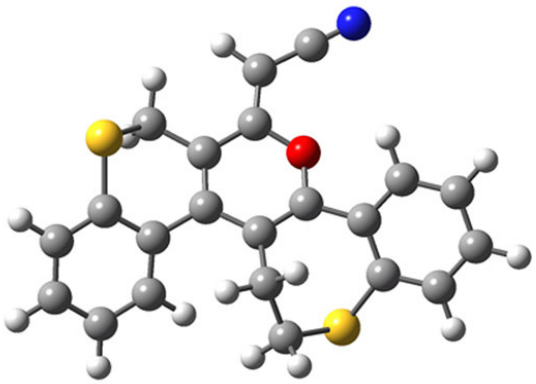
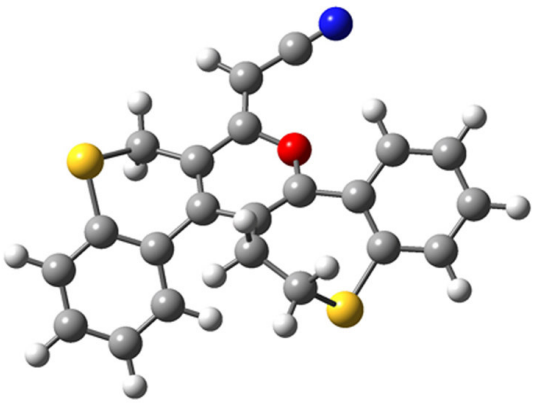
Supporting data

Non-catalytic Approach to the Synthesis of Partially Reduced 'S' Shaped Dioxathia-, and Oxadithiahelicenes Through Base Induced Inter-, and Intramolecular C-C Bond Formation

SUPPLEMENTARY INFORMATIONS



Ground State Optimized Structure of 9d



Transition State Optimized Structure of 9d

Ground state Optimized XYZ coordinates for 9d

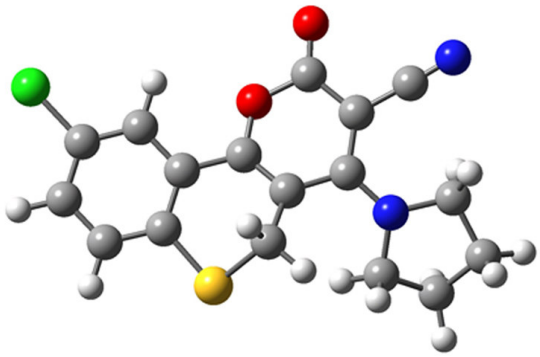
1	16	0	2.149175	-2.596687	-1.121865
2	16	0	-3.714757	1.604847	0.916960
3	8	0	1.146085	1.545444	-0.344805
4	7	0	2.345140	4.802374	-0.728185
5	6	0	-0.029316	2.241951	-0.395143
6	6	0	-1.246956	1.484138	-0.284421
7	6	0	-2.570940	2.192160	-0.389460
8	1	0	-3.043792	2.034157	-1.362832
9	1	0	-2.472909	3.261832	-0.224730
10	6	0	-3.660679	-0.101677	0.423058
11	6	0	-4.816144	-0.879725	0.517013
12	1	0	-5.717877	-0.441840	0.928719
13	6	0	-4.825276	-2.186883	0.044820
14	1	0	-5.730739	-2.778394	0.114679
15	6	0	-3.685845	-2.709951	-0.564217
16	1	0	-3.700664	-3.705998	-0.990536
17	6	0	-2.527832	-1.946169	-0.630931
18	1	0	-1.656376	-2.346733	-1.129832
19	6	0	-2.465828	-0.649066	-0.097169
20	6	0	-1.200494	0.122651	-0.099653
21	6	0	0.085117	-0.522690	0.159042
22	6	0	0.220527	-1.881687	0.827813
23	1	0	-0.738476	-2.177692	1.257311
24	1	0	0.904378	-1.757986	1.672109
25	6	0	0.749063	-3.048218	-0.017139
26	1	0	-0.004743	-3.441661	-0.701095
27	1	0	1.054117	-3.863423	0.642575
28	6	0	3.090222	-1.455547	-0.113599

29	6	0	4.420606	-1.784445	0.162695
30	1	0	4.787545	-2.760926	-0.128092
31	6	0	5.267722	-0.872013	0.783547
32	1	0	6.296847	-1.145398	0.986393
33	6	0	4.791683	0.388457	1.136216
34	1	0	5.446674	1.109316	1.610798
35	6	0	3.471222	0.727487	0.873333
36	1	0	3.104525	1.712700	1.130107
37	6	0	2.597493	-0.184140	0.259044
38	6	0	1.207876	0.230696	0.007366
39	6	0	0.084738	3.590020	-0.591682
40	1	0	-0.795970	4.203276	-0.697437
41	6	0	1.331725	4.242658	-0.672855

Transition State Optimized XYZ coordinates for 9d

1	16	0	1.896672	-2.847544	-0.547927
2	16	0	-3.852488	1.580223	0.756935
3	8	0	1.128848	1.503101	-0.296180
4	7	0	2.457600	4.723968	-0.391294
5	6	0	-0.010353	2.249193	-0.212010
6	6	0	-1.248255	1.519743	-0.150261
7	6	0	-2.554231	2.241069	-0.354528
8	1	0	-2.901697	2.164079	-1.389219
9	1	0	-2.472499	3.295817	-0.101968
10	6	0	-3.716972	-0.103002	0.195994
11	6	0	-4.867862	-0.883107	0.066627
12	1	0	-5.827584	-0.463750	0.344835
13	6	0	-4.788757	-2.169393	-0.453948
14	1	0	-5.688636	-2.764778	-0.556752
15	6	0	-3.560349	-2.668457	-0.886096
16	1	0	-3.498494	-3.648895	-1.343438
17	6	0	-2.411112	-1.903550	-0.734783
18	1	0	-1.460583	-2.288789	-1.085411
19	6	0	-2.452893	-0.626019	-0.149442
20	6	0	-1.210100	0.162231	0.032825
21	6	0	0.054327	-0.494111	0.388878
22	6	0	-0.002950	-1.740996	1.260351
23	1	0	-0.986071	-2.189565	1.151252
24	1	0	0.041013	-1.396721	2.301935
25	6	0	1.059344	-2.841170	1.083984
26	1	0	0.602541	-3.827060	1.191465
27	1	0	1.847360	-2.766377	1.832727
28	6	0	3.040179	-1.519426	-0.209116
29	6	0	4.405667	-1.798615	-0.311891
30	1	0	4.713098	-2.800366	-0.585958
31	6	0	5.355652	-0.815823	-0.059364
32	1	0	6.410350	-1.050555	-0.146344
33	6	0	4.944967	0.460998	0.317892
34	1	0	5.675223	1.233879	0.525970
35	6	0	3.592702	0.753375	0.414970
36	1	0	3.281040	1.756371	0.672412
37	6	0	2.611539	-0.221444	0.150558
38	6	0	1.198516	0.195976	0.122933

39	6	0	0.148056	3.603745	-0.285977
40	1	0	-0.711334	4.255820	-0.292294
41	6	0	1.418777	4.211355	-0.353403

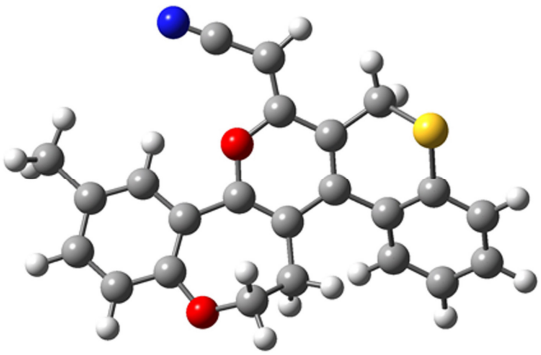


Ground State Optimized Structure of 4f

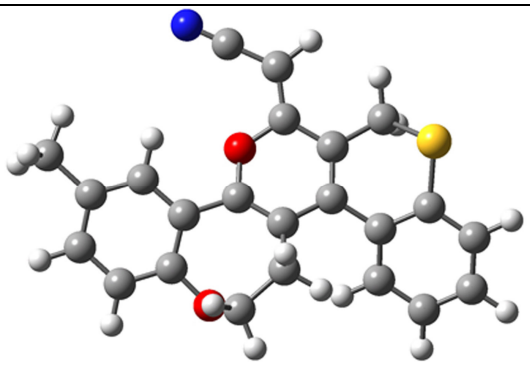
Ground state Optimized XYZ coordinates for 4f

1	16	0	-0.781725	-2.735331	0.244083
2	17	0	-5.616448	1.295305	-0.277118
3	8	0	-0.471946	1.668541	-0.280524
4	8	0	0.569196	3.634671	-0.198684
5	7	0	3.948056	3.242458	0.481124
6	7	0	3.016590	-0.486141	0.138512
7	6	0	-2.112121	-1.568290	0.094520
8	6	0	-3.413187	-2.053303	-0.051965
9	1	0	-3.589076	-3.122610	-0.048896
10	6	0	-4.487781	-1.183225	-0.177031
11	1	0	-5.495234	-1.564844	-0.280674
12	6	0	-4.257894	0.190850	-0.146605
13	6	0	-2.976472	0.697856	-0.019613
14	1	0	-2.804446	1.764803	-0.020914
15	6	0	-1.880483	-0.174500	0.090660
16	6	0	-0.521176	0.377704	0.091917
17	6	0	0.692008	2.448638	-0.084704
18	6	0	1.911162	1.698535	0.152837
19	6	0	1.905075	0.287877	0.221992
20	6	0	0.596645	-0.334799	0.409764
21	6	0	0.362882	-1.630916	1.150695
22	1	0	-0.089032	-1.422495	2.124065
23	1	0	1.263961	-2.202948	1.331771
24	6	0	4.383254	0.066020	-0.058044
25	1	0	4.715673	0.605720	0.826481
26	1	0	4.376357	0.766071	-0.897022
27	6	0	5.246809	-1.154402	-0.380647
28	1	0	5.602931	-1.627473	0.539438
29	1	0	6.118199	-0.882661	-0.977257
30	6	0	4.267758	-2.078459	-1.108926
31	1	0	4.105234	-1.732369	-2.133860
32	1	0	4.592015	-3.119510	-1.148149
33	6	0	2.990433	-1.911128	-0.284984

34	1	0	2.082683	-2.126448	-0.848436
35	1	0	3.032478	-2.575823	0.584758
36	6	0	3.050578	2.532504	0.308564



Ground State Optimized Structure of 9c



Transition State Optimized Structure of 9c

Ground State Optimized XYZ coordinates for 9c

1	16	0	3.829333	1.571070	1.055344
2	8	0	-1.056501	1.229243	-0.104925
3	8	0	-1.928571	-3.032533	0.705460
4	7	0	-2.667396	4.281439	-0.113644
5	6	0	1.409083	0.075738	-0.144188
6	6	0	2.741953	-0.536251	-0.374798
7	6	0	2.892788	-1.668580	-1.193204
8	6	0	4.126667	-2.280782	-1.371137
9	6	0	5.253520	-1.769370	-0.729833
10	6	0	5.147935	-0.609536	0.028540
11	6	0	3.912961	0.022607	0.184966
12	6	0	2.548878	2.306015	-0.031022
13	6	0	1.316918	1.443360	-0.054362
14	6	0	0.021707	2.056678	-0.034728
15	6	0	-1.003578	-0.132666	0.015381
16	6	0	-2.379988	-0.675770	0.060427
17	6	0	-3.433914	0.221471	-0.255992
18	6	0	-4.763678	-0.154228	-0.348703
19	6	0	-5.081885	-1.498700	-0.110096
20	6	0	-4.093463	-2.399355	0.232732
21	6	0	-2.751644	-2.012168	0.334833
22	6	0	-0.679714	-2.742151	1.319457
23	6	0	0.348173	-2.226488	0.321199
24	6	0	0.215070	-0.753125	0.011364
25	6	0	-0.257499	3.396625	-0.024771
26	6	0	-1.579911	3.881492	-0.070175
27	6	0	-5.832576	0.850842	-0.704588
28	1	0	2.027787	-2.066721	-1.706924
29	1	0	4.208210	-3.151957	-2.010290
30	1	0	6.218444	-2.247883	-0.851239
31	1	0	6.030328	-0.166690	0.475317
32	1	0	2.340521	3.284805	0.395053
33	1	0	2.974391	2.446853	-1.028992

34	1	0	0.539463	4.123127	-0.015482
35	1	0	-3.183811	1.254225	-0.444148
36	1	0	-6.111895	-1.834555	-0.174552
37	1	0	-4.323408	-3.434693	0.452322
38	1	0	-0.820280	-2.036994	2.146389
39	1	0	-0.352095	-3.698347	1.728533
40	1	0	1.340441	-2.405057	0.739851
41	1	0	0.274034	-2.853524	-0.573148
42	1	0	-6.651728	0.829649	0.020346
43	1	0	-5.429726	1.864535	-0.726903
44	1	0	-6.264473	0.638399	-1.688213

Transition State Optimized Coordinates for 9c

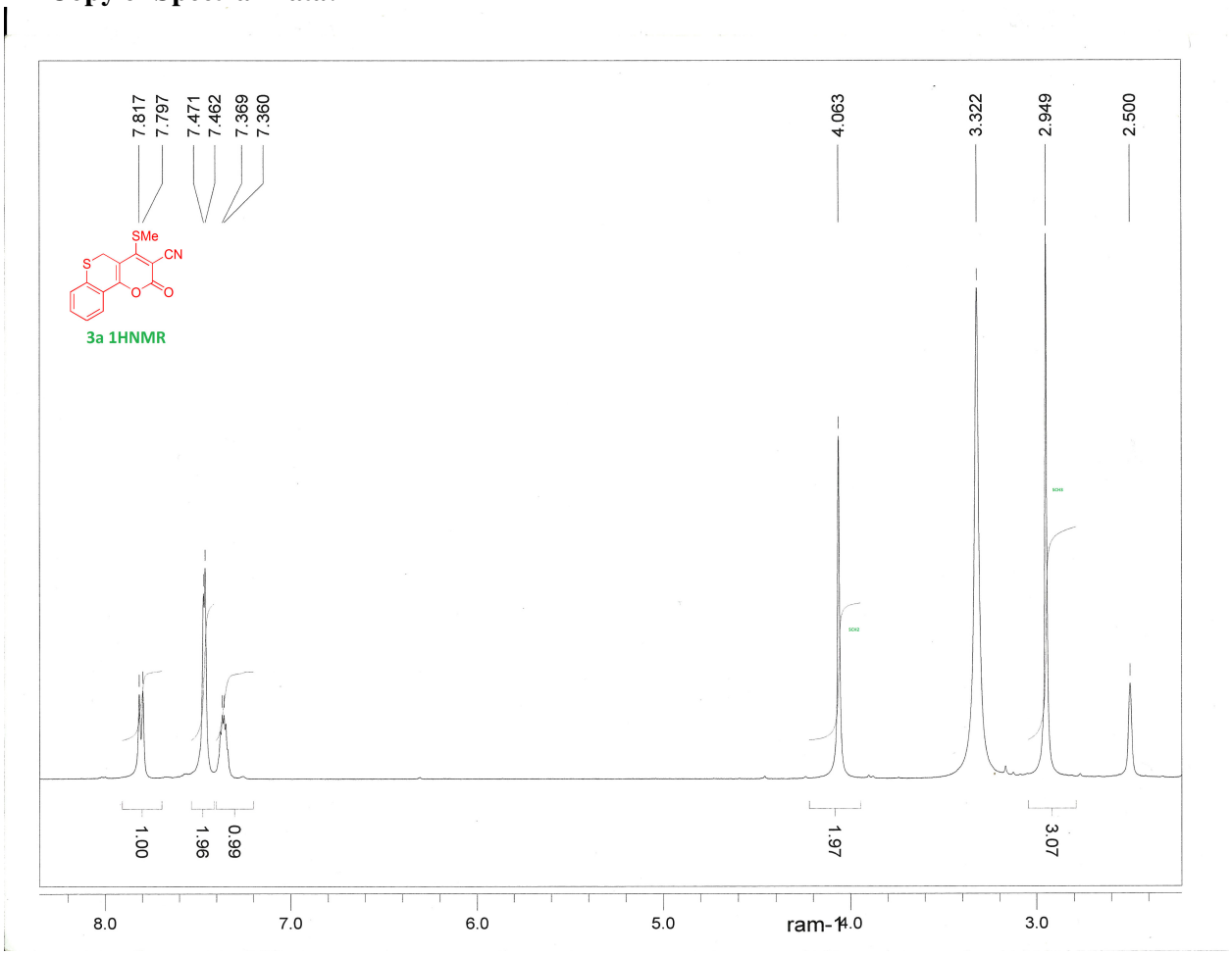
1	16	0	3.899611	1.694216	0.820553
2	8	0	-1.053158	1.277314	-0.294238
3	8	0	-1.554588	-2.856328	-0.293819
4	7	0	-2.633974	4.360860	-0.336757
5	6	0	1.383646	0.105521	0.006254
6	6	0	2.685524	-0.576400	-0.186993
7	6	0	2.749405	-1.828348	-0.823295
8	6	0	3.955137	-2.498187	-0.984861
9	6	0	5.135891	-1.924958	-0.513728
10	6	0	5.109808	-0.657330	0.055836
11	6	0	3.901144	0.027917	0.196494
12	6	0	2.565359	2.296595	-0.282491
13	6	0	1.316741	1.469428	-0.125717
14	6	0	0.027252	2.103432	-0.179949
15	6	0	-1.019745	-0.043499	0.069991
16	6	0	-2.374275	-0.603063	0.070661
17	6	0	-3.492700	0.247151	0.161169
18	6	0	-4.793946	-0.227103	0.028998
19	6	0	-4.977326	-1.593731	-0.219864
20	6	0	-3.892157	-2.456116	-0.309870
21	6	0	-2.595826	-1.971575	-0.164039
22	6	0	-0.790719	-3.025895	0.906065
23	6	0	0.287405	-1.942512	1.117523
24	6	0	0.172230	-0.657088	0.314614
25	6	0	-0.236951	3.443553	-0.218895
26	6	0	-1.553336	3.943824	-0.291415
27	6	0	-5.974493	0.706411	0.150614
28	1	0	1.836163	-2.269459	-1.205449
29	1	0	3.974230	-3.461248	-1.481174
30	1	0	6.079858	-2.446059	-0.624239
31	1	0	6.031222	-0.177734	0.364612
32	1	0	2.398897	3.330471	0.011814
33	1	0	2.930419	2.289926	-1.313969
34	1	0	0.566562	4.162890	-0.195813
35	1	0	-3.328266	1.305638	0.314817
36	1	0	-5.981213	-1.987427	-0.342645
37	1	0	-4.024691	-3.513074	-0.507126
38	1	0	-1.477206	-3.064314	1.757265
39	1	0	-0.319662	-4.005518	0.810926
40	1	0	0.281550	-1.654666	2.176908

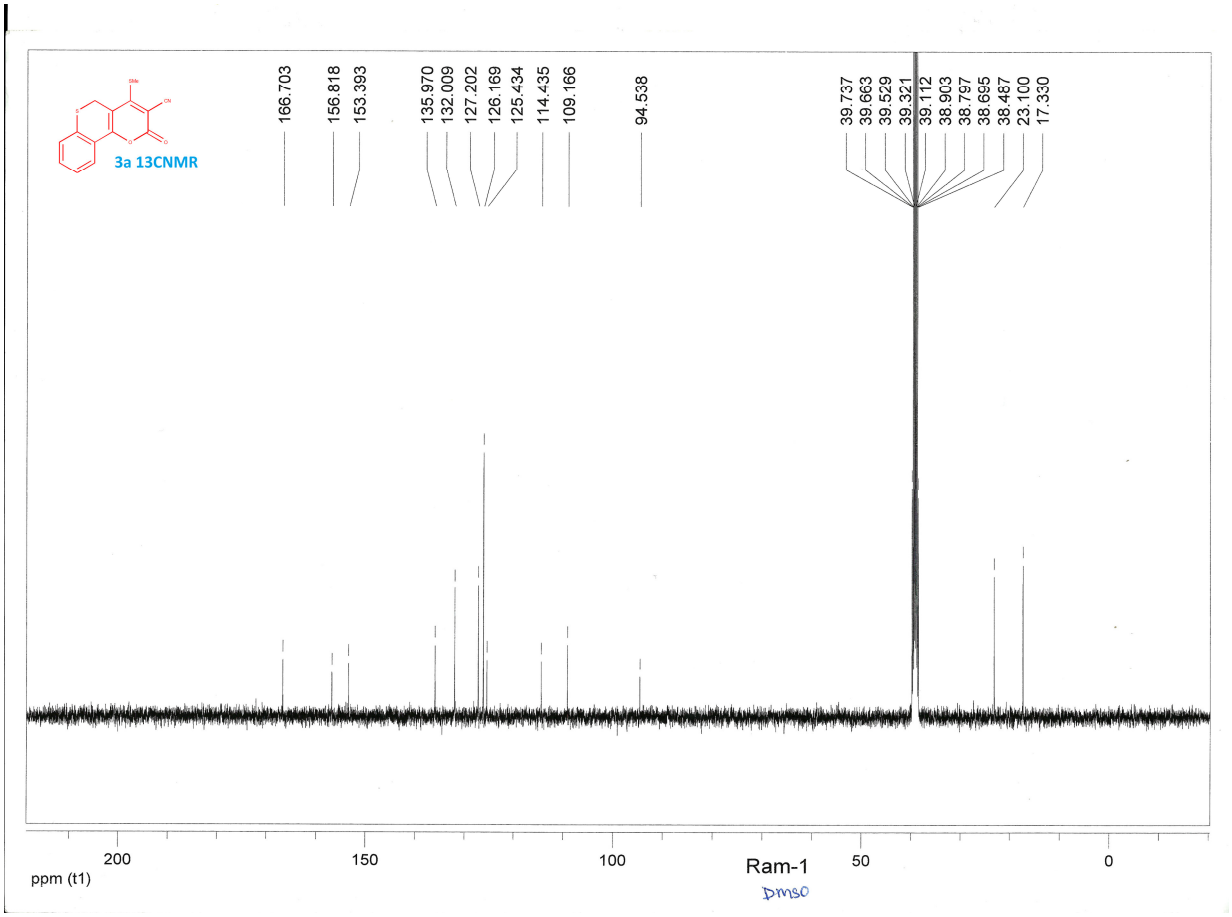
41	1	0	1.266250	-2.381863	0.947595
42	1	0	-6.714809	0.513079	-0.630260
43	1	0	-6.478097	0.580456	1.115035
44	1	0	-5.663621	1.749386	0.071984

Table S1. Selected Metric Parameters for the compounds **9d**, **9c** and **4f**

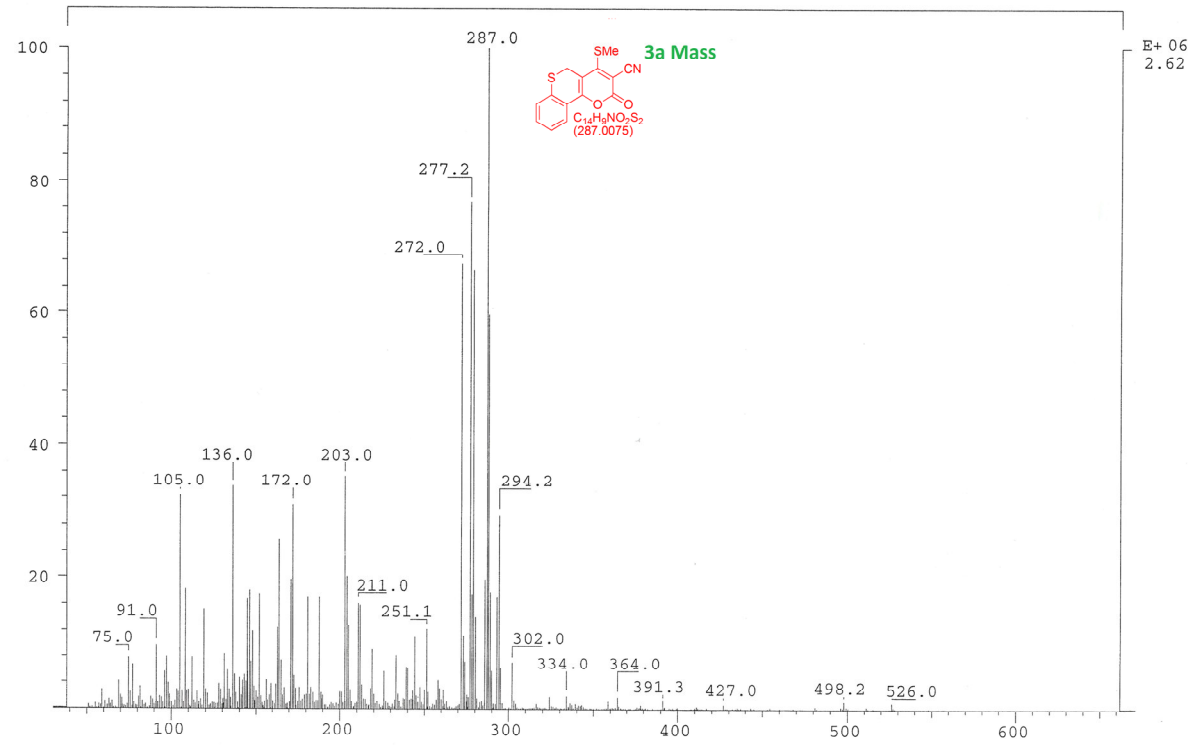
9d			
Torsion Angle	**Ground State**		**Transition State**
	Experimental	**Calculated**	
C8-C9-C10-C11	-38.71°	-38.48°	-36.63°
C9-C10-C11-C12	-10.86°	-10.21°	-32.26°
C10-C11-C12-C13	+110.52°	+112.60°	+148.36°
Twist Angle			
RingA-RingC	38.69°	36.96°	36.80°
RingC-RingE	44.95°	35.70	28.16
9c			
Torsion Angle			
C3-C2-C1-C20	38.01°	38.24°	36.63°
C2-C1-C20-C19	21.90°	16.92°	31.42°
C1-C20-C19-C18	149.46°	152.41°	152.86°
Twist Angle			
RingA-RingC	36.49°	37.40°	34.96°
RingC-RingE	4.13°	4.62°	18.66°
4f			
Torsion Angle			
C5-C6-C7-O1	16.21°	12.44°	
C6-C7-O1-C8	171.73°	167.01°	

Copy of Spectral Data:



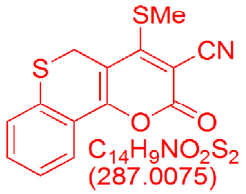

3a 13CNMR
166.703
156.818
153.393
135.970
132.009
127.202
126.169
125.434
114.435
109.166
94.538
39.737
39.663
39.529
39.321
39.112
38.903
38.787
38.695
38.487
23.100
17.330
200
150
100
50
0
ppm (t1)
Ram-1
DMSO

SPEC: kaz1754 21-Oct-09 Elapse: 00:26.9 3
Samp: RAM - 1 Start : 13:36:27 14
Mode: CI +VE +LMR BSCAN (EXP) UP HR NRM
Oper: Thomes Inlet :
Base: 287.0 Inten : 2619007 Masses: 50 > 650
Norm: 287.0 RIC : 38367119 #peaks: 919
Peak: 3000.00 mmu

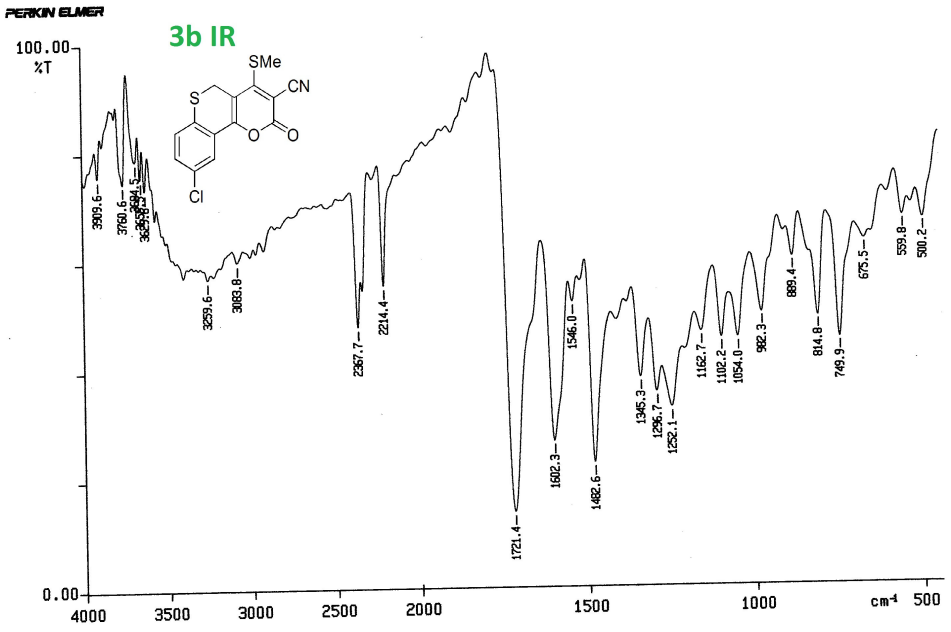


LIST: kazhr1754 21-Oct-09 Elapse: 00:58.9 8
Samp: RAM - 1 Start : 13:36:27 12
Mode: CI +VE +LMR BSCAN (EXP) UP HR NRM
Oper: Thomes Inlet
Limt: (110) . .N.O2.S2
: (1411) C100.H100.N.O2.S2
Peak: 3000.00 mmu R+D: -2.0 > 60.0
Data: CMASS : converted

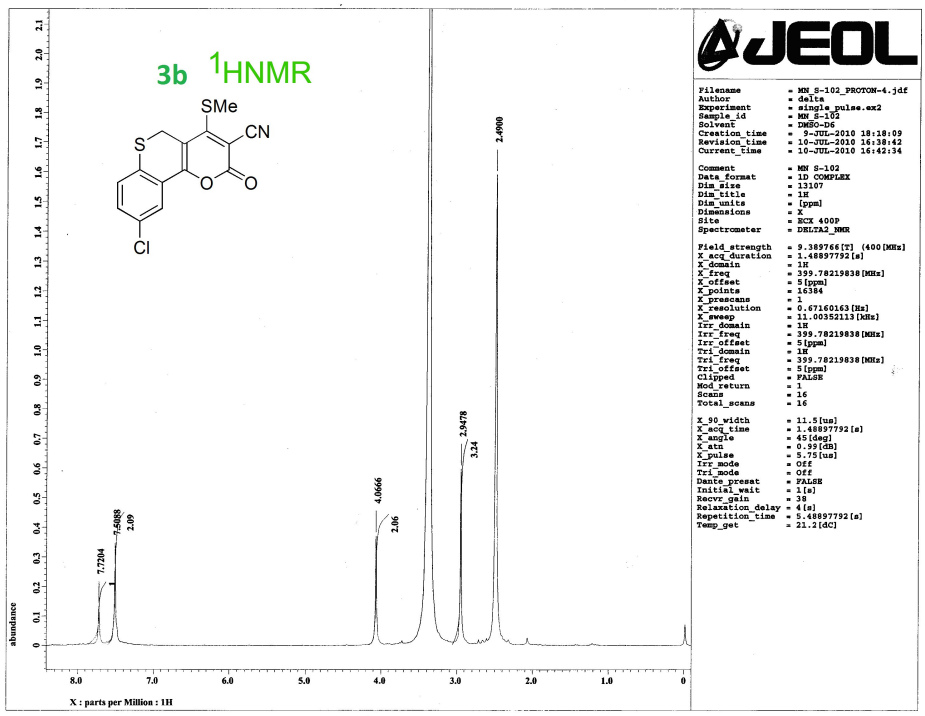
3a HRMS



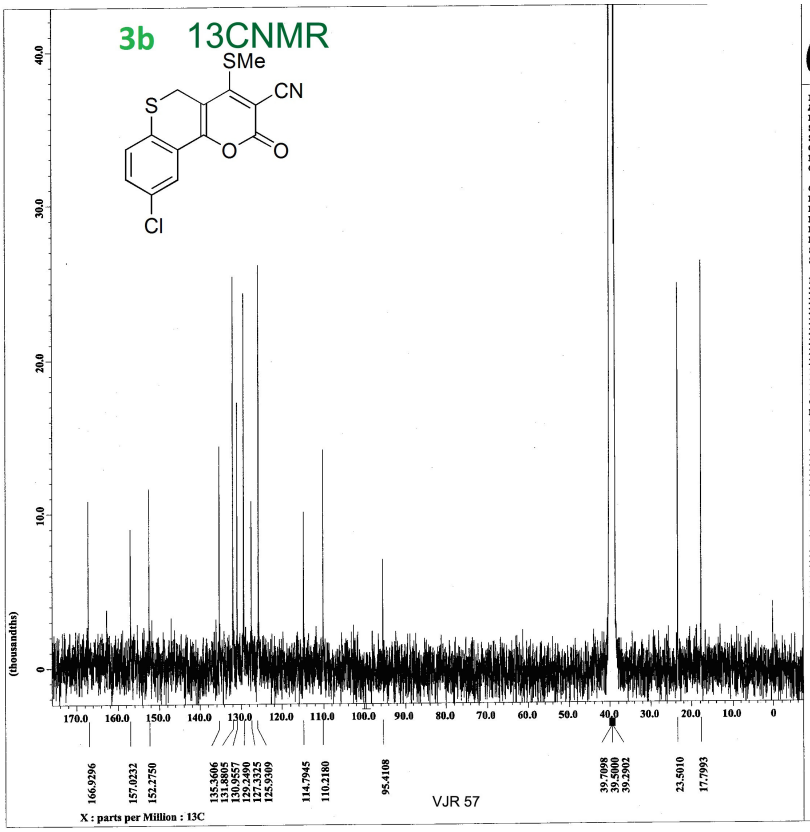
Mass	Intensity	%RA	Flags	(mmu) Delta	R+D	Composition
279.1420	2132797	42.77	F#			
280.1436	426833	8.56	F#	-3.1	0.5	C12.H26.N.O2.S2
281.1471	47800	0.96	F#	1.2	0.0	C12.H27.N.O2.S2
281.9914	36021	0.72	F#			
282.1499	4053	0.08	F#			
283.0490	59427	1.19	#			
284.0701	48686	0.98	F#			
285.0748	23938	0.48	#			
286.0023	832058	16.69	#	-2.7	11.5	C14.H8.N.O2.S2
287.0084	4986247	100.00	#	-0.9	11.0	C14.H9.N.O2.S2
288.0145	2744068	55.03	#	0.8	10.5	C14.H10.N.O2.S2
289.0117	852273	17.09	#			
290.0124	273603	5.49	F#			
290.1565	8536	0.17	F#			
291.0065	86962	1.74	F#			
291.1625	6814	0.14	F#			



10/05/20 10:41 CODE- VJR 57
X: 4 scans, 4.0cm-1, flat, smooth, abex



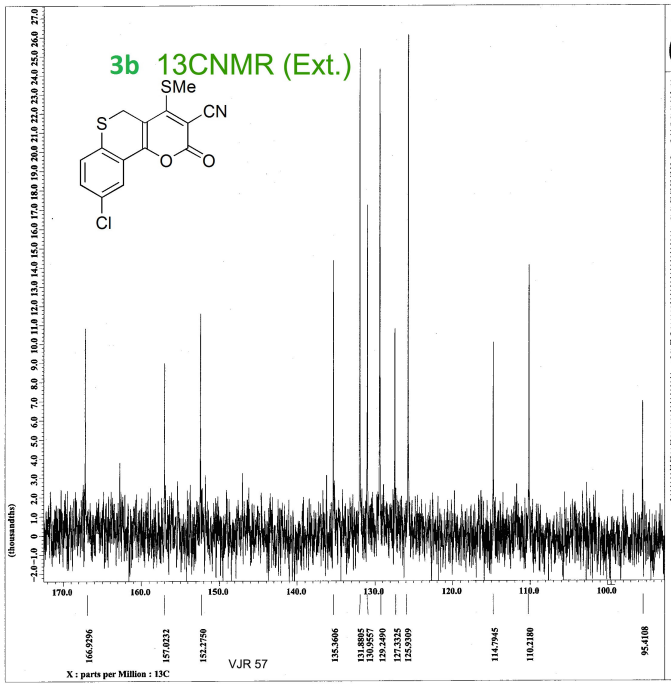
3b 13CNMR



JEOL

```
Filename          = MN_S-102_CARBON-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = MN_S-102
Solvent           = DMSO-D6
Creation_time     =  9-JUL-2010 20:02:48
Revision_time     = 10-JUL-2010 16:47:36
Current_time      = 10-JUL-2010 16:48:16

Comment           = MN S-102
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 2048
Total_scans       = 2048

X_90_width        = 9[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.4[dB]
X_pulse           = 3[us]
Irr_atn_dec       = 20.99[dB]
Irr_atn_noe       = 20.99[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 56
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 21.7[dC]
```

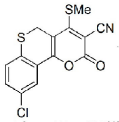
3b 13CNMR (Ext.)



JEOL

```
Filename          = MN_S-102_CARBON-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = MN_S-102
Solvent           = DMSO-D6
Creation_time     =  9-JUL-2010 20:02:48
Revision_time     = 10-JUL-2010 16:47:36
Current_time      = 10-JUL-2010 16:49:28

Comment           = MN S-102
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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             = 2048
Total_scans       = 2048

X_90_width        = 9[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.4[dB]
X_pulse           = 3[us]
Irr_atn_dec       = 20.99[dB]
Irr_atn_noe       = 20.99[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 56
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 21.7[dC]
```

3b HRMS



Data:9DEC125A
Sample Name:VJR-57
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Acquired:12/21/2009 12:38:26 PM
Operator:admin
Mass Calibration data:(Internal Mass Calibration Data)
Created:12/21/2009 12:41:50 PM
Created by:admin

Charge number:1 Tolerance:5.00(mmu)
Element:^{12}C:0 .. 14, ^{1}H:0 .. 9, ^{35}Cl:0 .. 1, ^{14}N:0 .. 1, ^{16}O:0 .. 2, ^{32}S:0 .. 2

Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

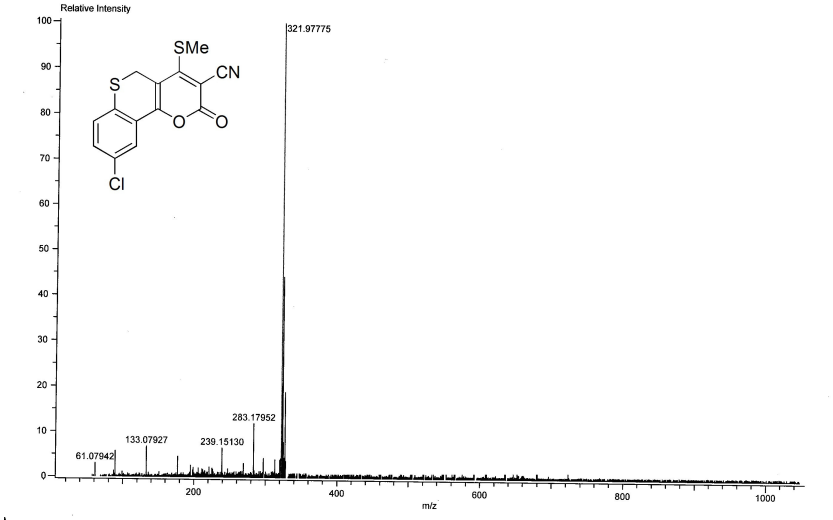
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
321.97775	82111.82	321.97632	1.42	$^{12}C_{14}{}^{1}H_{9}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{2}{}^{32}S_{2}$	12.5

3b HRMS

Acq. Data Name: 9DEC125A
Internal Sample Id: VJR-57
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.349..0.363);,1.0];Correct Base[5.0%];...
Experiment Date/Time: 12/21/2009 12:38:26 PM

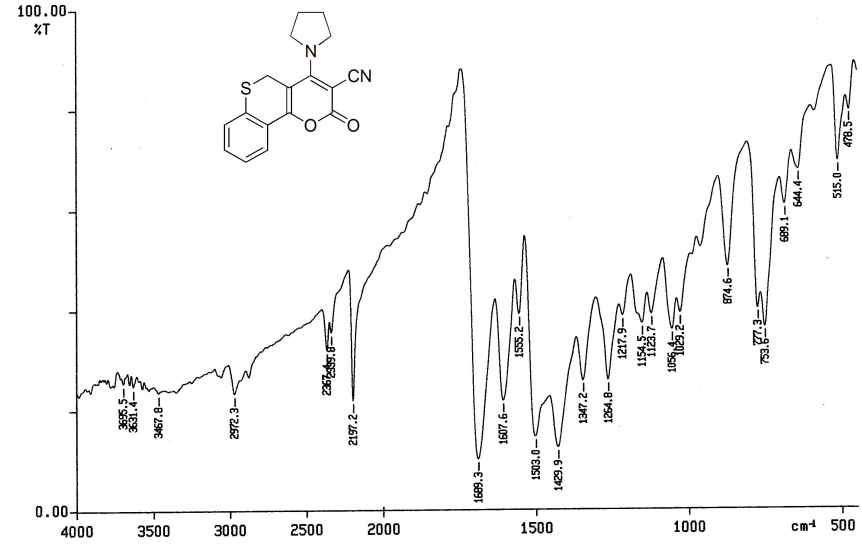
E:\CDRI\NOV09B/DEC09A:9DEC125A
Ion Guide RF Volt: 550V
Orifice1 Volt Sweep: 28V
Acquired m/z Range: 10.0..1050.0

Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 13[V]
Time of Maximum: 0.246[min]
Operator Name: admin



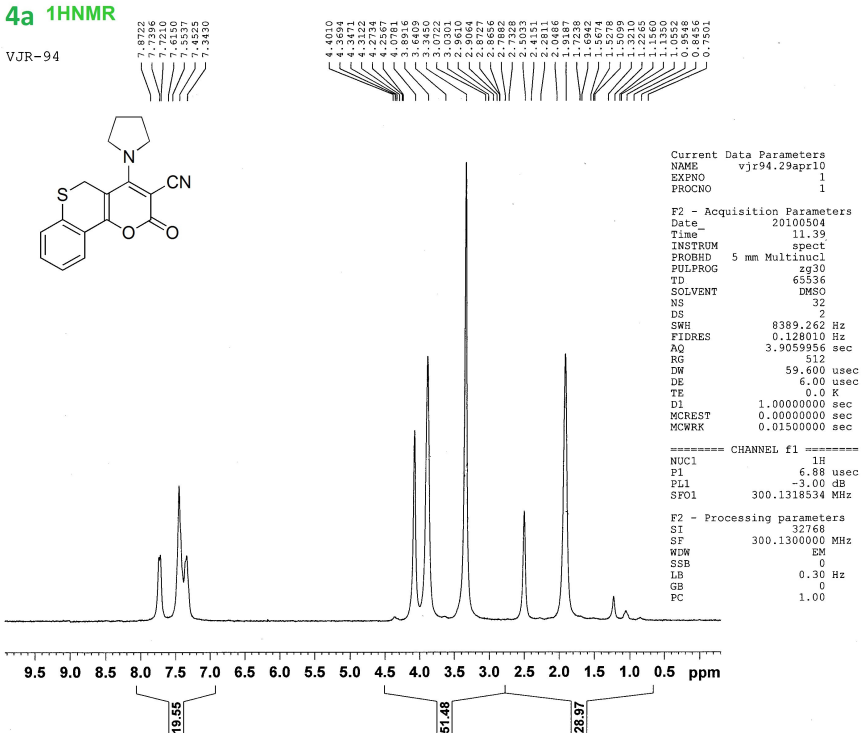
4a IR

PERKIN ELMER

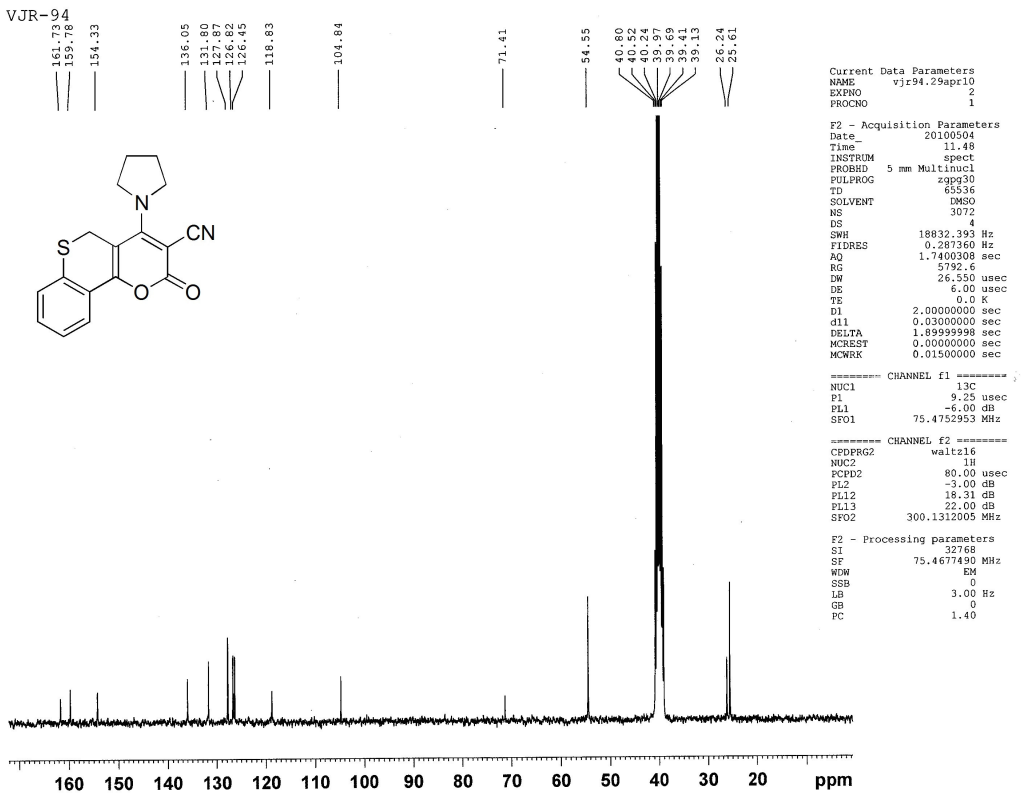


10/05/24 10:49 CODE- VJR-9Y
X: 4 scans, 4.0cm-1, smooth, abex

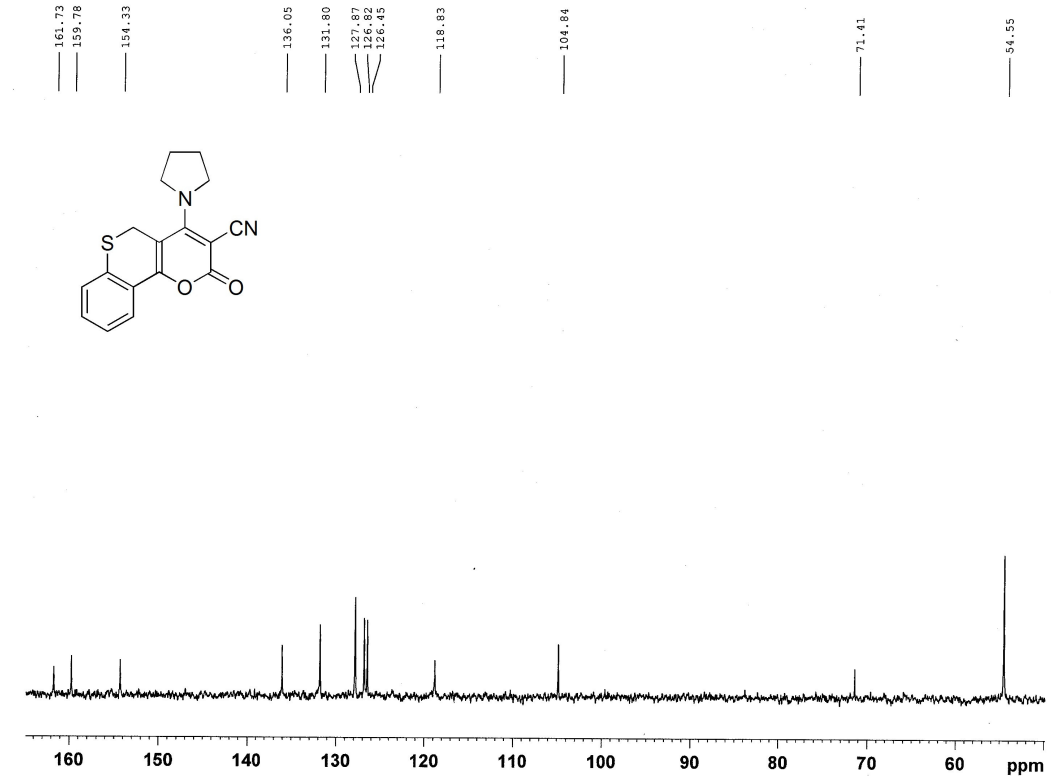
4a 1HNMR



4a 13CNMR

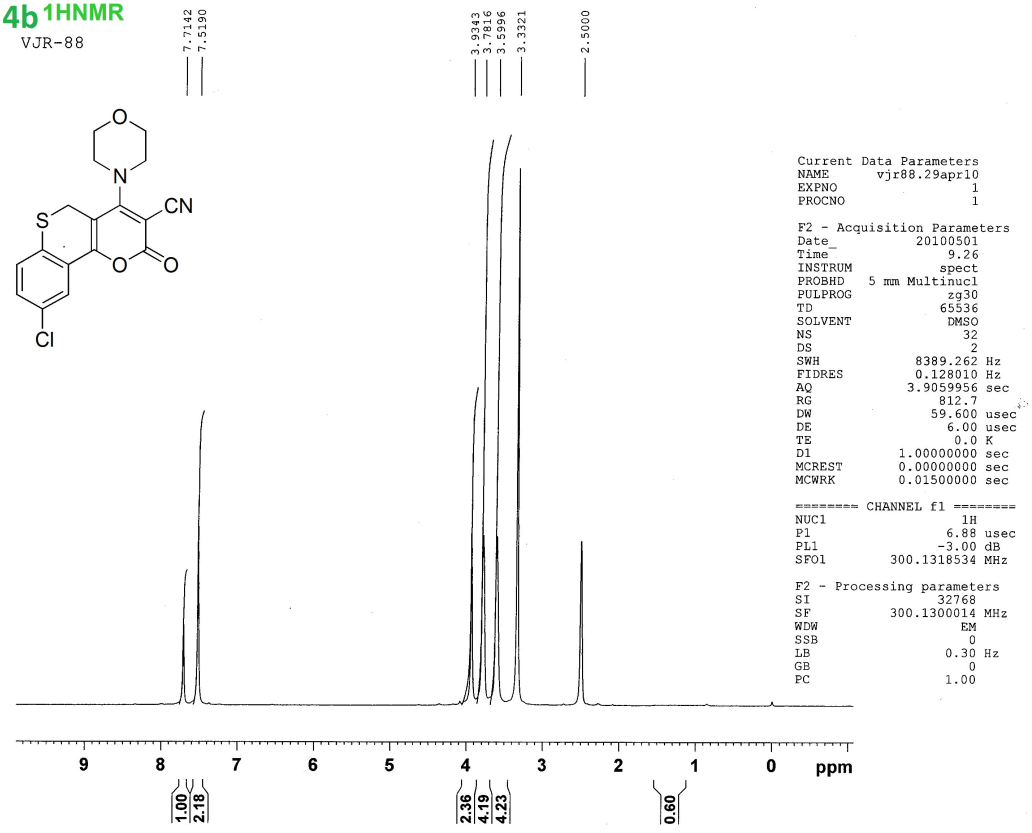


4a 13CNMR (Ext.)



4b 1HNMR

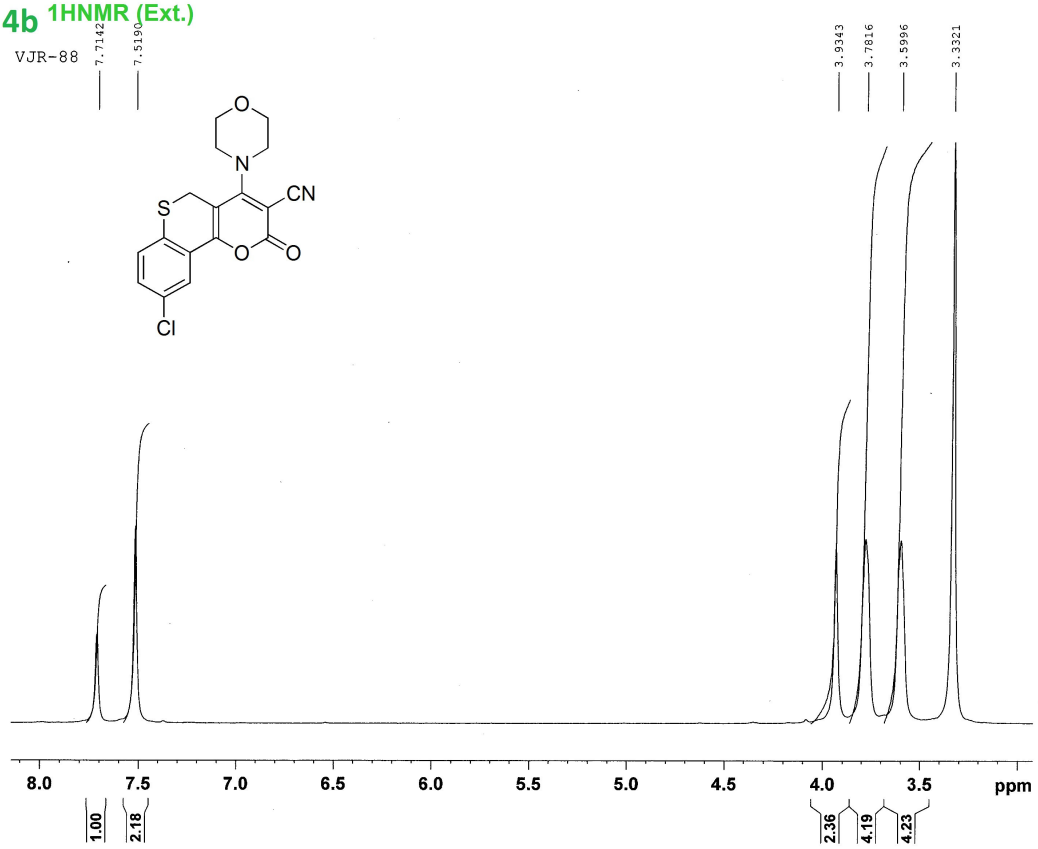
VJR-88




```
Current Data Parameters
NAME        vjr88.29apr10
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100501
Time                9.26
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    32
DS                     2
SWH             8389.262 Hz
FIDRES          0.128010 Hz
AQ             3.9059956 sec
RG                 812.7
DW                59.600 usec
DE                 6.00 usec
TE                  0.0 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  6.88 usec
PL1                -3.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300014 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

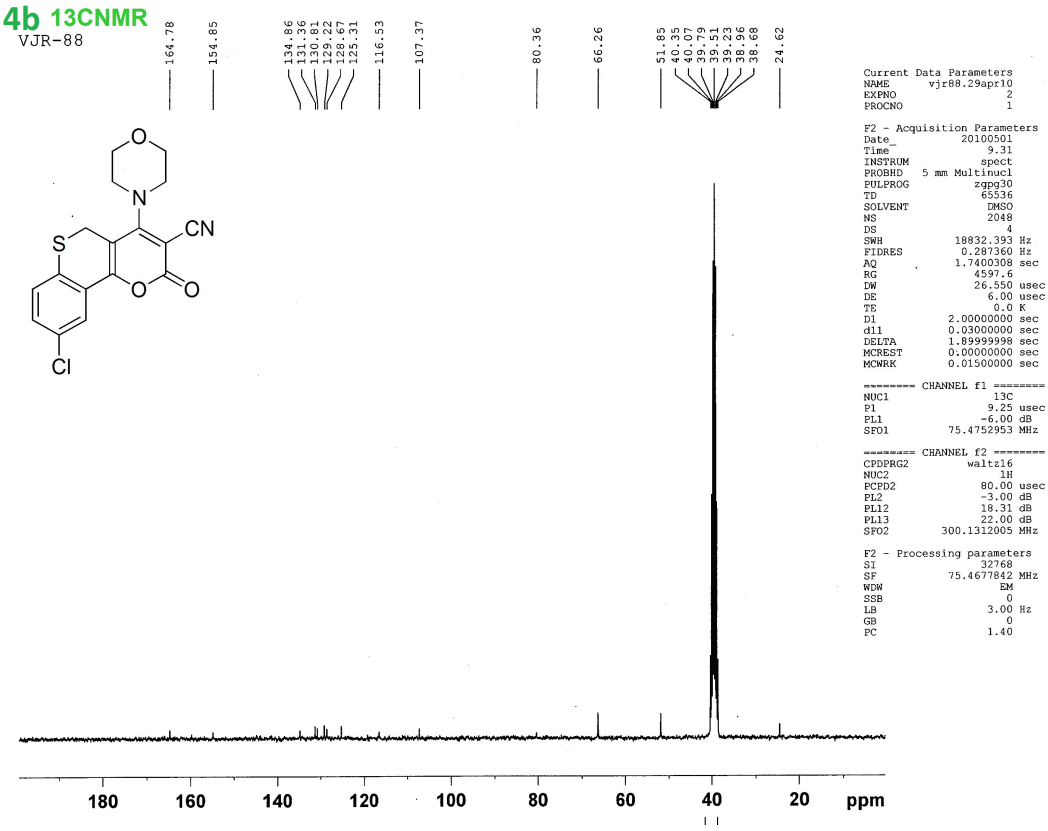
4b 1HNMR (Ext.)

VJR-88



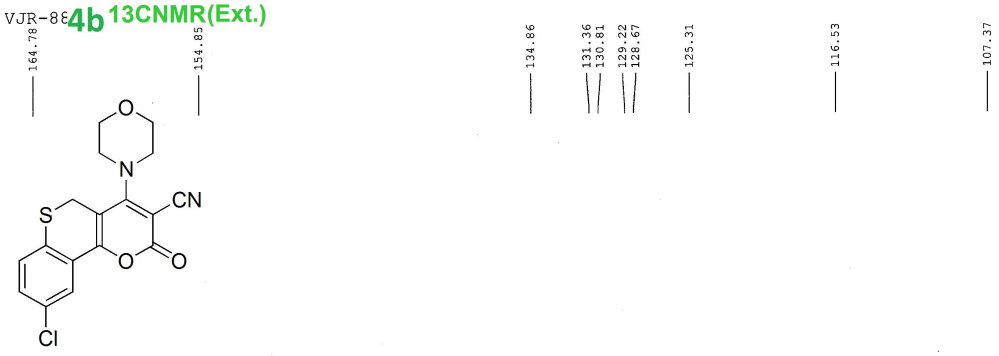
4b 13CNMR

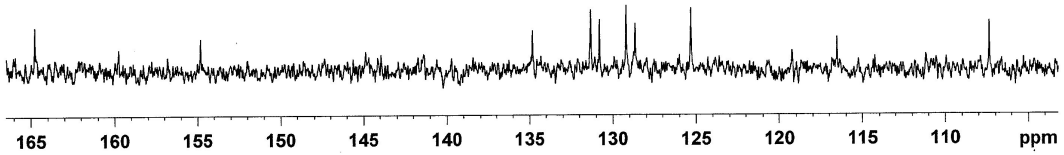
VJR-88



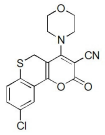

```
Current Data Parameters
NAME          vjr88.29apr10
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100501
Time                   9.31
INSTRUM               spect
PROBHD   5 mm Multinucl
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                   2048
DS                      4
SWH            18832.393 Hz
FIDRES          0.287360 Hz
AQ              1.7400308 sec
RG                 4597.6
DW                26.550 usec
DE                 6.00 usec
TE                    0.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.25 usec
PL1                -6.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             80.00 usec
PL2                -3.00 dB
PL12               18.31 dB
PL13               22.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF            75.4677842 MHz
WDW                      EM
SSB                       0
LB                 3.00 Hz
GB                        0
PC                     1.40
```

VJR-88 **4b** 13CNMR(Ext.)





4b HRMS



Data:10JULY129A
Sample Name:VJR-88
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

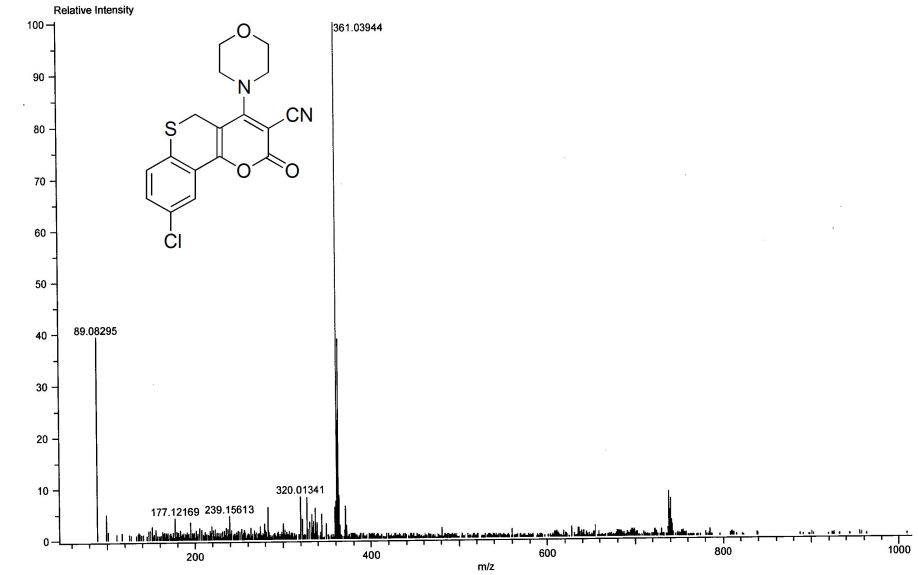
Acquired:7/6/2010 4:45:39 PM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:7/6/2010 5:09:25 PM
Created by:admin

Charge number:1
Tolerance:5.00(mmu)
Element:^{12}C:0 .. 17, ^{1}H:0 .. 14, ^{35}Cl:0 .. 1, ^{14}N:0 .. 2, ^{16}O:0 .. 3, ^{32}S:0 .. 1

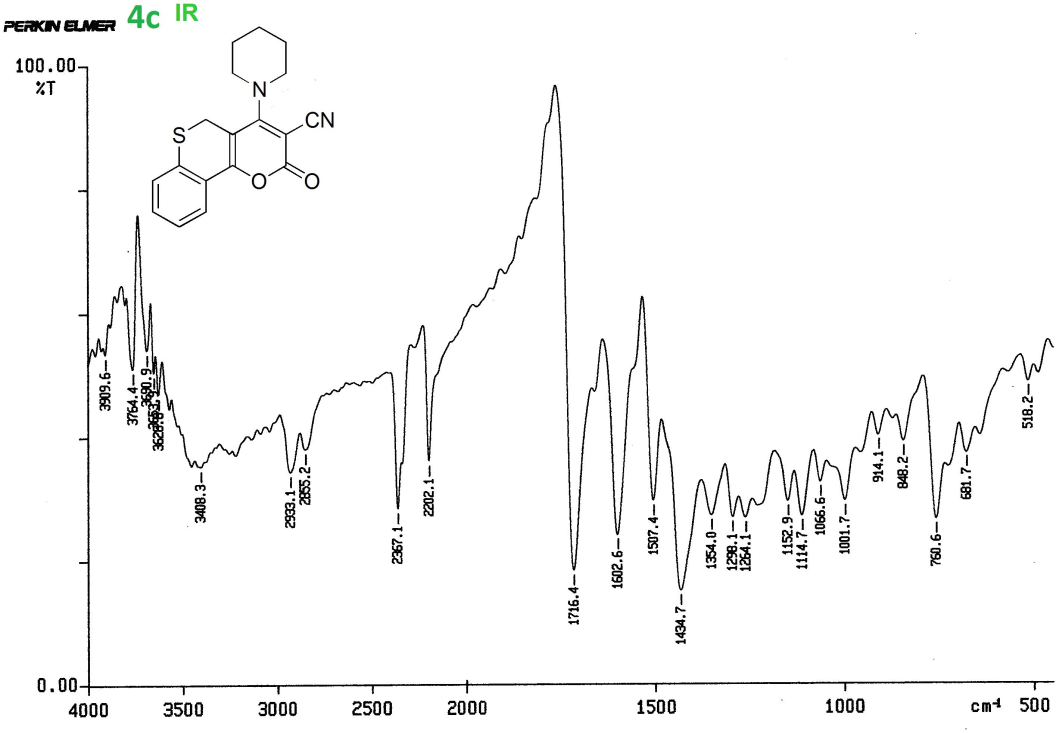
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
361.03944	42492.83	361.04137	-1.93	$^{12}C_{17}{}^{1}H_{14}{}^{35}Cl_{1}{}^{14}N_{2}{}^{16}O_{3}{}^{32}S_{1}$	12.5

Acq. Data Name: 10JULY129A **4b HRMS**
Internal Sample Id: VJR-88
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.229..0.237);,1.0];Correct Base[5.0%];.
Experiment Date/Time: 7/6/2010 4:45:39 PM
Orifice1 Volt Sweep: 15V
Acquired m/z Range: 50.0..1010.0
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.142[min]
Operator Name: admin



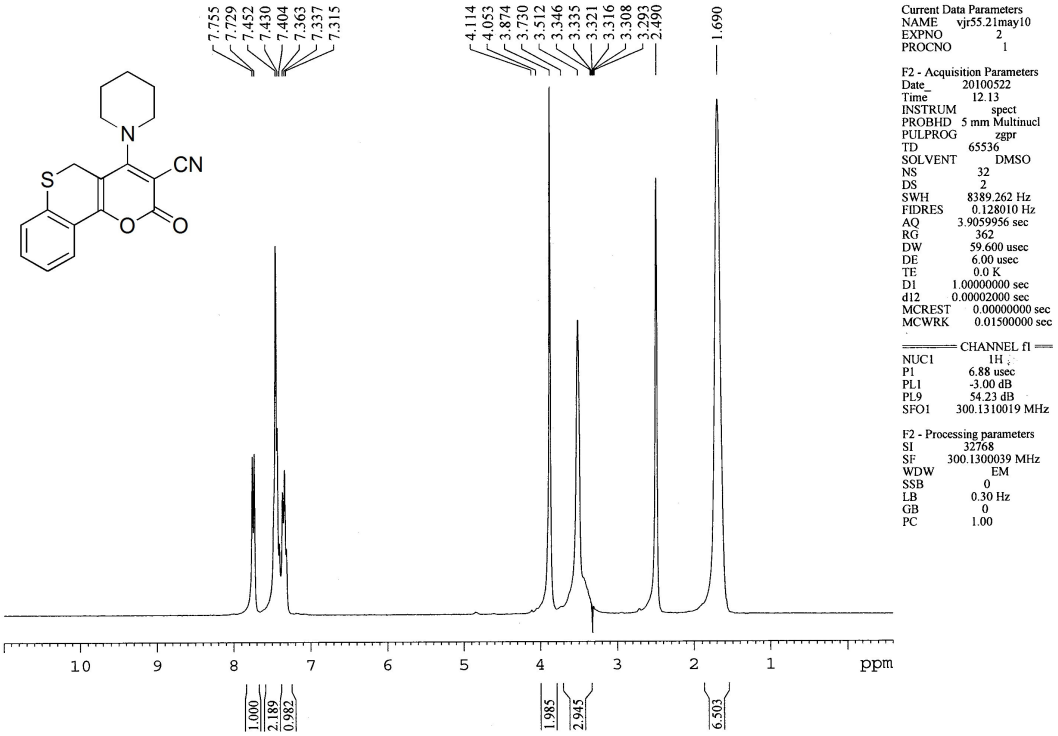
PERKIN ELMER **4c IR**



10/05/20 10:35 CODE-VJR-55
X: 4 scans, 4.0cm-1, flat, smooth, abex

4c 1HNMR

VJR-55



Current Data Parameters
NAME vjr55.21may10
EXPNO 2
PROCNO 1

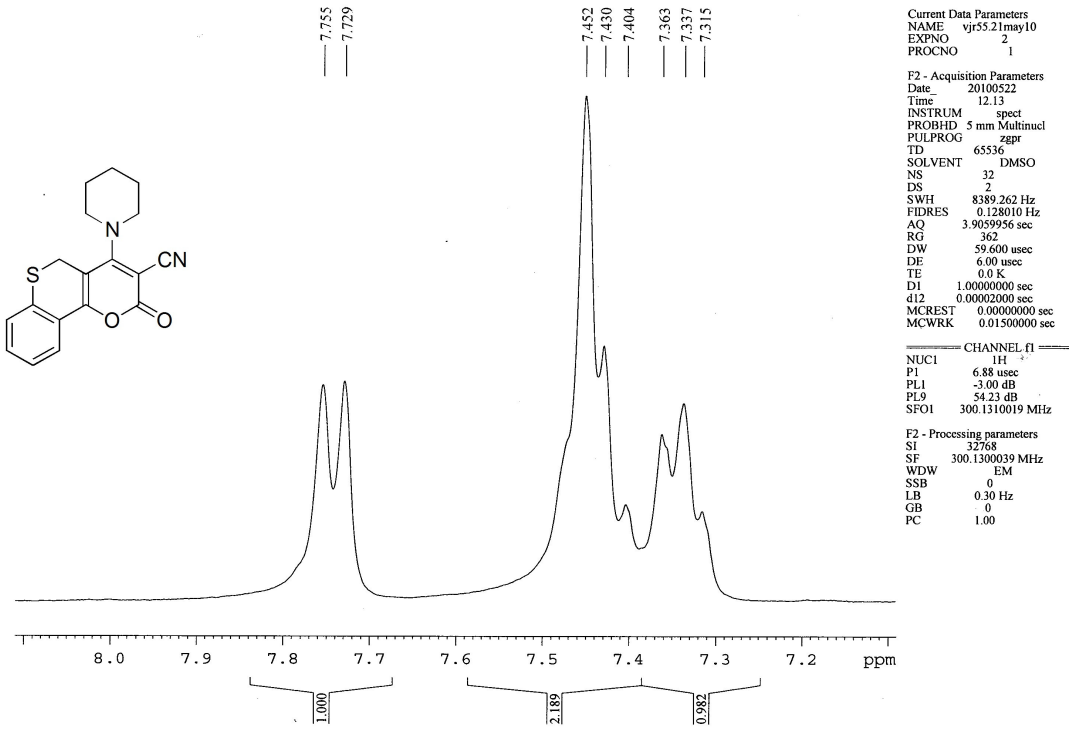
F2 - Acquisition Parameters
Date_ 20100522
Time 12.13
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpr
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 362
DW 59.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
d12 0.00002000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
PL9 54.23 dB
SFO1 300.1310019 MHz

F2 - Processing parameters
SI 32768
SF 300.1300039 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4c 1HNMR (Ext.)

VJR-55



Current Data Parameters
NAME vjr55.21may10
EXPNO 2
PROCNO 1

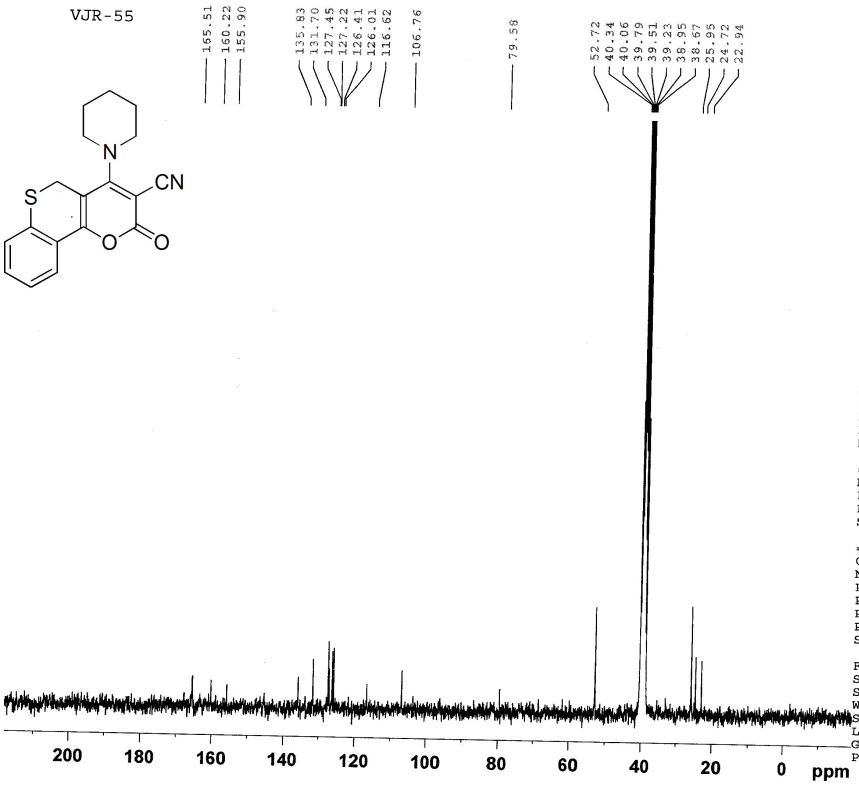
F2 - Acquisition Parameters
Date_ 20100522
Time 12.13
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpr
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 362
DW 59.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
d12 0.00002000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
PL9 54.23 dB
SFO1 300.1310019 MHz

F2 - Processing parameters
SI 32768
SF 300.1300039 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4c **13CNMR**

VJR-55



Current Data Parameters
NAME vjr55.21may10
EXPNO 3
PROCNO 1

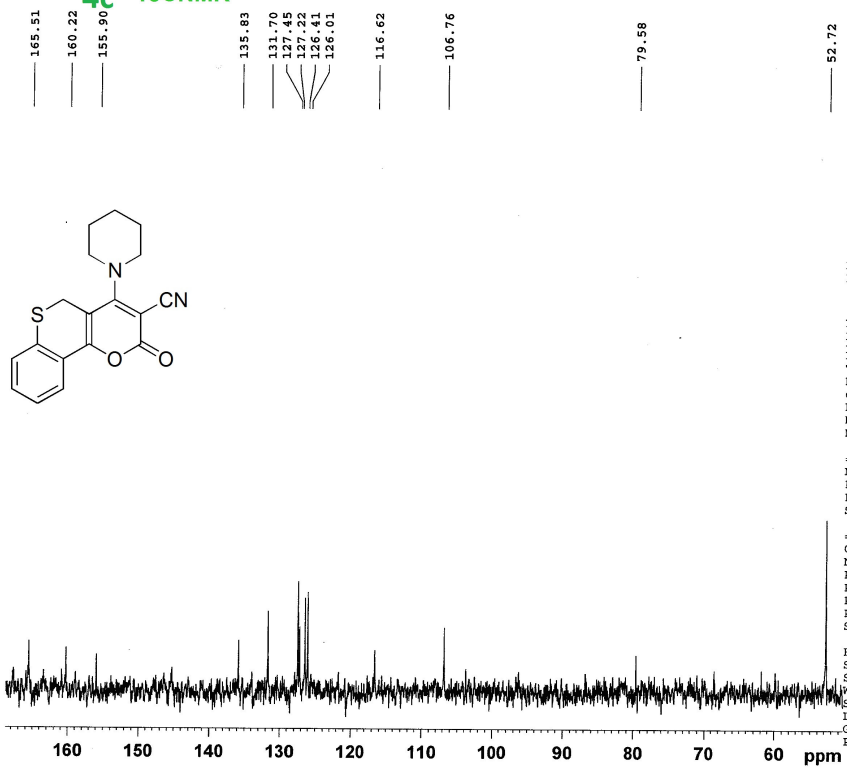
F2 - Acquisition Parameters
Date_ 20100522
Time 12.19
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1766
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 4597.6
DW 26.550 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PL1 -6.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 18.31 dB
PL13 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677854 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

VJR-55 **4c** **13CNMR**



Current Data Parameters
NAME vjr55.21may10
EXPNO 3
PROCNO 1

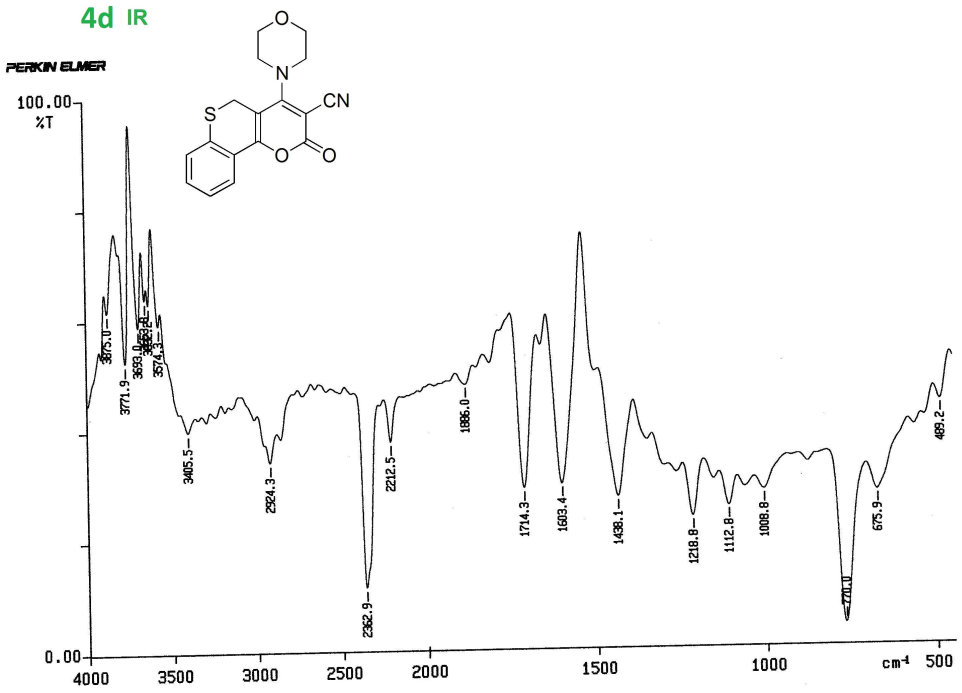
F2 - Acquisition Parameters
Date_ 20100522
Time 12.19
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1766
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 4597.6
DW 26.550 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PL1 -6.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 18.31 dB
PL13 22.00 dB
SFO2 300.1312005 MHz

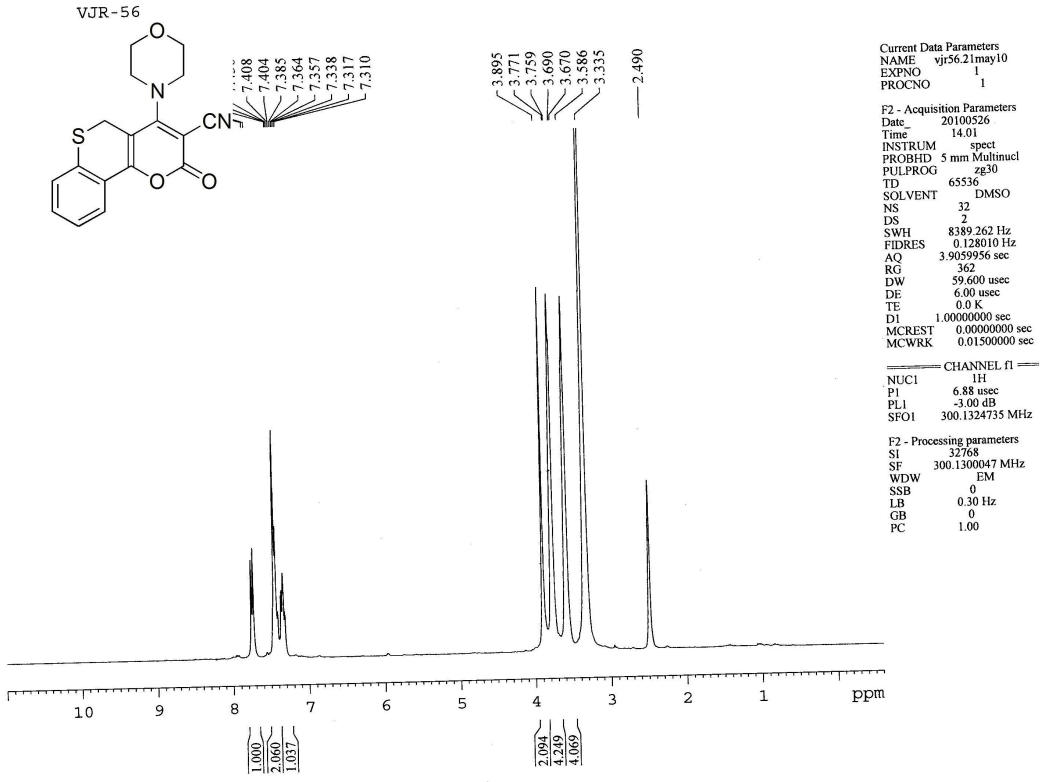
F2 - Processing parameters
SI 32768
SF 75.4677854 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

4d IR



10/05/20 10:50 CODE-VJR-56
X: 4 scans, 4.0cm-1, flat, smooth, abex

4d 1HNMR



Current Data Parameters
NAME vjr56.21may10
EXPNO 1
PROCNO 1

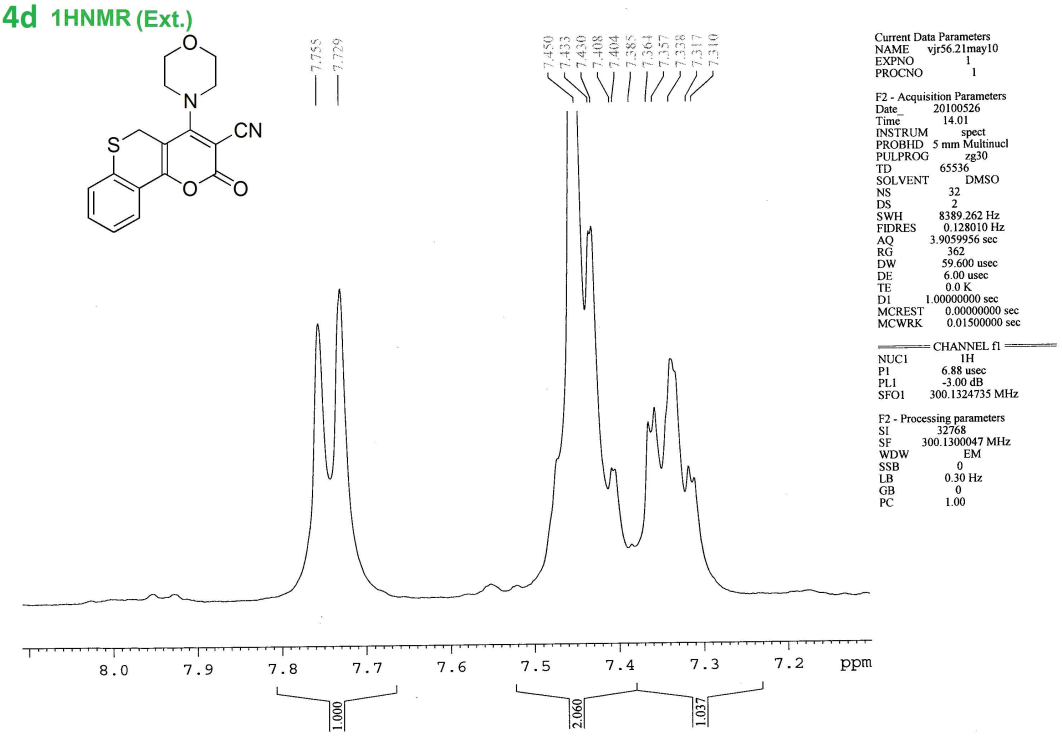
F2 - Acquisition Parameters
Date_ 20100526
Time 14.01
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 362
DW 59.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1324735 MHz

F2 - Processing parameters
SI 32768
SF 300.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

VJR-56

4d 1HNMR (Ext.)



Current Data Parameters
NAME vjr56.21may10
EXPNO 1
PROCNO 1

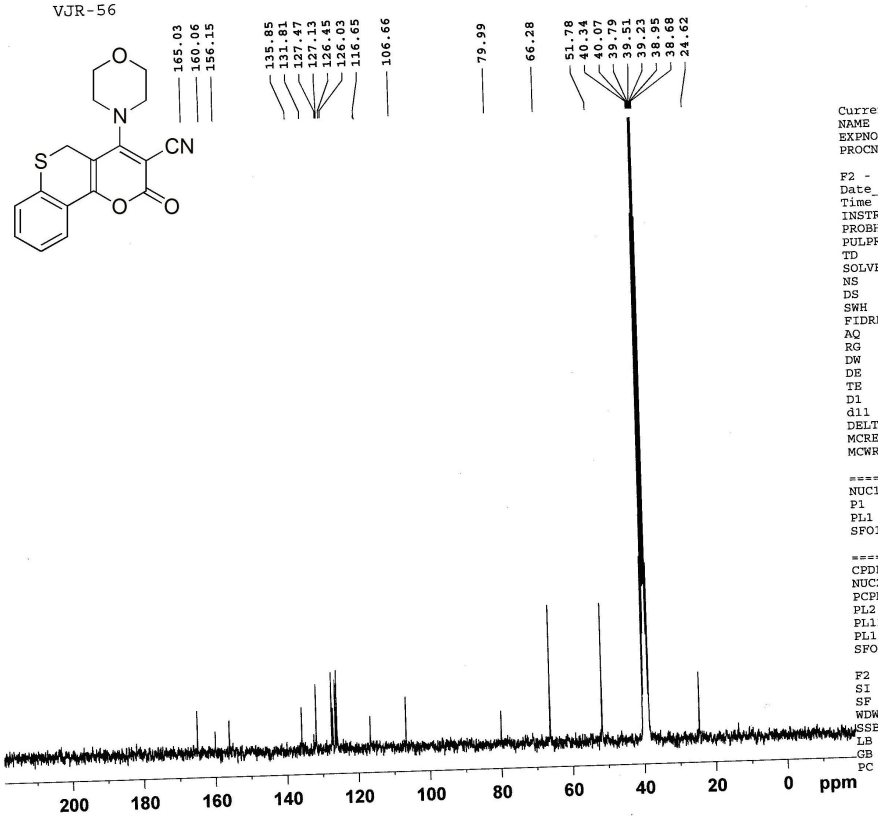
F2 - Acquisition Parameters
Date_ 20100526
Time 14.01
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 362
DW 59.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1324735 MHz

F2 - Processing parameters
SI 32768
SF 300.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4d 13CNMR

VJR-56



Current Data Parameters
NAME vjr56.21may10
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100526
Time 14.11
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1206
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 8192
DW 26.550 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

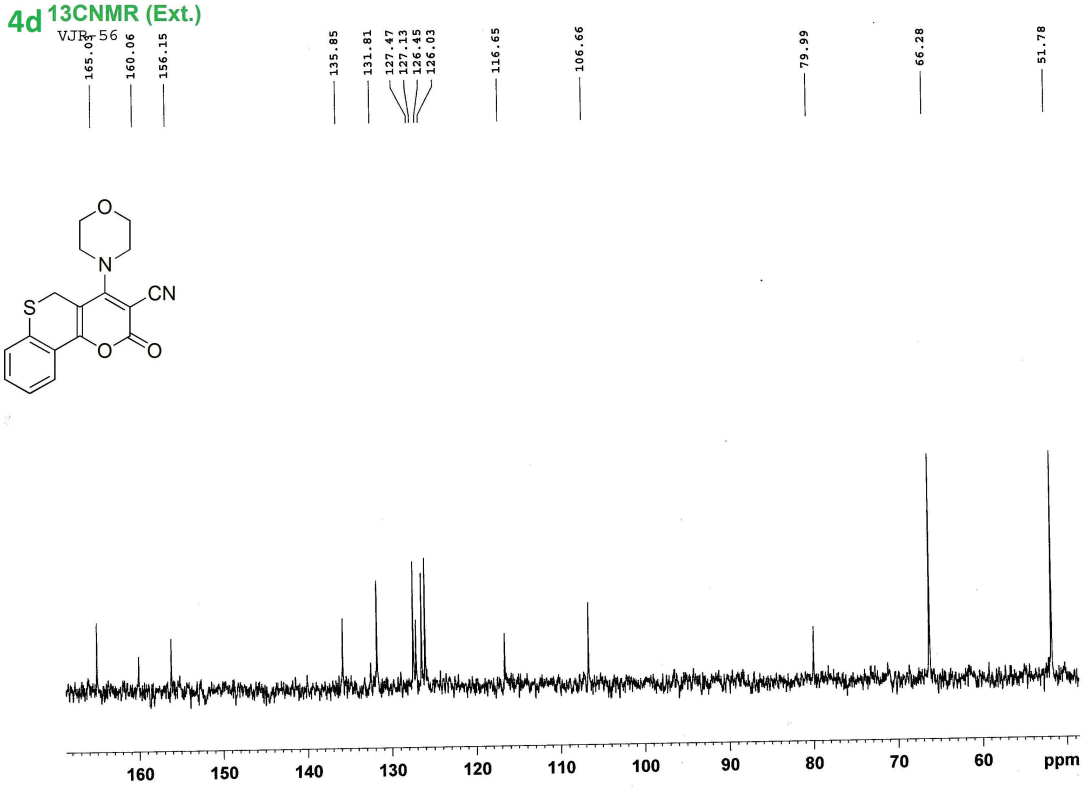
CHANNEL f1
NUC1 13C
P1 9.25 usec
PL1 -6.00 dB
SFO1 75.4752953 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 18.31 dB
PL13 22.00 dB
SFO2 300.1312005 MHz

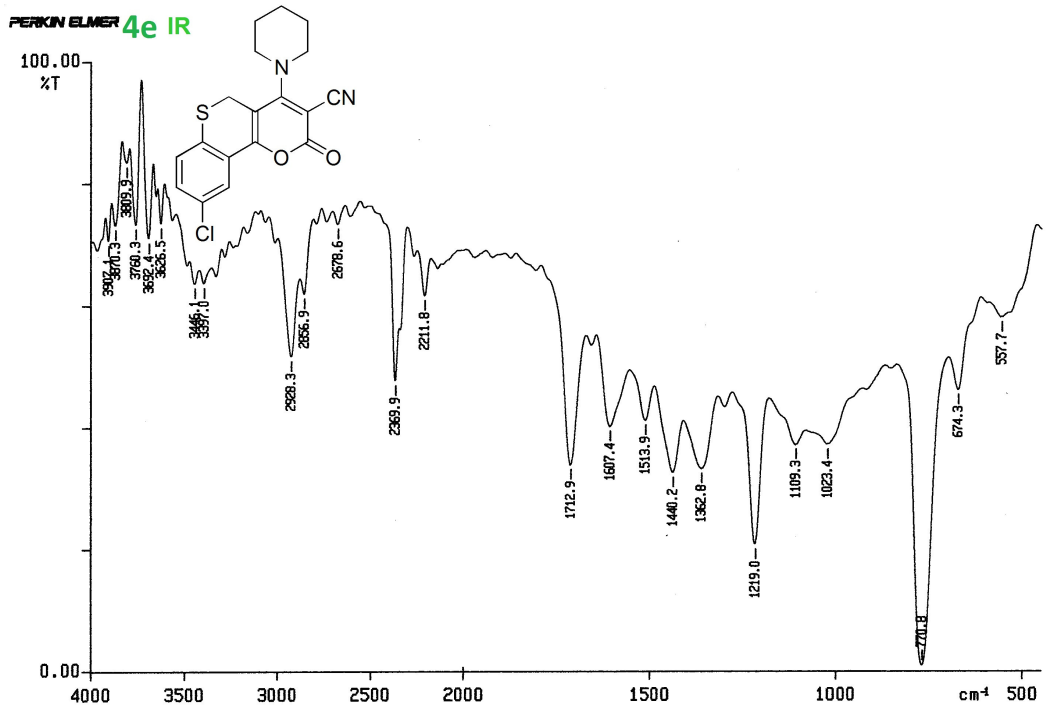
F2 - Processing parameters
SI 32768
SF 75.4677848 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

4d 13CNMR (Ext.)

VJR-56

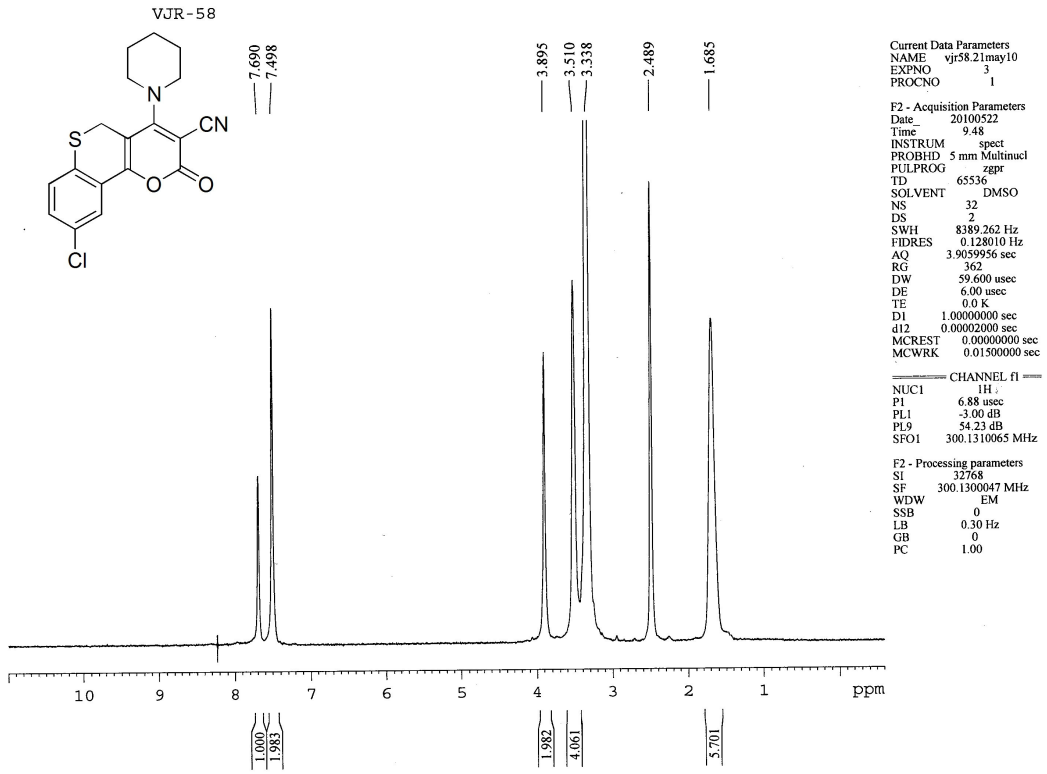


PERKIN ELMER **4e** IR



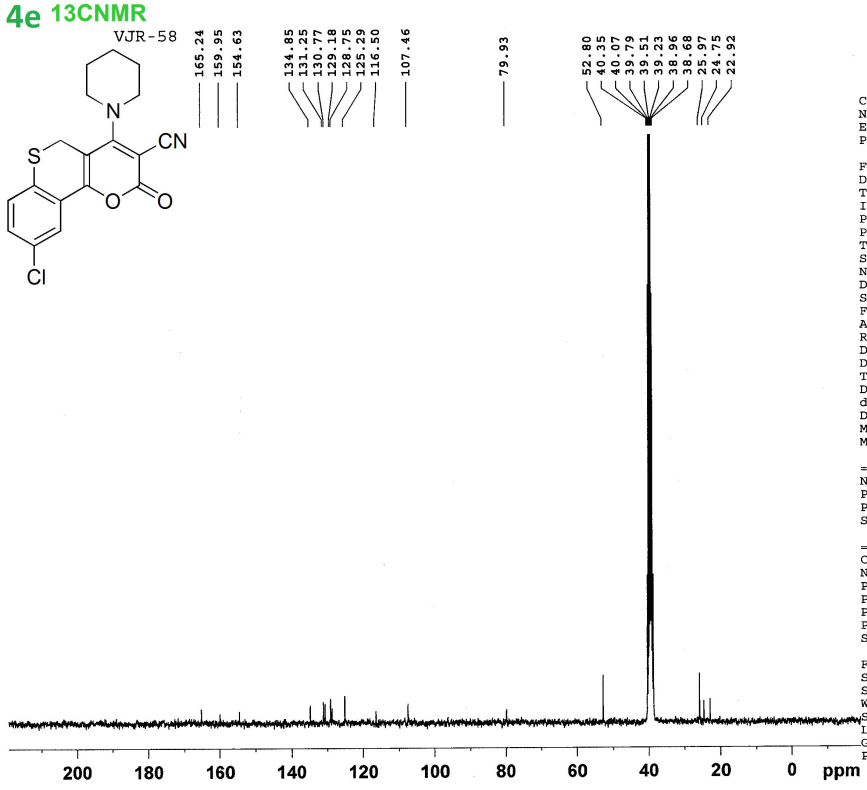
10/05/26 10:56 CODE-VJR-58
X: 4 scans, 4.0cm-1, flat, smooth, abex

4e 1HNMR



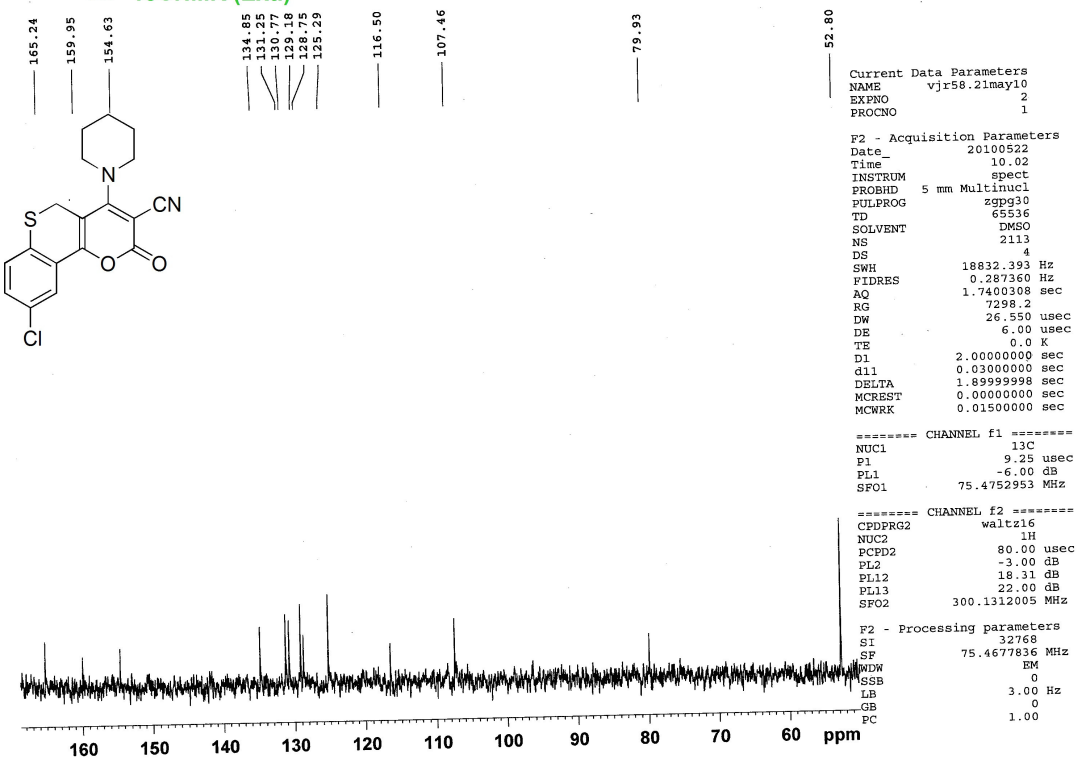

```
Current Data Parameters
NAME      vjr58.21may10
EXPNO              3
PROCNO             1

F2 - Acquisition Parameters
Date_          20100522
Time              9.48
INSTRUM          spect
PROBHD  5 mm Multinucl
PULPROG          zgpr
TD              65536
SOLVENT          DMSO
NS                32
DS                 2
SWH          8389.262 Hz
FIDRES       0.128010 Hz
AQ          3.9059956 sec
RG               362
DW            59.600 usec
DE             6.00 usec
TE              0.0 K
D1          1.00000000 sec
d12         0.00002000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

========== CHANNEL f1 ==========
NUC1               1H
P1              6.88 usec
PL1             -3.00 dB
PL9             54.23 dB
SFO1       300.1310065 MHz

F2 - Processing parameters
SI             32768
SF       300.1300047 MHz
WDW               EM
SSB                0
LB              0.30 Hz
GB                 0
PC              1.00
```

4e 13CNMR




```
Current Data Parameters
NAME       vjr58.21may10
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100522
Time               10.02
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  2113
DS                     4
SWH           18832.393 Hz
FIDRES         0.287360 Hz
AQ             1.7400308 sec
RG                7298.2
DW             26.550 usec
DE              6.00 usec
TE                 0.0 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1              9.25 usec
PL1             -6.00 dB
SFO1       75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2           80.00 usec
PL2             -3.00 dB
PL12            18.31 dB
PL13            22.00 dB
SFO2      300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF        75.4677836 MHz
WDW                   EM
SSB                    0
LB              3.00 Hz
GB                     0
PC                  1.00
```

VJR-58 **4e 13CNMR (Ext.)**




```
Current Data Parameters
NAME        vjr58.21may10
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_             20100522
Time                 10.02
INSTRUM              spect
PROBHD    5 mm Multinucl
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   2113
DS                      4
SWH           18832.393 Hz
FIDRES         0.287360 Hz
AQ             1.7400308 sec
RG                  7298.2
DW                26.550 usec
DE                 6.00 usec
TE                  0.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.25 usec
PL1                -6.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               18.31 dB
PL13               22.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677836 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.00
```

4e HRMS

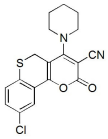
Data:9DEC124A
Sample Name:VJR-58
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%],Ave...

Acquired:12/21/2009 12:33:09 PM
Operator:admin
Mass Calibration data:(Internal Mass Calibration Data)
Created:12/21/2009 12:36:55 PM
Created by:admin

Charge number:1 Tolerance:5.00(mmu)
Element:^{12}C:0 .. 18, ^{1}H:0 .. 16, ^{35}Cl:0 .. 1, ^{14}N:0 .. 2, ^{16}O:0 .. 2, ^{32}S:0 .. 1

Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
359.06187	76375.08	359.06210	-0.23	$^{12}C_{18}{}^{1}H_{16}{}^{35}Cl_{1}{}^{14}N_{2}{}^{16}O_{2}{}^{32}S_{1}$	12.5

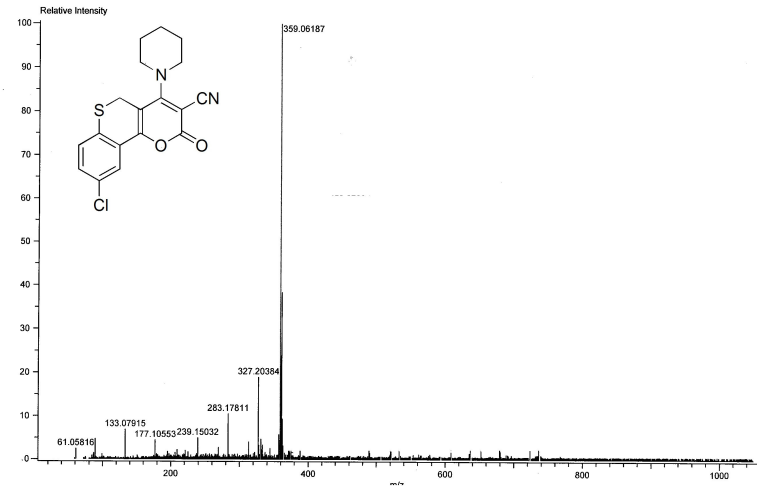


4e HRMS

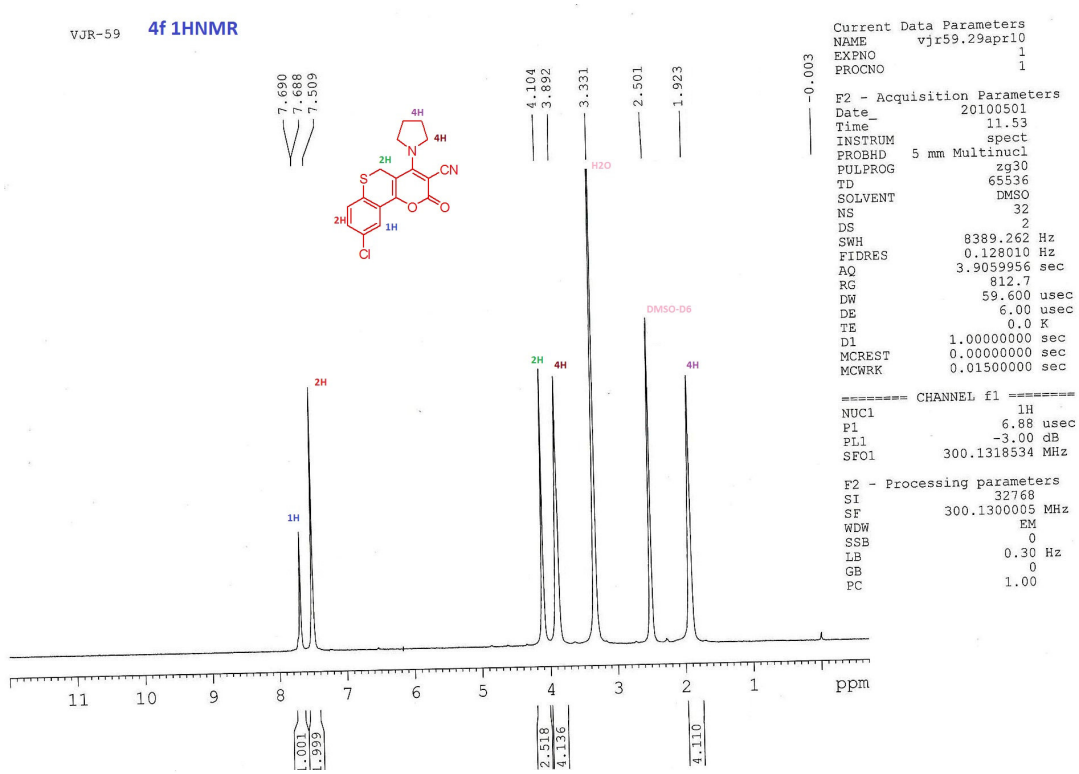
Acq. Data Name: 9DEC124A
Internal Sample Id: VJR-58
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.359..0.384),,1.0];Correct Base[5.0%];...
Experiment Date/Time: 12/21/2009 12:33:09 PM

E:\CDRI\NOV09B/DEC09A:9DEC124A
Ion Guide RF Volt: 550V
Orifice1 Volt Sweep: 28V
Acquired m/z Range: 10.0..1050.0

Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 13[V]
Time of Maximum: 0.269[min]
Operator Name: admin



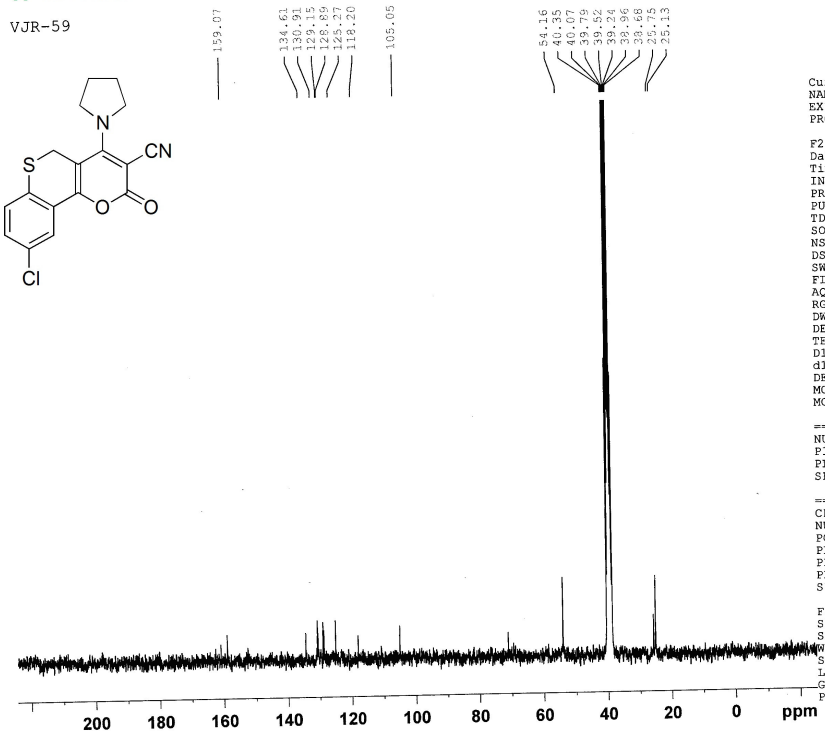
VJR-59 **4f 1HNMR**




```
Current Data Parameters
NAME        vjr59.29apr10
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20100501
Time                 11.53
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     32
DS                      2
SWH             8389.262 Hz
FIDRES          0.128010 Hz
AQ              3.9059956 sec
RG                  812.7
DW                 59.600 usec
DE                  6.00 usec
TE                   0.0 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  6.88 usec
PL1                -3.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF              300.1300005 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

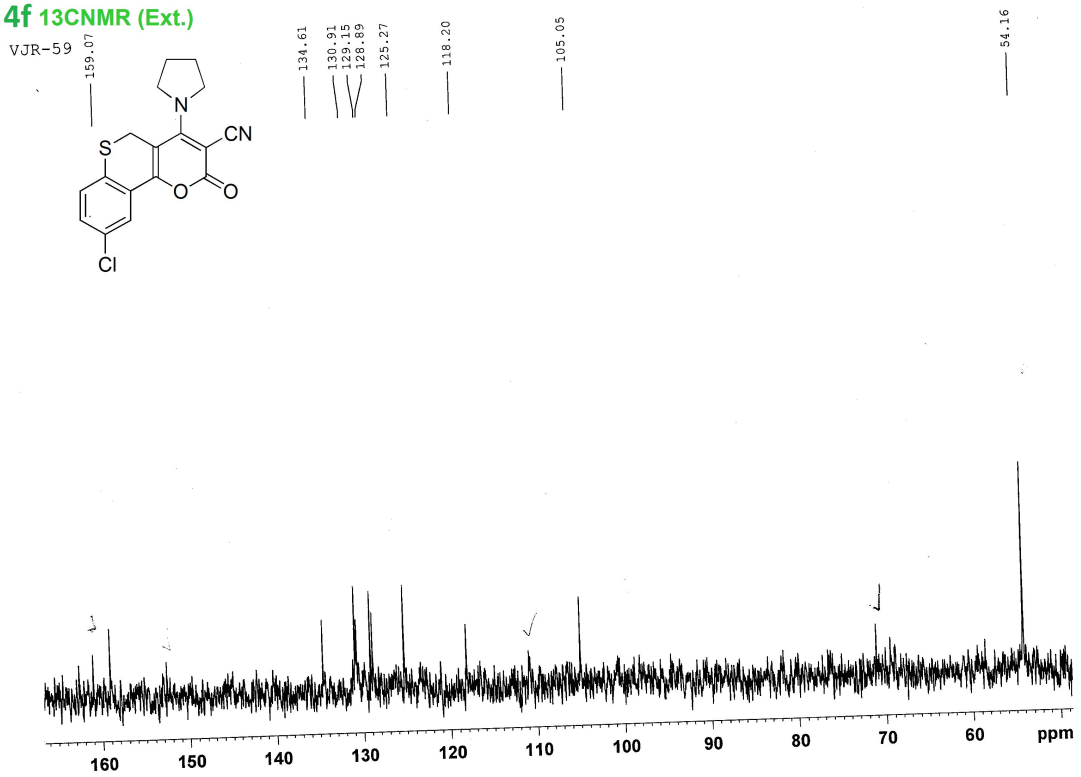
4f 13CNMR

VJR-59




```
Current Data Parameters
NAME        vjr59.29apr10
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_              20100501
Time                 12.11
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                   3072
DS                      4
SWH            18832.393 Hz
FIDRES          0.287360 Hz
AQ              1.7400308 sec
RG                  16384
DW                 26.550 usec
DE                  6.00 usec
TE                   0.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.25 usec
PL1                -6.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               18.31 dB
PL13               22.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF              75.4677840 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.40
```

4f 13CNMR (Ext.)

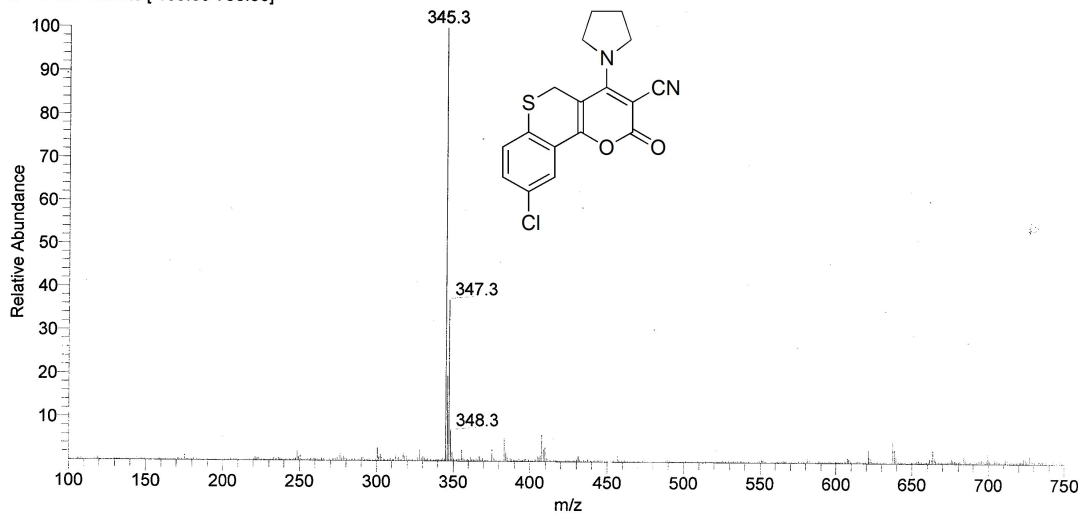


4f Mass

MSAIF, CDRI LUCKNOW

Original Data Path: 10I5APR17204050172_172903.RAW
Current Data Path: C:\Data2010\APR10\
Sample ID:
Acquisition Date: 4/5/2010 5:59:20 PM
Vial: B:32

10I5APR17204050172_172903 #18-50 RT: 0.30-0.70 AV: 33 SB: 2 0.00 , 0.00 NL: 2.06E7
T: + c ESI Full ms [100.00-750.00]



4f HRMS

Data:9DEC123A
Sample Name:VJR-59
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Acquired:12/21/2009 12:26:19 PM
Operator:admin
Mass Calibration data:(Internal Mass Calibration Data)
Created:12/21/2009 12:31:08 PM
Created by:admin

Charge number:1 Tolerance:5.00(mmu)
Element:^{12}C:0 .. 17, ^{1}H:0 .. 14, ^{35}Cl:0 .. 1, ^{14}N:0 .. 2, ^{16}O:0 .. 2, ^{32}S:0 .. 1

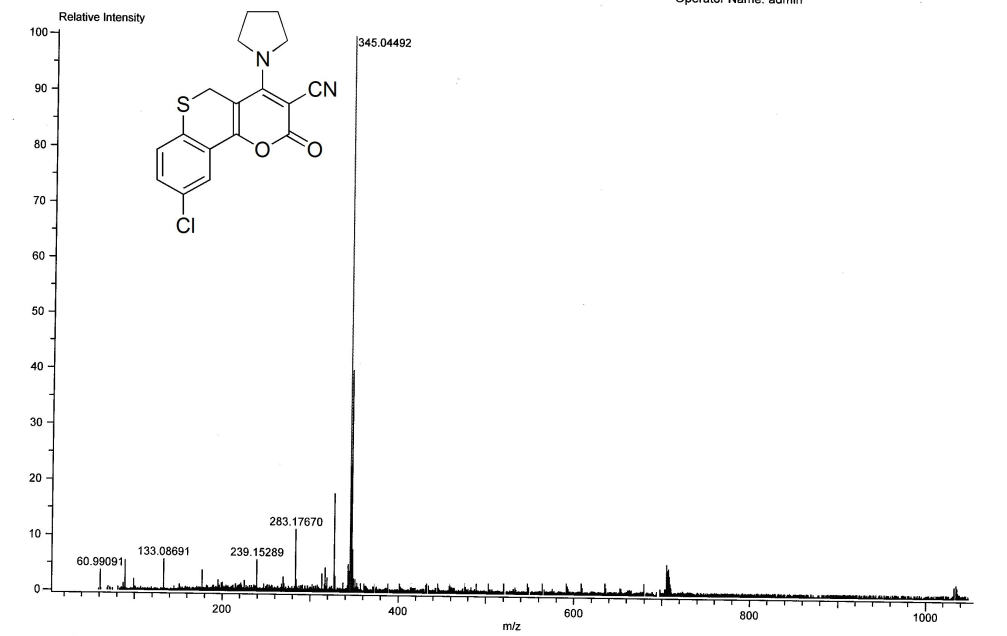
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
345.04492	75037.32	345.04645	-1.53	$^{12}C_{17}{}^{1}H_{14}{}^{35}Cl_{1}{}^{14}N_{2}{}^{16}O_{2}{}^{32}S_{1}$	12.5

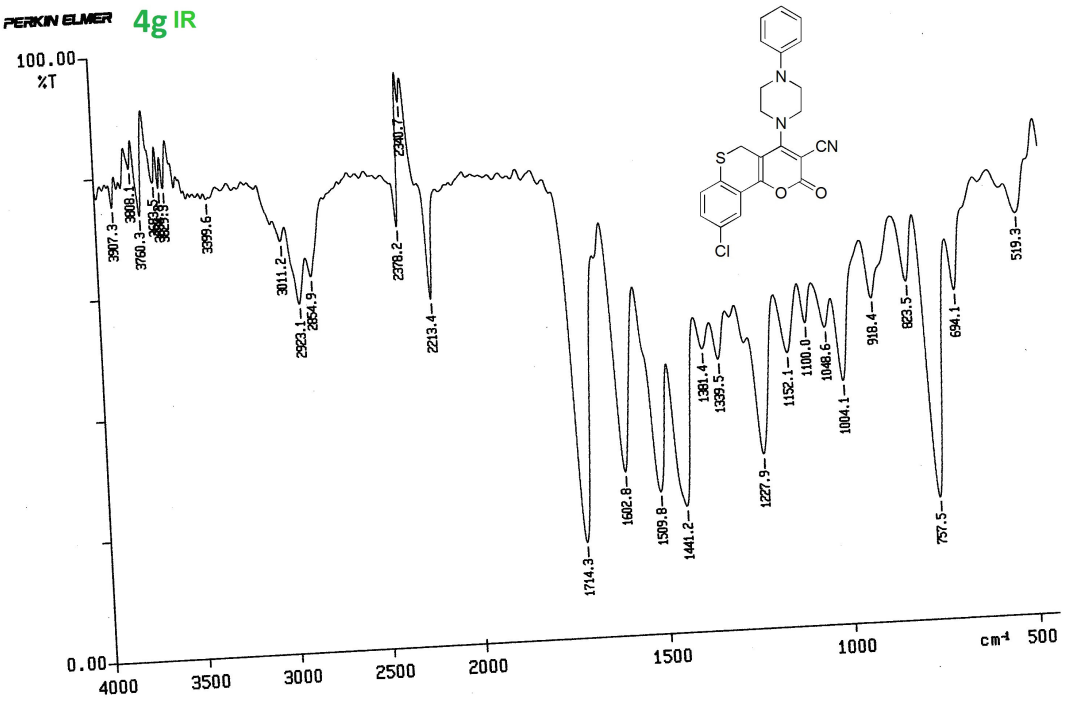
Acq. Data Name: 9DEC123A **4f HRMS**
Internal Sample Id: VJR-59
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect{Centroid,50,Area};Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average{MS[1] 0.316..0.330);,1.0];Correct Base[5.0%];...
Experiment Date/Time: 12/21/2009 12:26:19 PM

E:\CDRI\NOV09B/DEC09A:9DEC123A
Ion Guide RF Volt: 550V
Orifice1 Volt Sweep: 28V
Acquired m/z Range: 10.0..1050.0

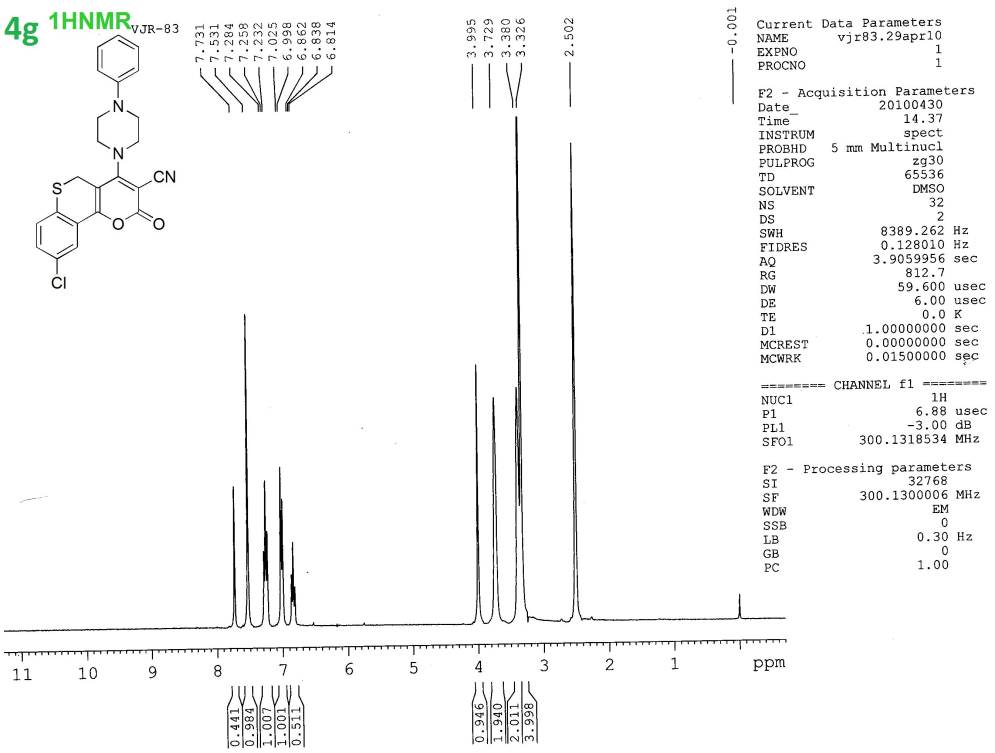
Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 13[V]
Time of Maximum: 0.202[min]
Operator Name: admin

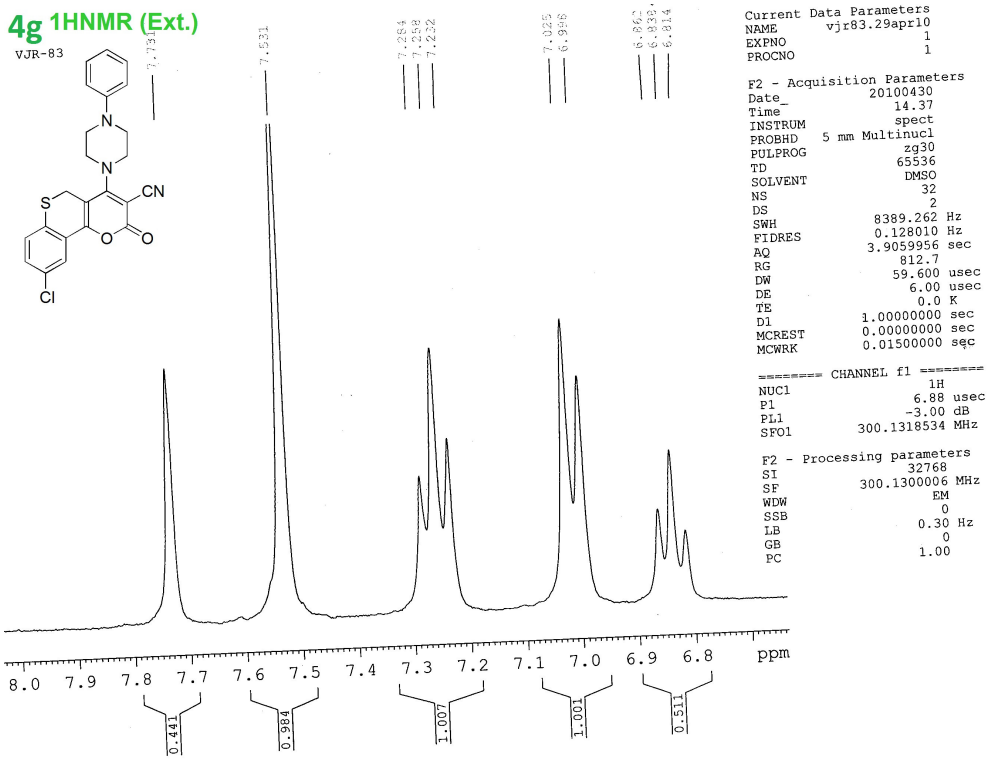


PERKIN ELMER **4g IR**



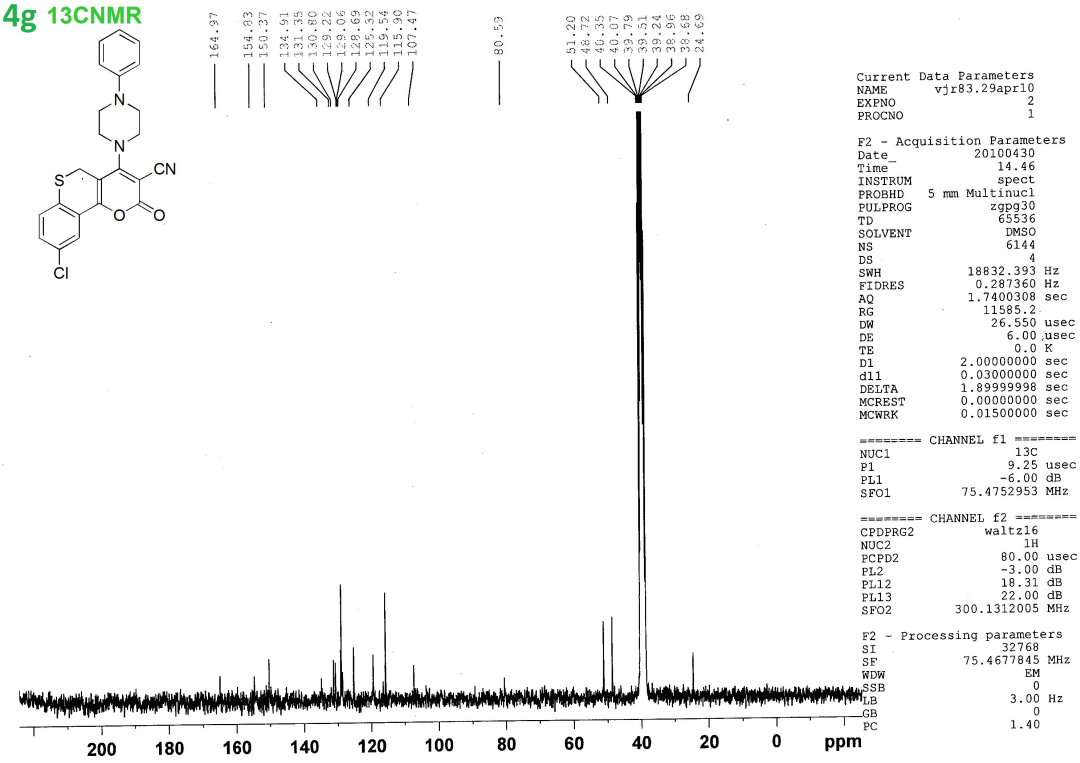
10/05/25 10:58 CODE- VJR-83
X: 4 scans, 4.0cm-1, apod weak, flat, smooth, abex


4g 1HNMR VJR-83
7.731
7.531
7.284
7.258
7.232
7.025
6.998
6.862
6.838
6.814
3.995
3.729
3.380
3.326
2.502
-0.001
N
N
S
CN
O
O
Cl
11 10 9 8 7 6 5 4 3 2 1 ppm
0.441
0.984
1.007
1.001
0.511
0.946
1.940
2.011
3.998
Current Data Parameters
NAME vjr83.29apr10
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100430
Time 14.37
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 812.7
DW 59.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300006 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


4g 1HNMR (Ext.)
VJR-83
7.731
7.531
7.284
7.258
7.232
7.025
6.946
6.862
6.838
6.814
N
N
S
CN
O
O
Cl
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm
0.441
0.984
1.007
1.001
0.511
Current Data Parameters
NAME vjr83.29apr10
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100430
Time 14.37
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 812.7
DW 59.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300006 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

VJR-83

4g 13CNMR




```
Current Data Parameters
NAME        vjr83.29apr10
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100430
Time                14.46
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  6144
DS                     4
SWH          18832.393 Hz
FIDRES        0.287360 Hz
AQ            1.7400308 sec
RG              11585.2
DW               26.550 usec
DE                6.00 usec
TE                 0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.25 usec
PL1                 -6.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -3.00 dB
PL12             18.31 dB
PL13             22.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677845 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.40
```

4g HRMS

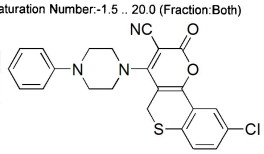
Data:10JULY131A
Sample Name:VJR-83
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Acquired:7/6/2010 4:48:29 PM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:7/6/2010 5:12:51 PM
Created by:admin

Charge number:1
Tolerance:5.00(mmu)
Element:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{35}Cl:0 .. 1, ^{14}N:0 .. 3, ^{16}O:0 .. 2, ^{32}S:0 .. 1

Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
436.08769	13945.65	436.08865	-0.96	$^{12}C_{23}{}^{1}H_{18}{}^{35}Cl_{1}{}^{14}N_{3}{}^{16}O_{2}{}^{32}S_{1}$	16.5

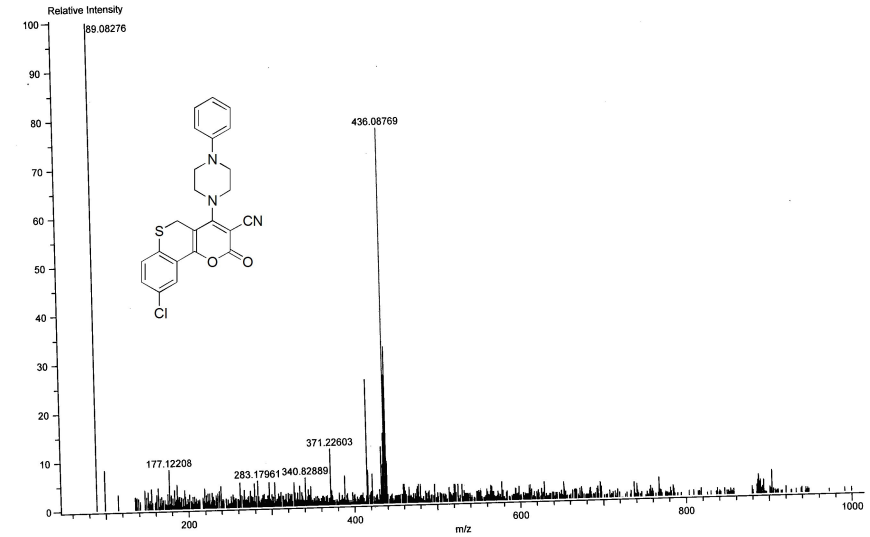


4g HRMS

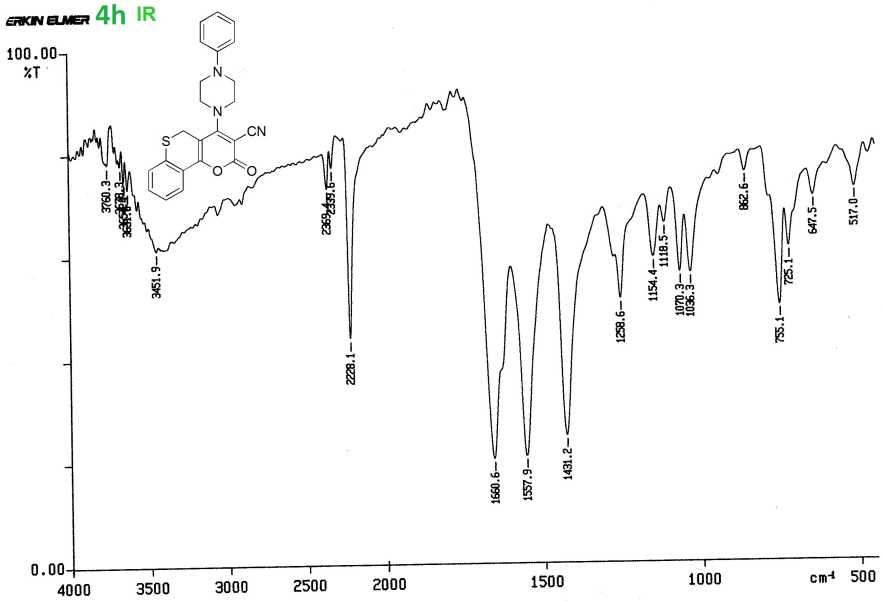
Acq. Data Name: 10JULY131A
Internal Sample Id: VJR-83
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.269..0.291);,1.0];Correct Base[5.0%];...
Experiment Date/Time: 7/6/2010 4:48:29 PM

Orifice1 Volt Sweep: 15V
Acquired m/z Range: 50.0..1010.0

Spec. Record Interval: 0.4[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.189[min]
Operator Name: admin

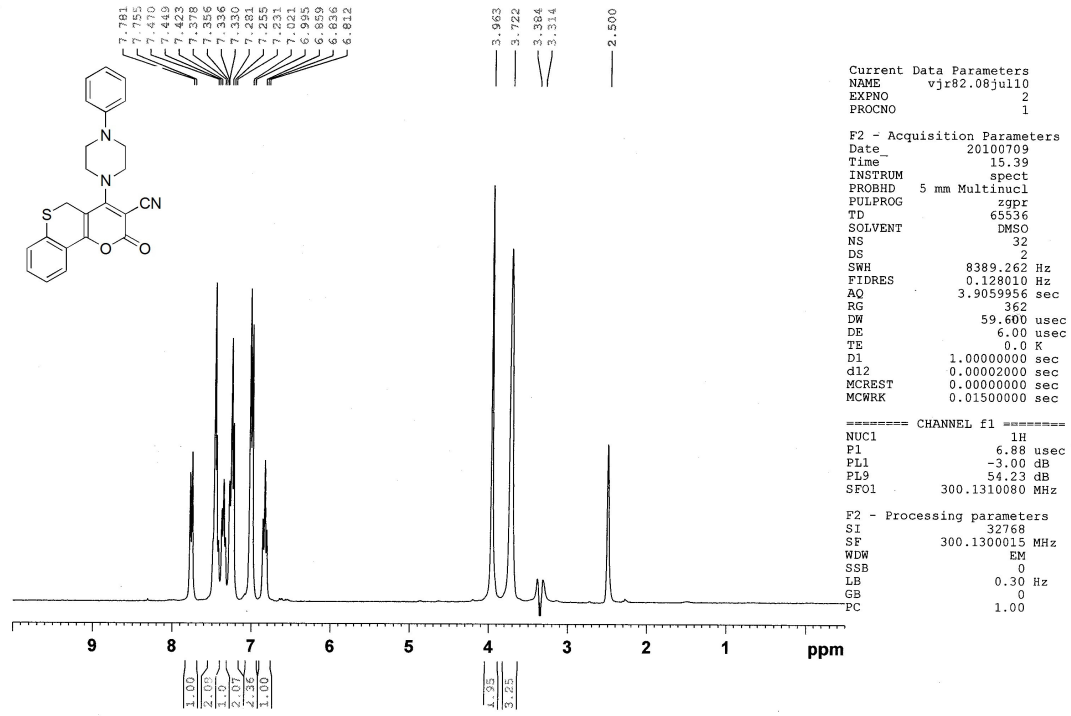


PERKIN ELMER **4h IR**



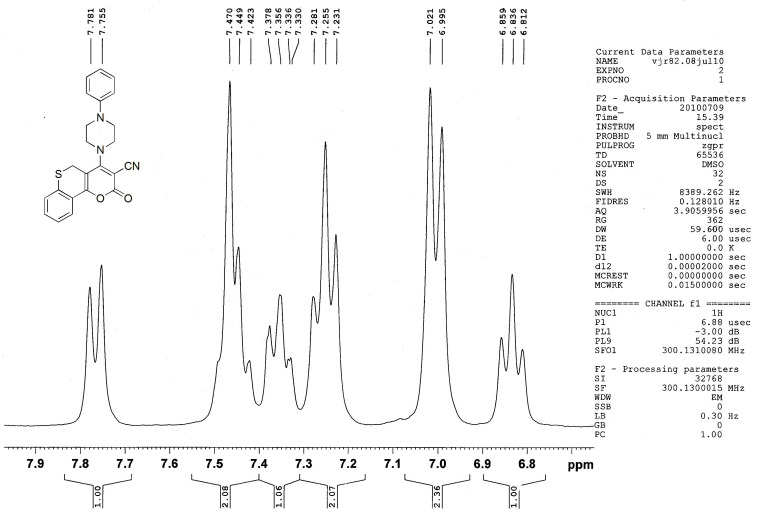
10/05/17 10:28 CODE- VJR-82
X: 4 scans, 4.0cm-1, flat, smooth, abex

VJR-82 **4h 1HNMR**



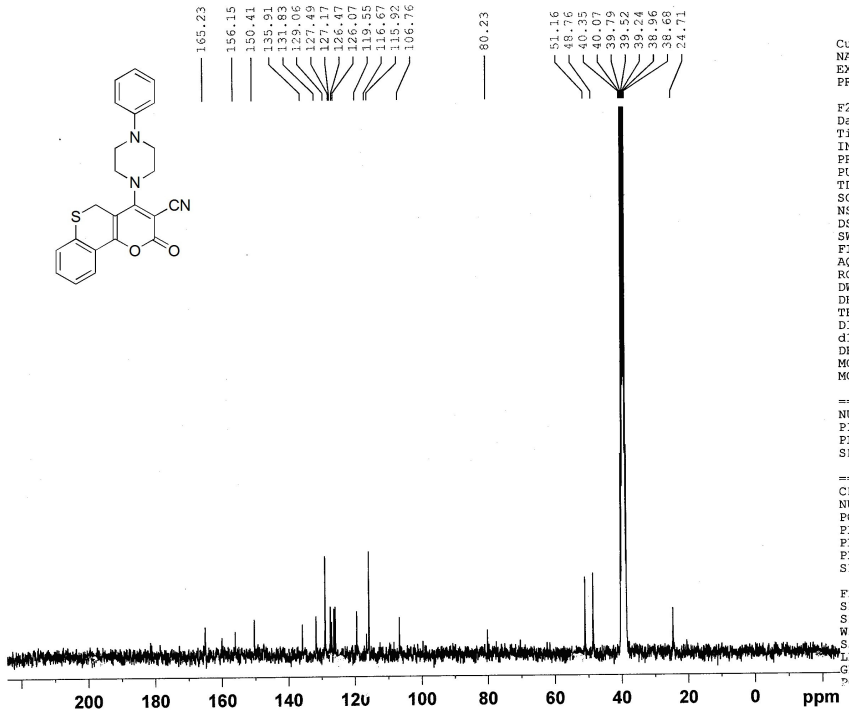

```
Current Data Parameters
NAME        vjr82.08jul10
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100709
Time               15.39
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG             zgpr
TD                 65536
SOLVENT             DMSO
NS                    32
DS                     2
SWH             8389.262 Hz
FIDRES          0.128010 Hz
AQ              3.9059956 sec
RG                   362
DW                59.600 usec
DE                 6.00 usec
TE                  0.0 K
D1             1.00000000 sec
d12            0.00002000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  6.88 usec
PL1                -3.00 dB
PL9                54.23 dB
SFO1         300.1310080 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300015 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

VJR-82 **4h** **1HNMR (Ext.)**



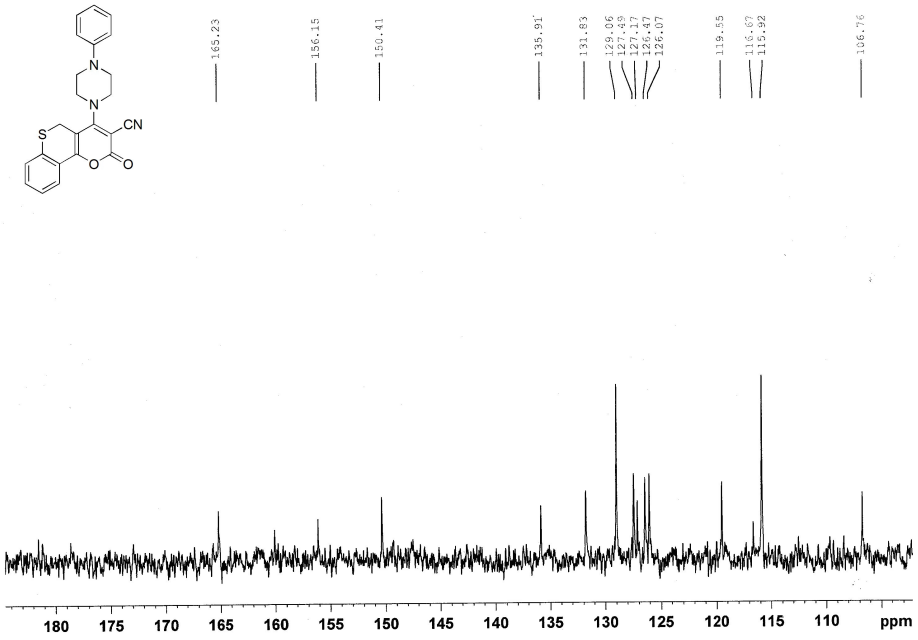

```
Current Data Parameters
NAME        vjr82.08jul10
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100709
Time                15.39
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG             zgpr
TD                 65536
SOLVENT             DMSO
NS                    32
DS                     2
SWH             8389.262 Hz
FIDRES          0.128010 Hz
AQ              3.9059956 sec
RG                   362
DW                59.600 usec
DE                 6.00 usec
TE                  0.0 K
D1           1.00000000 sec
d12          0.00002000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  6.88 usec
PL1                -3.00 dB
PL9                54.23 dB
SFO1        300.1310080 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300015 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

VJR-82 **4h** **13CNMR**




```
Current Data Parameters
NAME        vjr82.08jul10
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100710
Time                15.01
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1855
DS                     4
SWH            18832.393 Hz
FIDRES          0.287360 Hz
AQ              1.7400308 sec
RG                9195.2
DW                26.550 usec
DE                 6.00 usec
TE                  0.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.25 usec
PL1                -6.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               18.31 dB
PL13               22.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                  32768
SF          75.4677840 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```

VJR-82 **4h 13CNMR**

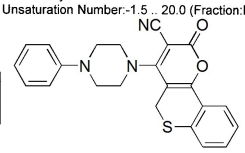


4h HRMS

Data:10MAY058A
Sample Name:VJR-82
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Charge number:1
Element:^{12}C:0 .. 23, ^{1}H:0 .. 20, ^{14}N:0 .. 3, ^{16}O:0 .. 2, ^{32}S:0 .. 1
Tolerance:5.00(mmu)

Acquired:5/4/2010 1:50:13 PM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:5/4/2010 2:00:01 PM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)



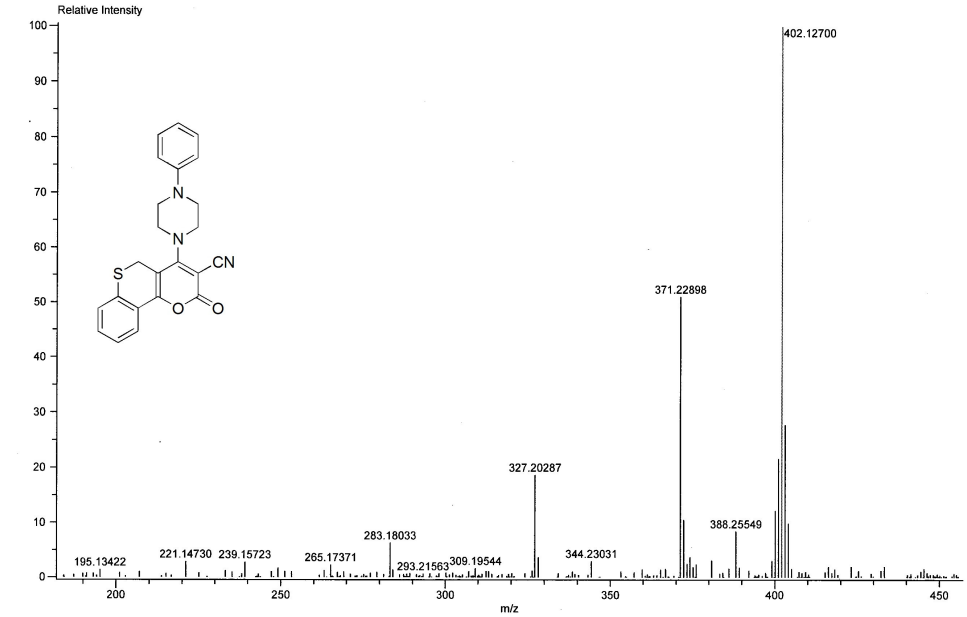
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
402.12700	70947.69	402.12762	-0.63	$^{12}C_{23}{}^{1}H_{20}{}^{14}N_{3}{}^{16}O_{2}{}^{32}S_{1}$	16.5

4h HRMS

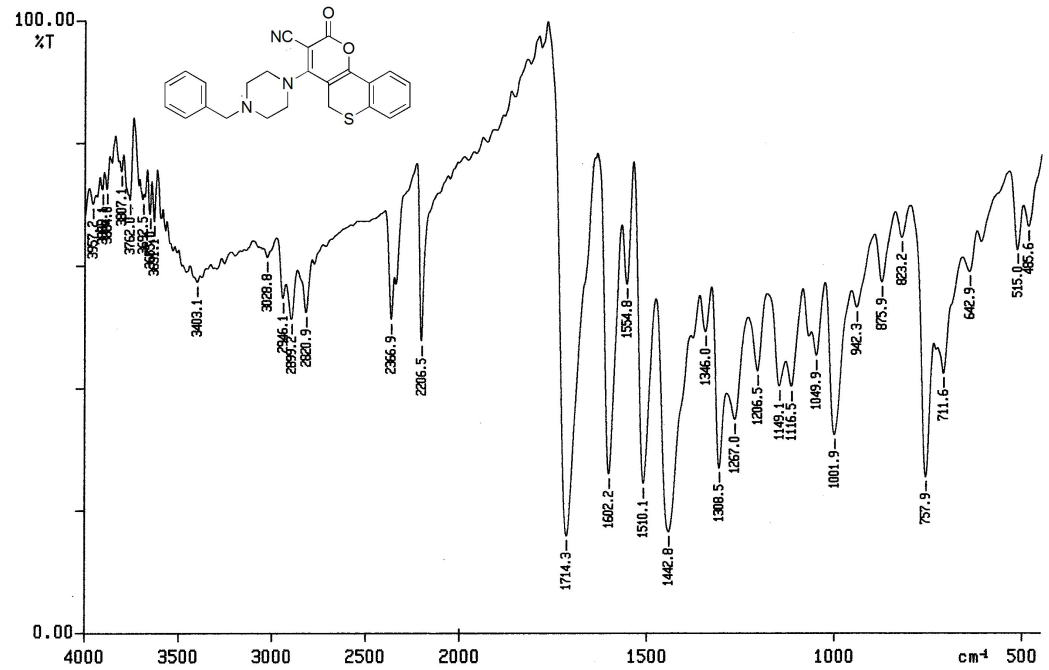
Acq. Data Name: 10MAY058A
Internal Sample Id: VJR-82
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.189..0.198);,1.0];Correct Base[5.0%];...
Experiment Date/Time: 5/4/2010 1:50:13 PM

E:\CDRI\MAY10A/MAY10A:10MAY058A
Ion Guide RF Volt: 550V
Orifice1 Volt Sweep: 25V
Acquired m/z Range: 10.0..1050.0

Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 15[V]
Time of Maximum: 0.127[min]
Operator Name: admin

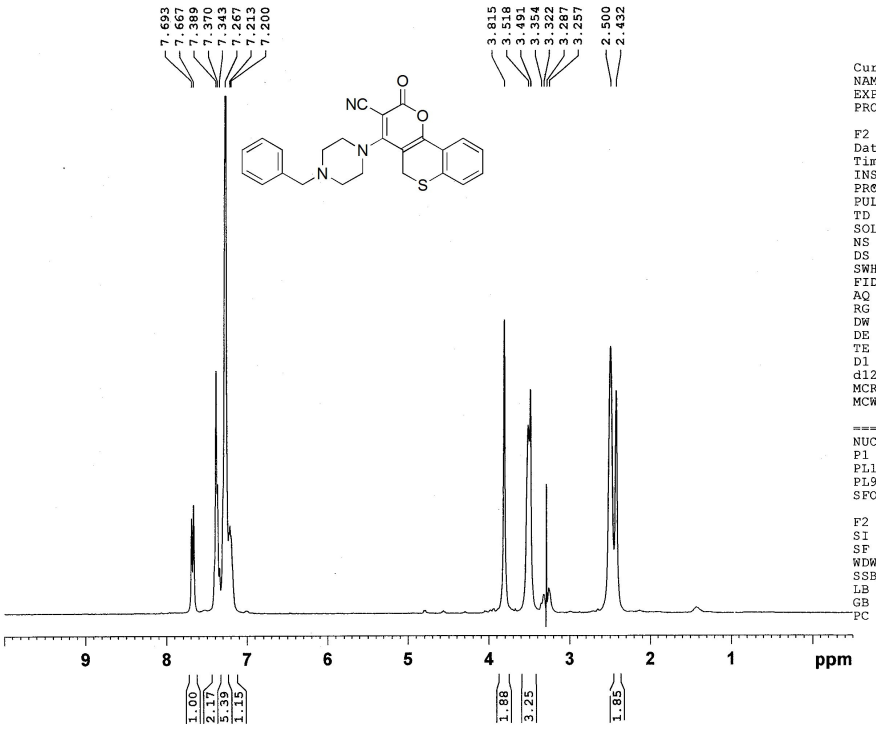


PERKIN ELMER **4i IR**



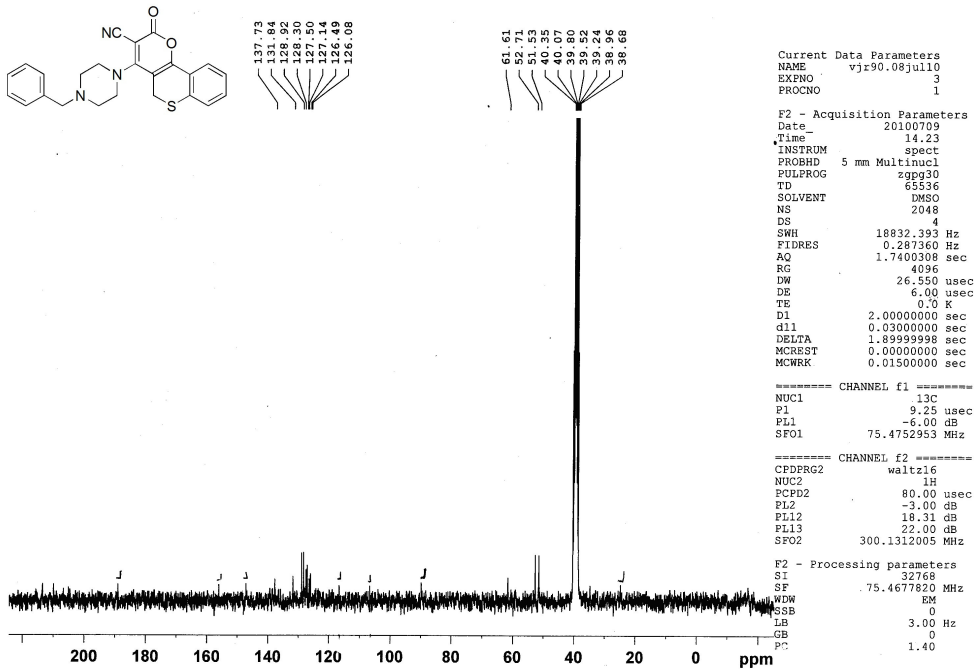
10/05/24 10:43 CODE-VJR-90
X: 4 scans, 4.0cm-1, flat, smooth, abex

VJR-90 **4i 1HNMR**




```
Current Data Parameters
NAME                 vjr90.08jul10
EXPNO                            2
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20100709
Time                         14.12
INSTRUM                      spect
PROBHD    5 mm Multinucl
PULPROG                      zgpr
TD                          65536
SOLVENT                      DMSO
NS                             32
DS                              2
SWH                    8389.262 Hz
FIDRES                 0.128010 Hz
AQ                   3.9059956 sec
RG                            512
DW                       59.600 usec
DE                        6.00 usec
TE                           0.0 K
D1                  1.00000000 sec
d12                 0.00002000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                        6.88 usec
PL1                      -3.00 dB
PL9                      54.23 dB
SFO1               300.1310096 MHz

F2 - Processing parameters
SI                           32768
SF                 300.1300221 MHz
WDW                             EM
SSB                              0
LB                        0.30 Hz
GB                               0
PC                            1.00
```

VJR-90 **4i 13CNMR**



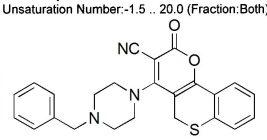

```
Current Data Parameters
NAME        vjr90.08jul10
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100709
Time               14.23
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2048
DS                    4
SWH           18832.393 Hz
FIDRES         0.287360 Hz
AQ             1.7400308 sec
RG                 4096
DW               26.550 usec
DE                6.00 usec
TE                 0.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PL1               -6.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              18.31 dB
PL13              22.00 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677820 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                1.40
```

HRMS 4i

Data:10JULY128A
Sample Name:VJR-90
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Acquired:7/6/2010 4:44:18 PM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:7/6/2010 5:05:34 PM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Charge number:1 Tolerance:5.00(mmu)
Element:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{14}N:0 .. 3, ^{16}O:0 .. 2, ^{32}S:0 .. 1



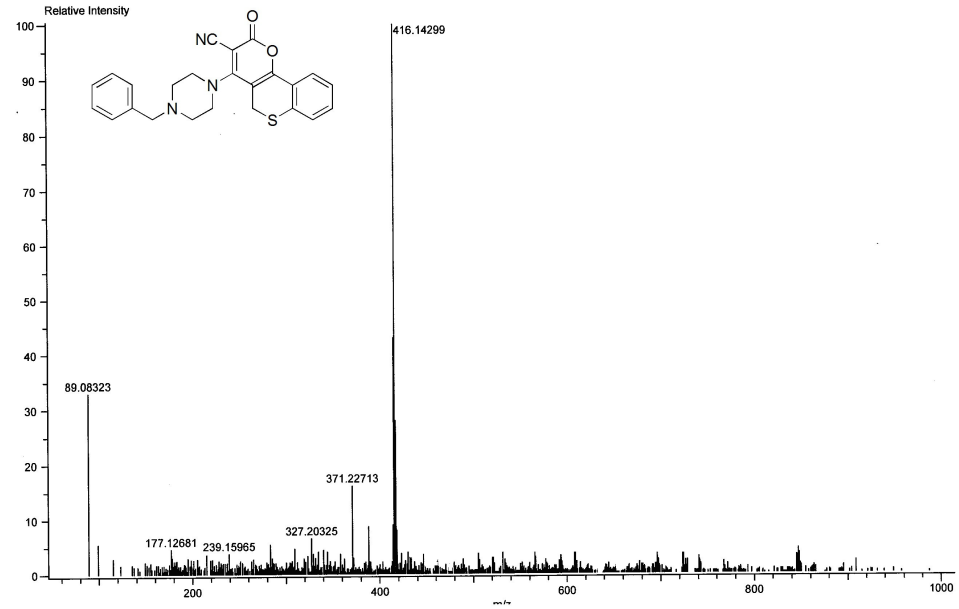
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
416.14299	26995.56	416.14327	-0.28	$^{12}C_{24}{}^{1}H_{22}{}^{14}N_{3}{}^{16}O_{2}{}^{32}S_{1}$	16.5

4i HRMS

Acq. Data Name: 10JULY128A
Internal Sample Id: VJR-90
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.217..0.229);,1.0];Correct Base[5.0%];..
Experiment Date/Time: 7/6/2010 4:44:18 PM

Orifice1 Volt Sweep: 15V
Acquired m/z Range: 50.0..1010.0

Spec. Record Interval: 0.4[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.137[min]
Operator Name: admin



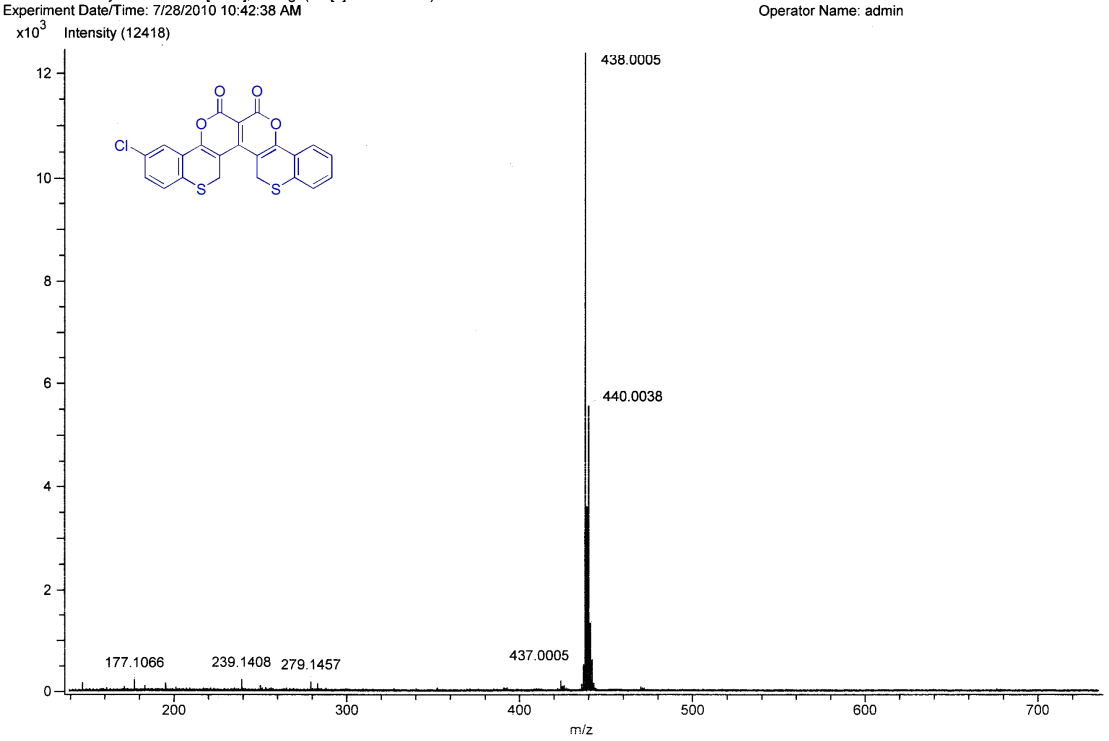
Acq. Data Name: 10JULY332A
Internal Sample Id: VJR-100B
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Correct Base[5.0%];Average(MS[1] 0.168..0.186)
Experiment Date/Time: 7/28/2010 10:42:38 AM

8 HRMS

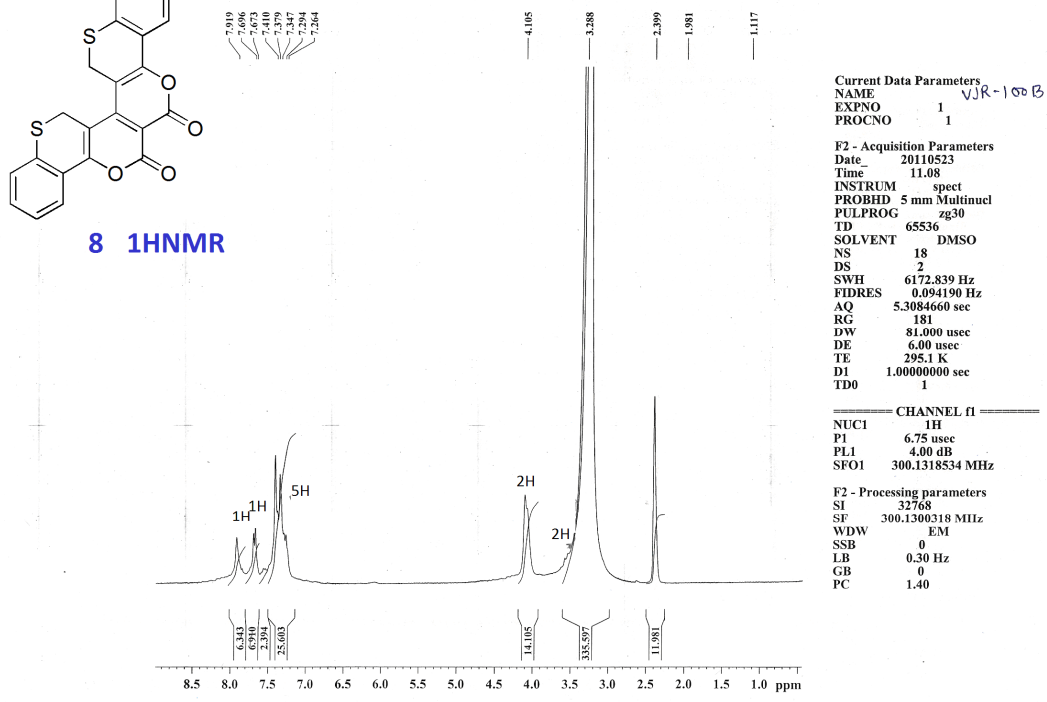
Orifice1 Volt Sweep: 15V
Acquired m/z Range: 50.0..1000.0

Spec. Record Interval: 0.4[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.183[min]

Operator Name: admin



8 1HNMR

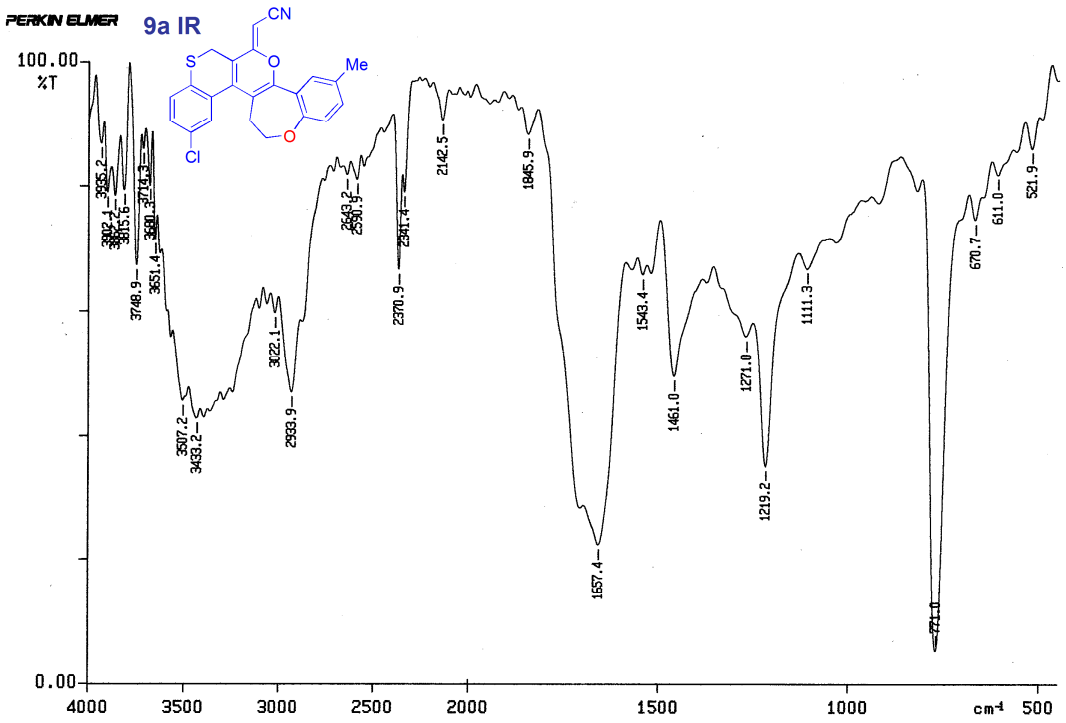


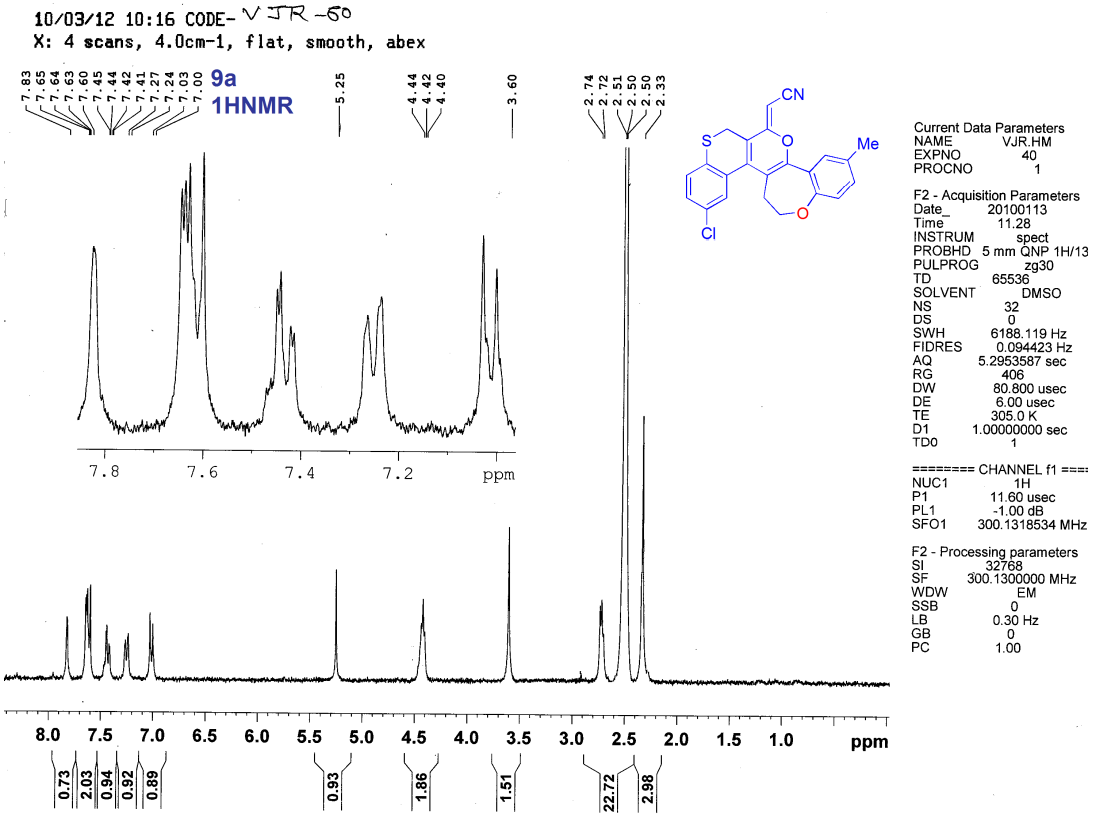
Current Data Parameters
NAME VJR-100B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110523
Time 11.08
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 18
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 6.75 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300318 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40


PERKIN ELMER
9a IR
100.00
%T
0.00
4000
3500
3000
2500
2000
1500
1000
cm-1
500
3935.2
3748.9
3651.4
3507.2
3433.2
3022.1
2933.9
2643.2
2370.9
2142.5
1845.9
1657.4
1543.4
1461.0
1271.0
1219.2
1111.3
771.0
670.7
611.0
521.9
CN
S
O
Me
Cl
O


10/03/12 10:16 CODE- VJR -60
X: 4 scans, 4.0cm-1, flat, smooth, abex
9a
1HNMR
7.83
7.65
7.64
7.63
7.60
7.45
7.44
7.42
7.41
7.27
7.24
7.03
7.00
5.25
4.44
4.42
4.40
3.60
2.74
2.72
2.51
2.50
2.50
2.33
CN
S
O
Me
Cl
O
7.8
7.6
7.4
7.2
ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.73
2.03
0.94
0.92
0.89
0.93
1.86
1.51
22.72
2.98
Current Data Parameters
NAME VJR.HM
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100113
Time 11.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 0
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 406
DW 80.800 usec
DE 6.00 usec
TE 305.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ====
NUC1 1H
P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

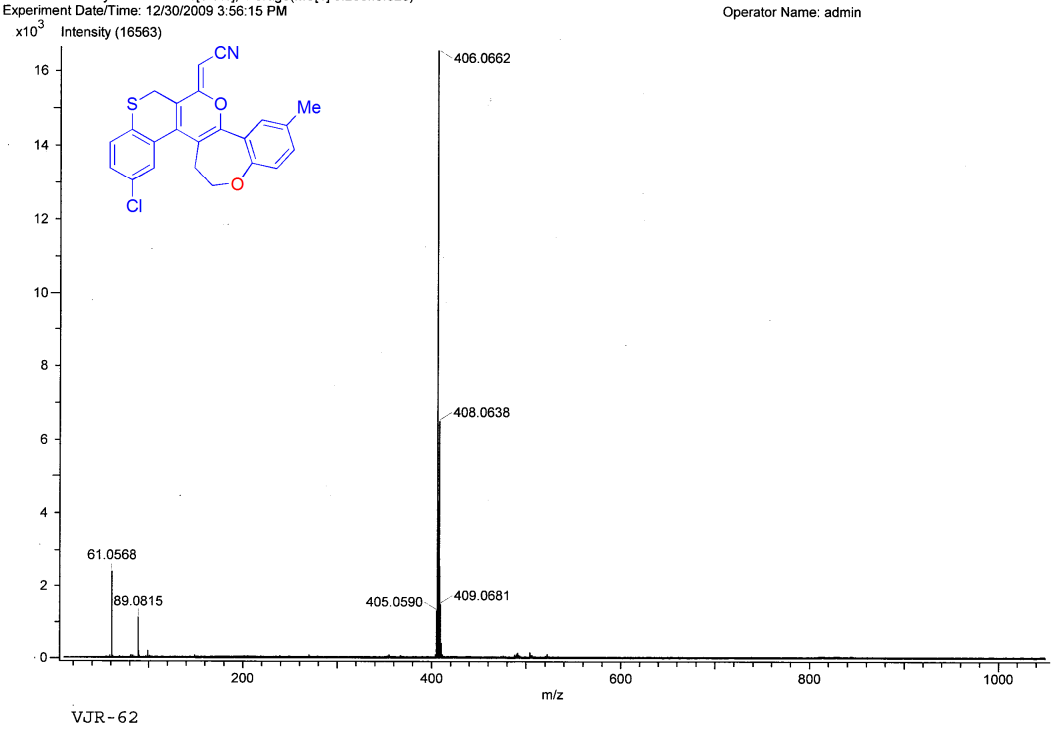
9a HRMS

Acq. Data Name: 9DEC162A
Internal Sample Id: VJR-60
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Correct Base[5.0%];Average(MS[1] 0.283..0.320)
Experiment Date/Time: 12/30/2009 3:56:15 PM

E:\CDRI\NOV09B/DEC09A:9DEC162A
Ion Guide RF Volt: 550V
Orifice1 Volt Sweep: 28V
Acquired m/z Range: 10.0..1050.0

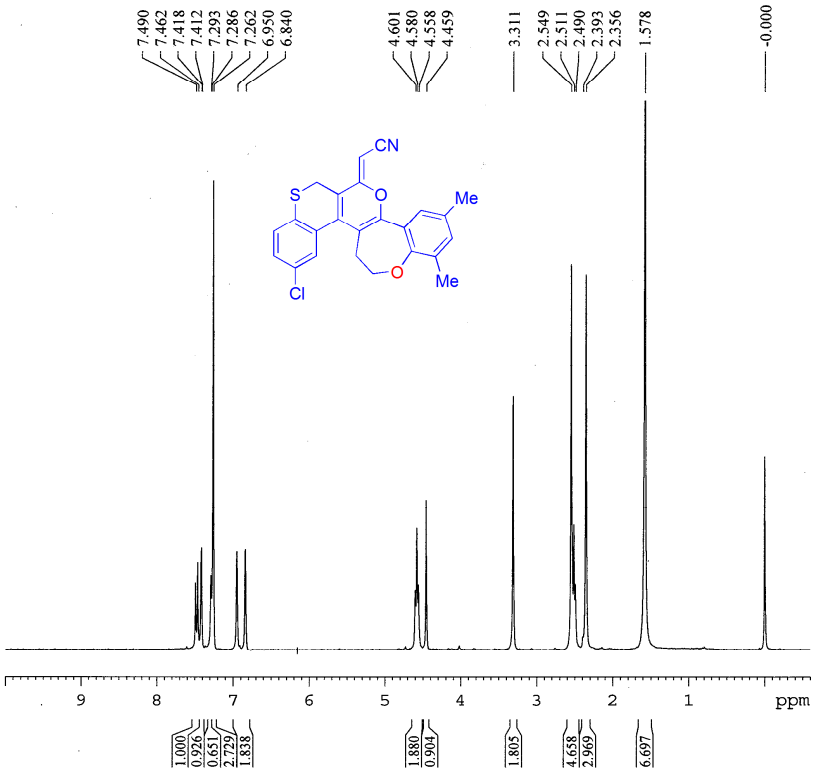
Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 13[V]
Time of Maximum: 0.296[min]

Operator Name: admin



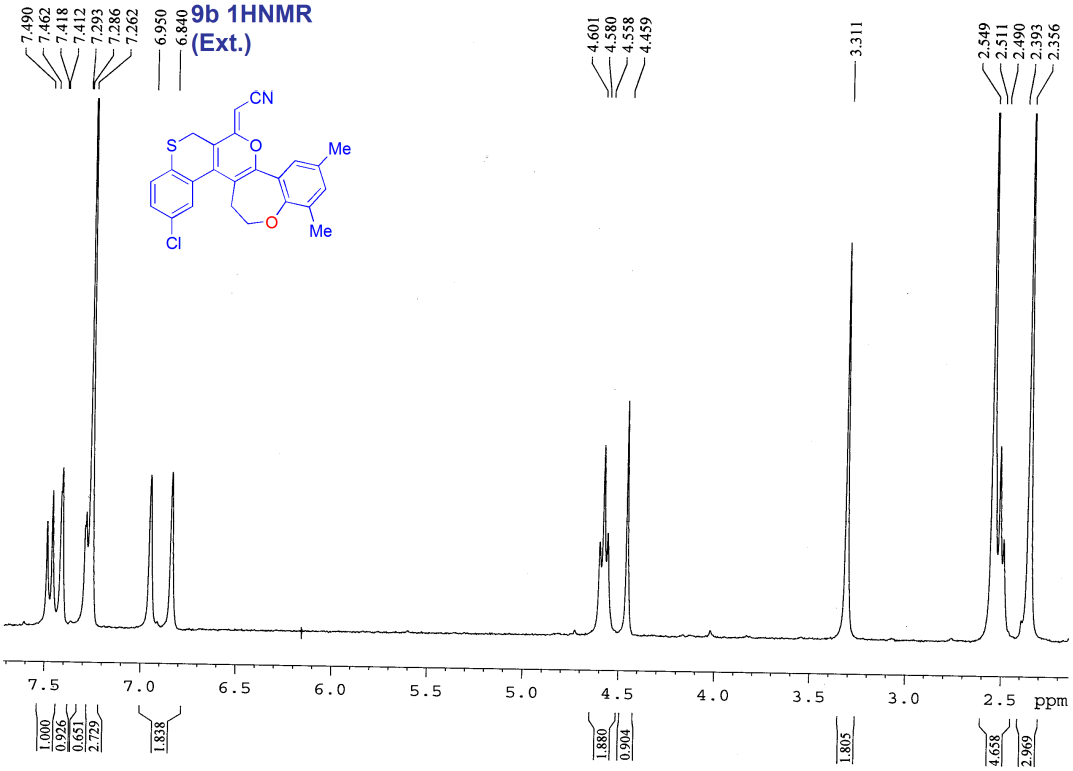
VJR-62

9b 1HNMR




```
Current Data Parameters
NAME          vjr62.temp
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100317
Time               12.02
INSTRUM            spect
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH            9578.544 Hz
FIDRES         0.146157 Hz
AQ             3.4210291 sec
RG                1149.4
DW                52.200 usec
DE                 6.00 usec
TE                296.6 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 6.88 usec
PL1               -3.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300060 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

9b 1HNMR (Ext.)

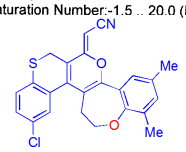


9b HRMS

Data:10JAN030A
Sample Name:VJR-62
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Acquired:1/12/2010 12:00:26 PM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:1/12/2010 12:04:20 PM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Charge number:1
Tolerance:5.00(mmu)
Element:^{12}C:0 .. 24, ^{1}H:0 .. 19, ^{35}Cl:0 .. 1, ^{14}N:0 .. 1, ^{16}O:0 .. 2, ^{32}S:0 .. 1



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
420.08117	33504.99	420.08250	-1.34	$^{12}C_{24}{}^{1}H_{19}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{2}{}^{32}S_{1}$	16.5

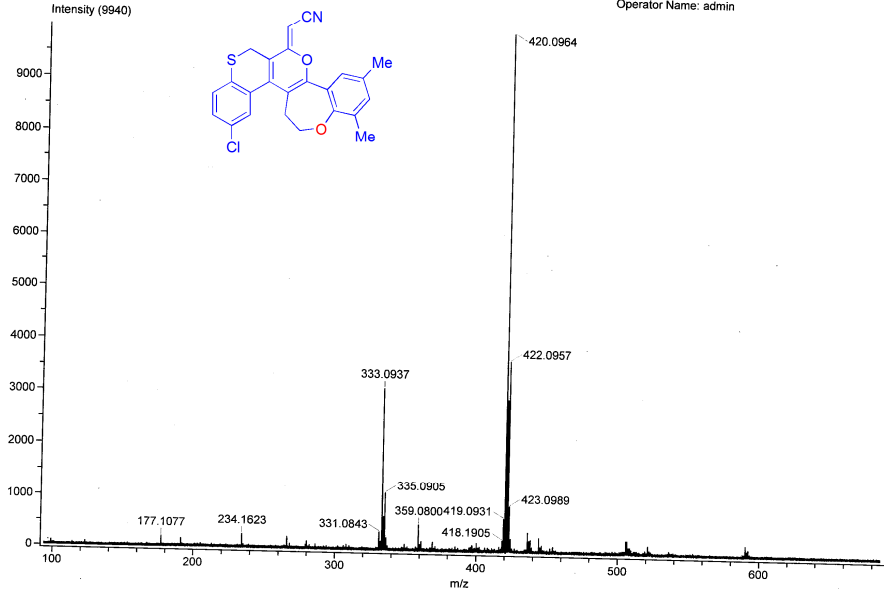
9b HRMS

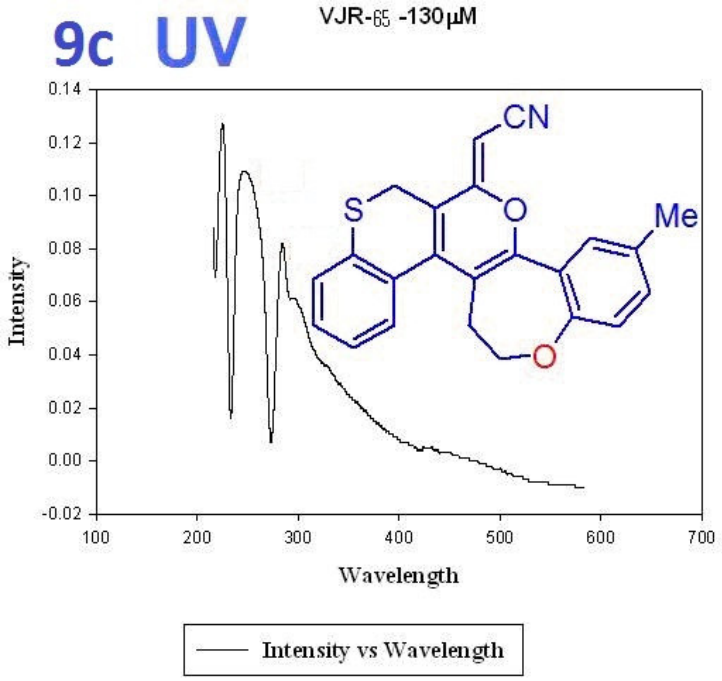
Acq. Data Name: 10JAN030A
Internal Sample Id: VJR-62
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Correct Base[5.0%];Average(MS[1] 0.425..0.441)
Experiment Date/Time: 1/12/2010 12:00:26 PM

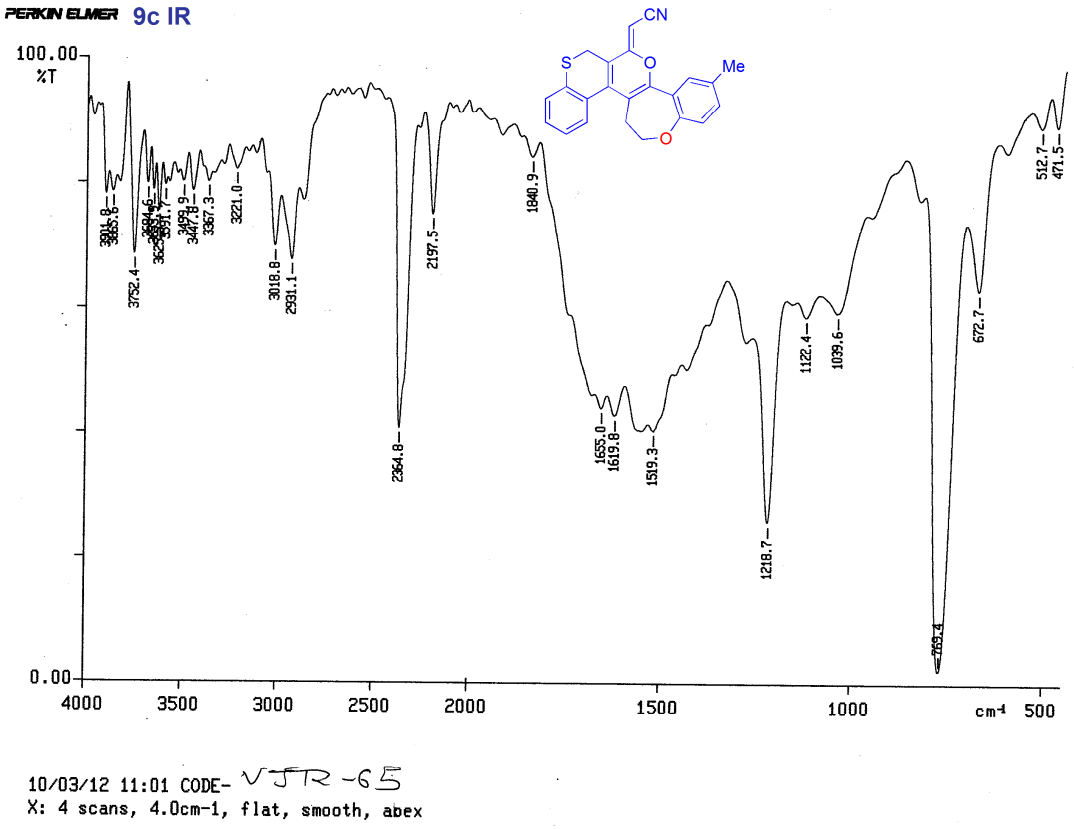
E:\JAN10A\JAN10A:10JAN030A
Ion Guide RF Volt: 300V
Orifice1 Volt Sweep: 18V
Acquired m/z Range: 10.0..1050.0

Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 13[V]
Time of Maximum: 0.430[min]

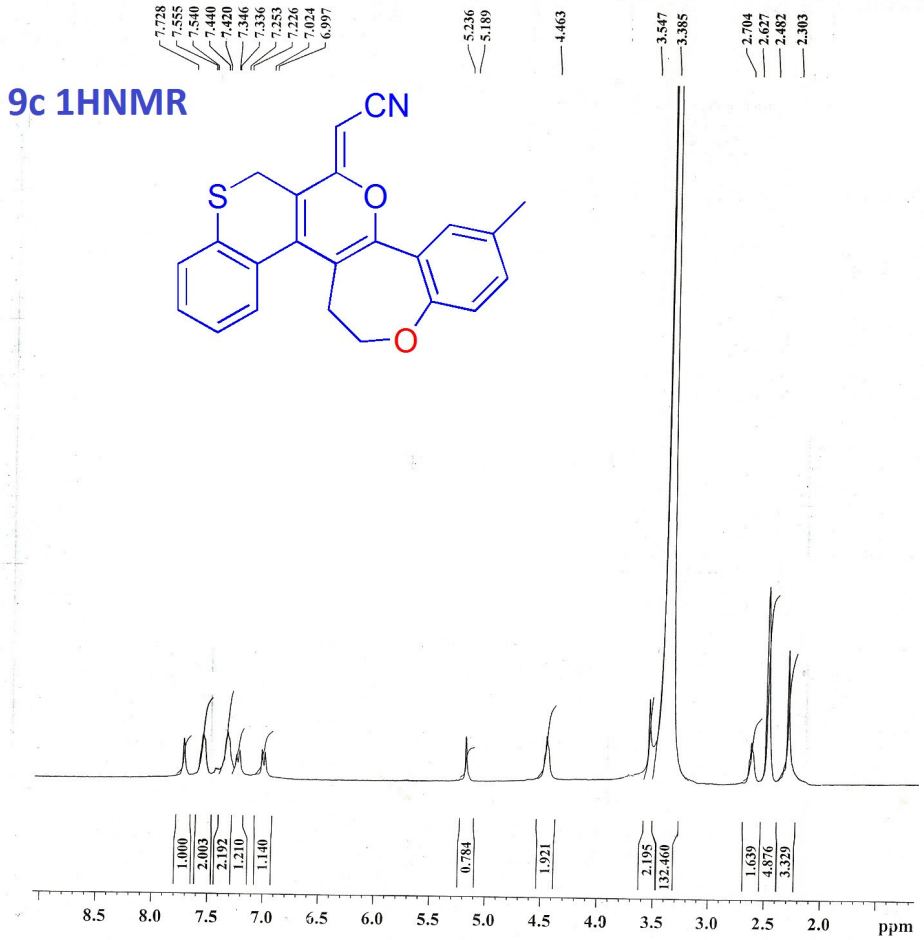
Operator Name: admin







10/03/12 11:01 CODE- VJR-65
X: 4 scans, 4.0cm-1, flat, smooth, abex



Current Data Parameters
NAME VJR-65
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110523
Time 15.32
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 143.7
DW 81.000 usec
DE 6.00 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 6.75 usec
PL1 4.00 dB
SFO1 300.1318534 MHz

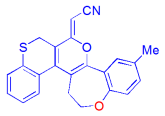
F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

9c HRMS

Data:10JAN029A
Sample Name:VJR-65
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Charge number:1 Tolerance:5.00(mmu)
Element:^{12}C:0 .. 23, ^{1}H:0 .. 18, ^{14}N:0 .. 1, ^{16}O:0 .. 2, ^{32}S:0 .. 1

Acquired:1/12/2010 11:55:29 AM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:1/12/2010 11:59:01 AM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
372.10409	32305.62	372.10582	-1.73	$^{12}C_{23}{}^{1}H_{18}{}^{14}N_{1}{}^{16}O_{2}{}^{32}S_{1}$	16.5

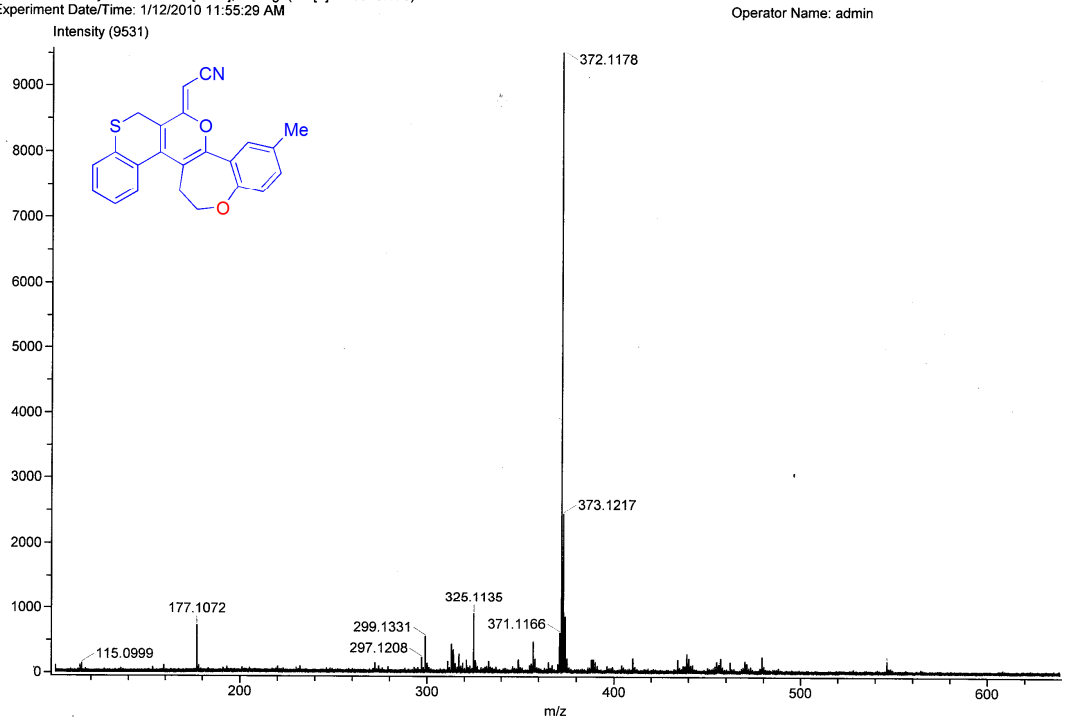
9c HRMS

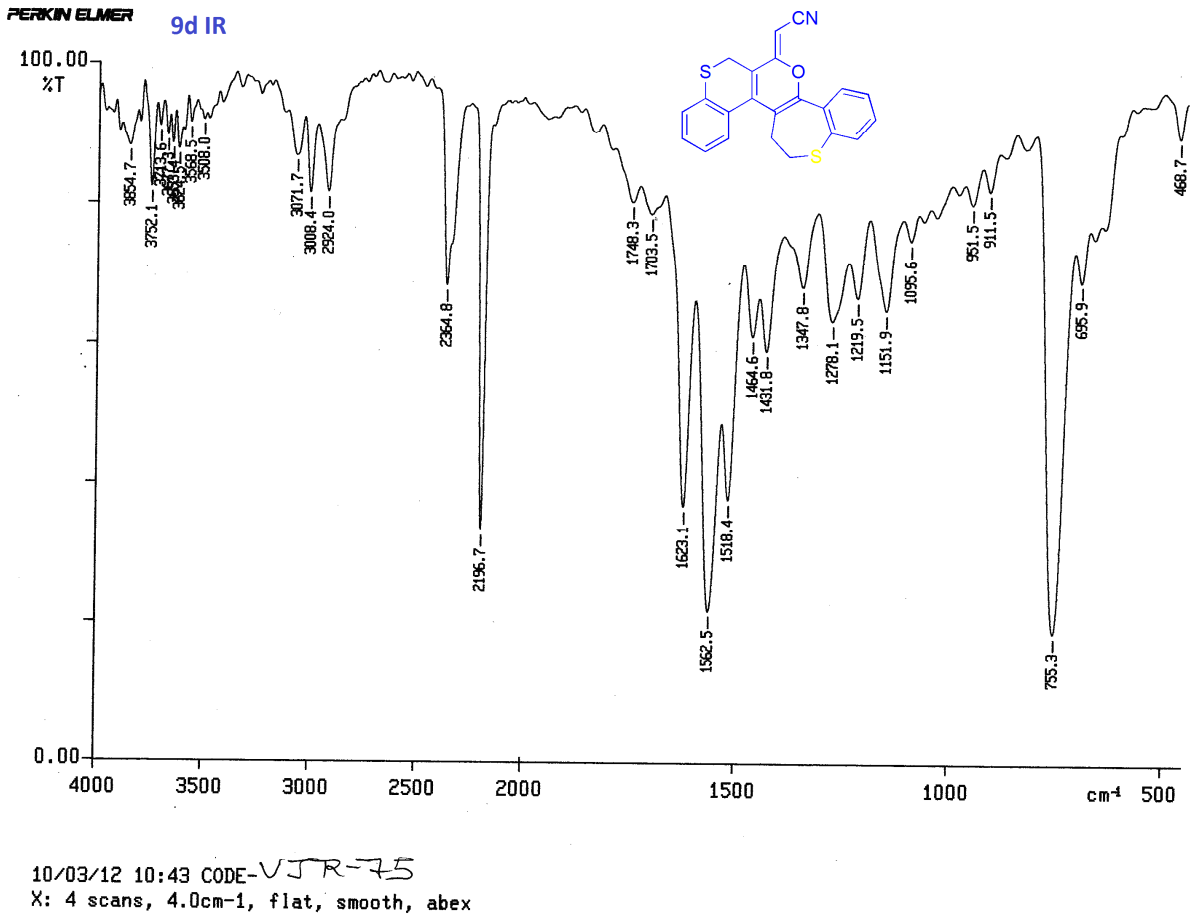
Acq. Data Name: 10JAN029A
Internal Sample Id: VJR-65
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Correct Base[5.0%];Average(MS[1] 0.155..0.176)
Experiment Date/Time: 1/12/2010 11:55:29 AM

E:\JAN10A\JAN10A:10JAN029A
Ion Guide RF Volt: 300V
Orifice1 Volt Sweep: 18V
Acquired m/z Range: 10.0..1050.0

Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 13[V]
Time of Maximum: 0.168[min]

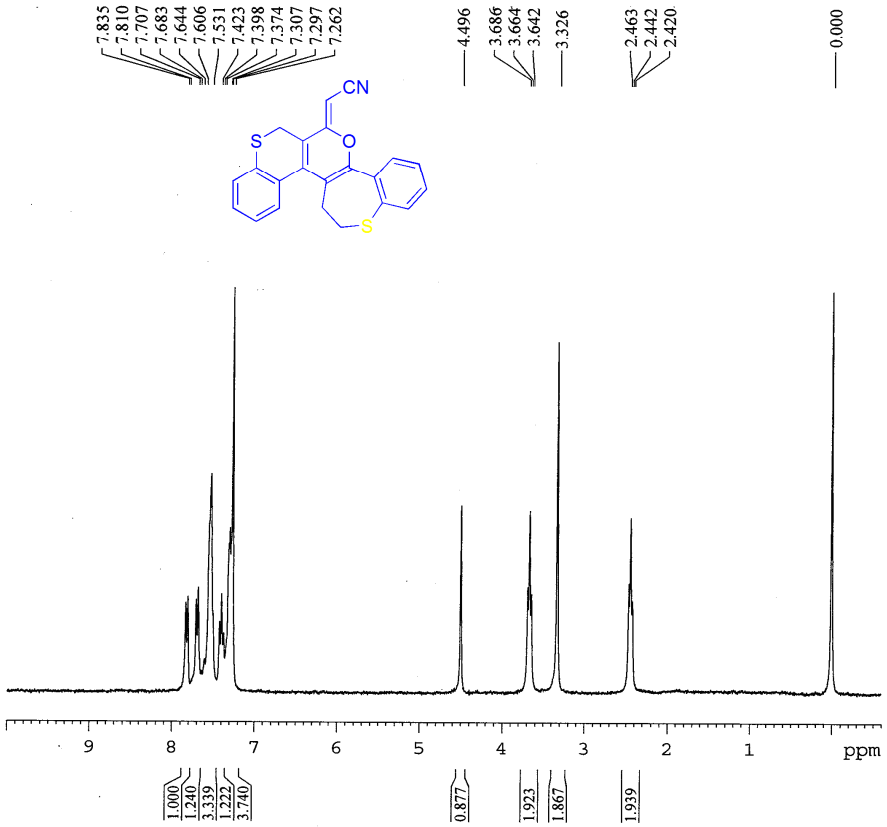
Operator Name: admin




PERKIN ELMER
9d IR
100.00
%T
0.00
4000
3500
3000
2500
2000
1500
1000
cm-1
500
3854.7
3752.1
3508.0
3071.7
3008.4
2924.0
2364.8
2196.7
1748.3
1703.5
1623.1
1562.5
1518.4
1464.6
1431.8
1347.8
1278.1
1219.5
1151.9
1095.6
951.5
911.5
755.3
695.9
468.7
CN
S
O
S
10/03/12 10:43 CODE-VJR-75
X: 4 scans, 4.0cm-1, flat, smooth, abex

VJR-75

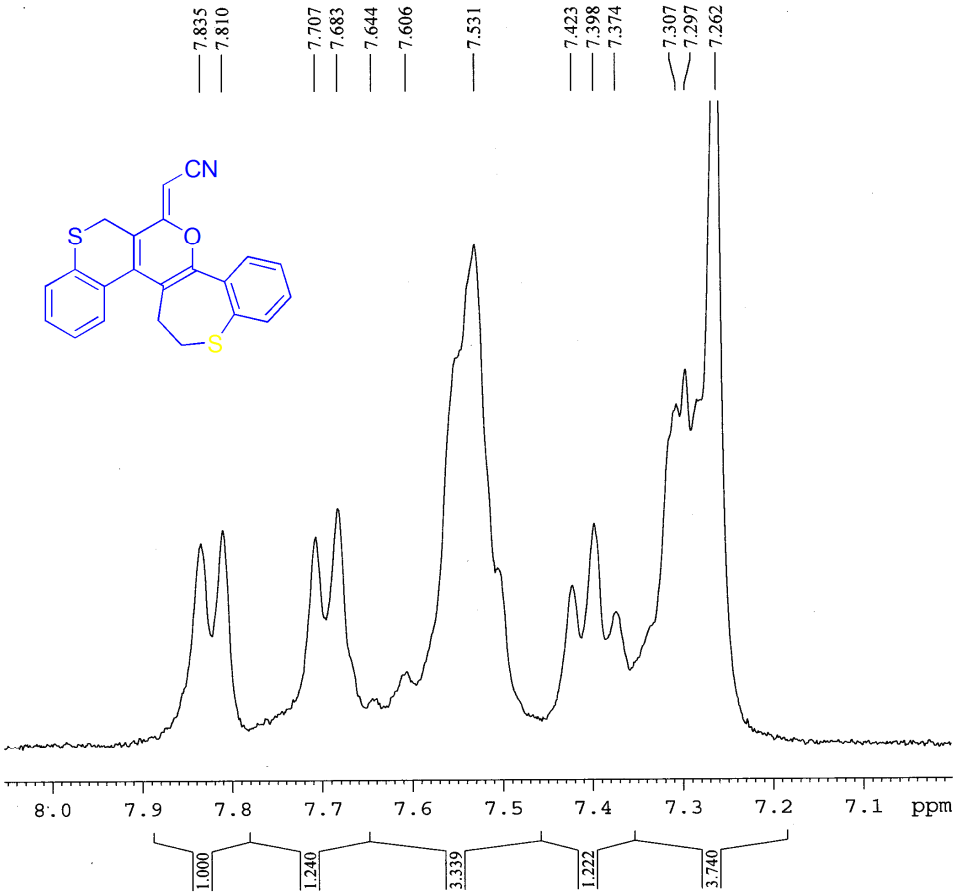
9d 1HNMR




```
Current Data Parameters
NAME                 vjr75.temp
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20100402
Time                      10.22
INSTRUM                   spect
PROBHD    5 mm Multinucl
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          32
DS                           2
SWH                   9578.544 Hz
FIDRES                0.146157 Hz
AQ                    3.4210291 sec
RG                       2580.3
DW                       52.200 usec
DE                        6.00 usec
TE                       299.0 K
D1                    1.00000000 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                        6.88 usec
PL1                      -3.00 dB
SFO1                300.1313246 MHz

F2 - Processing parameters
SI                       32768
SF                  300.1300054 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

VJR-75

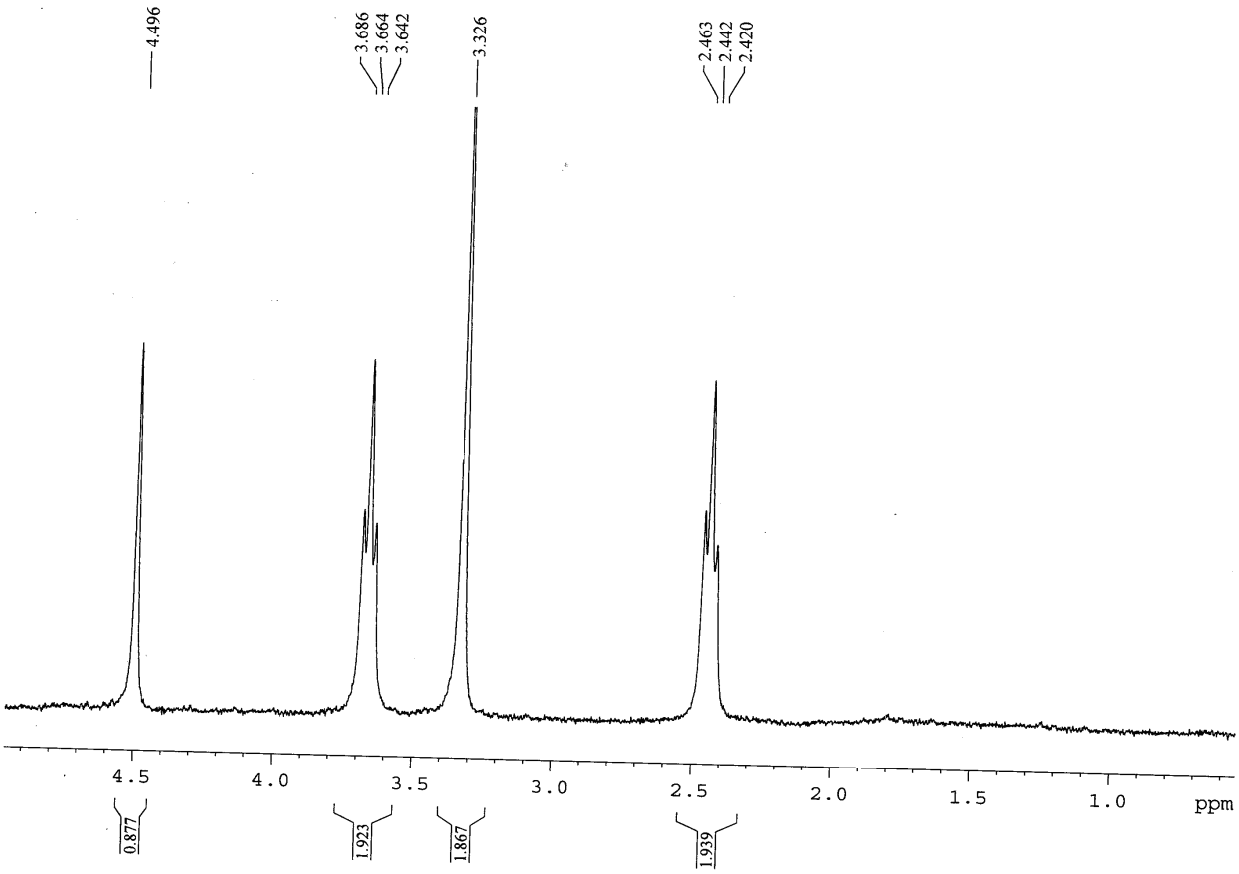
9d 1HNMR (Ext.)




```
Current Data Parameters
NAME          vjr75.temp
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100402
Time              10.22
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH            9578.544 Hz
FIDRES        0.146157 Hz
AQ            3.4210291 sec
RG               2580.3
DW               52.200 usec
DE                6.00 usec
TE               299.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                6.88 usec
PL1              -3.00 dB
SFO1        300.1313246 MHz

F2 - Processing parameters
SI                32768
SF          300.1300054 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

VJR-75

9d 1HNMR (Ext. 2)

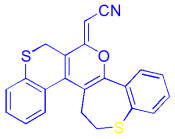


9d HRMS

Data:10FEB010A
Sample Name:VJR-75
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Charge number:1 Tolerance:5.00(mmu)
Element:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{14}N:0 .. 1, ^{16}O:0 .. 1, ^{32}S:0 .. 2

Acquired:2/3/2010 11:01:33 AM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:2/3/2010 11:10:06 AM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)



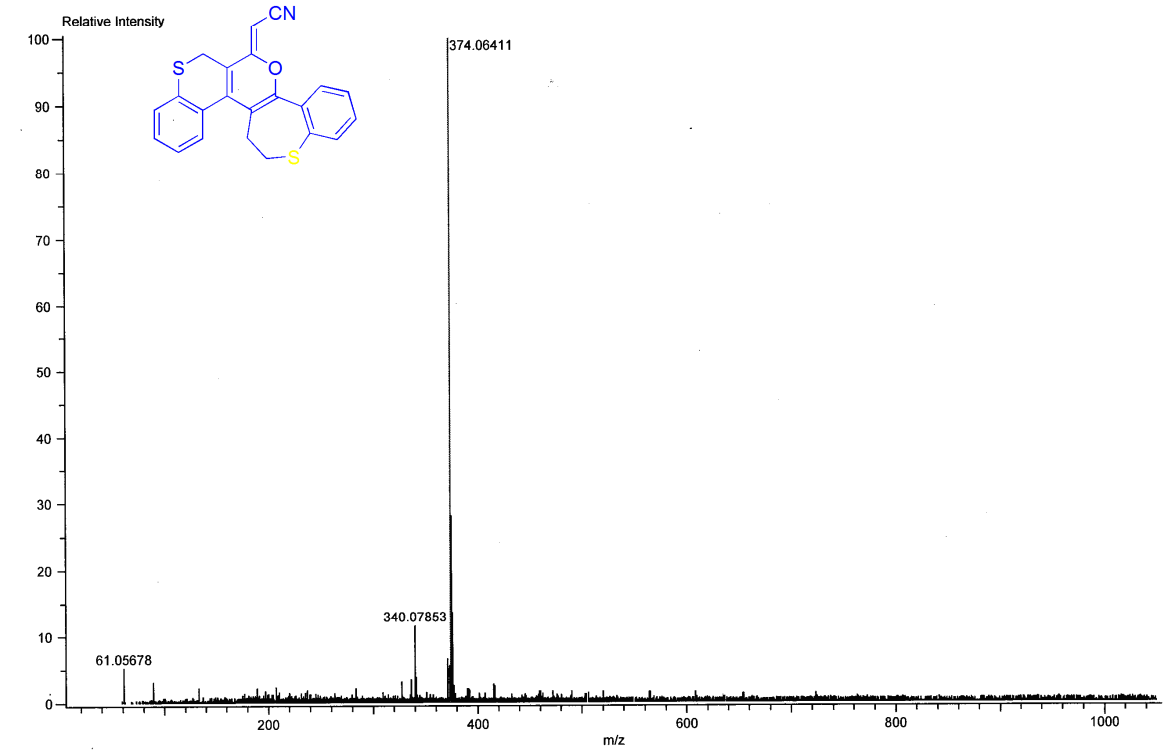
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
374.06411	64954.54	374.06733	-3.22	$^{12}C_{22}{}^{1}H_{16}{}^{14}N_{1}{}^{16}O_{1}{}^{32}S_{2}$	17.5

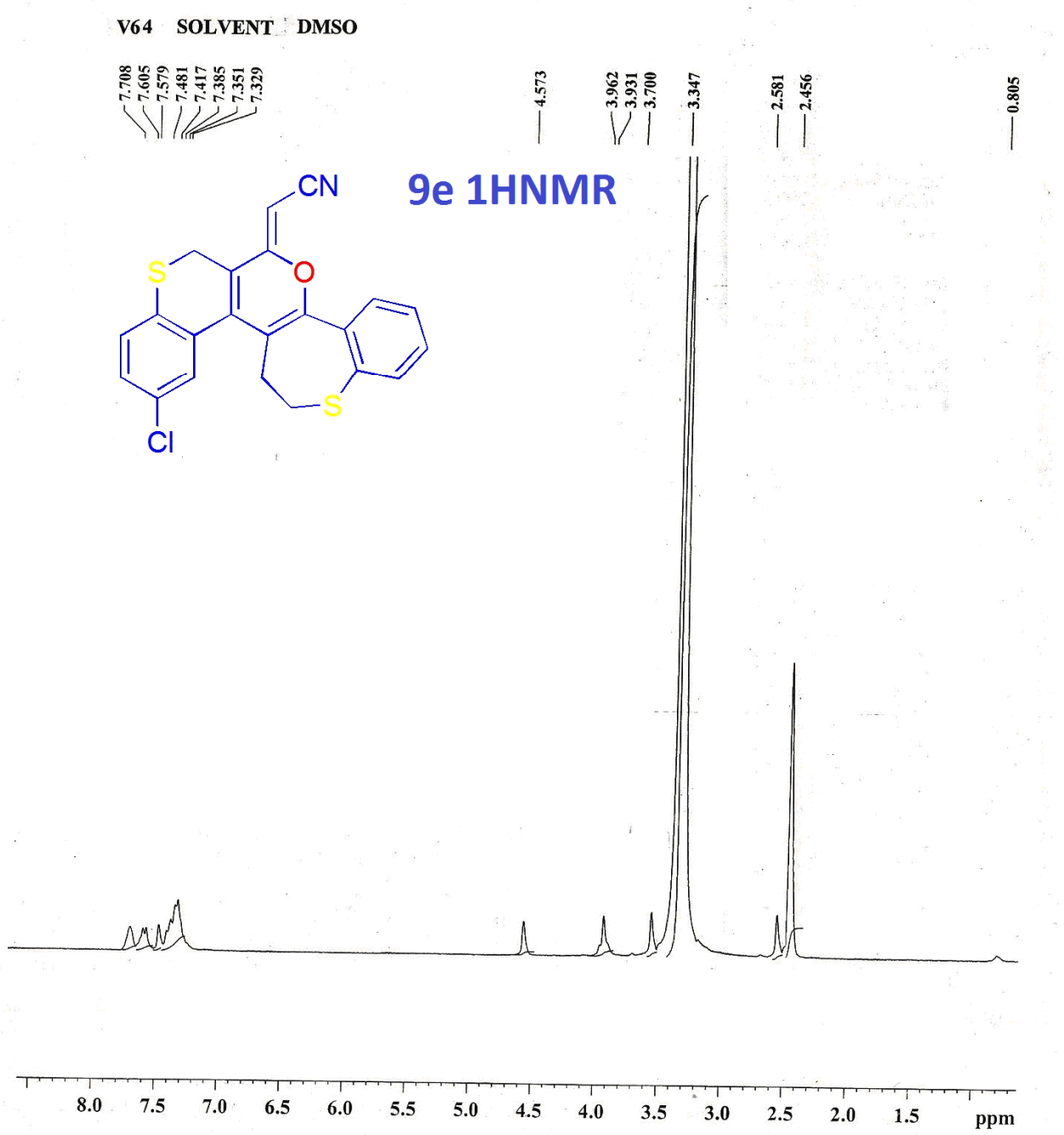
9d HRMS

Acq. Data Name: 10FEB010A
Internal Sample Id: VJR-75
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.206..0.219);,1.0];Average(MS[1] 0.35...
Experiment Date/Time: 2/3/2010 11:01:33 AM

Acq. Data Name(FullPath): E:\JAN10A/FEB10:10FEB010A
Ion Guide RF Volt: 550V
Orifice1 Volt Sweep: 28V
Acquired m/z Range: 10.0..1050.0

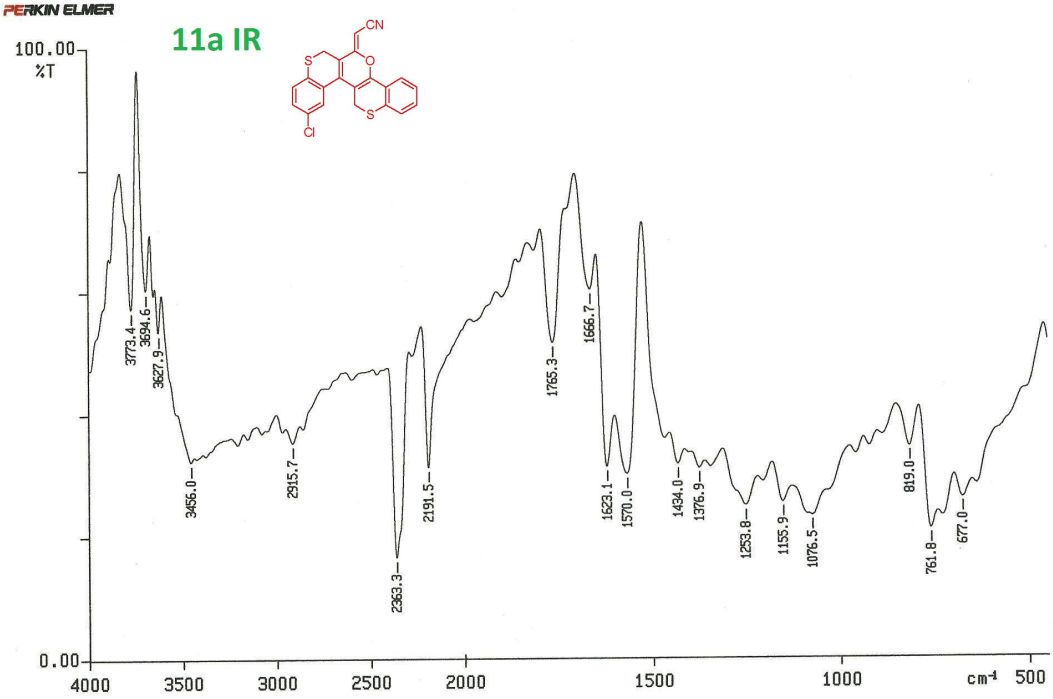
Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 13[V]
Time of Maximum: 0.363[min]
Operator Name: admin





PERKIN ELMER

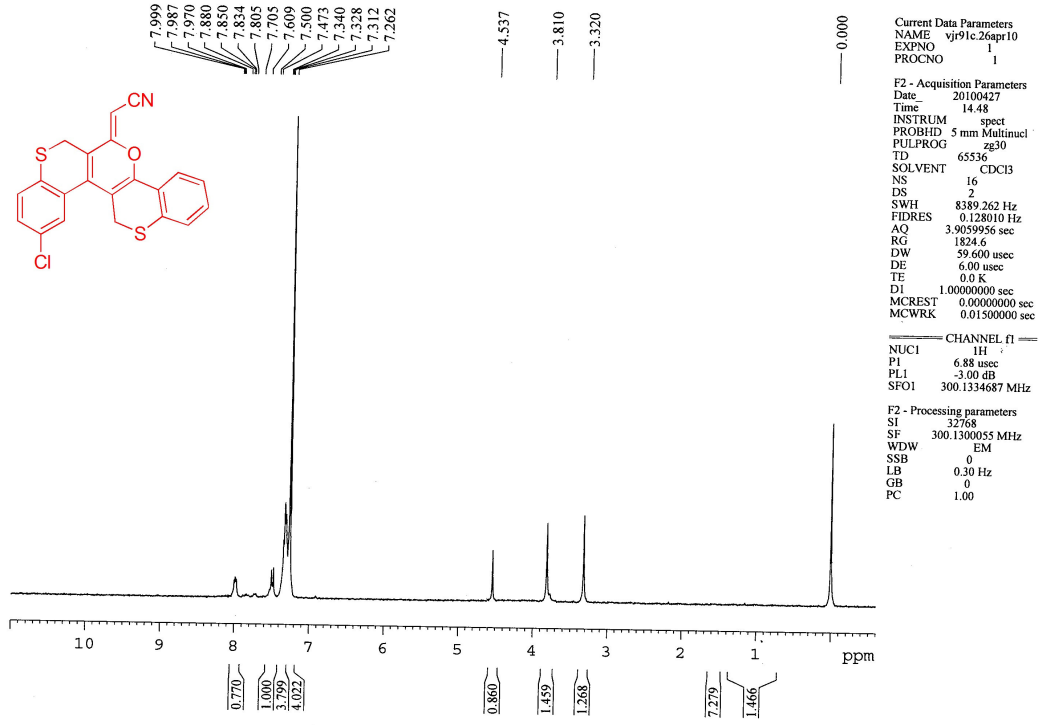
11a IR



10/05/24 10:47 CODE- VJR-91C
X: 4 scans, 4.0cm-1, flat, smooth, abex

11a ^{1}HNMR

VJR-91C



Current Data Parameters
NAME vjr91c.26apr10
EXPNO 1
PROCNO 1

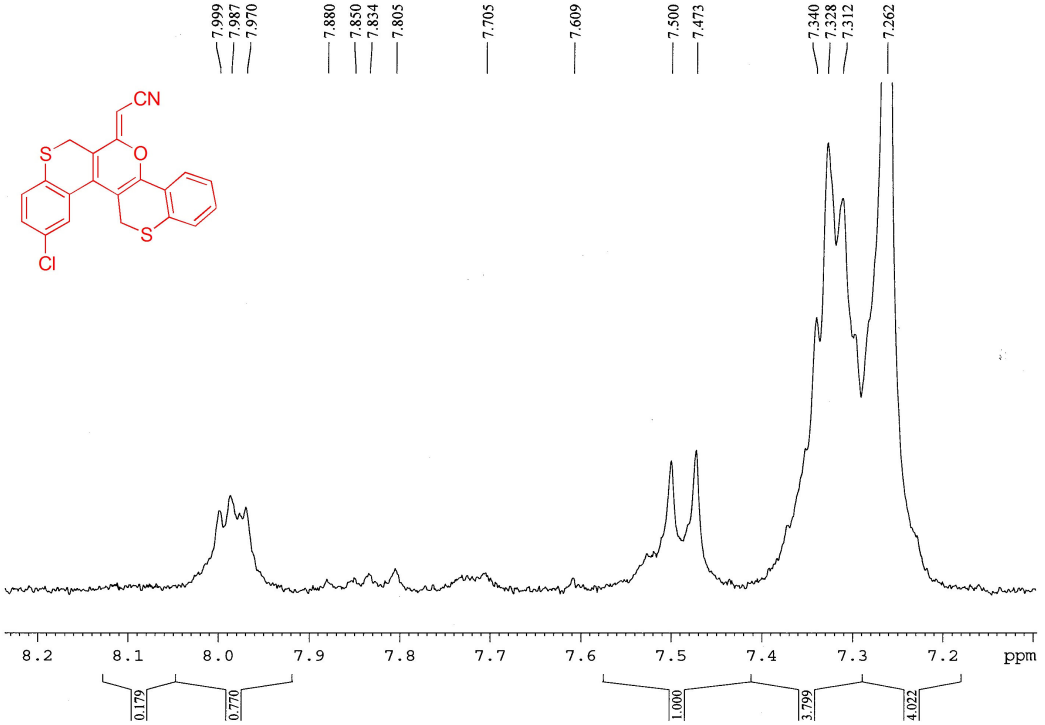
F2 - Acquisition Parameters
Date_ 20100427
Time 14.48
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 1824.6
DW 59.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1334687 MHz

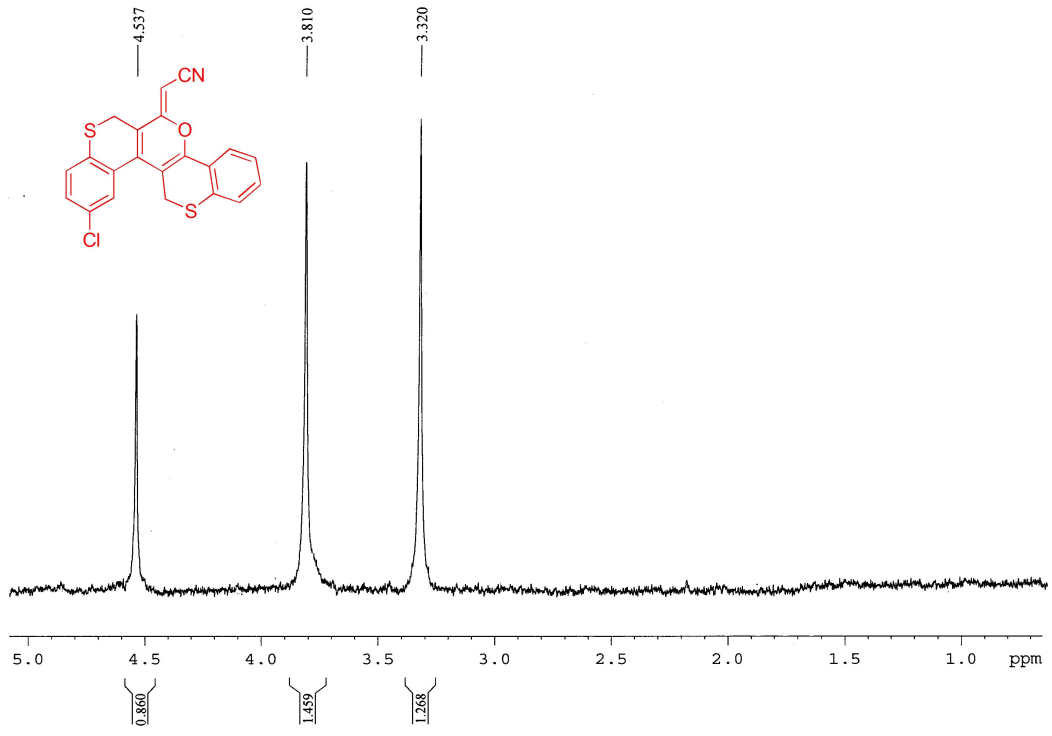
F2 - Processing parameters
SI 32768
SF 300.1300055 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

VJR-91C

11a 1HNMR (Ext.)



VJR-91C **11a 1HNMR (Ext. 2)**



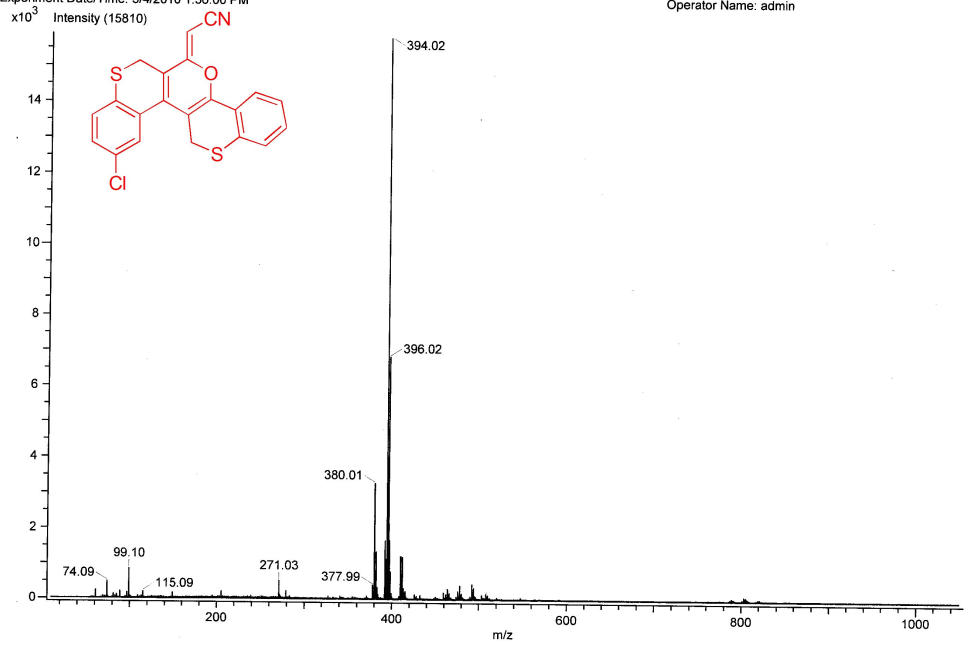
Acq. Data Name: 10MAY061A
Internal Sample Id: VJR-91C
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Correct Base[5.0%];Average(MS[1] 0.098..0.126)
Experiment Date/Time: 5/4/2010 1:56:00 PM

11a Mass

E:\CDRI\MAY10A/MAY10A:10MAY061A
Ion Guide RF Volt: 550V
Orifice1 Volt Sweep: 25V
Acquired m/z Range: 10.0..1050.0

Sample Comments: DART
Spec. Record Interval: 0.4[s]
Ring Lens Volt: 15[V]
Time of Maximum: 0.110[min]

Operator Name: admin

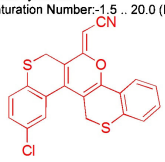


11a HRMS

Data:10JULY132A
Sample Name:VJR-91C
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Acquired:7/6/2010 4:49:50 PM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:7/6/2010 5:14:55 PM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Charge number:1
Tolerance:5.00(mmu)
Element:^{12}C:0 .. 100, ^{1}H:0 .. 200, ^{35}Cl:0 .. 1, ^{14}N:0 .. 1, ^{16}O:0 .. 1, ^{32}S:0 .. 2



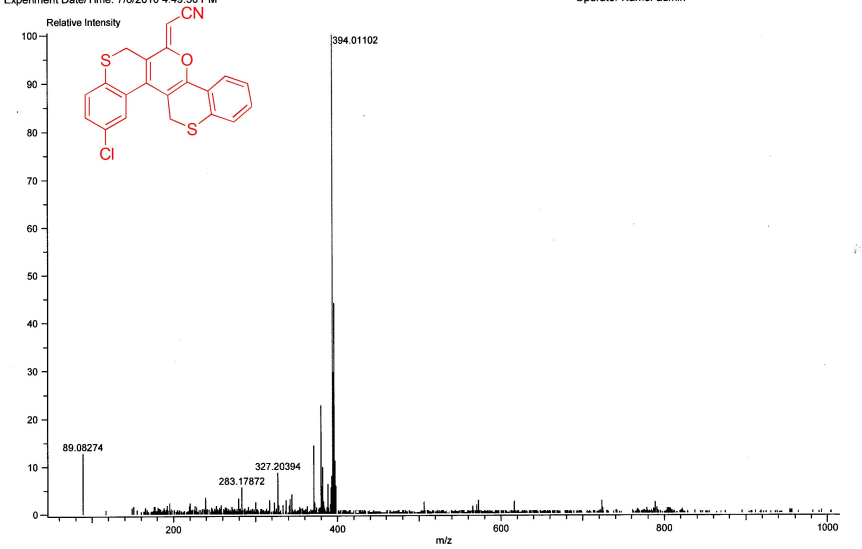
Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
394.01102	47669.90	394.01271	-1.68	$^{12}C_{21}{}^{1}H_{13}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{1}{}^{32}S_{2}$	17.5

Acq. Data Name: 10JULY132A
Internal Sample Id: VJR-91C
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.235..0.243);,1.0];Correct Base[5.0%],...
Experiment Date/Time: 7/6/2010 4:49:50 PM

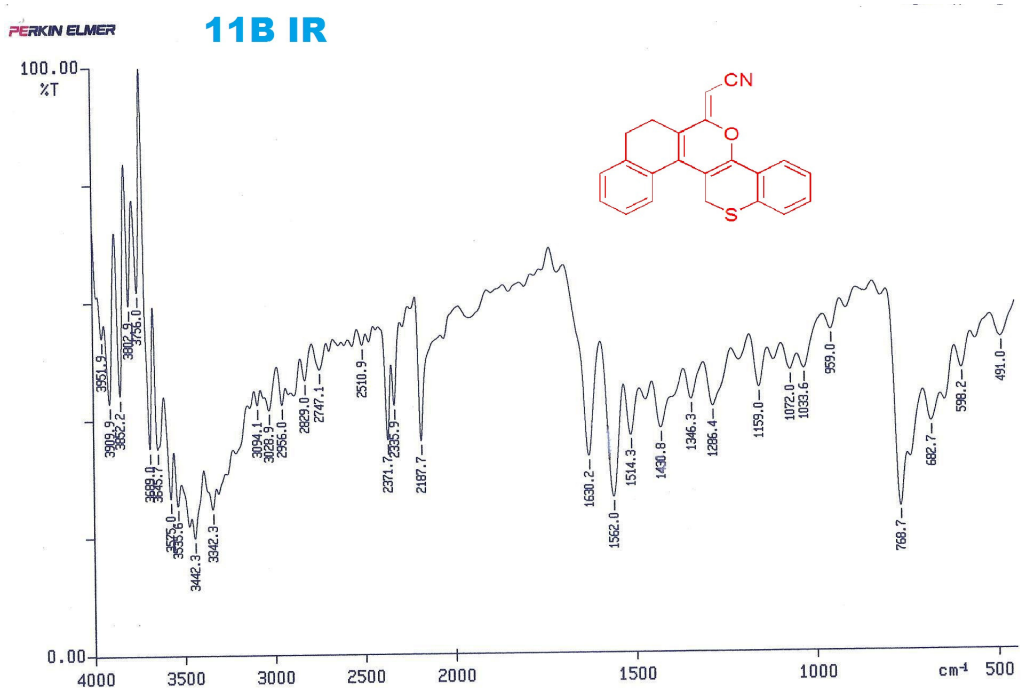
11a HRMS

Orifice1 Volt Sweep: 15V
Acquired m/z Range: 50.0..1010.0

Spec. Record Interval: 0.4[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.164[min]
Operator Name: admin



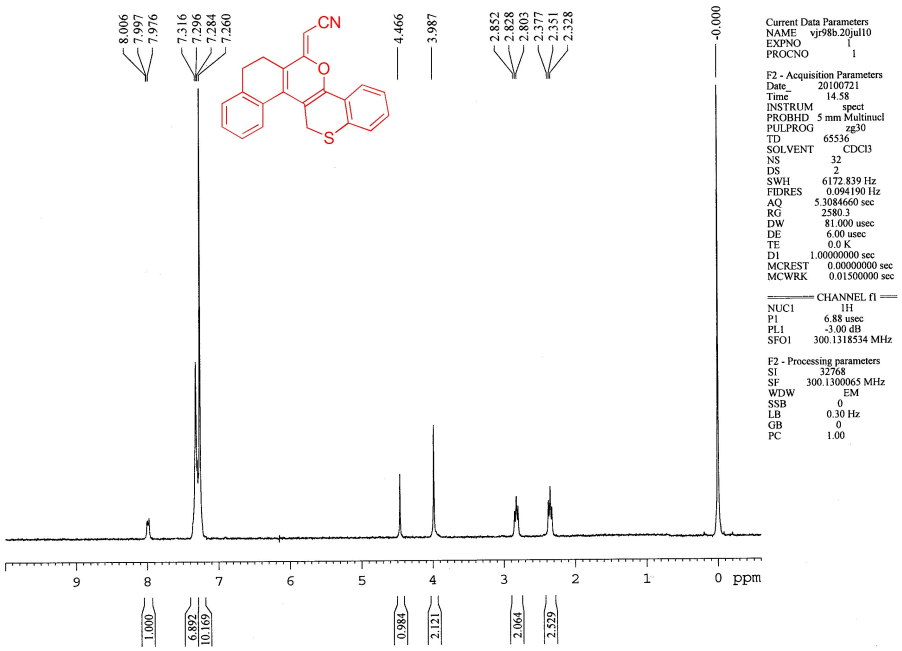
11B IR



10/08/25 10:25 CODE- VJR-98B
X: 4 scans, 4.0cm-1, flat, smooth, abex

VJR-98B

11b 1HNMR



Current Data Parameters
NAME vjr98b.20jul10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100721
Time 14.58
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 2580.3
DW 81.000 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

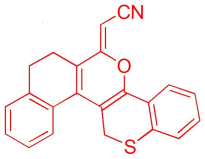
11b HRMS

Data:10JULY331A
Sample Name:VJR-98B
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

Acquired:7/28/2010 10:41:13 AM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:7/28/2010 12:05:23 PM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Charge number:1 Tolerance:3.00(mmu)
Element:^{12}C:0 .. 22, ^{1}H:0 .. 16, ^{14}N:0 .. 1, ^{16}O:0 .. 1, ^{32}S:0 .. 1

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
342.09509	115717.53	342.09526	-0.17	$^{12}C_{22}{}^{1}H_{16}{}^{14}N_{1}{}^{16}O_{1}{}^{32}S_{1}$	16.5

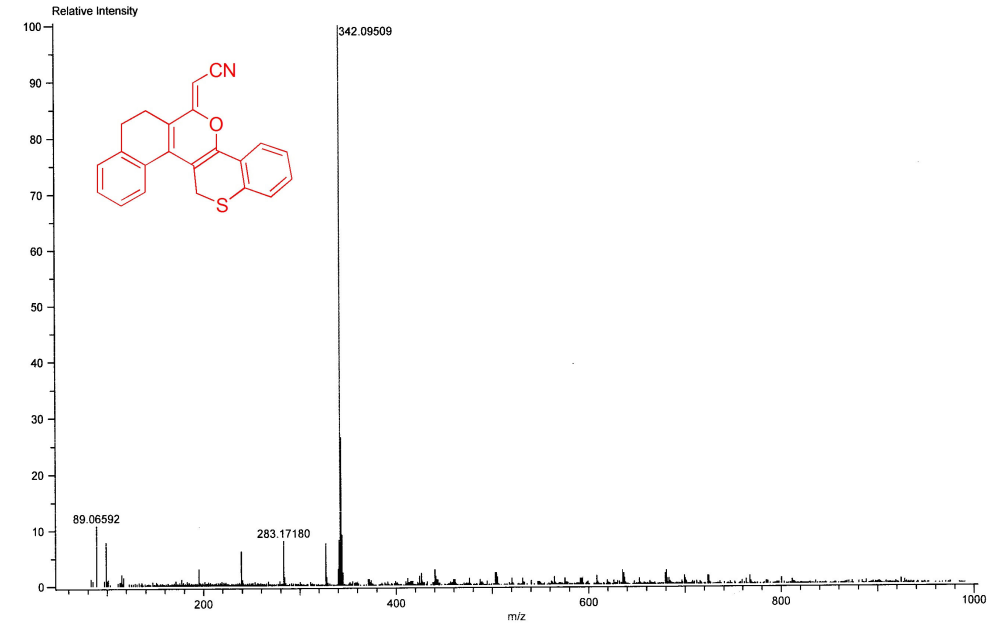


Acq. Data Name: 10JULY331A
Internal Sample Id: VJR-98B
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.216..0.231);,1.0];Correct Base[5.0%];..
Experiment Date/Time: 7/28/2010 10:41:13 AM

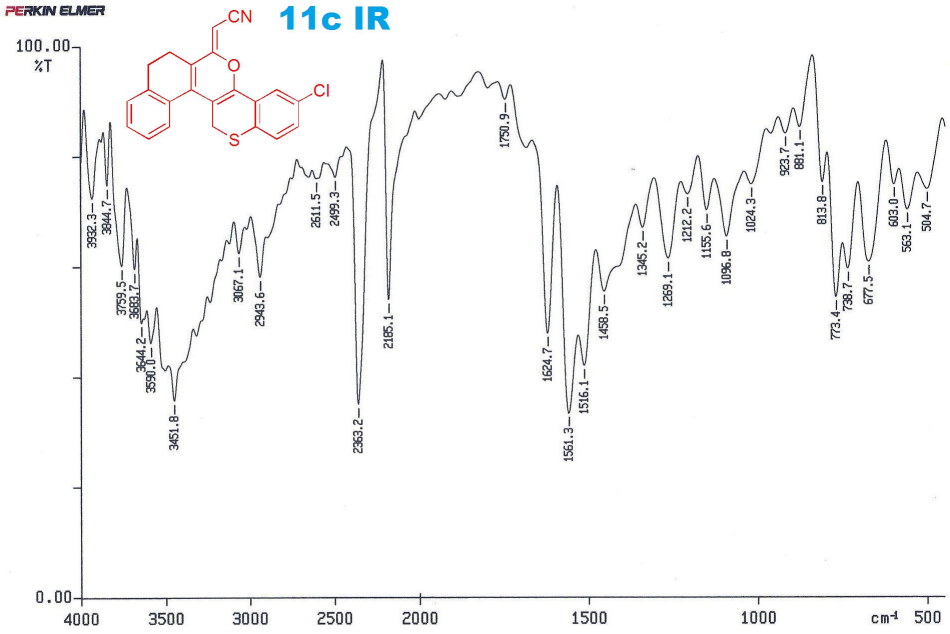
11b HRMS

Orifice1 Volt Sweep: 15V
Acquired m/z Range: 50.0..1000.0

Spec. Record Interval: 0.4[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.124[min]
Operator Name: admin



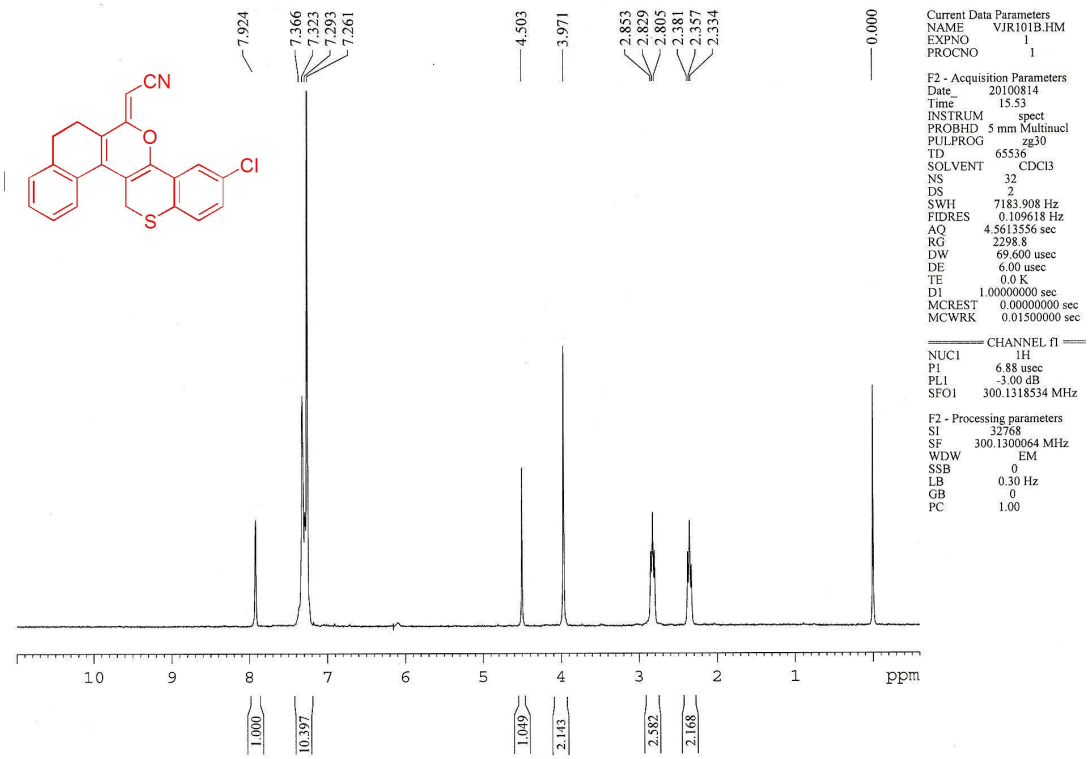
11c IR



10/08/23 10:50 CODE- VJR 101A
X: 4 scans, 4.0cm-1, flat, smooth, abex

VJR-101B

11c 1HNMR



Current Data Parameters
NAME VJR101B.HM
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100814
Time 15.53
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 7183.908 Hz
FIDRES 0.109618 Hz
AQ 4.5613556 sec
RG 2298.8
DW 69.600 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

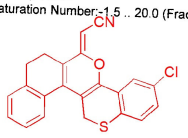
Data:10JULY333A
Sample Name:VJR-101A
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Ave...

11c HRMS

Acquired:7/28/2010 10:44:14 AM
Operator:admin
Mass Calibration data:YOKUDELNA_ES+_2000
Created:7/28/2010 12:13:23 PM
Created by:admin
Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Charge number:1
Element:^{12}C:0 .. 22, ^{1}H:0 .. 15, ^{35}Cl:0 .. 1, ^{14}N:0 .. 1, ^{16}O:0 .. 1, ^{32}S:0 .. 1
Tolerance:5.00(mmu)

Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
376.05452	101999.24	376.05629	-1.77	$^{12}C_{22}{}^{1}H_{15}{}^{35}Cl_{1}{}^{14}N_{1}{}^{16}O_{1}{}^{32}S_{1}$	16.5



Acq. Data Name: 10JULY333A
Internal Sample Id: VJR-101A
Ionization Mode: ESI+
MS Calibration Name: YOKUDELNA_ES+_2000
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%];Smooth[3]];Add[Correct Base[5.0%];Average(MS[1] 0.220..0.231);,1.0];Correct Base[5.0%];...
Experiment Date/Time: 7/28/2010 10:44:14 AM

11c HRMS

Orifice1 Volt Sweep: 15V
Acquired m/z Range: 50.0..1000.0

Spec. Record Interval: 0.4[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.124[min]
Average(MS[1] 0.220..0.231);,1.0];Correct Base[5.0%];...
Operator Name: admin