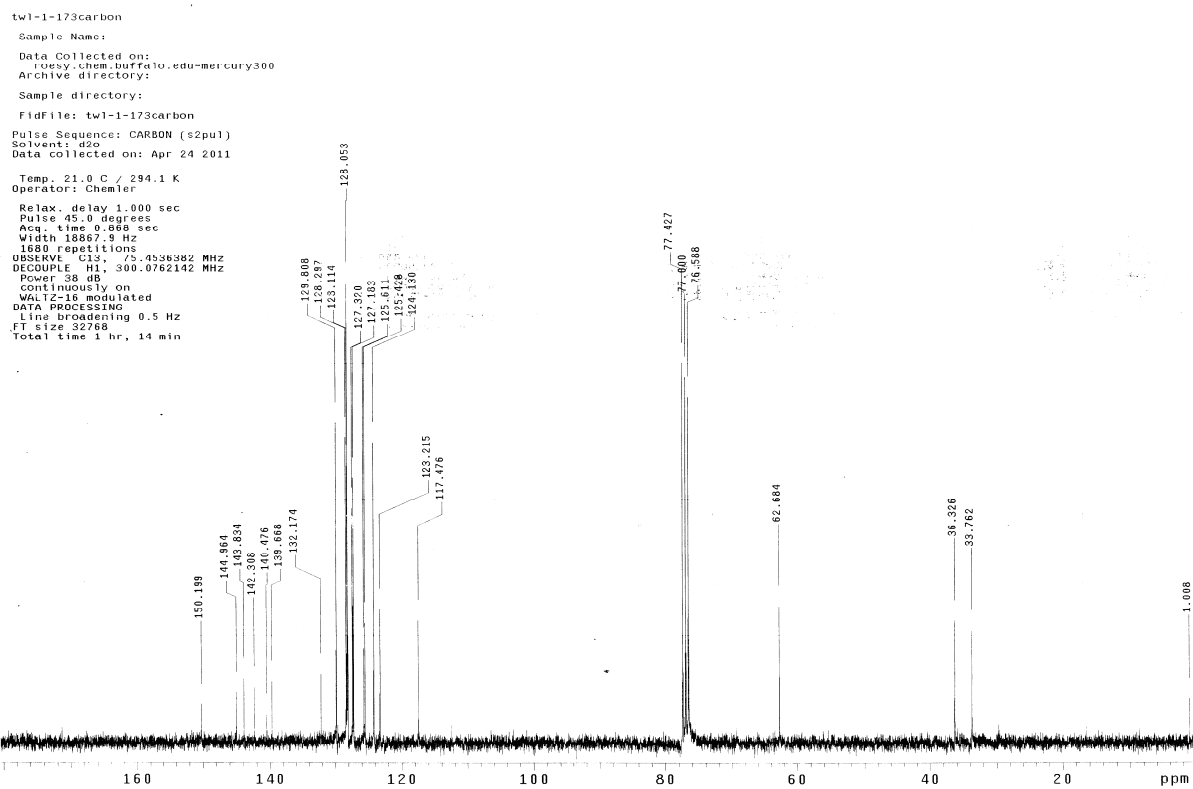
Total time 2 hr, 28 min

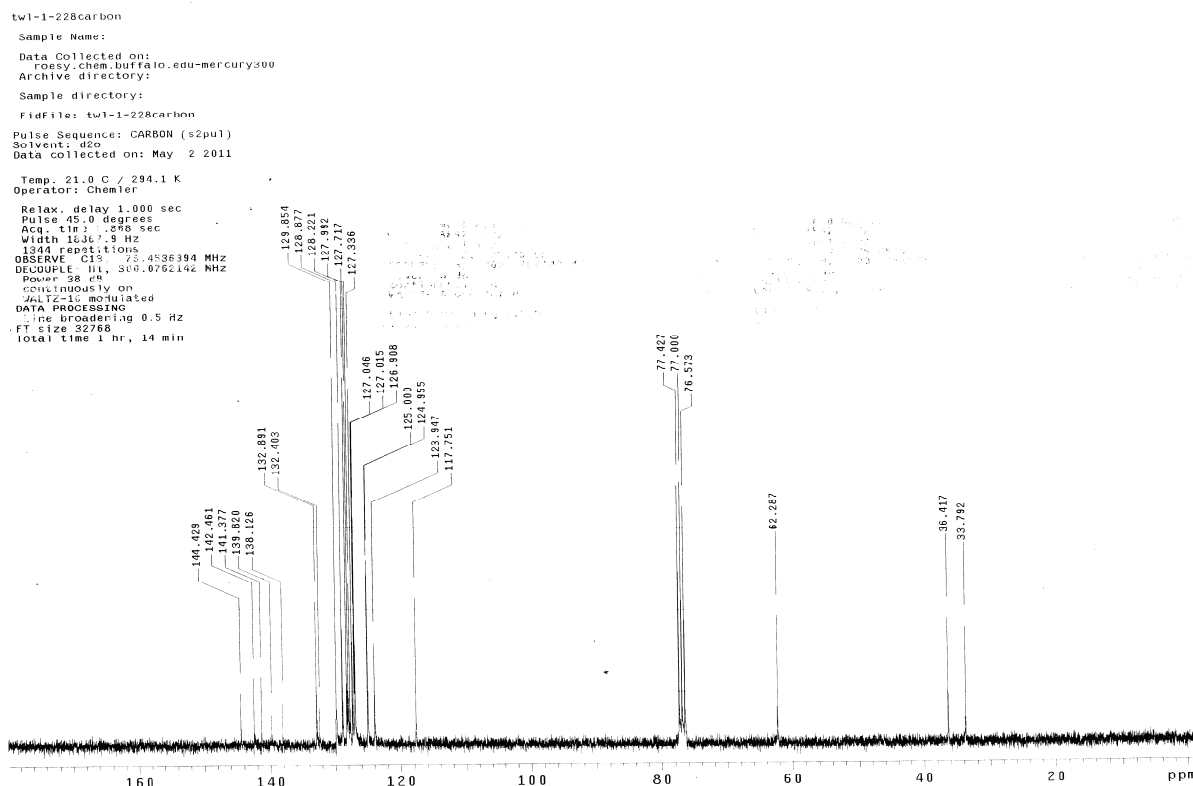
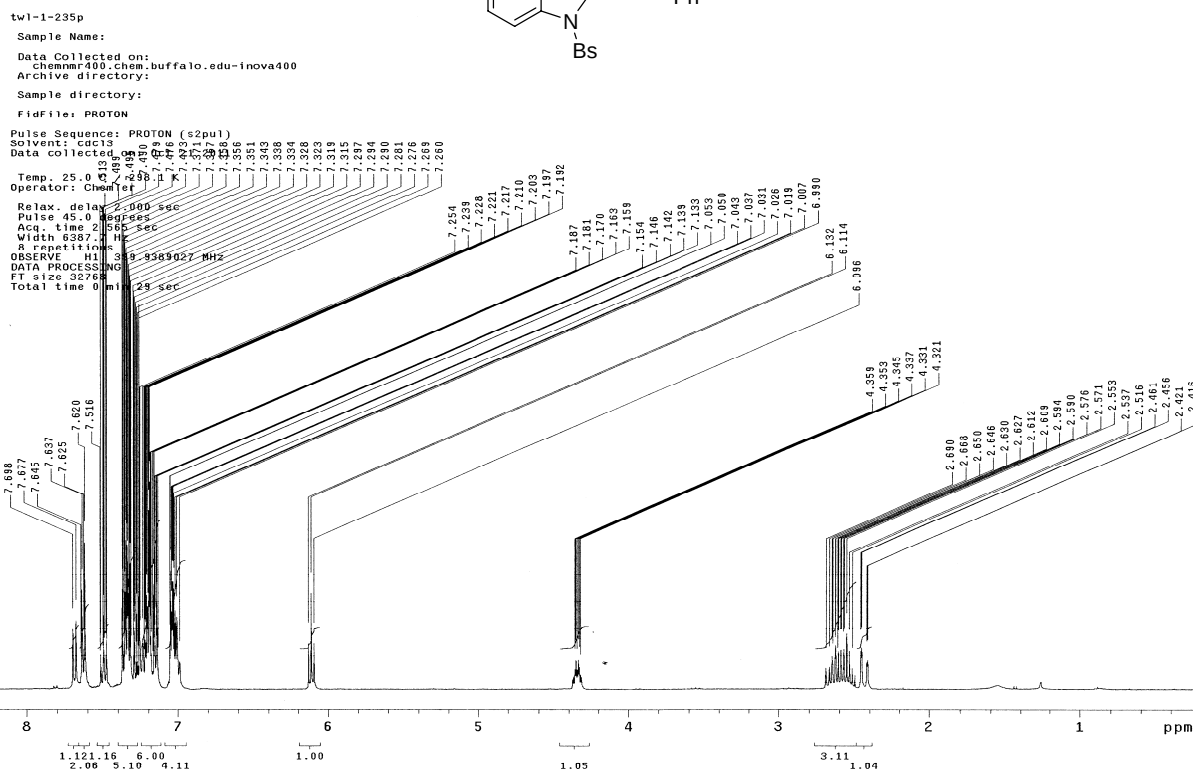
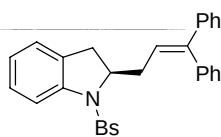












tw1-1-111prepped

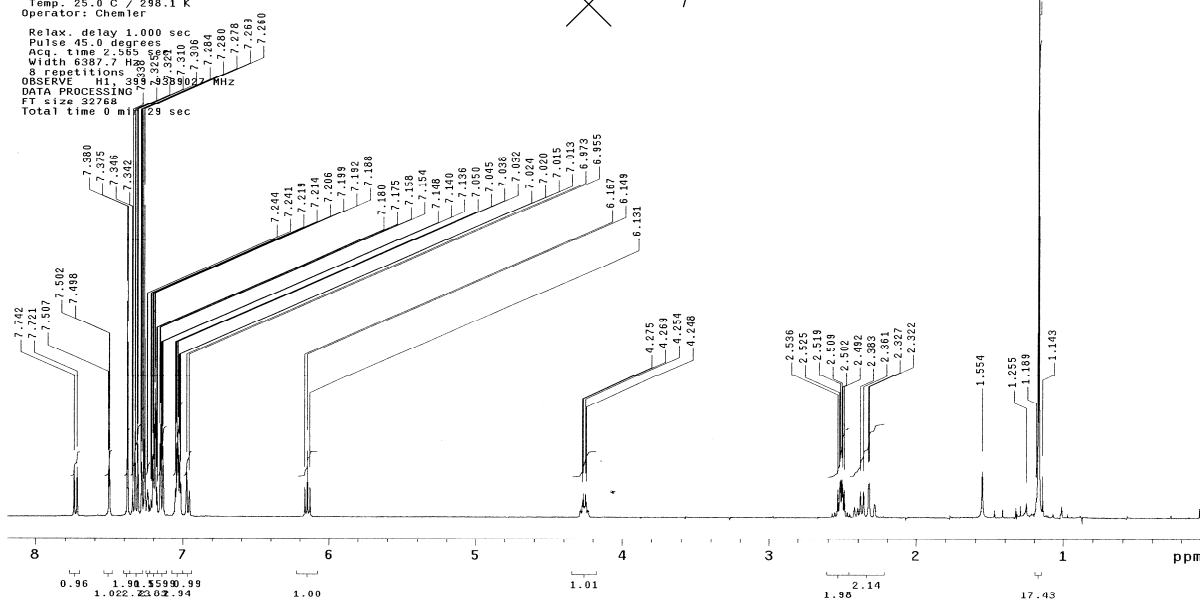
Sample Name:

Data Collected on:
Chemnar400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 30 2011Temp. 25.0 C / 298.1 K
Operator: ChemlerRelax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.585 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9389032 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 29 sec

tw1-1-116carbon

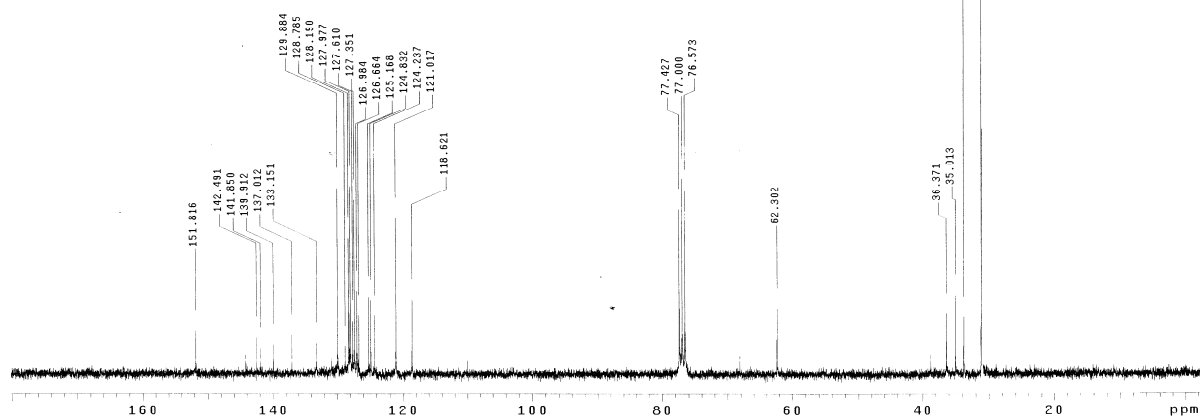
Sample Name:

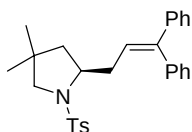
Data Collected on:
roesy.chem.buffalo.edu-mercury300

Archive directory:

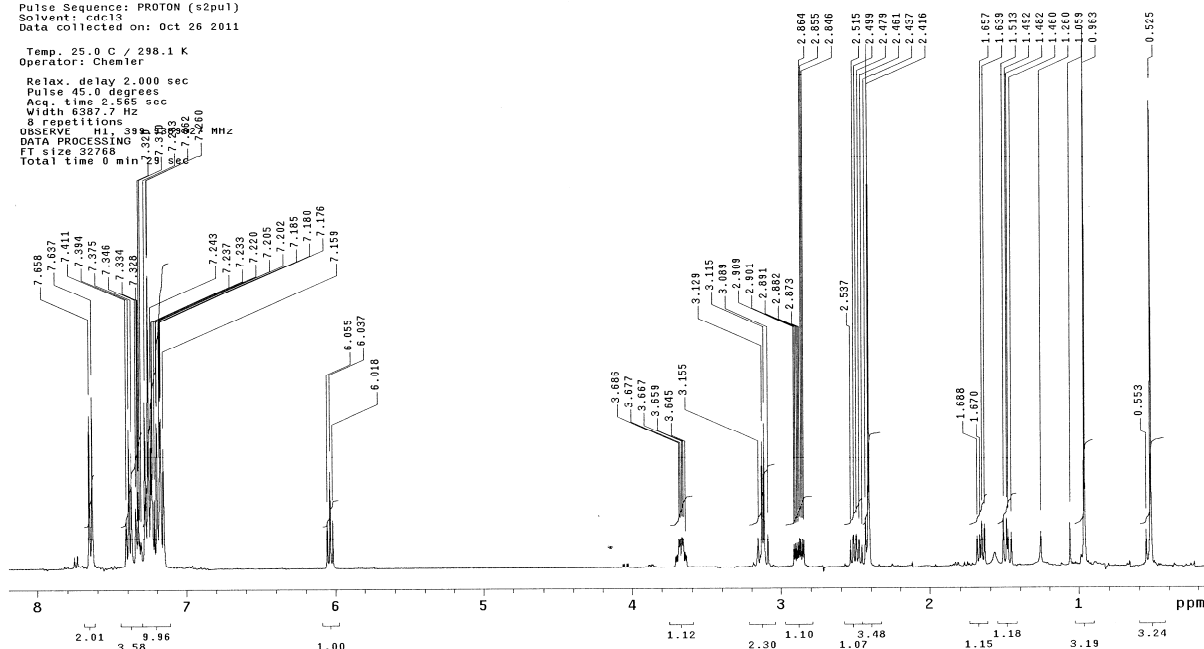
Sample directory:

FidFile: tw1-1-116carbon

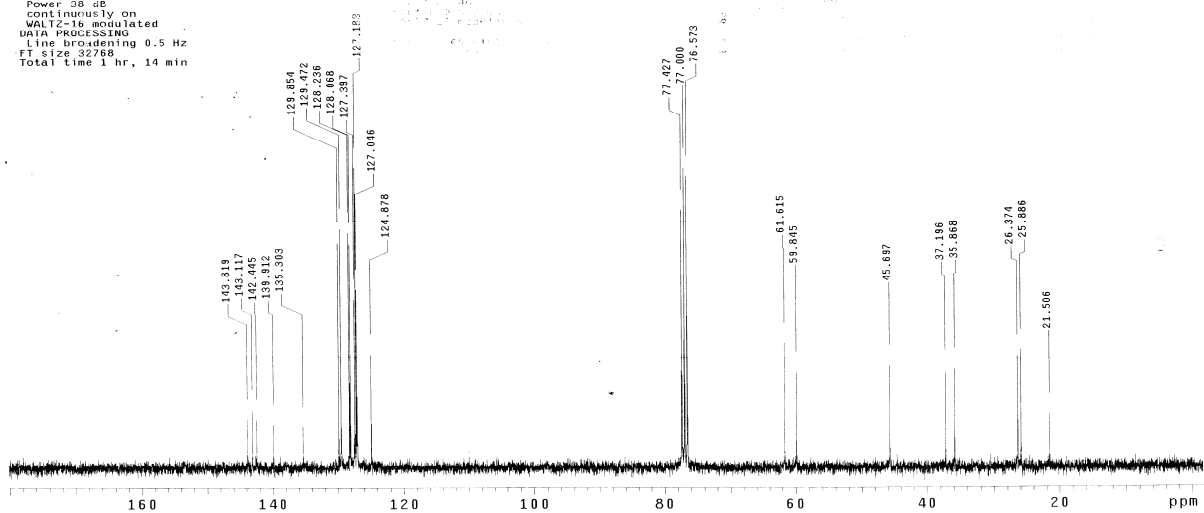
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 25 2011Temp. 21.0 C / 294.1 K
Operator: ChemlerRelax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.5 Hz
1544 repetitions
OBSERVE C13, 78.4536388 MHz
DECOUPLE H1, 300.0754430 MHz
Power 39 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 14 min



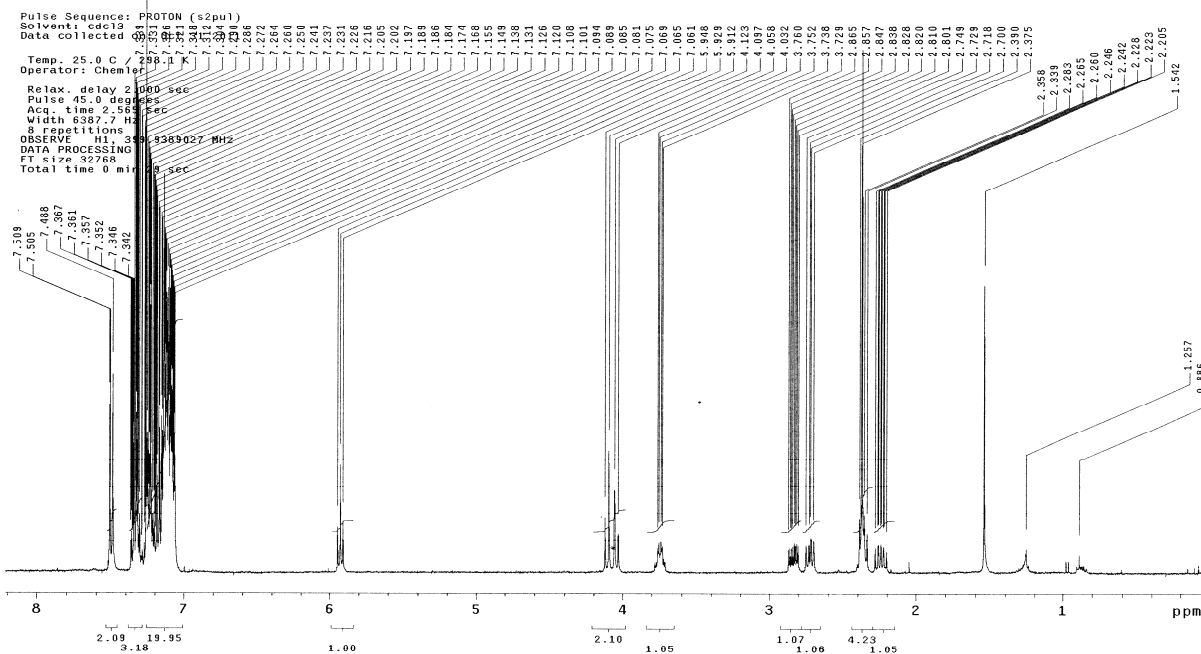
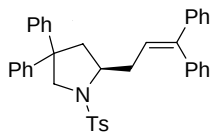
tw1-1-064p
 Sample Name:
 Data Collected on:
 chemmm400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdc13
 Data collected on: Oct 26 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 5.565 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 399.999999 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



tw1-1-064carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: tw1-1-064carbon
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdc13
 Data collected on: Apr 25 2011
 Temp. 21.0 C / 294.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 1624 repetitions
 OBSERVE C13, 75.4536389 MHz
 DECOUPLE H1, 300.0754430 MHz
 Power 38 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 1 hr, 14 min



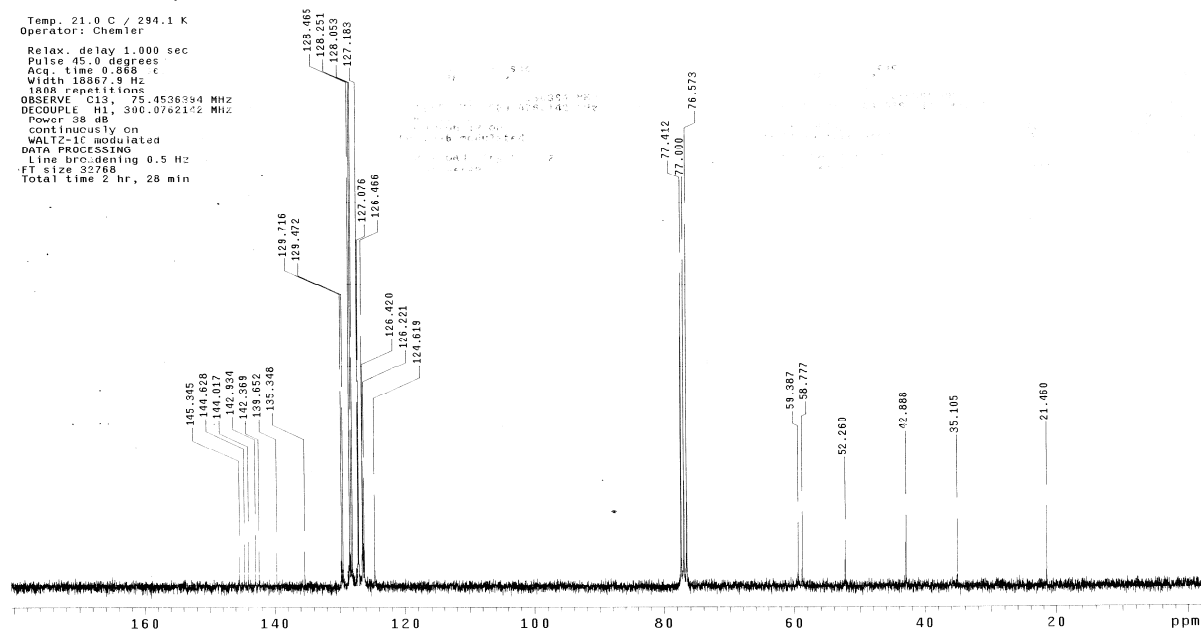
tw1-1-210prepped
 Sample Name:
 Data Collected on:
 chemnmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 FidFile: PROTON



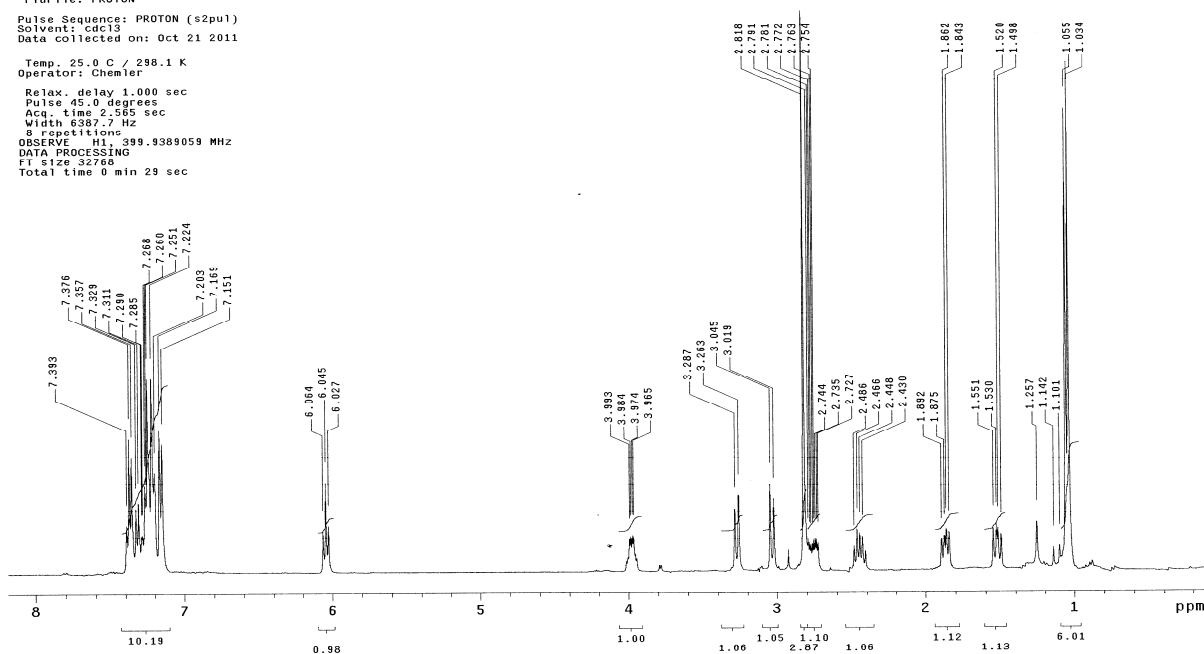
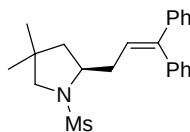
tw1-1-211carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: tw1 1 211carbon

Pulse Sequence: CARBON (s2pul)
 Solvent: d2o
 Data collected on: May 2 2011

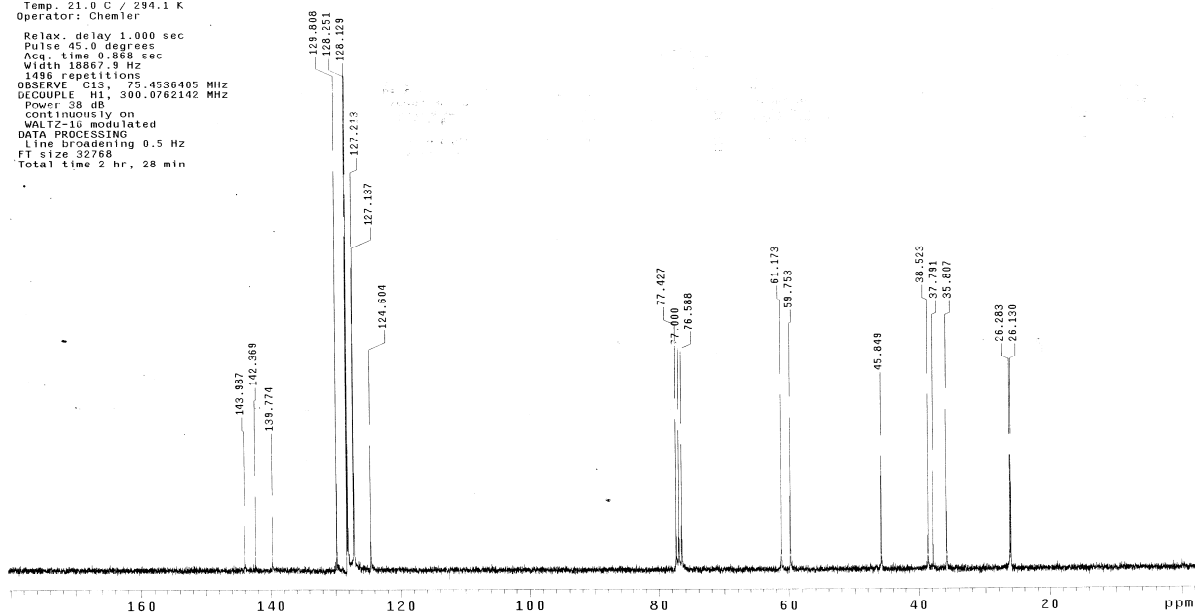
Temp. 21.0 C / 294.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.888 sec
 Width 18867.9 Hz
 1800 repetitions
 OBSERVE C13, 75.4536394 MHz
 DECOUPLE H1, 300.0762162 MHz
 Power 58 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 2 hr, 28 min

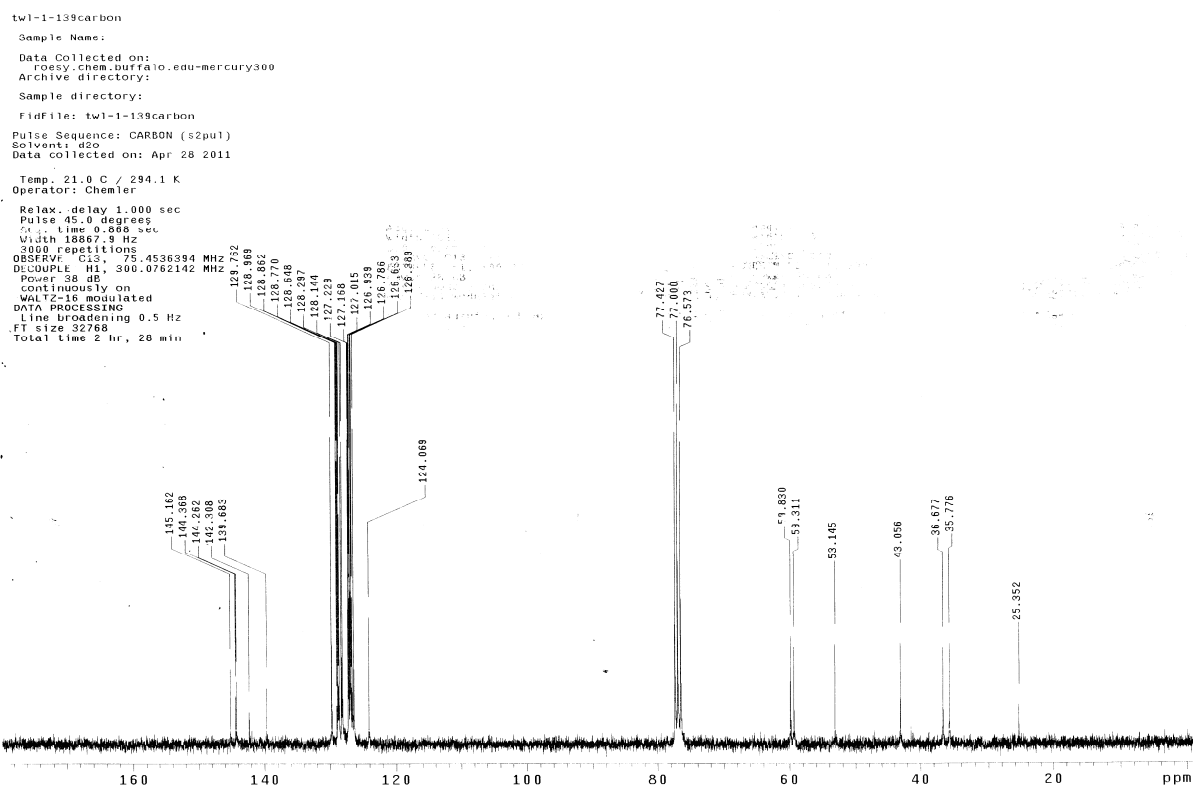
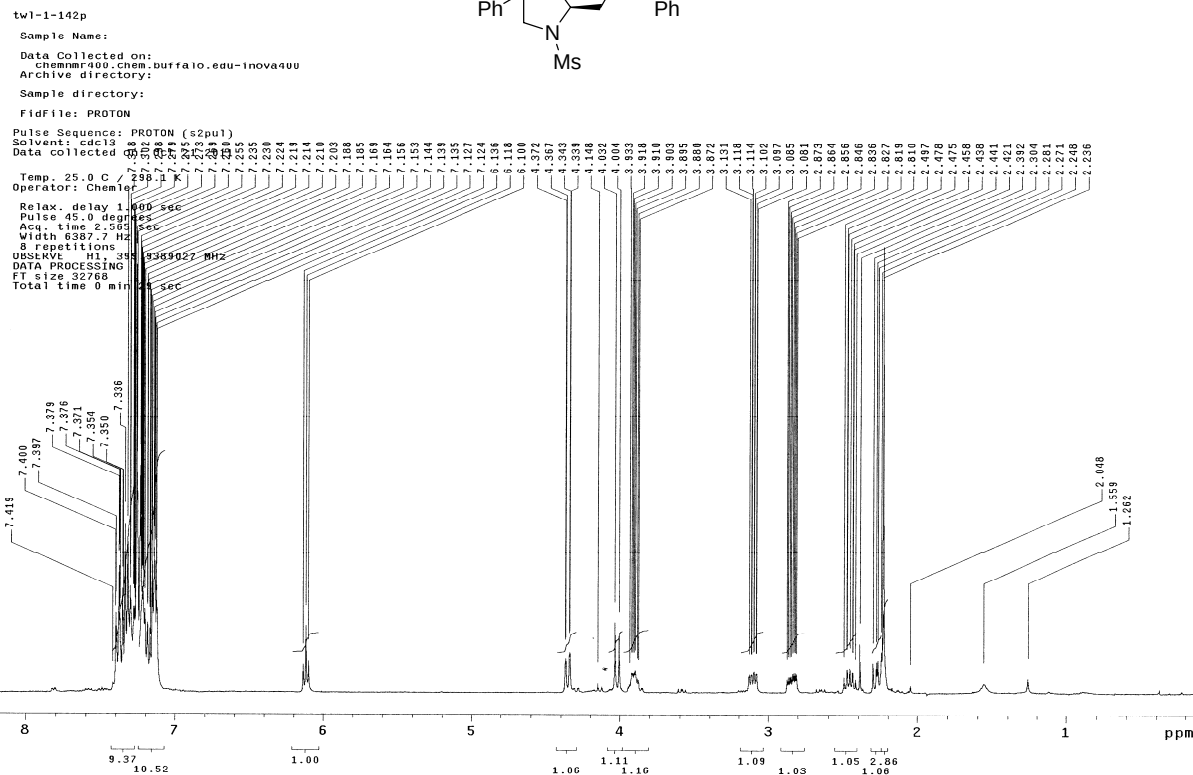
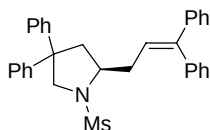


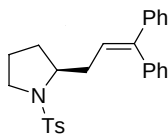
tw1-1-135p
 Sample Name:
 Data Collected on: chemmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 FIDfile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdc13
 Data collected on: Oct 21 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.505 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 399.9389059 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



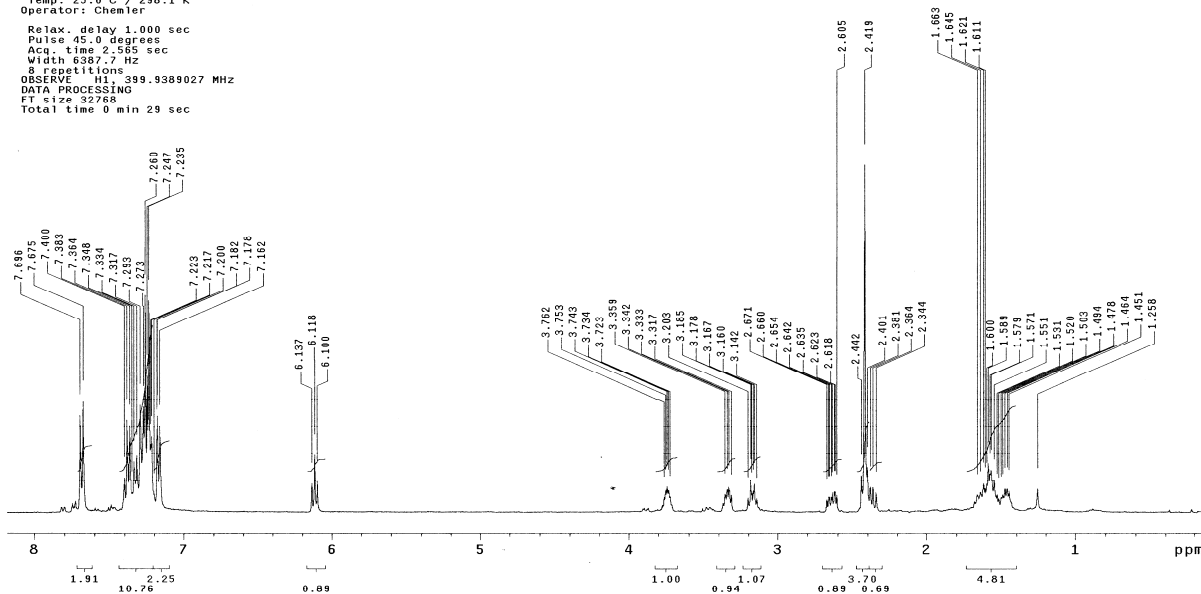
tw1-1-139carbon
 Sample Name:
 Data Collected on: roscy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FIDfile: tw1-1-135carbon
 Pulse Sequence: CARBON (s2pul)
 Solvent: d2o
 Data collected on: Apr 26 2011
 Temp. 21.0 C / 294.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 1496 repetitions
 OBSERVE G13, 75.4536405 MHz
 DECOUPLE H1, 300.0762142 MHz
 Power 38 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 2 hr, 28 min



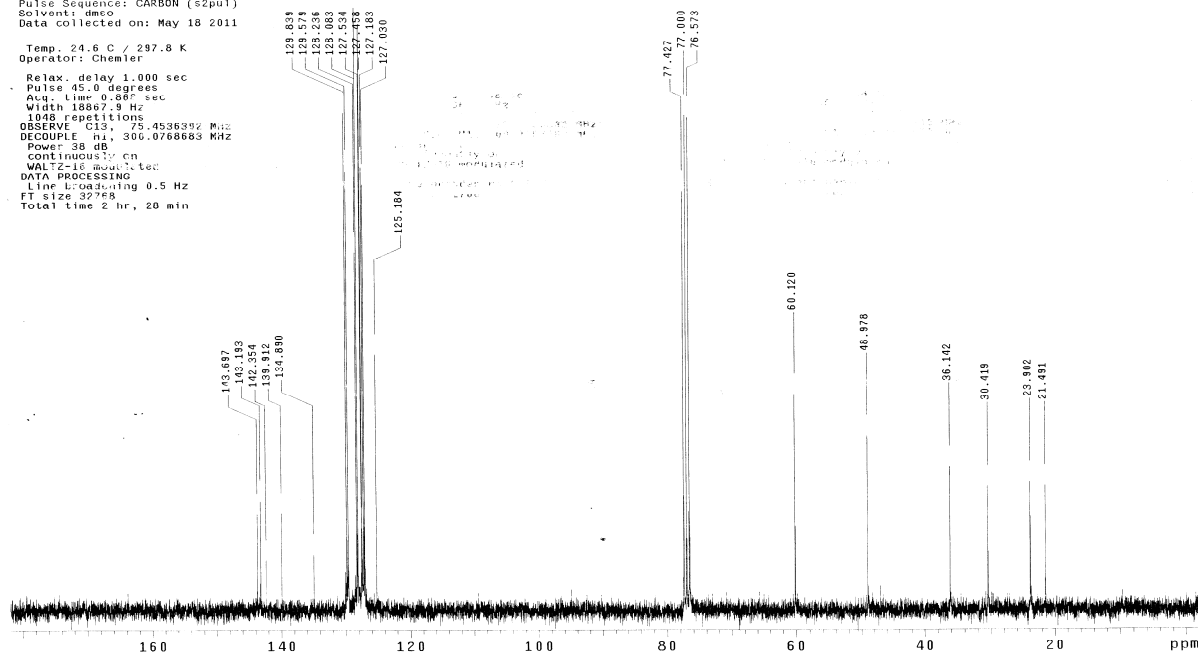




tw1-1-131p
 Sample Name:
 Data Collected on:
 chemmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Oct 22 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.565 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 399.9389027 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



tw1-1-127carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pul)
 Solvent: dmso
 Data collected on: May 18 2011
 Temp. 24.6 C / 297.8 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.867 sec
 Width 18867.9 Hz
 1048 repetitions
 OBSERVE C13, 75.4536392 MHz
 DECOUPLE H1, 300.0766653 KHz
 Power 38 dB
 Continuous: on
 WALTZ-16 subroutines
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 2 hr, 20 min



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 25 2004

Temp. 25.0 C / 298.15 K
Operator: Chemist
Relax. delay 2.700 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1 399.9389027 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 29 sec

Chemical structure: CC(C)(C)c1ccc(cc1)CC(=O)CCc2ccc(cc2)C(C)(C)C

Peak list (ppm): 7.648, 7.644, 7.608, 7.604, 7.600, 7.591, 7.584, 7.555, 7.245, 7.234, 7.221, 7.214, 7.202, 7.157, 7.181, 7.177, 7.160, 6.138, 6.110, 6.102, 3.851, 3.842, 3.812, 3.802, 3.333, 3.321, 3.317, 3.308, 3.303, 3.294, 3.283, 3.205, 3.187, 3.178, 3.169, 3.161, 2.615, 2.614, 2.607, 2.599, 2.598, 2.582, 2.569, 2.565, 2.438, 2.417, 2.389, 1.665, 1.656, 1.646, 1.635, 1.619, 1.594, 1.583, 1.580, 1.560, 1.541, 1.523, 1.520, 1.510, 1.492, 1.471, 1.461, 1.443, 1.433, 1.412, 1.355, 1.348, 1.337, 1.304, 1.276, 1.256, 1.236, 1.178.

Integration values: 1.62, 0.99, 4.21, 6.17, 1.00, 0.87, 0.95, 0.95, 0.77, 0.75, 28.55.

Sample directory:
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data Collected on: May 16 2011

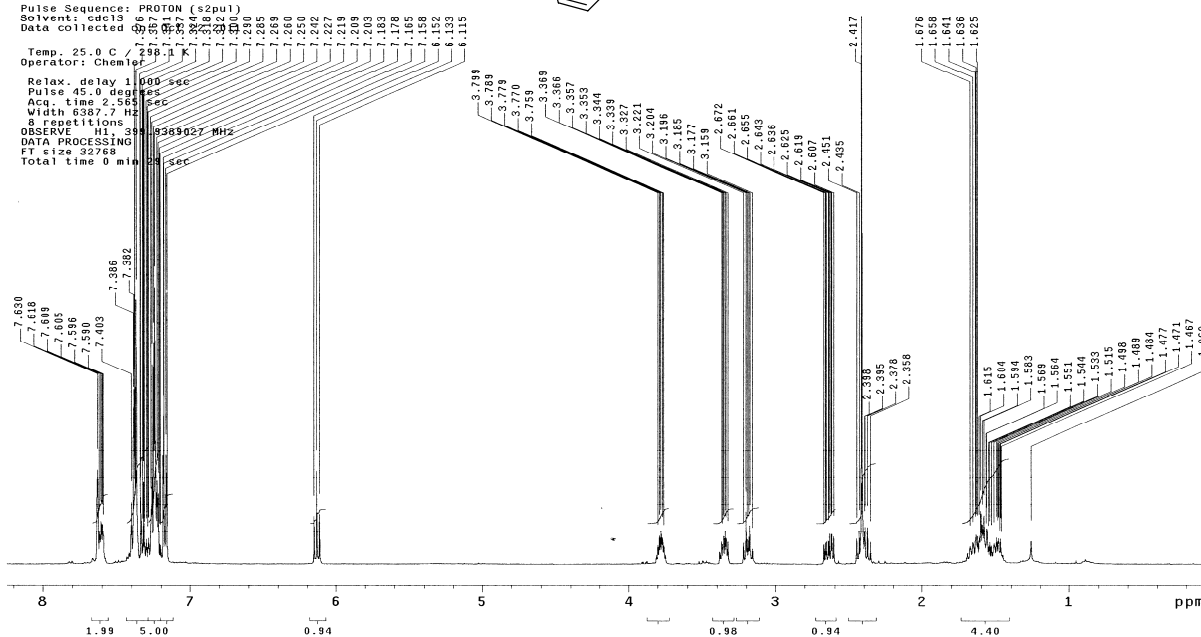
Temp. 23.0 C / 296.1 K
Operator: Chemier

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
364 repetitions
OBSERVE C13, 75.4536410 MHz
DECOUPLE H1, 300.0754436 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
Data PROCESSING
Line broadening 0.5 Hz
F1 size 32768
Total time 2 hr, 28 min

151.98
143.621
142.323
139.927
137.378
129.808
126.221
118.068
127.152
127.010
126.405
125.153
121.444
77.427
77.000
76.573
60.196
48.226
36.112
35.019
30.343
23.832

ppm

```
Pulse Sequence: gzgpg007 - PROTON (szpul)
Solvent: cdc13
Data collected: 60 sec
Temp. 25.0 C / 298.1 K
Operator: Chemist
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1
DATA PROCESSING
ft 121 32768
Total time 0 min 24.5 sec
```



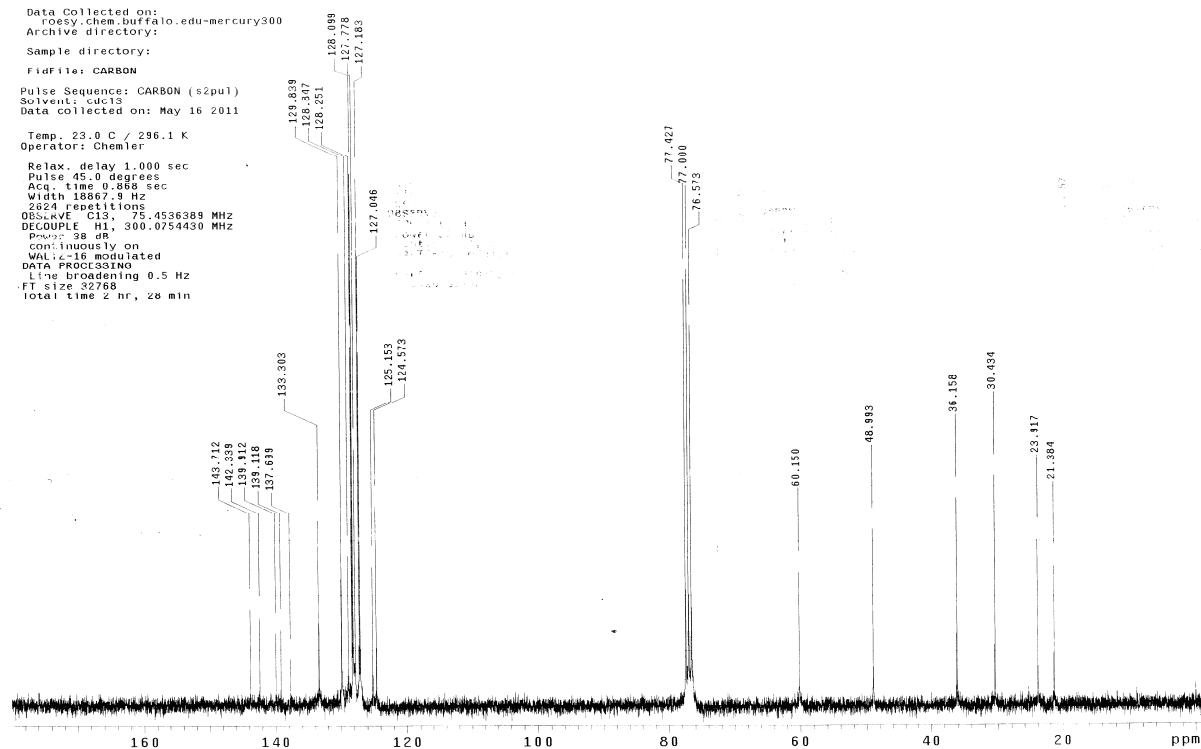
```

FidFile: CARBON
Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: May 16 2011

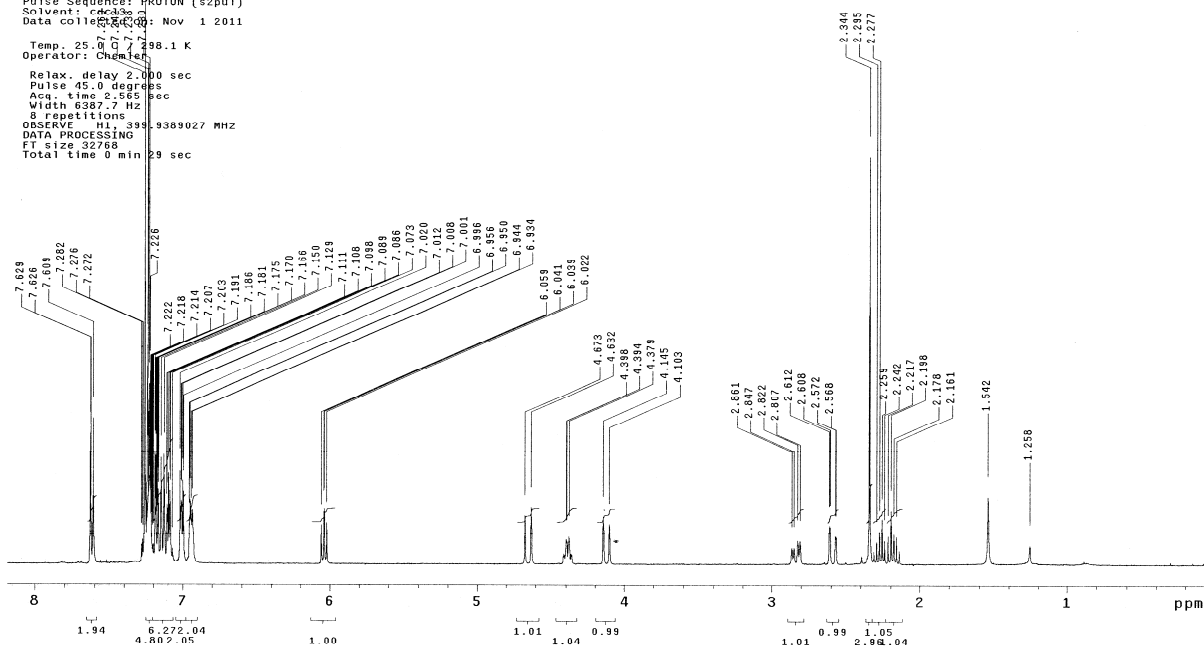
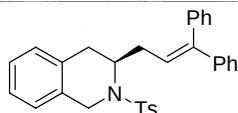
Temp. 23.0 C / 296.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 4.00 sec 0.065
Acq. time 0.868 sec
Width 18867.9 HZ
2624 repetitions
F1 400.14536389 MHz
DECOUPLE H1, 300.0754430 MHz
P2PROG 98 R8
Cont: continuously on
WALTZ-16 modulated
PROG333ING
Line broadening 0.5 HZ
FT size 32768
FID file: 20110516_08.mn

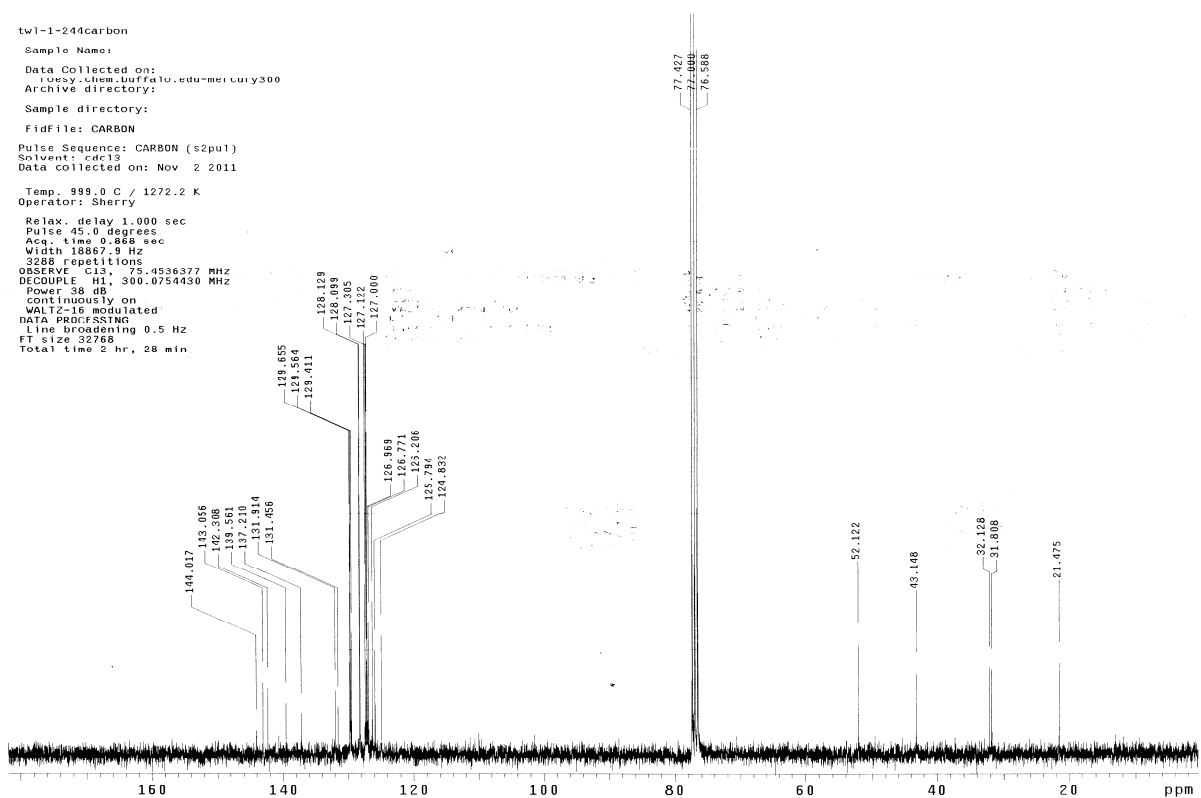
```



tw1-1-244prepped
 Sample Name:
 Data Collected on:
 chemm400.chem.buffalo.edu-tnova400
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdc13
 Data collected on: Nov 1 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemist
 Relax. delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 2.565 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 399.9389027 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



tw1-1-244carbon
 Sample Name:
 Data Collected on:
 rusey.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdc13
 Data collected on: Nov 2 2011
 Temp. 99.0 C / 1272.2 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 3288 repetitions
 OBSERVE C13, 75.4536377 MHz
 DECOUPLE H1, 300.0754430 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 2 hr, 28 min



Ts-o-allylaniline styrene

Sample Name:

Data Collected on:
rossy.chem.buffalo.edu-mercury300

Archive directory:

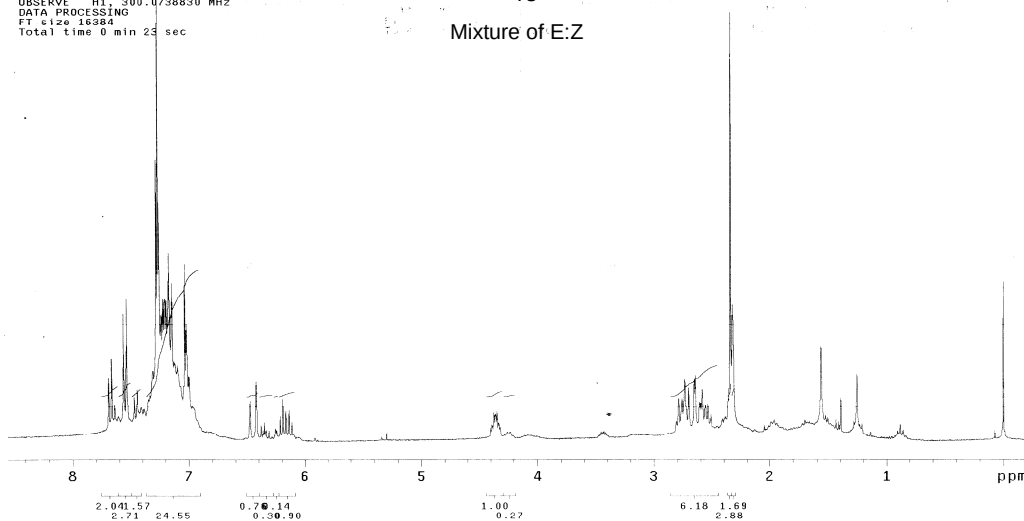
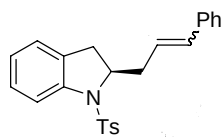
Sample directory:

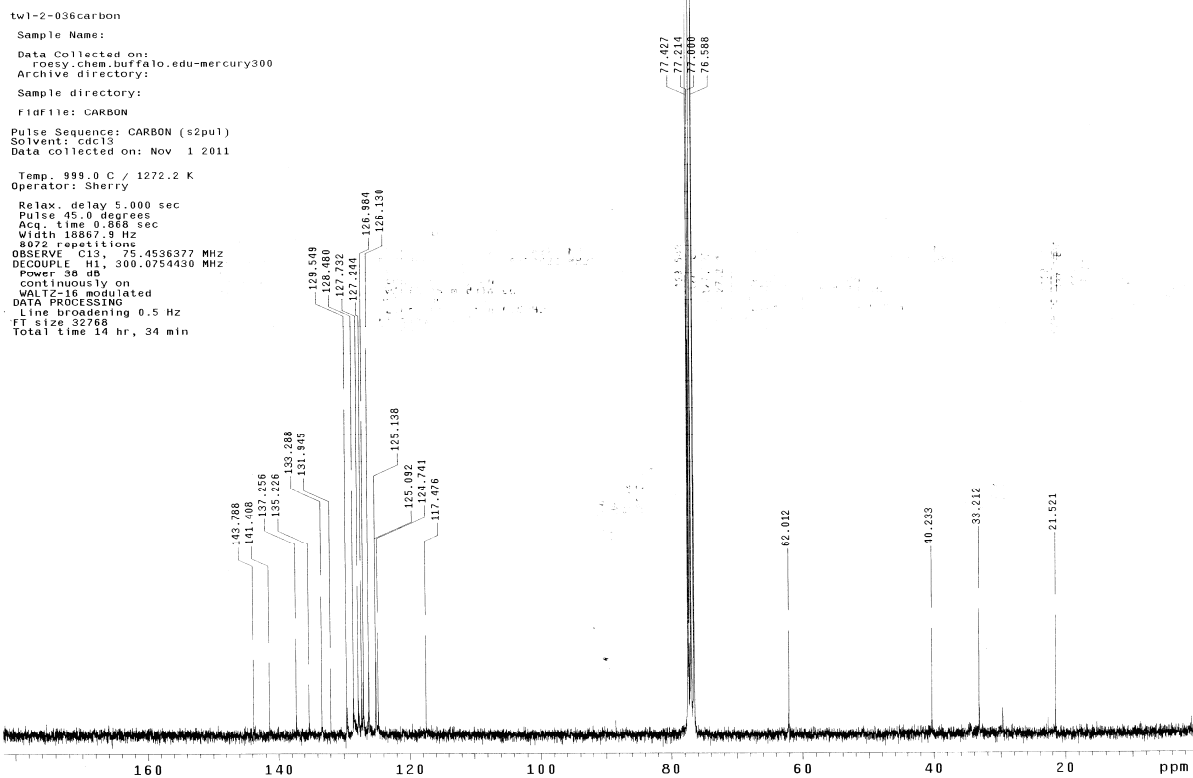
FidFile: PROTON

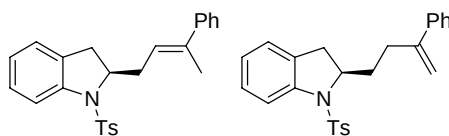
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 25 2011Temp. 21.0 C / 294.1 K
Operator: ChemierRelax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.705 sec
Width 4810.0 Hz
8 repetitions
OBSERVE H1, 300.0738830 MHz
DATA PROCESSING
FT size 16384
Total time 0 min 23 sec

Chanté

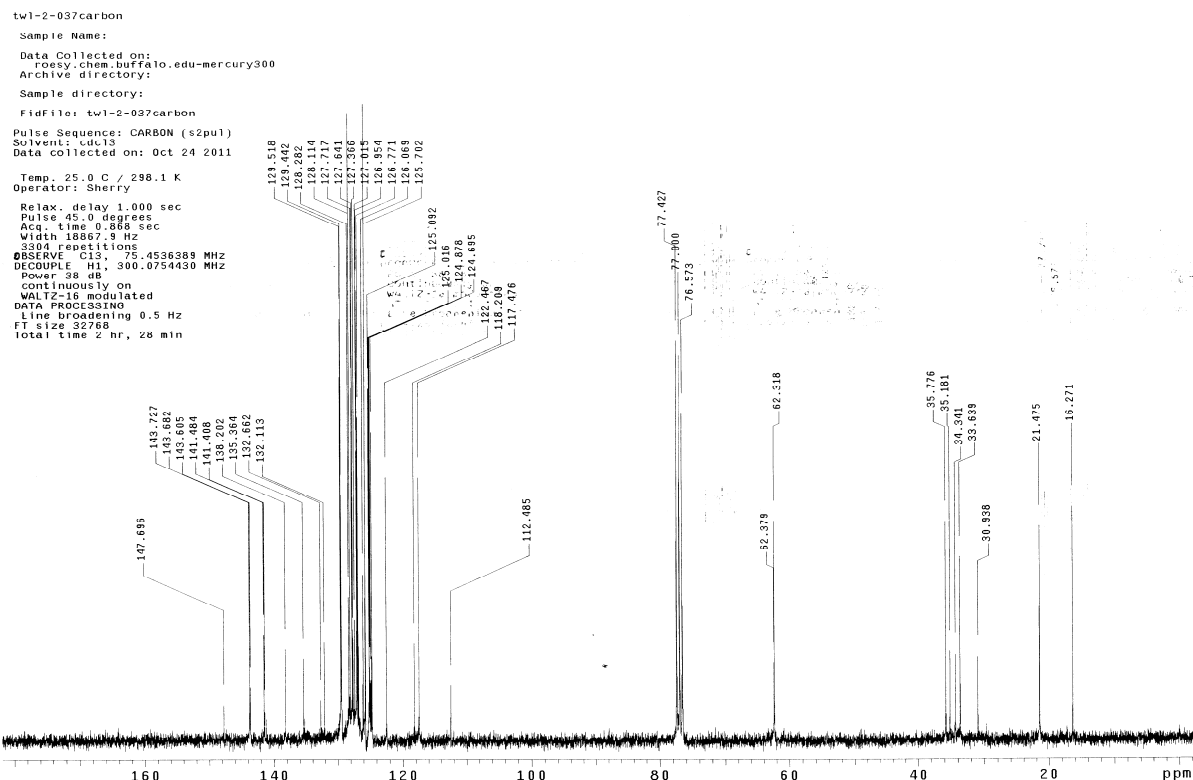
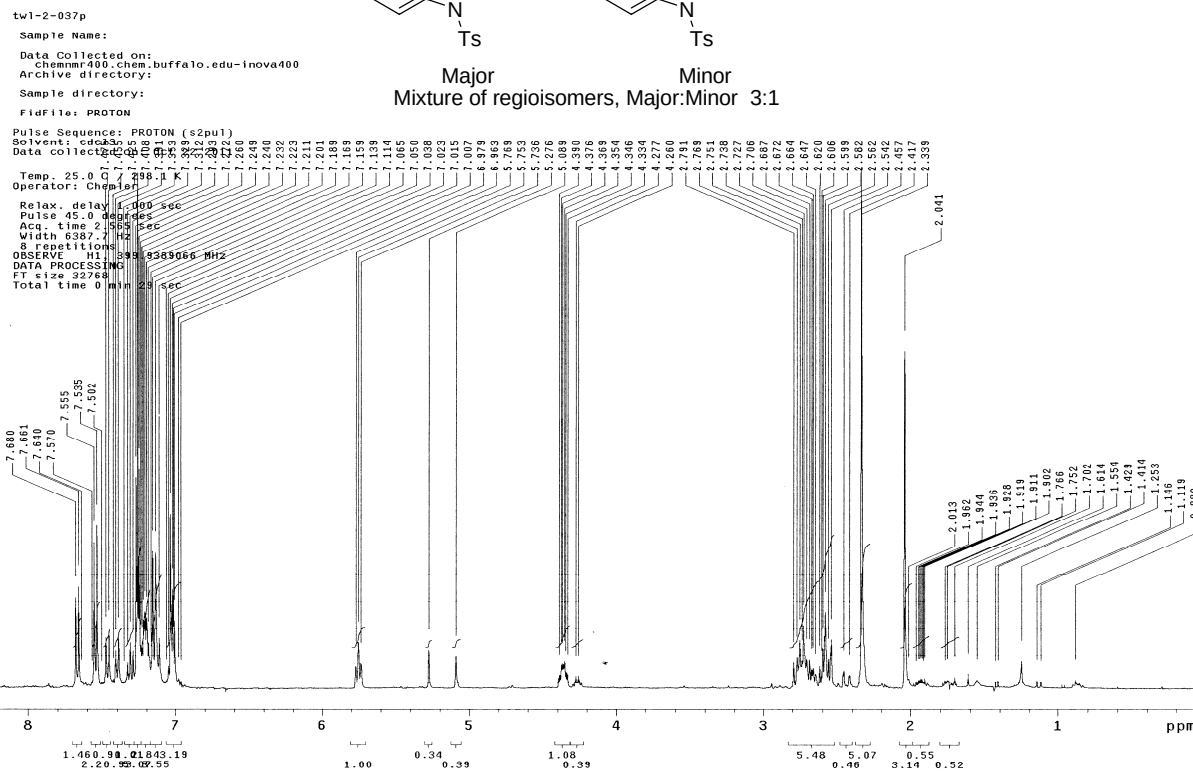
(37)



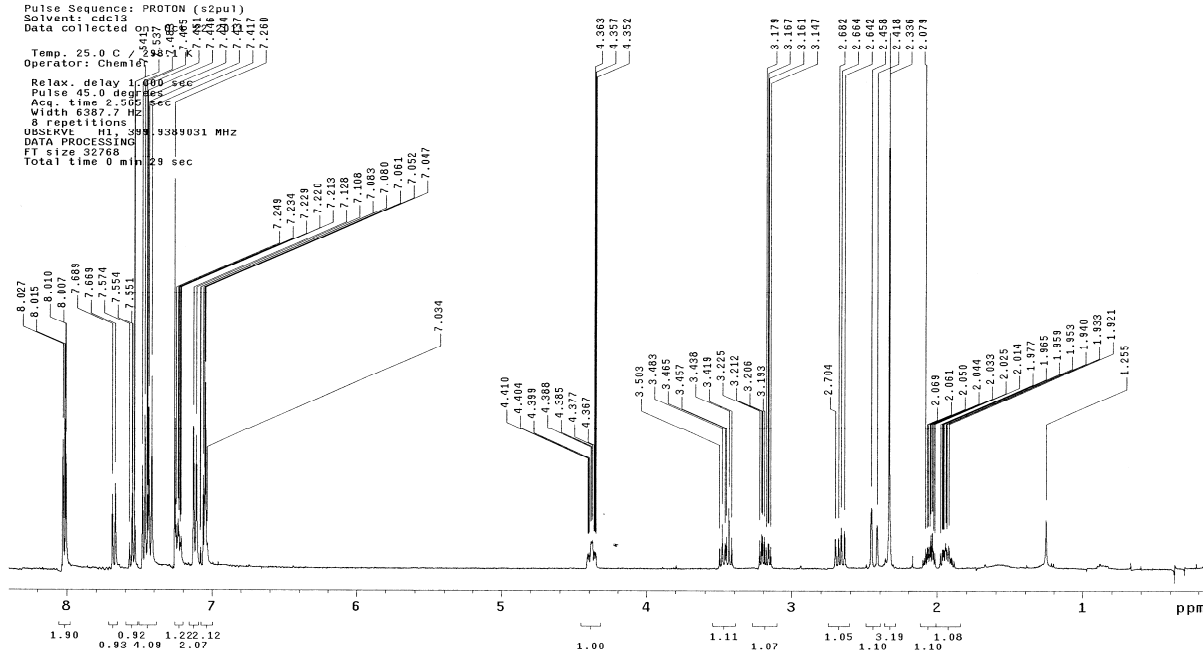
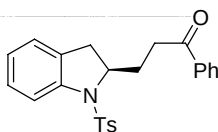




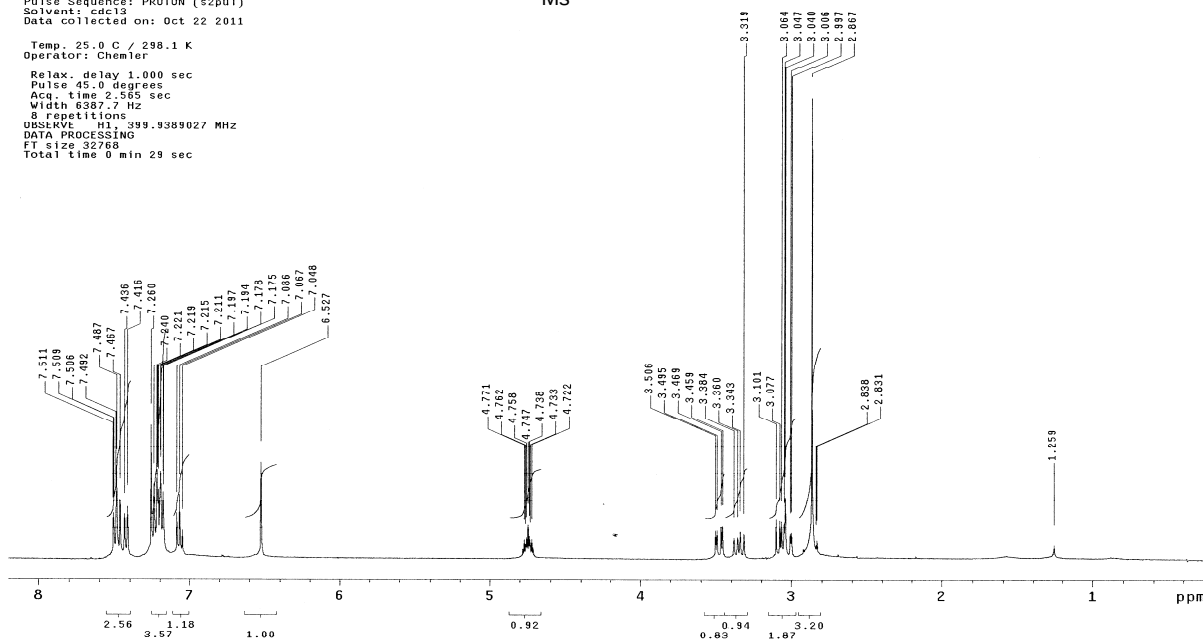
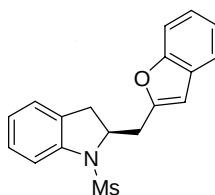
Mixture of regioisomers, Major:Minor 3:1



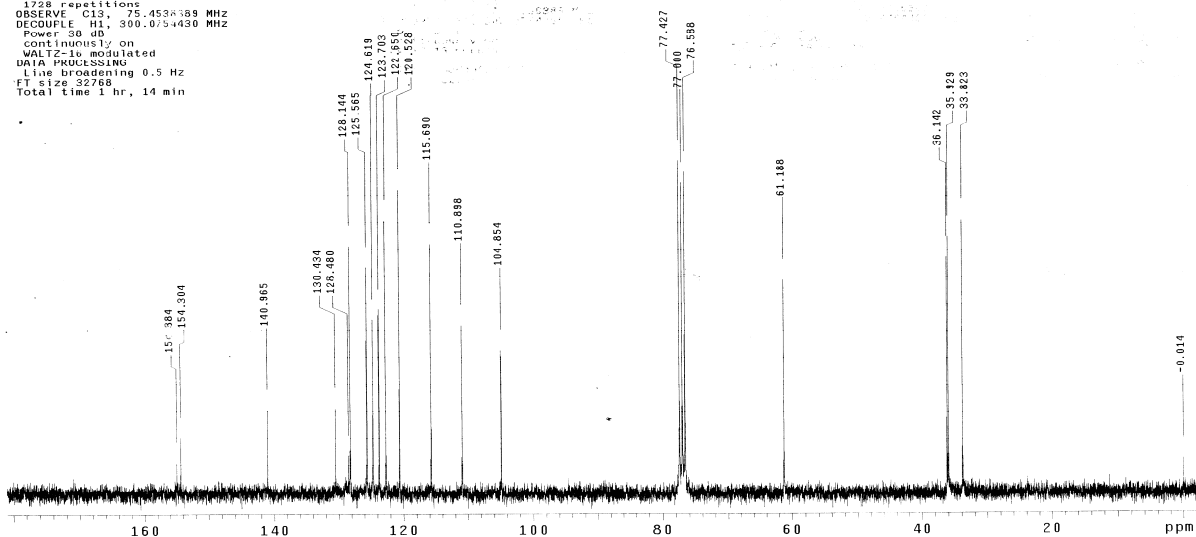
twl-1-281p
 Sample Name:
 Data Collected on:
 chemnmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 Fldfile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdc13
 Data collected on: Aug 21 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.505 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 300.1389031 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



tw1-1-193p
 Sample Name:
 Data Collected on:
 chemmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Oct 22 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.565 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 399.9389027 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec

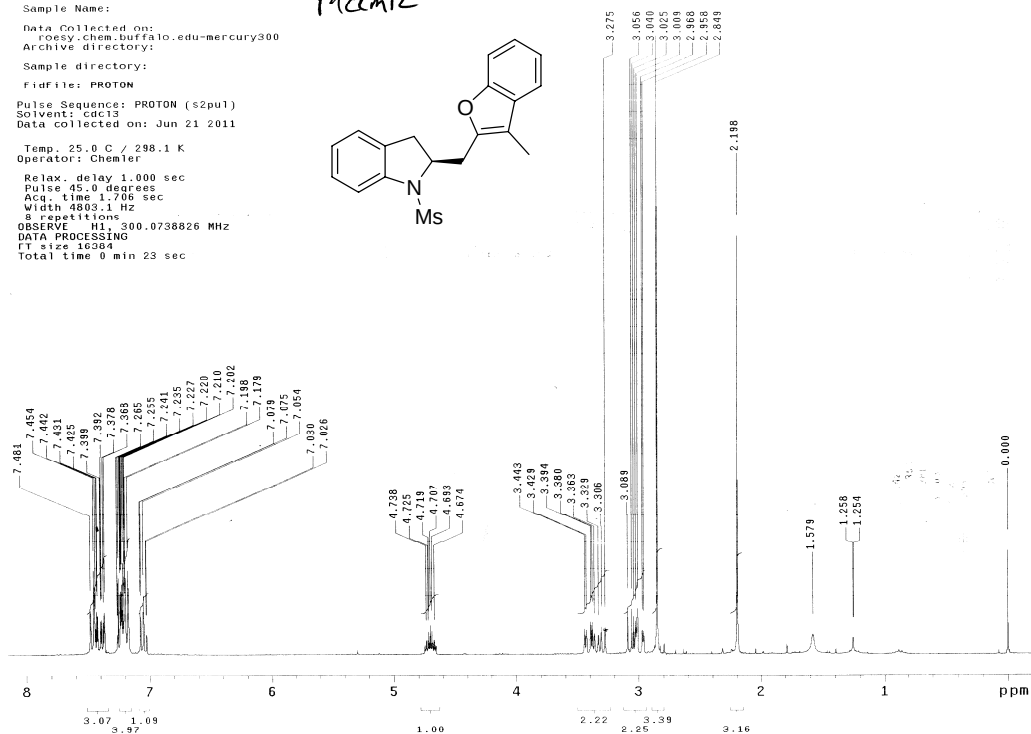
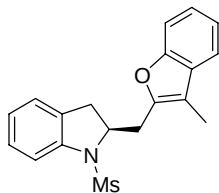


tw1-1-190carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: May 7 2011
 Temp. 23.0 C / 296.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.665 sec
 Width 18867.9 Hz
 1728 repetitions
 OBSERVE C13, 75.4534389 MHz
 DECOUPLE H1, 300.0154389 MHz
 Power 30 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 1 hr, 14 min

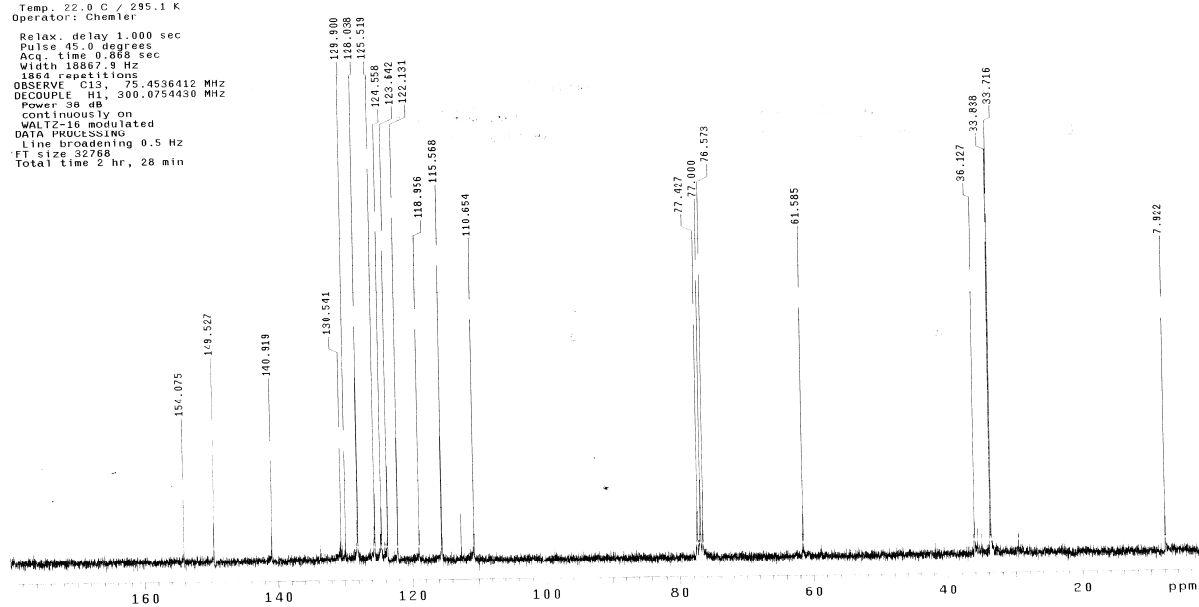


tw1-1-282p
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FID file: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdc13
 Data collected on: Jun 21 2011
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.706 sec
 Width 4803.1 Hz
 8 repetitions
 OBSERVE H1, 300.0738826 MHz
 DATA PROCESSING
 FT size 16384
 Total time 0 min 23 sec

racemic



tw1-1-282carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FID file: tw1-1-282carbon
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdc13
 Data collected on: Aug 21 2011
 Temp. 22.0 C / 295.1 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 1864 repetitions
 OBSERVE C13, 75.4536412 MHz
 DECOUPLE H1, 300.0754430 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 2 hr, 28 min



1

