ELECTRONIC SUPPORTING INFORMATION

A one-pot, three-component reaction for the synthesis of novel 7-arylbenzo[*c*]acridine-5,6-diones

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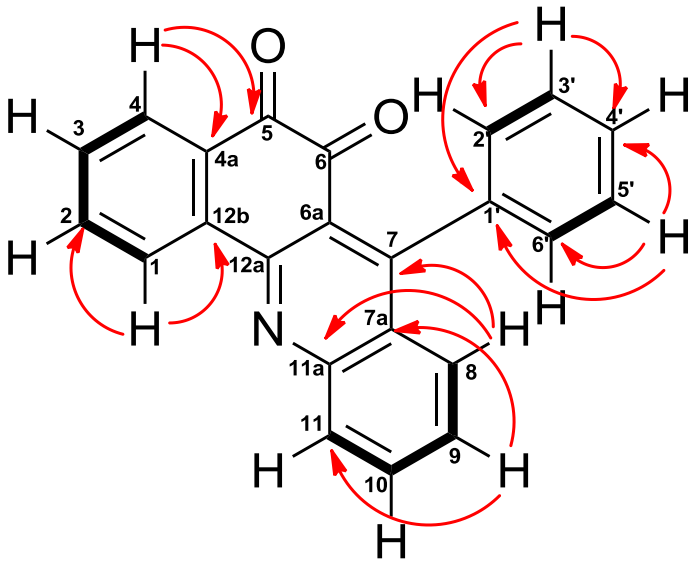
Additional Information on communication

Structure elucidation of compound 5

In IR spectrum, signal at 1684 cm^{-1} revealed the presence of carbonyl group. The molecular formula was established as $C_{23}H_{13}NO_2$ on the basis of ESIHRMS data *m/z*: 358.0818 $[M + Na]^+$ (calcd *m/z* 358.0844 for $[M + Na]^+$). Combined analysis of the ^1H, ^{13}C and DEPT-135 NMR spectroscopic data revealed the presence of thirteen aromatic protons and thirteen sp^2 tertiary (δ 127.2, 128.0, 128.2, 128.6, 128.6, 129.0, 130.0, 131.2, 133.0, 136.1), eight sp^2 quaternary carbons (δ 122.2, 128.0, 131.9, 136.2, 137.8, 151.5, 154.7) and two carbonyl carbon (δ 180.7, 181.3). The proton at δ 9.01 was assigned as H-8 on the basis of splitting patterns of this proton on 10-substituted compounds (**5a**-**n**). The ^1H-^1H COSY correlations H-8 with H-9, H-9 with H-10, H-1 with H-2, H-2 with H-3, H-3 with H-4, H-2′ with H-3′ and H-5′ with H-6′ showed the connectivity of adjacent proton. In the HMBC spectrum two protons resonating at δ 8.18 (H-4 and H-9) presented different HMBC correlations. H-4 was correlated with two carbonyl carbons at δ 180.7 (C-6) and 181.3(C-5) and with a quaternary carbon at δ 128.0 (C-4a) while, H-1 was correlated with quaternary carbon at δ 149.7 (C-12b) and CH at δ 136.0 (C-2). Three Protons (H-3′, 4′ and 5′) at δ 7.55 of phenyl ring attached at C-7 were correlated with two methine carbons at δ 128.0 (C-2′, 6′) and protons at δ 7.18 (H-2′) were correlated with two methine carbons at δ 128.6 (2C, C-3′, 5′) and a methine carbon at 128.6 (C-4′). Proton at δ 9.04 (H-8) was correlated with two quaternary carbon at δ 151.5 (C-11a) and 131.9 (C-7). Proton at δ 7.83 (H-9) was correlated with a quaternary carbon at δ 137.8 (C-7a) and with an aromatic CH at δ 128.2 (C-11). The structure was confirmed by single crystal X-ray crystallography of single crystal.



5

Table S1. ^{1}H (400 MHz) and ^{13}C (100 MHz) data for **5** in $CDCl_3$

	δ_H ppm	δ_c ppm
1	8.17-8.22, m (overlapped with H-4)	130.0
2	7.83-7.90, m (overlapped with H-9)	136.1
3	7.60-7.64, dt (J = 7.8, 0.9 Hz)	131.2
4	8.17-8.22 (overlapped)	129.0
8	9.01, d, 1H, J = 7.9 Hz	127.2
9	7.83-7.90 (overlapped)	133.0
10	7.46-7.52, m (overlapped with H-11)	128.0
11	7.46-7.52 (overlapped)	128.2
2′	7.18, m (overlapped with H-6′)	127.9
3′	7.55, m (overlapped with H-4′, 5′)	128.6
4′	7.55 (overlapped)	128.6
5′	7.55 (overlapped)	128.6
6′	7.18 (overlapped)	127.9

Table S2. Selected bond distances and angles for **5**

Bond distances (Å)

N1-C8	1.328(5)	C9---C11	1.381(5)
N1-C13	1.361(5)	C9---C10	1.479(6)
O1-C10	1.202(5)	C11---C12	1.415(6)
O2-C1	1.203(5)	C11---C18	1.496(5)
C1-C2	1.464(6)	C12---C17	1.412(6)
C1-C10	1.521(6)	C12---C13	1.415(5)
C2-C3	1.392(6)	C13---C14	1.410(5)
C2-C7	1.393(6)	C14---C15	1.358(6)
C3-C4	1.359(7)	C15---C16	1.396(6)
C4-C5	1.376(7)	C16---C17	1.349(6)
C5-C6	1.378(7)	C18---C19	1.377(4)
C6-C7	1.395(6)	C19---C20	1.394(5)
C7-C8	1.481(6)	C20---C21	1.362(4)
C8-C9	1.427(5)	C21---C20	1.362(4)

Bond angles (°)

C8	N1	C13	118.2(4)	O1	C10	C1	116.4(4)
O2	C1	C2	123.1(4)	C9	C10	C1	119.6(4)
O2	C1	C10	118.6(4)	C9	C11	C12	118.5(4)
C2	C1	C10	118.3(4)	C9	C11	C18	122.9(4)
C3	C2	C7	120.1(4)	C12	C11	C18	118.5(4)
C3	C2	C1	119.3(4)	C17	C12	C11	123.9(4)
C7	C2	C1	120.7(4)	C17	C12	C13	117.7(4)
C4	C3	C2	120.9(5)	C11	C12	C13	118.4(4)
C3	C4	C5	119.5(5)	N1	C13	C14	117.3(4)
C4	C5	C6	120.8(5)	N1	C13	C12	122.8(4)
C5	C6	C7	120.4(5)	C14	C13	C12	119.9(4)
C6	C7	C2	118.3(4)	C15	C14	C13	119.7(4)
C6	C7	C8	120.0(4)	C14	C15	C16	120.9(4)
C2	C7	C8	121.7(4)	C17	C16	C15	120.4(4)
N1	C8	C9	123.0(4)	C16	C17	C12	121.3(4)
N1	C8	C7	116.1(4)	C19	C18	C19	119.3(4)
C9	C8	C7	120.9(4)	C19	C18	C11	120.4(2)
C11	C9	C8	119.2(4)	C19	C18	C11	120.4(2)
C11	C9	C10	122.0(4)	C18	C19	C20	120.1(3)
C8	C9	C10	118.8(4)	C21	C20	C19	120.0(4)
O1	C10	C9	124.1(4)	C20	C21	C20	120.5(5)

Reaction optimization

The model reaction of 2-hydroxynaphthalene-1,4-dione (**1**), benzaldehyde (**2**) and aniline (**3**) was investigated to optimize the reaction conditions (Scheme 1). For optimization purpose, the reaction yields were determined using HPLC analysis.

Solvent screening

A range of solvents starting from polar (protic and aprotic) to non polar were screened to achieve the best results. Polar protic solvents (MeOH, EtOH, 1-BuOH, 2-PrOH, *t*-BuOH, PEG Table S1) mainly resulted in **6** with only traces of **5**. Water as a solvent yielded 10% of the desired product, but investigation of water in combination with other reagents like polyphosphoric acid, PEG 6000, acetic acid did not result the desired product. The polar aprotic solvent (Table S2) like DMF, DMSO and THF also produced trace amount of desired product, while ethyl acetate yielded good result (12%, entry 10, Table S2). Toluene yielded 96% of **5** (single spot), while xylene, 1,4-dioxane, 1,1-dichlroethane, dibromomethane, 1,3-dibrmopropane and 1,2-dibromopropane resulted in traces of desired product. The solvent screening depicted (Table S1, S2, S3) chloroform as solvent of choice to move ahead. In most of the cases, the major product obtained was **6**. Formation of **6** was an obstacle for the progress of reaction to yield **5** as the substrates **1** and **3** were used up for its formation.

Table S3. List of polar protic solvents used for the screening in model reaction

S. No.	Solvent	Time (h)	Temperature (°C)	%age of 5[a]	%age of 6[a]
1.	Water	12	100	10	49
2.	Methanol	12	80	-	22
3.	Ethanol	12	80	-	90
4.	1-Butanol	12	120	-	39
5.	2-Propanol	12	90	5	29
6.	t-Butanol	12	80	5	14
7.	Water+ PPA	12	100	-	-
8.	Water+Acetic acid	12	100	-	55
9.	Water+PEG 6000	12	100	-	-
10.	PEG 6000	12	80	-	60
11.	Butan-2-one	12	80	8	14

[a]yield determined using HPLC analysis

Table S4. List of polar aprotic solvents used for the screening in model reaction

S. No.	Solvent	Time (h)	Temperature (°C)	%age of 5[a]	%age of 6[a]
1.	DMF	12	120	5	60
2.	NMP	12	120	-	80
3.	DMSO	12	120	7	-
4.	ACN	12	80	-	-
5.	ACN+PPA	12	80	-	12
6.	Benzonitrile	12	120	-	-
7.	Nitromethane	12	120	-	48
8.	Nitrobenzene	12	120	-	-
9.	DCM	12	40	-	25
10.	EtOAc	12	70	12	21
11.	Acetone	12	40	-	13
12.	THF	12	70	5	15

[a]yield determined using HPLC analysis

Table S5. Non-polar solvents used for the screening in model reaction

S. No.	Solvent	Time (h)	Temperature (°C)	%age of 5[a]	%age of 6[a]
1.	Xylene	12	120	-	23
2.	Toluene	12	110	-	96
3.	Heptane	12	100	-	27
4.	Carbon tetrachloride	12	80	-	30
5	1,4-Dioxane	12	80	5	45
6	Diethyl ether	12	35	-	7
7	Dibutyl ether	12	120	-	7
8	Chloroform	12	50	16	30
9	1,1-Dichloroethene	12	60	9	30
10	Dibromomethane	12	100	-	21
11	Bromobenzene	12	120	-	51
12	1,3-Dibromopropane	12	120	7	7
13	1,2-Dibromoethane	12	120	-	36
14	Chlorobenzene	12	130	-	72

[a]yield determined using HPLC analysis

Considering other optimization parameters, screening of time of addition of **2** to the reaction mixture containing **1**, **3** and *p*-TSA in refluxing $CHCl_3$ was summarized in Table S4.[1] Here, the best results were obtained when all the three reactants **1**, **2** and **3** were mixed together in 20 mol % *p*-TSA using chloroform as solvent under refluxing for 12 h (entry 7, Table S4).

Table S6. Effect of time of addition of reagent[a]

S.No.	Time of addition[a] (min)	Time (h)	%age of 5[b]	%age of 6[b]
1	180	12	-	74
2	120	12	-	70
3	60	12	-	64
4	30	12	16	37
5	15	12	57	-
6	10	12	64	-
7	0	12	75	-

[a]time at which **2** was added to the reaction mixture of **1** and **3** in *p*-TSA; [b]yield determined using HPLC analysis

The progress of reaction was studied with respect to time and the results are summarized in Table S5. The optimized time for completion of the reaction was 6 h as both decreased and increased reaction times led to the reduced yields.

Table S7. Time study of the reaction

S. No.	Time (h)	%age of Intermediate IV[a]	%age of 5[a]
1	0.0	-	-
2	0.5	23	6
3	1.0	56	11
4	1.5	55	15
5	2.0	53	19
6	2.5	45	22
7	3.0	42	34
8	3.5	42	42
9	4.0	40	43
10	4.5	31	49
11	5.0	27	45
12	5.5	33	50
13	6.0	-	92

[a]yield determined using HPLC analysis

A variety of Lewis acid were investigated under refluxing condition in various solvents and summarized in Table S6. Lewis acid screening resulted $NbCl_5$ as a surrogate catalyst for the model reaction.

Table S8. Lewis acid Screening

S.No.	Time (h)	Solvent	Lewis acid	%age of 5[a]	%age of 6[a]
1	6	Water	$AlCl_3$	-	-
2	6	toluene	$AlCl_3$	-	-
3	6	Water	$AlCl_3$	7	39
4	6	Chloroform	$AlCl_3$	7	-
5	6	Water	$BF_3.Et_2O$	7	74
6	6	Chloroform	$BF_3.Et_2O$	25	10
7	6	Water	$ZnCl_2$	41	24
8	6	Chloroform	$ZnCl_2$	35	51
9	6	Water	$SnCl_2$	-	76
10	6	Chloroform	$SnCl_2$	12	-
11	6	Water	$TiCl_4$	-	-
12	6	Chloroform	$TiCl_4$	22	-
13	6	Water	$FeCl_3$	70	43
14	6	Chloroform	$FeCl_3$	50	-
15	6	Water	$NbCl_5$	-	66
16	6	Chloroform	$NbCl_5$	78	-
17	6	Water	CsCl	7	82
18	6	Chloroform	CsCl	46	-

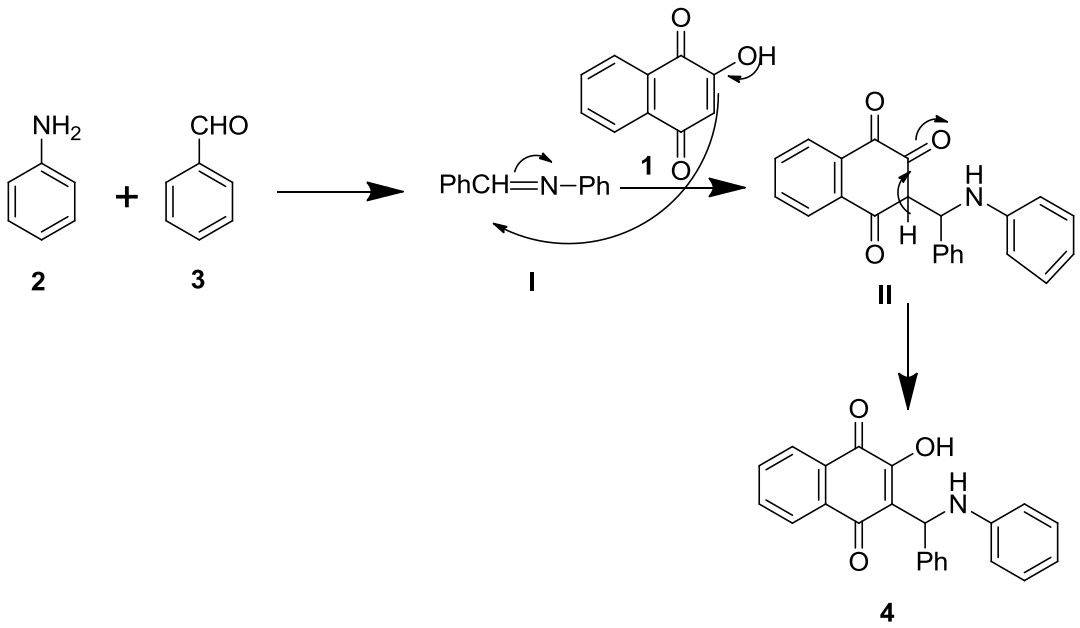
[a]yield determined using HPLC analysis

Acidic catalyst screening (Table S7) includes the investigation of methane sulphonic acid, sulphuric acid, acetic acid, hydrochloric acid, nitric acid, phosphoric acid, formic acid in comparison to *p*-TSA in both water and chloroform, but only *p*-TSA was able to give the desired product. The reaction worked well with only *p*-TSA while failed with all other acids.

Table S9. Screening of various acidic catalyst for reaction optimization

S. No.	Time (h)	Solvent	Catalyst	%age of 5[a]	%age of 6[a]
1	6	Water	*p*-TSA	-	75
2	6	Chloroform	*p*-TSA	94	-
3	6	Water	Methane sulphonic acid	-	-
4	6	Chloroform	Methane sulphonic acid	-	50
5	6	Water	Sulphuric acid	-	21
6	6	Chloroform	Sulphuric acid	-	-
7	6	Water	Acetic acid	-	-
8	6	Chloroform	Acetic acid	-	-
9	6	Water	Hydrochloric acid	-	-
10	6	Chloroform	Hydrochloric acid	-	-
11	6	Water	Nitric acid	-	-
12	6	Chloroform	Nitric acid	-	-
13	6	Water	Phosphoric acid	-	70
14	6	Chloroform	Phosphoric acid	-	12
15	6	Water	Formic acid	-	80
16	6	Chloroform	Formic acid	-	-

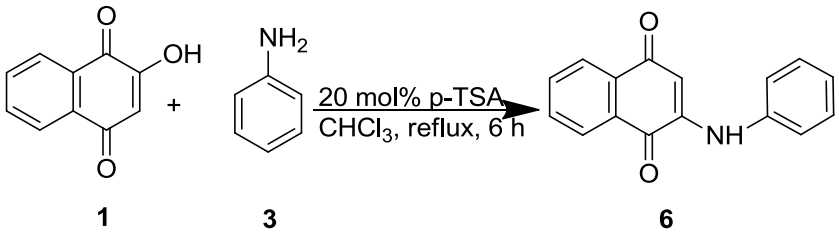
[a]yield determined using HPLC analysis



Scheme S1. Plausible mechanism for the formation of 4.[2]

To discard the possibility of reaction proceeding via 1,4-conjugate addition (Doebner–Miller reaction)

2-Hydroxynaphthalene-1,4-dione **1**, upon reaction with aniline **3**, yielded compound **6** (isolated and characterized). The compound **6** was reacted, *ex-situ*, with benzaldehyde under different reaction conditions (Table S8) to yield product **5**. The failure of these reactions led to conclusion of ruling out this possibility.



1 **3** **6**

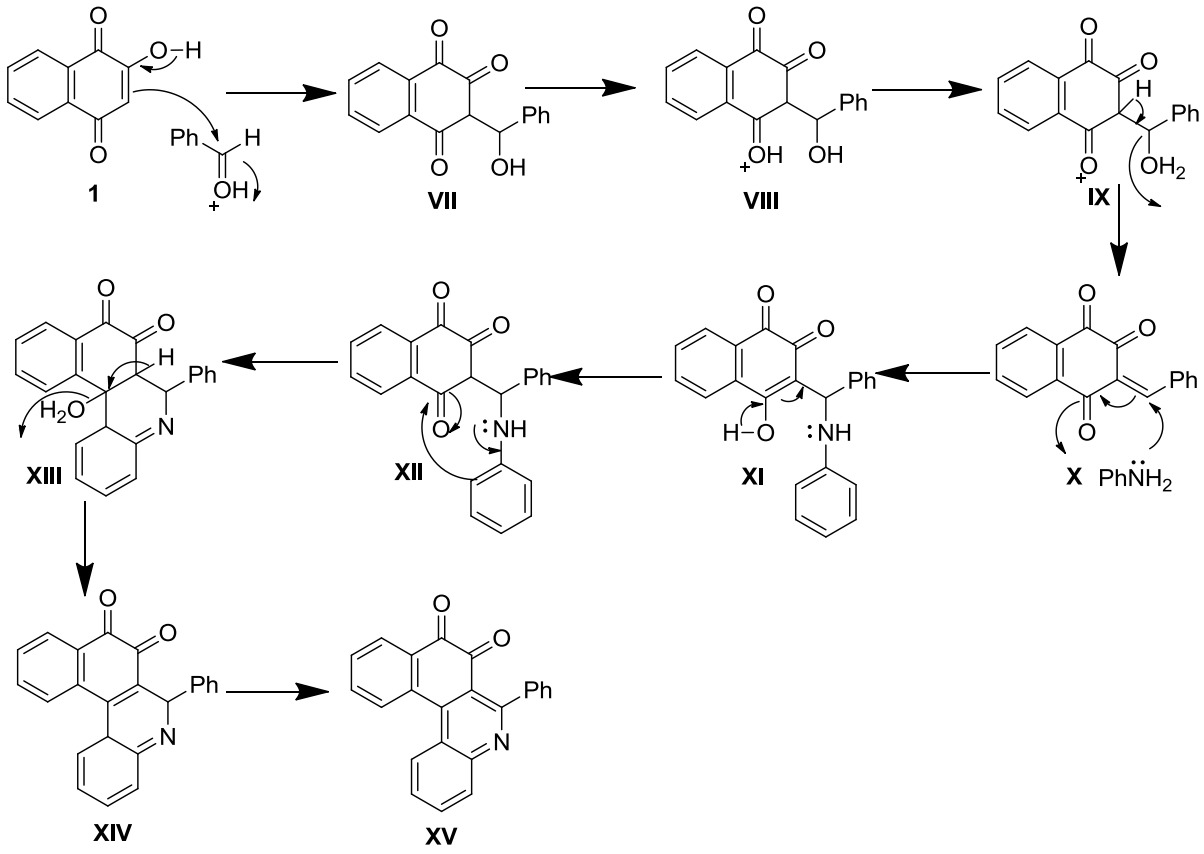
Scheme S2. Reaction of 2-hydroxynaphthalene-1,4-dione **1** with aniline **3** via 1,4-conjugate addition.

Table S10. *Ex situ* reaction trials

S.No.	Solvent	Catalyst[a]	Time (h)	Temperature (°C)
1.	Chloroform	*p*-TSA	12	60
2.	Toluene	*p*-TSA	12	100
3.	Water	*p*-TSA	12	100
4.	Dichloromethane	*p*-TSA	12	40
5.	Polyethylene glycol 6000	*p*-TSA	12	100
6.	Chloroform	$BF_3.Et_2O$	6	40
7.	Chloroform	$ZnCl_2$	6	40
8.	Water	$ZnCl_2$	6	100
9.	Chloroform	$SnCl_2$	6	40
10.	Chloroform	$TiCl_4$	6	40
11.	Chloroform	$FeCl_3$	6	40
12.	Chloroform	$NbCl_5$	6	40
13.	Chloroform	CsCl	6	40

[a]20 mol%

Moreover as shown in Scheme 4, aniline does not react with intermediate **IX** through conjugate addition, even if aniline would have reacted with *α,β*-unsaturated carbonyl intermediate **X** through conjugate addition, it would have led to a different product **XV** (Scheme S3).



Scheme S3. Product formation considering the case of Doebner–Miller reaction.

LCMS analysis of mixture containing compound 5 and 6

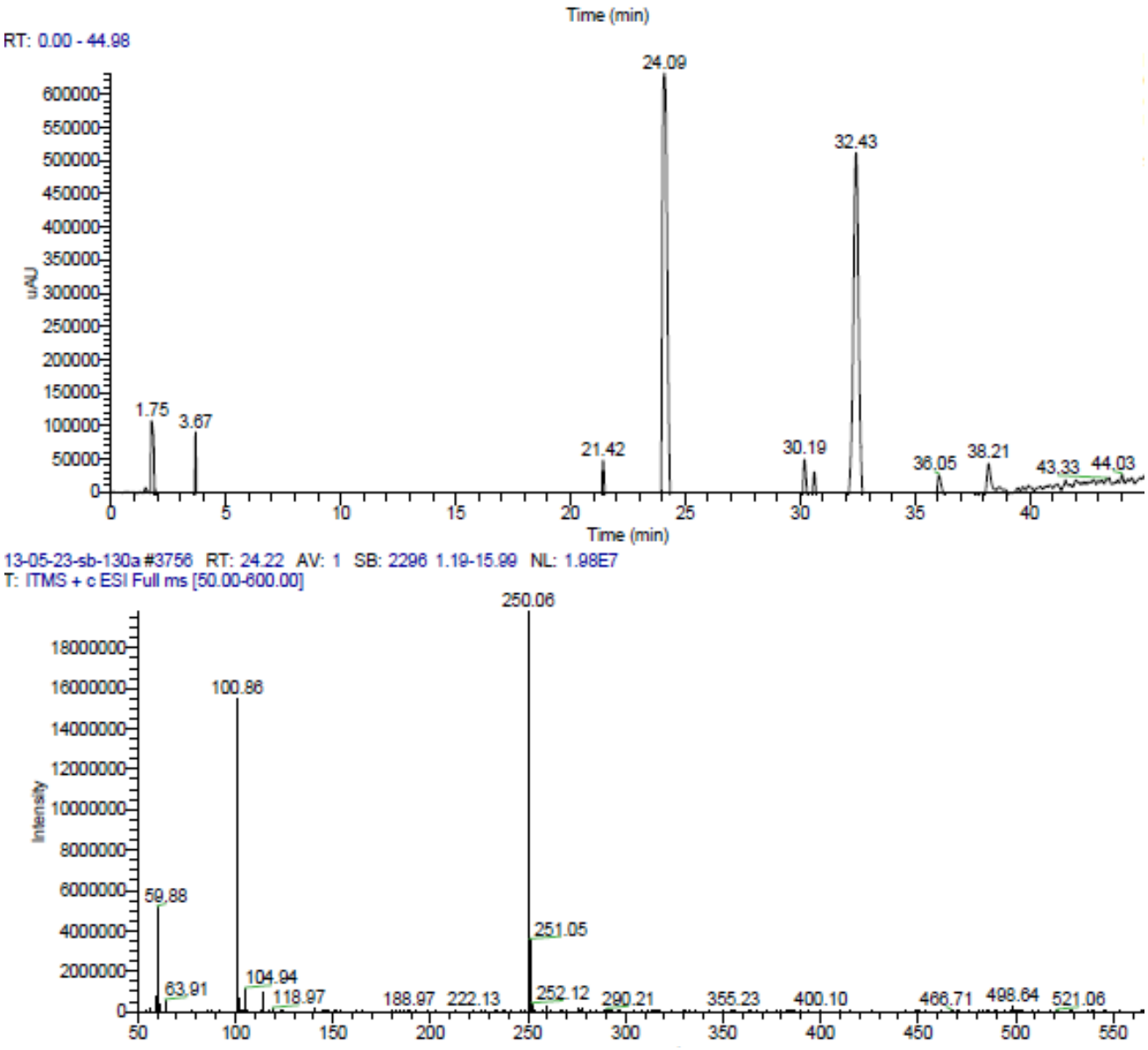


Figure S1a. LCMS analysis of mixture containing compound 5 and 6.

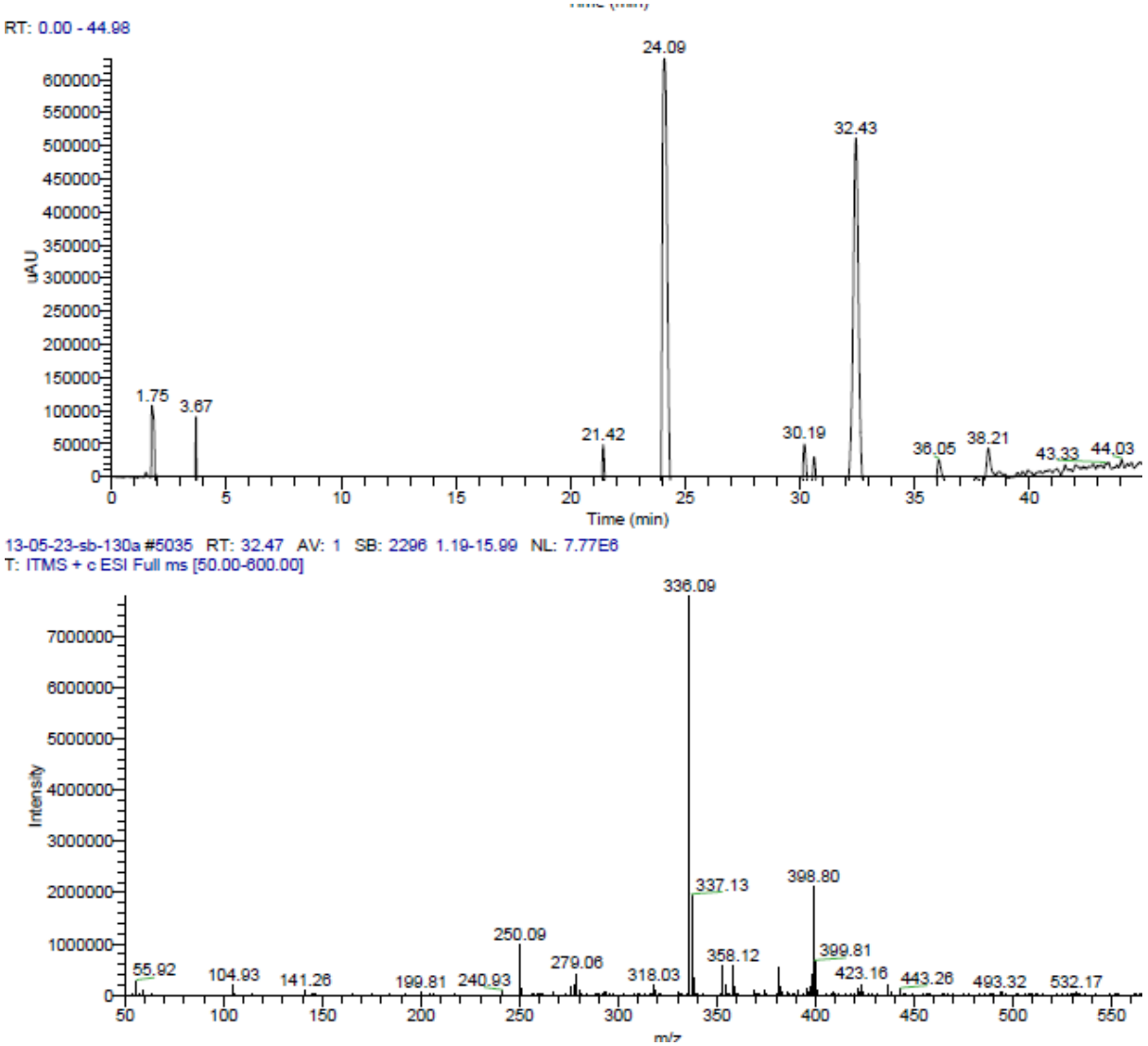


Figure S1b. LCMS analysis of mixture containing compound **5** and **6.**

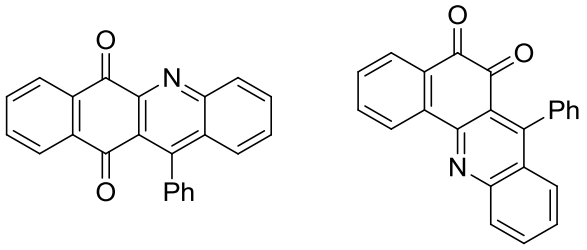


Figure S2. Two possible structures of **5.**

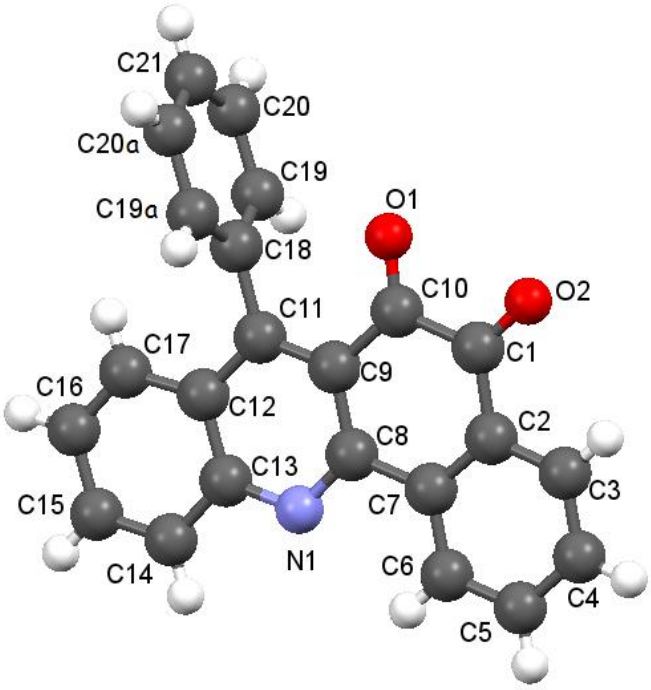


Fig. S3. Fully labelled ORTEP drawing of **5**.

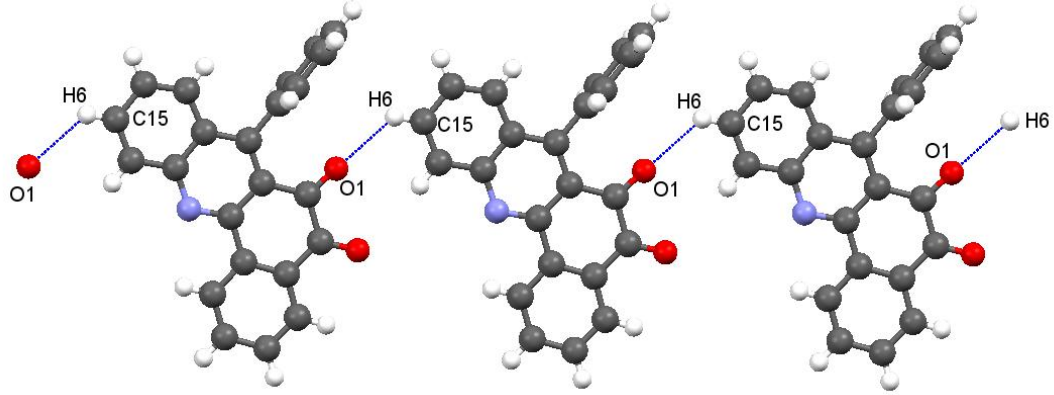


Fig. S4. Supramolecular assembly of **5** via C-H...O interactions.

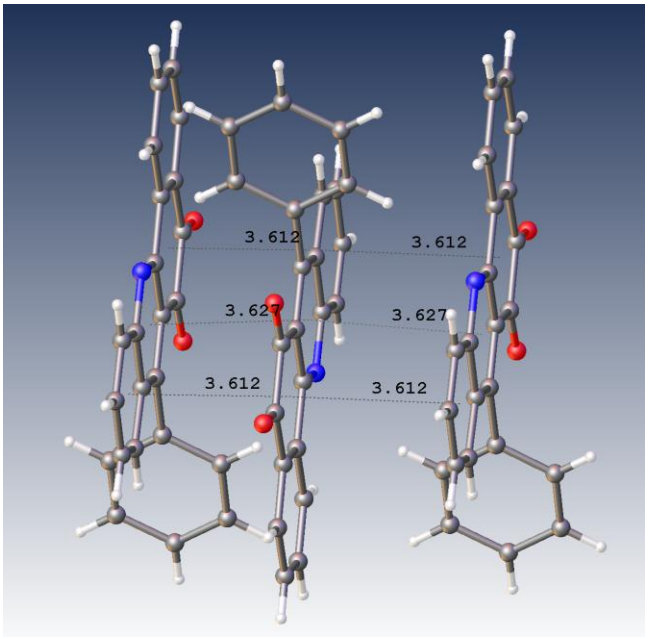


Fig. S5. π-π interactions in **5**.

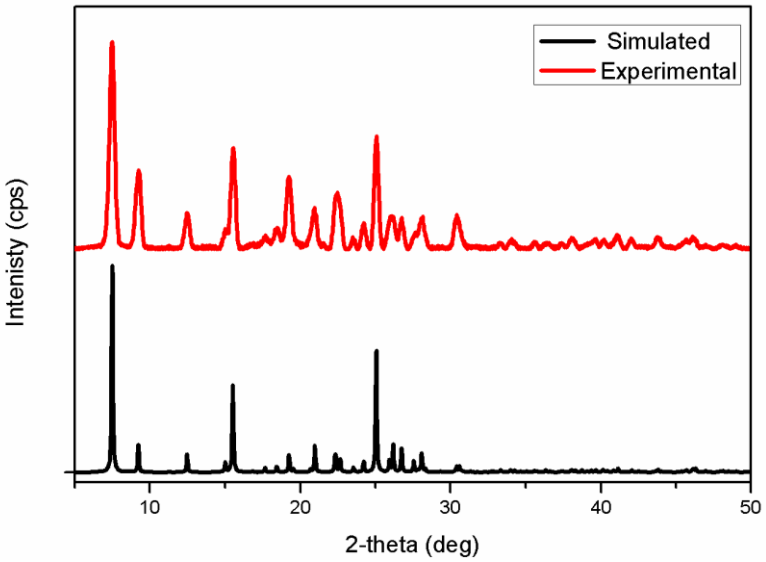


Fig. S6. Simulated and experimental X-ray powder diffractograms of **5**.

Mass Spectrum List Report

Analysis Info

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Sample Name	IPSM-INTER23	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

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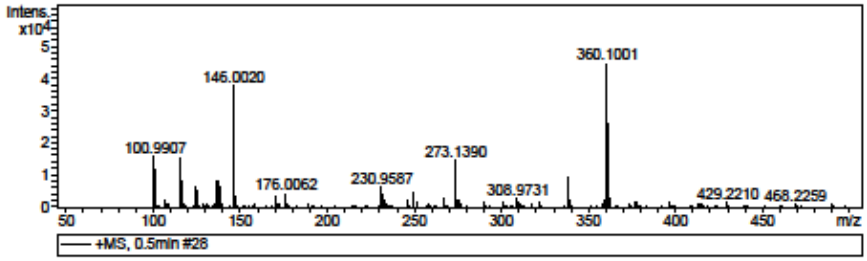
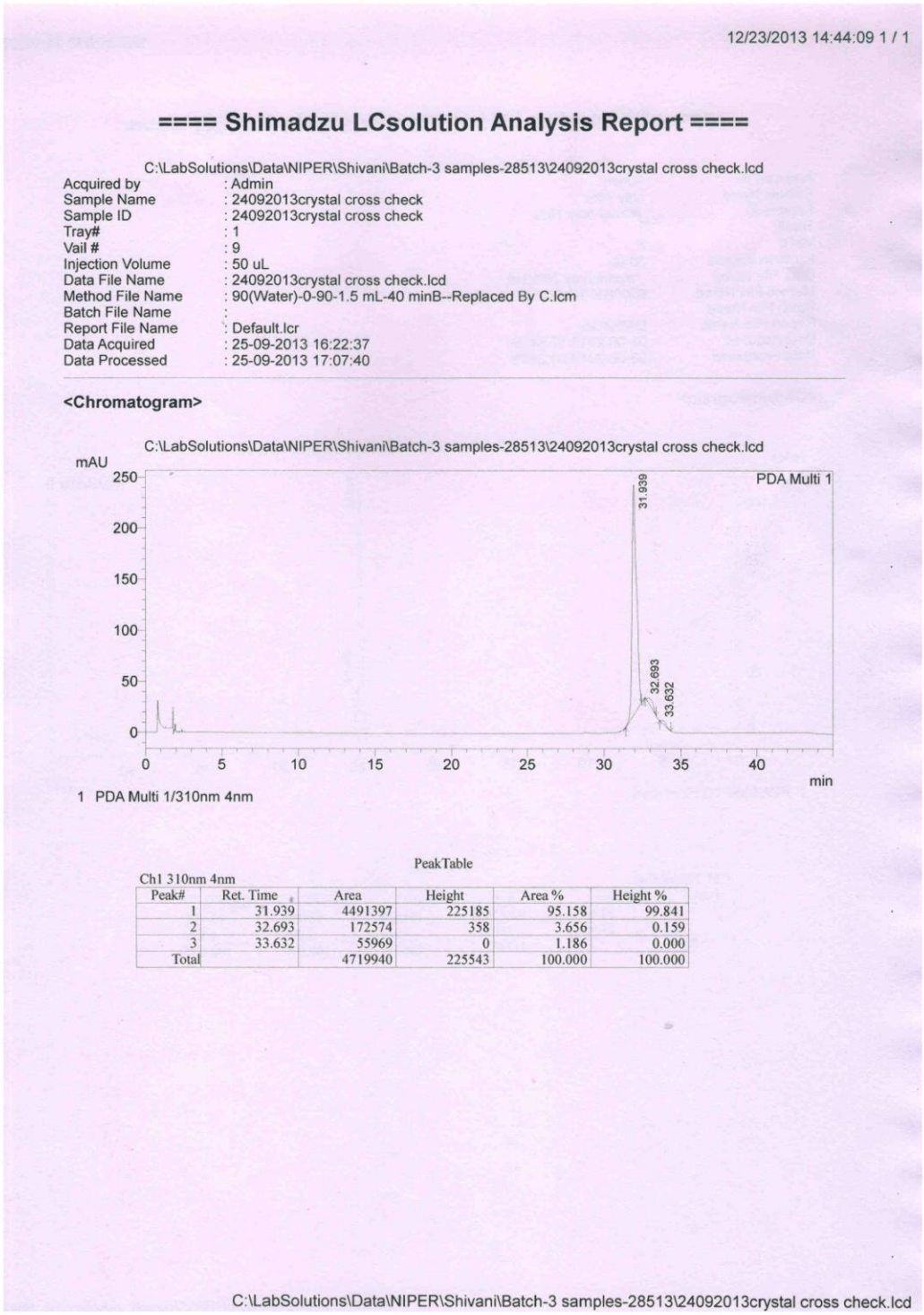


#	m/z	Res.	S/N	I	FWHM
1	100.9907	18222	203.4	15757	0.0055
2	115.9958	17433	124.2	15290	0.0067
3	125.0026	18178	43.9	6420	0.0069
4	136.9955	19364	49.4	8226	0.0071
5	146.0020	18184	207.4	37760	0.0080
6	170.0935	17376	29.6	3651	0.0098
7	176.0062	19308	44.8	4480	0.0091
8	230.9587	19103	96.3	6228	0.0121
9	248.9694	20116	52.7	4889	0.0124
10	266.5504	19737	28.8	2967	0.0135
11	273.1390	19456	136.2	14524	0.0140
12	289.1700	18728	15.4	1401	0.0154
13	301.1417	21072	22.2	1710	0.0143
14	308.9731	19727	38.9	2774	0.0157
15	338.1179	21703	126.0	9371	0.0156
16	360.1001	20504	289.4	44662	0.0176
17	376.0850	7886	11.1	1614	0.0477
18	396.0986	18798	19.7	1337	0.0211
19	413.2667	20406	19.8	1268	0.0203
20	415.2185	20330	19.5	1253	0.0204
21	429.2210	17576	21.9	1455	0.0244
22	440.4210	19629	9.7	587	0.0224
23	468.2259	21099	20.7	1036	0.0222
24	480.1844	25421	3.7	183	0.0189
25	490.2368	23421	9.9	480	0.0209

Figure S7. HRMS spectrum of intermediate t_R = 23 min.

HPLC Chromatogram of Compound 5



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==== Shimadzu LCsolution Analysis Report ====

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Sample ID	: 24092013crystal cross check
Tray#	: 1
Vail #	: 9
Injection Volume	: 50 uL
Data File Name	: 24092013crystal cross check.lcd
Method File Name	: 90(Water)-0-90-1.5 mL-40 minB--Replaced By C.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 25-09-2013 16:22:37
Data Processed	: 25-09-2013 17:07:40

<Chromatogram>

C:\LabSolutions\Data\NIPER\Shivani\Batch-3 samples-28513\24092013crystal cross check.lcd

1 PDA Multi 1/310nm 4nm

PeakTable

Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	31.939	4491397	225185	95.158	99.841
2	32.693	172574	358	3.656	0.159
3	33.632	55969	0	1.186	0.000
Total		4719940	225543	100.000	100.000

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Figure S8. HPLC Chromatogram of Compound 5.

.

HPLC Chromatogram of Compound 6

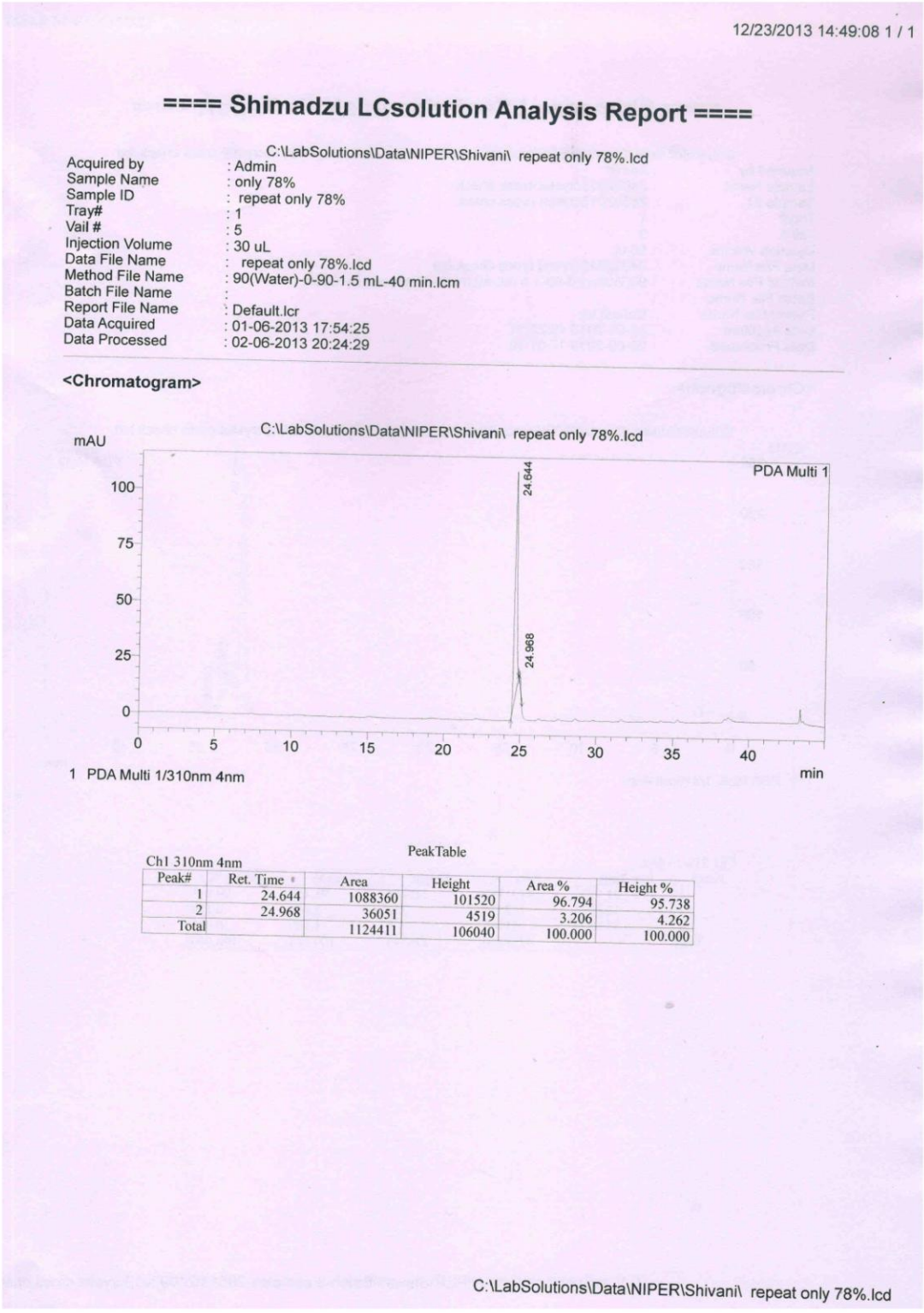


Figure S9. HPLC Chromatogram of Compound 6.

Experimental

General Information: Unless otherwise noted, all reagents and solvents were purchased from commercial sources and used as received. Unless specified, the proton and carbon NMR spectra were obtained in $CDCl_3$ using a 400 MHz spectrometer and are reported in δ units. Coupling constants (*J* values) are reported in Hz. Column chromatography was performed on silica gel (60-120 or 230-400 mesh). High Resolution Mass Spectra (HRMS) were obtained using Bruker-Maxis. IR spectra were obtained using Perkin Elmer-Spectrum II instrument. All melting points were taken using a melting point apparatus equipped with a calibrated thermometer and are uncorrected. New compounds were characterized by melting point, ^{1}H NMR, $^{13}CNMR$, IR, and HRMS data. Purity of all the synthesized compounds was confirmed using qNMR and all the compounds were found more than 96% pure.[3]

HPLC analyses were performed on Phenomenex C18 column (250 X 4.6 mm) connected to a Shimadzu (USA manufacturing Inc.) UFLC system consisting of a model LC-10AD fitted with SIL-20AC HT autosampler and SPD-M20A diode array detector. All the samples were analysed at 310 nm wavelength with the flow rate of 1.5 mL/min. HPLC grade acetonitrile (JT Baker) and ultra pure water (Elga®) were used for sample preparation and in HPLC mobile phases. Mobile phase composition used throughout the analyses was Acetonitrile:Water gradient from 10:90 at 0 min to 100:0 at 40 min. Preparative HPLC was performed on Luna C18 column (250 × 30 mm) connected to a preparative HPLC system (Shimadzu, CBM-20A) equipped with LC-8A binary gradient pump, SPD-20AV UV-Vis detector, FRC-10A fraction collector.

LC-ESI/MS analysis was performed using a Thermo Scientific, Germany, LTQ-XL instrument equipped with Xcalibur software. The column conditions of HPLC system described above were used. Sample (1 mg/mL) in acetonitrile was used for analysis. Injection volume used was 10 µL and flow rate was 1.0 mL/min. The instrument was operated under the following conditions: capillary voltage 18 V, spray voltage 5 kV, tube lens offset 150 V, capillary temperature 245°C, sheath gas (nitrogen) flow rate 60 arbitrary units, spray current 0.12, Aux gas flow rate 18 and sweep gas flow rate -0.06. Data were acquired in the MS scanning modes with scan ranges of 100–1000 *m/z*, the maximum injection time was 50 ms, and the number of microscans was three.

General experimental procedure for the synthesis of 7-arylbenzo[*c*]acridine-5,6-diones

Chloroform (3-5 mL) was added to a mixture of 2-hydroxynaphthalene-1,4-dione (500 mg, 2.87 mmol, 1.0 equiv), benzaldehyde (292.96 µL, 2.87 mmol, 1.0 equiv), aniline (262.14 µL, 2.87 mmol, 1.0 equiv) and *p*-TSA (109.21 mg, 20 mol %) with stirring. The resulting mixture was refluxed for 6 h. After completion of the reaction, the reaction mixture was allowed to cool to room temperature and extracted three times with $CHCl_3$. The combined organic layers were washed with saturated NaCl (aq) twice and dried over anhydrous Na_2SO_4. The organic layer was then concentrated under vacuum, and the crude residue was purified by silica gel (#60-120 mesh size) column chromatography (hexanes/EtOAc) to afford 7-phenylbenzo[*c*]acridine-5,6-dione (**5**). The products were soluble in $CHCl_3$ or CH_2Cl_2 and were precipitated from methanol.

Details of qNMR analysis

The purity of the synthesized compounds was determined by qNMR,[3] for the same, a known amount of the analyte and internal standard 1,4-dioxane (amount taken for all the fifteen analytes and for their internal standards are provided in Table S11) were dissolved in 700 µL of deuterated solvent and 600 µL of the solution was taken in the NMR tube for analysis. All the samples were prepared immediately before analysis. Here, the internal standard was analysed using peak at δ value 3.72 ppm and the details of δ value of peak used for analysis of samples (**5, 5a-5r**) are discussed in Table S11. The purity was determined from qNMR using the equation: $P_x = (A_x/A_s)\ (N_s/N_x)\ (W_s/W_x)\ (M_x/M_s)\ P_s$

Where A_x and A_s are area under the peak of sample and internal standard, N_x and N_s are number of protons of the sample and internal standard, W_x and W_s are amount taken for sample and internal standard (in mg), M_x and M_s are molar masses of sample and internal standard, respectively.

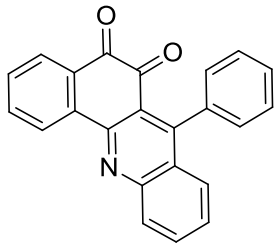
Table S11. Experimental details of qNMR analyses

S. No.	Compound	δ^a(ppm)	W_s	W_x	A_x	A_s	N_s	N_x	M_s	M_x	P_s	P_x
1	**5**	9.04	5.16	10.13	1	15.57	8	1	88.11	335.35	99	98.62
2	**5a**	9.00	5.16	9.25	1	20.36	8	1	88.11	399.82	99	98.47
3	**5b**	8.94	5.16	9.69	1	18.68	8	1	88.11	383.82	99	98.35
4	**5c**	9.01	5.16	8.47	1	24.68	8	1	88.11	444.27	99	98.58
5	**5d**	8.99	5.16	14.64	1	13.67	8	1	88.11	428.27	99	99.26
6	**5e**	9.01	3.16	8.19	1	13.79	8	1	88.11	390.39	99	98.18
7	**5f**	9.01	3.16	10.22	1	10.57	8	1	88.11	374.39	99	98.44
8	**5g**	9.01	3.16	15.42	1	8.14	8	1	88.11	433.37	99	98.07
9	**5h**	8.96	3.16	10.71	1	11.2	8	1	88.11	417.37	99	98.83
10	**5i**	8.96	3.16	10.92	1	10.99	8	1	88.11	415.43	99	98.33
11	**5j**	9.07	3.16	12.69	1	9.13	8	1	88.11	399.44	99	97.93
12	**5k**	8.86	5.16	9.98	1	18.13	8	1	88.11	383.37	99	98.27
13	**5l**	8.97	5.16	10.75	1	16.13	8	1	88.11	367.37	99	98.27
14	**5m**	9.01	5.16	8.39	1	23.13	8	1	88.11	410.37	99	98.08
15	**5n**	9.03	5.16	12.6	1	14.54	8	1	88.11	394.37	99	99.84
16	**5o**	8.95	3.16	10.52	1	10.98	8	1	88.11	379.08	99	96.83
17	**5p**	9.10	3.16	10.59	1	10.57	8	1	88.11	385.11	99	97.72
18	**5q**	9.05	3.16	8.58	1	12.07	8	1	88.11	353.08	99	96.84
19	**5r**	8.99	3.16	9.87	1	11.01	8	1	88.11	369.05	99	96.46

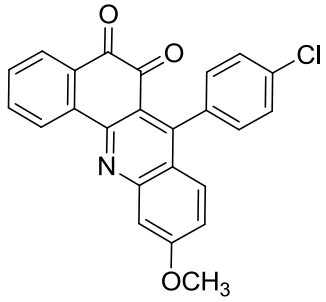
$^a\delta$ ^{1}H of compound used for analysis

Characterization Data

7-phenylbenzo[*c*]acridine-5,6-dione (**5**) orange solid, Yield 92%, mp = 265-268 °C, IR (KBr) υ_{max} 2924, 1684, 1457, 1075 cm^{-1}, ^{1}H NMR ($CDCl_3$) 9.04 (d, 1H, *J* = 7.9 Hz, H-8), 8.22-8.17 (m, 2H, H-1,4), 7.90-7.83 (m, 2H, H-2, 9), 7.62 (td,1H, *J* = 7.8, 0.9 Hz, H-3), 7.57-7.53 (m, 3H, H-3′, 4′, 5′), 7.52-7.46 (m, 2H, H-10, 11), 7.26-7.23 (m, 2H, H-2′, H-6′); ^{13}C NMR ($CDCl_3$) 181.3, 180.7, 154.7, 151.5, 149.7, 137.8, 136.2, 136.1, 133.0, 131.9, 131.2, 130.0, 129.0, 128.6, 128.6, 128.2, 128.0, 128.0, 127.9, 127.2, 122.2; HRMS (ESI) *m/z* calcd for $C_{23}H_{13}NO_2$ $[M+Na]^+$: 358.0844, found: 358.0818.

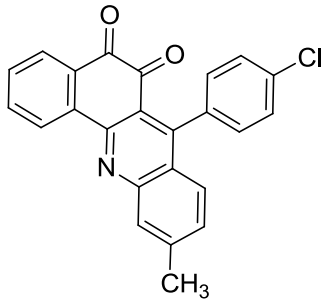


7-(4-chlorophenyl)-10-methoxybenzo[*c*]acridine-5,6-dione (**5a**) yellow solid, Yield 91%, mp = 283-285 °C, IR (KBr) υ_{max} 2948, 1650, 1454, 1412, 1219, 1113, 1032, 1020 cm^{-1}, ^1H NMR ($CDCl_3$) 9.00 (d, 1H, *J* = 7.5 Hz), 8.19 (dd, 1H, *J* = 7.8, 1.0 Hz), 7.87 (td, 1H, *J* = 7.9, 1.4 Hz), 7.63 (td, 1H, *J* = 7.5, 1.1 Hz), 7.54-7.52 (m, 3H), 7.39 (d, 1H, *J* = 9.3 Hz), 7.18 (dt, 2H, *J* = 6.5, 1.9 Hz), 7.13 (dd, 1H, *J* = 9.3, 2.6 Hz), 4.07 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.7, 180.6, 163.9, 152.9, 152.3, 152.1, 137.7, 136.0, 134.9, 134.3, 131.9, 131.2, 129.5, 129.4, 129.1, 128.9 , 127.1, 122.9, 121.5, 120.5, 108.0, 56.0; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}ClNO_3$ $[M+Na]^+$: 422.0559, found: 422.0559; $C_{24}H_{16}ClNO_3$ $[M+Na+2]^+$: 424.0530, found: 424.0536.



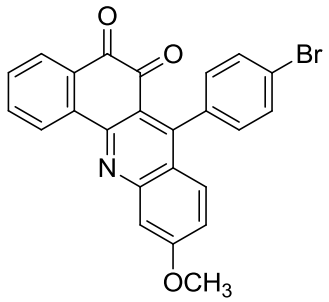
7-(4-chlorophenyl)-10-methylbenzo[*c*]acridine-5,6-dione (**5b**) yellow solid, Yield 87%, mp = 250-252 °C, IR (KBr) υ_{max} 2947, 1654, 1453, 1412, 1219, 1113, 1032, 771 cm^{-1}, ^1H NMR ($CDCl_3$) 8.94 (d, 1H, *J* = 8.0 Hz), 8.10 (dd, 1H, *J* = 7.7, 1.2 Hz), 7.94 (s, 1H), 7.82 (td, 1H, *J* = 8.5, 1.3 Hz), 7.57 (td, 1H, *J* = 6.9, 1.1 Hz), 7.49 (d, 1H, *J* = 1.8 Hz), 7.47 (d, 1H, *J* = 1.9 Hz), 7.31 (d, 1H, *J* = 8.6 Hz), 7.28-7.26 (m, 1H), 7.15 (d, 1H, *J* = 1.8 Hz), 7.13 (d, 1H, *J* = 1.8 Hz), 2.55 (s, 3H); ^{13}C NMR ($CDCl_3$) 181.1, 180.5, 153.0, 151.6, 149.9, 144.6, 137.7, 136.1, 134.8, 134.1, 131.7, 131.1, 130.5, 129.4, 129.2, 128.9, 128.8, 127.9, 127.1, 125.7, 121.5, 22.0; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}ClNO_2$ $[M+Na]^+$: 406.0610, found: 406.0610; $C_{24}H_{16}ClNO_2$ $[M+Na+2]^+$: 408.0581, found: 408.0587.

.

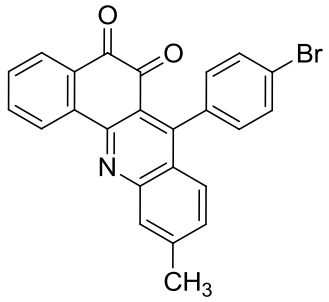


7-(4-bromophenyl)-10-methoxybenzo[c]acridine-5,6-dione (**5c**) yellow solid, Yield 82%, mp = 323-324 °C, IR (KBr) υ_{max} 2981, 1639, 1412, 1219, 1054, 1032, 1015, 772 cm^{-1}, ^1H NMR

($CDCl_3$) 9.01 (dd, 1H, *J* = 8.0, 0.8 Hz), 8.18 (dd, 1H, *J* = 7.8, 1.1 Hz), 7.88 (td, 1H, *J* = 7.4, 1.4 Hz), 7.68 (dt, 2H, *J* = 8.9, 2.4 Hz), 7.63 (td, 1H, *J* = 7.6, 1.1 Hz), 7.54 (d, 1H, *J* = 2.6 Hz), 7.40 (d, 1H, *J* = 9.3 Hz), 7.15 (d, 1H, *J* = 2.6 Hz), 7.14-7.13 (m, 1H), 7.12-7.11 (m, 1H), 4.07 (s, 3H); ^{13}C NMR ($CDCl_3$) 181.1, 180.5, 153.0, 151.6, 149.9, 144.6, 137.8, 136.1, 135.3, 132.1, 131.8, 131.2, 130.6, 129.7, 129.3, 129.1, 127.9, 127.1, 125.7, 122.4, 121.4, 56.0; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}BrNO_3$ $[M+Na]^+$: 466.0054, found: 466.0054; $C_{24}H_{16}BrNO_3$ $[M+Na+2]^+$: 468.0034, found: 468.0038.

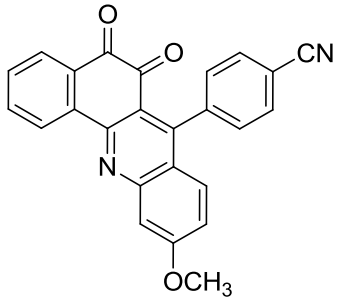


7-(4-bromophenyl)-10-methylbenzo[*c*]acridine-5,6-dione (**5d**) yellow solid, Yield 80%, mp = 196-198 °C, IR (KBr) υ_{max} 2950, 1648, 1406, 1219, 1054, 1032, 1016, 673 cm^{-1}, ^{1}H NMR ($CDCl_3$) 8.99 (dd, 1H, *J* = 8.0, 0.6 Hz), 8.17 (dd, 1H, *J* = 7.8, 1.0 Hz), 7.99 (s, 1H), 7.86 (td, 1H, *J* = 8.0, 1.4 Hz), 7.69 (dt, 2 H, *J* = 8.8, 2.2 Hz), 7.60 (td, 1H, *J* = 7.6, 1.1 Hz), 7.39-7.36 (m, 1H), 7.32 (dd, 1H, *J* = 8.6, 1.5 Hz), 7.13 (dt, 2H, *J* = 8.8, 2.2 Hz), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$) 181.1, 180.6, 153.0, 151.6, 150.0, 144.6, 137.8, 136.1, 135.3, 132.1, 131.8, 131.2, 130.6, 129.7, 129.3, 129.1, 127.9, 127.1, 125.7, 122.4, 121.5, 22.1; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}BrNO_2$ $[M+Na]^+$: 450.0105, found: 450.0105; $C_{24}H_{16}BrNO_2$ $[M+Na+2]^+$: 452.0085, found: 452.0091.

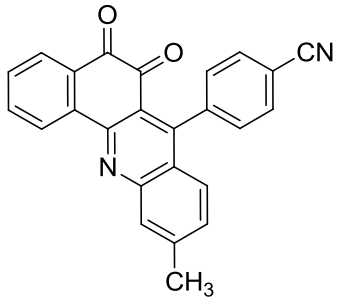


4-(10-methoxy-5,6-dioxo-5,6-dihydrobenzo[*c*]acridin-7-yl)benzonitrile (**5e**) yellow solid, Yield 91%, mp = 310-312 °C, IR (KBr) υ_{max} 2972, 2076, 1638, 1454, 1219, 1054, 1032, 1015 cm^{-1}, ^{1}H NMR ($CDCl_3$) 9.01 (dd, 1H, *J* = 8.0, 0.8 Hz), 8.20 (dd, 1H, *J* = 7.8, 1.1 Hz), 7.90 (dd, 1H, *J* = 8.0, 1.3 Hz), 7.85 (dt, 2H, *J* = 8.4, 1.9 Hz), 7.64 (td, 1H, *J* = 7.5, 1.1 Hz), 7.55 (d, 1H, *J* = 2.5 Hz), 7.37 (dt, 2H, *J* = 6.6, 1.8 Hz), 7.25 (d, 1H, *J* = 9.3 Hz), 7.15 (dd, 1H, *J* =

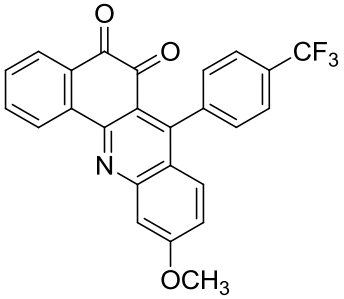
9.3, 2.6 Hz), 4.08 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.4, 180.2, 164.1, 152.3, 152.2, 151.7, 141.8, 137.5, 136.2, 132.4, 131.9, 131.4, 129.2, 129.0, 128.8, 127.0, 126.5, 122.2, 122.0, 118.7, 112.1, 108.2, 56.0; HRMS (ESI) *m/z* calcd for $C_{25}H_{14}N_2O_3$ $[M+Na]^+$: 413.0902, found: 413.0902.



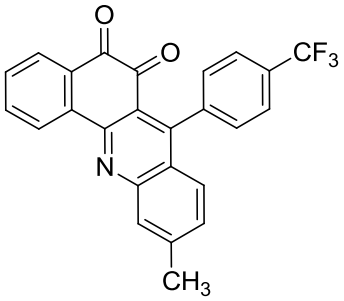
4-(10-methyl-5,6-dioxo-5,6-dihydrobenzo[*c*]acridin-7-yl)benzonitrile (**5f**) yellow solid, Yield 88%, mp = 262-265 °C, IR (KBr) υ_{max} 2948, 2052, 1654, 1453, 1412, 1219, 1113, 1032 cm^{-1}, ^{1}H NMR ($CDCl_3$) 9.01 (dd, 1H, *J* = 8.0, 0.7 Hz), 8.19 (dd, 1H, *J* = 7.8, 1.1 Hz), 8.03 (s, 1H), 7.90-7.88 (m, 1H), 7.86 (dt, 2H, *J* = 8.4, 1.8 Hz), 7.73 (d, 1H, *J* = 0.8 Hz), 7.64 (td, 1H, *J* = 7.6, 1.2 Hz), 7.37 (dt, 2H, *J* = 8.5, 1.8 Hz), 7.23-7.25 (m, 1H), 2.62 (s, 3H); ^{13}C NMR ($CDCl_3$) 181.8, 180.0, 151.7, 137.6, 136.2, 132.4, 131.4, 131.2, 130.9, 129.4, 129.2, 129.1, 128.8, 128.7, 128.5, 127.9, 127.4, 127.1, 125.1, 124.9, 121.1, 118.7, 22.1; HRMS (ESI) *m/z* calcd for $C_{25}H_{14}N_2O_2$ $[M+Na]^+$: 397.0953, found: 397.0963.



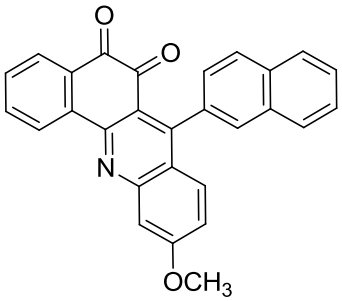
10-methoxy-7-(4-(trifluoromethyl)phenyl)benzo[c]acridine-5,6-dione (**5g**) yellow solid, Yield 79%, mp = 297-298 °C, IR (KBr) υ_{max} 2949, 1648, 1454, 1412, 1219, 1054, 1032, 1016 cm^{-1}, ^{1}H NMR ($CDCl_3$) 9.01 (dd, 1H, *J* = 8.0, 0.7 Hz), 8.20 (dd, 1H, *J* = 7.8, 1.1 Hz), 7.88 (td, 1H, *J* = 7.4, 1.4 Hz), 7.82 (d, 2H, J = 8.0 Hz), 7.64 (td, 1H, *J* = 7.6, 1.2 Hz), 7.54 (d, 1H, *J* = 2.6 Hz), 7.37 (d, 1H, *J* = 8.0 Hz), 7.31 (d, 1H, *J* = 9.3 Hz), 7.14 (dd, 1H, *J* = 9.3, 2.6 Hz), 4.07 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.5, 180.4, 164.0, 152.5, 152.3, 152.2, 140.4, 137.6, 136.1, 131.9, 131.3, 130.4, 129.3, 129.2, 128.3, 127.0, 125.6 (CF_3), 124.4, 122.6, 121.7, 120.3, 108.1, 56.0; HRMS (ESI) *m/z* calcd for $C_{25}H_{14}F_3NO_3$ $[M+Na]^+$: 456.0823, found: 456.0829.



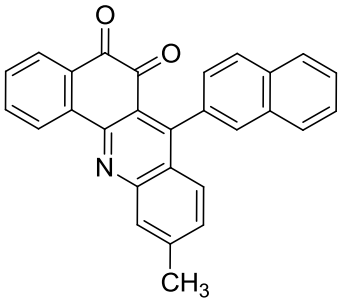
10-methyl-7-(4-(trifluoromethyl)phenyl)benzo[*c*]acridine-5,6-dione (**5h**) yellow solid, Yield 81%, mp = 260-262 °C, IR (KBr) υ_{max} 2946, 1655, 1453, 1413, 1113, 1032 cm^{-1}, ^{1}H NMR ($CDCl_3$) 8.96 (dd, 1H, *J* = 8.0, 0.7 Hz), 8.13 (dd, 1H, *J* = 7.8, 1.1 Hz), 7.96 (s, 1H), 7.86-7.81 (m, 3H), 7.60 (td, 1H, *J* = 7.6, 1.1 Hz), 7.38 (d, 1H, *J* = 7.9 Hz), 7.31-7.29 (m, 1H), 7.26 (d, 1H, *J* = 8.6 Hz), 2.59 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.8, 180.2, 152.6, 151.6, 150.0, 144.7, 140.4, 137.6, 136.1, 131.8, 131.3, 130.7, 130.5, 130.2, 129.3, 129.1, 128.4, 127.7, 127.1, 125.6 (CF_3), 122.8, 121.3, 22.1; HRMS (ESI) *m/z* calcd for $C_{25}H_{14}F_3NO_2$ $[M+Na]^+$: 440.0874, found: 440.0876.



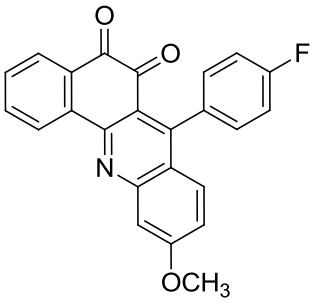
10-methoxy-7-(naphthalen-2-yl)benzo[*c*]acridine-5,6-dione (**5i**) orange solid, Yield 84%, mp = 269-272 °C, IR (KBr) υ_{max} 2948, 1654, 1454, 1412, 1113, 1032 cm^{-1}, ^{1}H NMR ($CDCl_3$) 8.96 (dd, 1H, *J* = 8.0, 0.6 Hz), 8.13 (dd, 1H, *J* = 7.7, 1.0 Hz), 8.03 (d, 1H, *J* = 8.4 Hz), 8.00 - 7.97 (m, 2H), 7.89-7.86 (m, 1H), 7.82 (td, 1H, *J* = 8.2, 1.3 Hz), 7.70 (s, 1H), 7.59-7.55 (m, 3H), 7.47 (d, 1H, *J* = 2.6 Hz), 7.40-7.36 (m, 2H), 7.00 (dd, 1H, *J* = 9.3, 2.6 Hz), 4.01 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.6, 180.5, 163.7, 154.2, 152.9, 152.0, 137.7, 135.9, 134.1, 133.2, 133.0, 131.9, 131.0, 130.0, 129.0, 128.2, 128.1, 128.0, 127.0, 126.7, 126.5, 126.4, 126.2, 123.2, 121.2, 120.7, 108.0, 55.9; HRMS (ESI) *m/z* calcd for $C_{28}H_{17}NO_3$ $[M+Na]^+$: 438.1106, found: 438.1109.



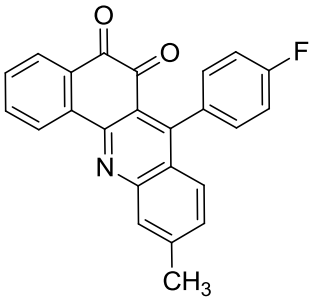
10-methyl-7-(naphthalen-2-yl)benzo[*c*]acridine-5,6-dione (**5j**) orange solid, Yield 73%, mp = 251-252 °C, IR (KBr) υ_{max} 2949, 1648, 1406, 1219, 1052, 1032, 1019 cm^{-1}, ^{1}H NMR ($CDCl_3$) 9.07 (d, 1H, *J* = 8.0 Hz), 8.19 (dd, 1H, *J* = 7.7, 1.1 Hz), 8.05-7.97 (m, 3H), 7.91-7.85 (m, 2H), 7.78-7.73 (m, 1H), 7.70 (s, 1H), 7.45 (d, 1H, *J* = 8.6 Hz), 7.37 (dd, 1H, *J* = 8.4, 1.7 Hz), 2.62 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.6, 180.5, 154.3, 150.1, 144.1, 138.1, 135.7, 133.9, 133.3, 133.2, 132.2, 130.9, 130.2, 129.2, 128.8, 128.3, 128.1, 128.0, 127.9, 127.1, 127.0, 126.7, 126.6, 126.4, 126.3, 21.8; HRMS (ESI) *m/z* calcd for $C_{28}H_{17}NO_2$ $[M+Na]^+$: 422.1157, found: 422.1157.



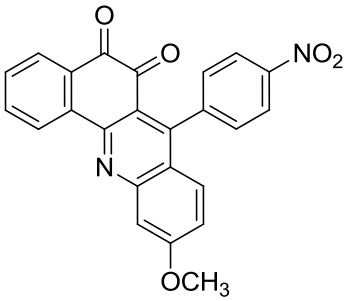
7-(4-fluorophenyl)-10-methoxybenzo[*c*]acridine-5,6-dione (**5k**) orange solid, Yield 76%, mp = 210-213 °C, IR (KBr) υ_{max} 2949, 1448, 1454, 1412, 1219, 1054, 1032, 1017 cm^{-1}, ^{1}H NMR ($CDCl_3$) 8.86 (d, 1H, *J* = 7.9 Hz), 8.06 (d, 1H, *J* = 7.7 Hz), 7.76 (dd, 1H, *J* =7.6 Hz), 7.52 (dd, 1H, *J* = 7.5 Hz), 7.41 (s, 1H), 7.30 (dd, 1H, *J* = 9.2, 0.9 Hz), 7.25-7.15 (m, 4H), 7.02 (d, 1H, *J* = 9.3 Hz), 3.99 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.7, 180.6, 163.9, 163.7, 153.0, 137.6, 135.7, 135.7, 132.2, 132.2, 131.9, 131.0, 129.9, 129.8, 129.5, 128.8, 127.0, 123.0, 121.2, 120.7, 115.7, 115.5, 108.2, 55.8; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}FNO_3$ $[M+Na]^+$:406.0855, found: 406.0855.



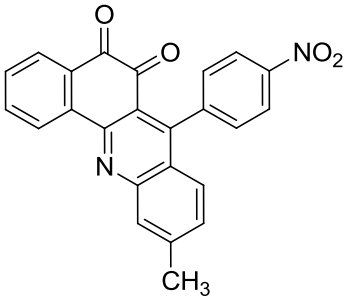
7-(4-fluorophenyl)-10-methylbenzo[*c*]acridine-5,6-dione (**5l**) orange solid, Yield 72%, mp = 221-222 °C, IR (KBr) υ_{max} 2947, 1654, 1452, 1412, 1220, 1193, 1113, 1031 cm^{-1}, ^{1}H NMR ($CDCl_3$) 8.97 (dd, 1H, *J* = 7.6, 0.7 Hz), 8.15 (dd, 1H, *J* = 7.8, 1.1 Hz), 7.96 (s, 1H), 7.85 (td, 1H, *J* = 7.4, 1.4 Hz), 7.60 (td, 1H, *J* = 7.7, 1.2 Hz), 7.37 (d, 1H, *J* = 8.6 Hz), 7.31 (d, 1H, *J* = 1.6 Hz), 7.26-7.22 (m, 4H), 2.60 (s 3H), ^{13}C NMR ($CDCl_3$) 181.1, 180.6, 163.7 (d), 153.3, 151.6, 149.9, 144.4, 137.7, 136.0, 134.1, 131.8, 131.1, 130.4, 129.9, 129.8, 129.2, 128.9, 128.0, 127.1, 126.0, 121.7, 115.8, 115.6, 22.0; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}FNO_2$ $[M+Na]^+$: 390.0906, found: 390.0915.



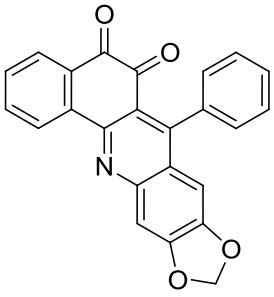
10-methoxy-7-(4-nitrophenyl)benzo[*c*]acridine-5,6-dione (**5m**) brown solid, Yield 87%, mp = 192-193 °C, IR (KBr) υ_{max} 2947, 1654, 1452, 1412, 1219, 1113, 1031 cm^{-1}, ^{1}H NMR ($CDCl_3$) 9.03 (d, 1H, *J* = 7.9 Hz), 8.43 (dd, 2H, *J* = 6.9, 1.8 Hz), 8.21 (dd, 1H, *J* = 7.7, 1.0 Hz), 7.90 (td, 1H, *J* = 7.8, 1.3 Hz), 7.66 (td, 1H, *J* = 7.6, 1.0 Hz), 7.57 (d, 1H, *J* = 2.5 Hz), 7.43 (dt, 2H, *J* = 6.9, 1.8 Hz), 7.26 (d,1H, *J* = 9.4 Hz), 7.16 (dd, 1H, *J* = 9.3, 2.5 Hz), 4.08 (s, 3H); ^{13}C NMR ($CDCl_3$) 182.5, 180.0, 151.7, 151.6, 137.5, 136.3, 134.8, 134.4, 131.8, 131.4, 131.3, 131.0, 130.6, 130.1, 129.5, 129.3, 129.0, 127.3, 127.1, 127.0, 126.7, 122.4, 55.9; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}N_2O_5$ $[M+Na]^+$: 433.0800, found: 433.0792.



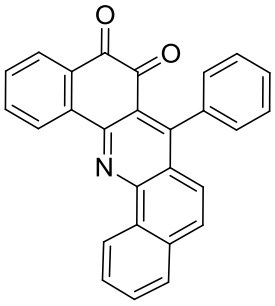
10-methyl-7-(4-nitrophenyl)benzo[*c*]acridine-5,6-dione (**5n**) yellow solid, Yield 86%, mp = 316-317 °C, IR (KBr) υ_{max} 2995, 1659, 1436, 1407, 1314, 1031 cm^{-1}, ^{1}H NMR ($CDCl_3$) 9.03 (dd, 1H, *J* = 8.0, 0.7 Hz), 8.43 (dt, 2H, *J* = 8.8, 2.0 Hz), 8.21 (dd, 1H, *J* = 7.8, 1.1 Hz), 8.06 (s, 1H), 7.90 (td, 1H, *J* = 7.3, 1.4 Hz), 7.81-7.79 (m, 1H), 7.44 (dt, 2H, *J* = 6.8, 2.0 Hz), 7.36 (dd, 1H, *J* = 8.7, 1.6 Hz), 7.26 (d, 1H, *J* = 8.6 Hz), 2.64 (s, 3H); ^{13}C NMR ($CDCl_3$) 182.5, 180.0, 151.7, 151.6, 137.5, 136.3, 134.8, 134.4, 131.8, 131.4, 131.3, 130.9, 130.6, 130.1, 129.5, 129.3, 129.0, 127.3, 127.1, 127.0, 126.8, 122.4, 22.1; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}N_2O_4$ $[M+Na]^+$: 417.0851, found: 417.0856.



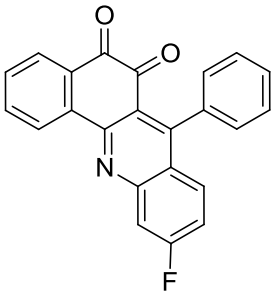
7-phenylbenzo[*h*][1,3]dioxolo[4,5-*b*]acridine-5,6-dione (**5o**) yellow solid, Yield 90%, mp = 105-107 °C, IR (KBr) υ_{max} 2928, 1659, 1384, 1219, 1107, 772 cm^{-1}, ^{1}H NMR ($CDCl_3$) 8.95 (d, 1H, *J* = 7.9 Hz), 8.29 (d, H, *J* = 7.8 Hz), 8.21-8.23 (m, 3H), 8.04-8.-8 (m, 2H), 7.75-7.79 (m, 4H, 1H), 6.15 (s, 2H); ^{13}C NMR ($CDCl_3$) 183.5, 182.6, 160.5, 159.6, 149.0, 135.6, 134.7, 134.6, 134.1, 130.7, 131.4, 129.0, 128.8, 128.7, 128.0, 128.0, 127.8, 127.7, 123.7, 106.3; HRMS (ESI) *m/z* calcd for $C_{24}H_{14}NO_4$ $[M+H]^+$: 380.0922, found: 380.0928.



7-phenyldibenzo[*c*,*h*]acridine-5,6-dione (**5p**) orange solid, Yield 83%, mp = 126-129 °C, IR (KBr) 2922, 1956, 1607, 1572, 1384, 1300, 1107 cm^{-1}, ^1H NMR ($CDCl_3$) 9.10 (d, 1H, *J* = 7.9 Hz), 8.19 (d, 1H, *J* = 7.6 Hz), 8.07 (s, 1H), 8.01 (dd, 2H, *J* = 16.5, 8.3 Hz), 7.91 (t, 1H, *J* = 7.8 Hz), 7.63 (t, 2H, *J* = 8.8 Hz), 7.49 (t, 1H, *J* = 7.5 Hz), 7.22-7.26 (m, 4H), 7.13 (d, 1H, *J* = 8.5 Hz), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$) 180.3, 179.7, 163.91, 152.9, 152.4, 152.2, 137.9, 135.6, 134.5, 133.6, 132.2, 131.7, 130.9, 129.9, 128.9, 128.5, 128.4, 127.1, 126.4, 125.9, 125.3, 125.3, 124.8, 123.7, 121.8, 121.2, 108.2, 21.8; HRMS (ESI) *m/z* calcd for $C_{27}H_{16}NO_2$ $[M+H]^+$: 386.1181, found: 386.1182.

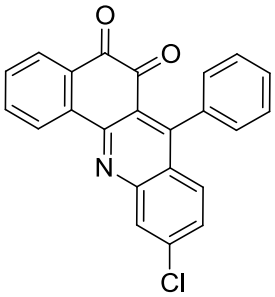


10-Fluoro-7-phenylbenzo[*c*]acridine-5,6-dione (**5q**) yellow solid, Yield 85%, mp = 271-273 °C, IR (KBr) υ_{max} 2928, 1961, 1695, 1384, 1275, 1108, 764 cm^{-1}, ^1H NMR ($CDCl_3$) 9.03 (d, 1H, *J* = 7.7 Hz), 8.21 (dd, 1H, *J* = 7.7, 1.1 Hz), 7.84-7.90 (m, 2H), 7.66 (td, 1H, *J* = 7.3, 1.0 Hz), 7.54-7.58 (m, 4H), 7.27-7.29 (m, 1H), 7.22-7.25 (m, 2H); ^{13}C NMR ($CDCl_3$) 180.4, 180.2, 165.5, 151.2, 148.1, 137.4, 136.1, 135.9, 131.9, 131.5, 131.4, 131.2, 129.1, 128.6, 128.3, 127.8, 127.3, 119.7, 118.3, 113.8, 113.6; HRMS (ESI) *m/z* calcd for $C_{23}H_{13}FNO_2$ $[M+H]^+$: 354.0930, found: 354.0933.



10-Chloro-7-phenylbenzo[*c*]acridine-5,6-dione (**5r**) yellow solid, Yield 82%, mp = 225-229 °C, IR (KBr) 2928, 1659, 1384, 1275, 1108, 764 cm^{-1}, ^1H NMR ($CDCl_3$) 8.99 (d, 1H, *J* = 7.5 Hz), 8.19 (dd, 1H, *J* = 7.8, 1.0 Hz), 7.87 (td, 1H, *J* = 7.9, 1.4 Hz), 7.63 (td, 1H, *J* = 7.5, 1.1 Hz), 7.54-7.52 (m, 3H), 7.39 (d, 1H, *J* = 9.3 Hz), 7.18 (dt, 2H, *J* = 6.5, 1.9 Hz), 7.13 (dd, 1H,

J = 9.3, 2.6 Hz); ^{13}C NMR ($CDCl_3$) 182.7, 182.6, 162.8, 152.9, 152.3, 152.1, 137.7, 136.0, 134.9, 134.3, 131.9, 131.2, 129.5, 129.4, 129.1, 128.9, 127.1, 122.9, 121.5, 120.5; HRMS (ESI) *m/z* calcd for $C_{23}H_{13}ClNO_2$ $[M+H]^+$: 370.0634, found: 370.0637 and $C_{23}H_{13}ClNO_2$ $[M+H+2]^+$: 372.0605, found: 372.0611.



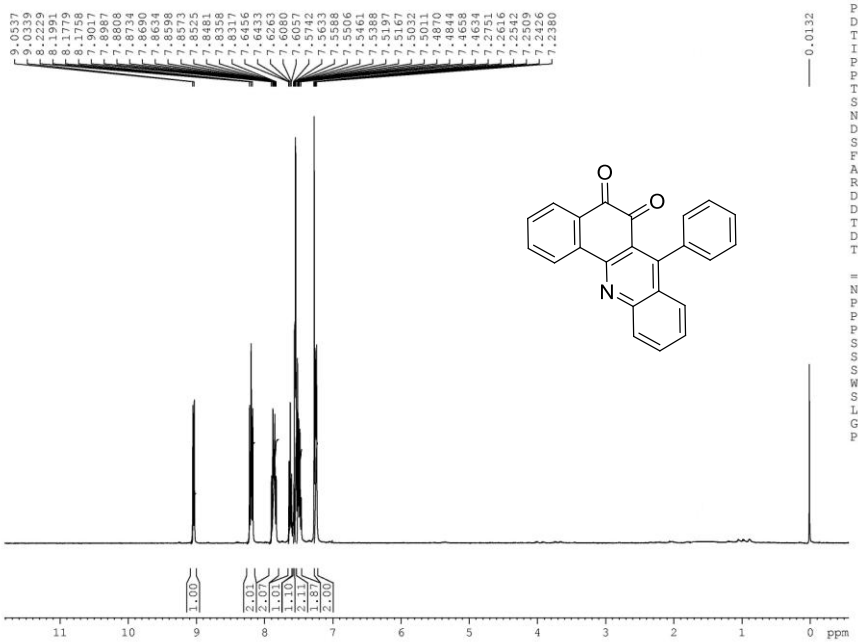
References

1. *p*-TSA was added to the mixture containing **1** and **3** in chloroform under refluxing conditions. To the above mixture, **2** was added at different intervals of time.

2. M. Dabiri, Z. N. Tisseh and A. Bazgir, *Dyes Pigment*, 2011, **89**, 63-69.

3. S. Mahajan and I. P. Singh, *Magn. Reson. Chem.*, 2013, **51**, 76-81.

ipsm−237.32
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Jun} niper 9



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PROCNO	1
Date_	20130604
Time	11.04
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PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
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NUC1	1H
P1	12.20 usec
PL1	−2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
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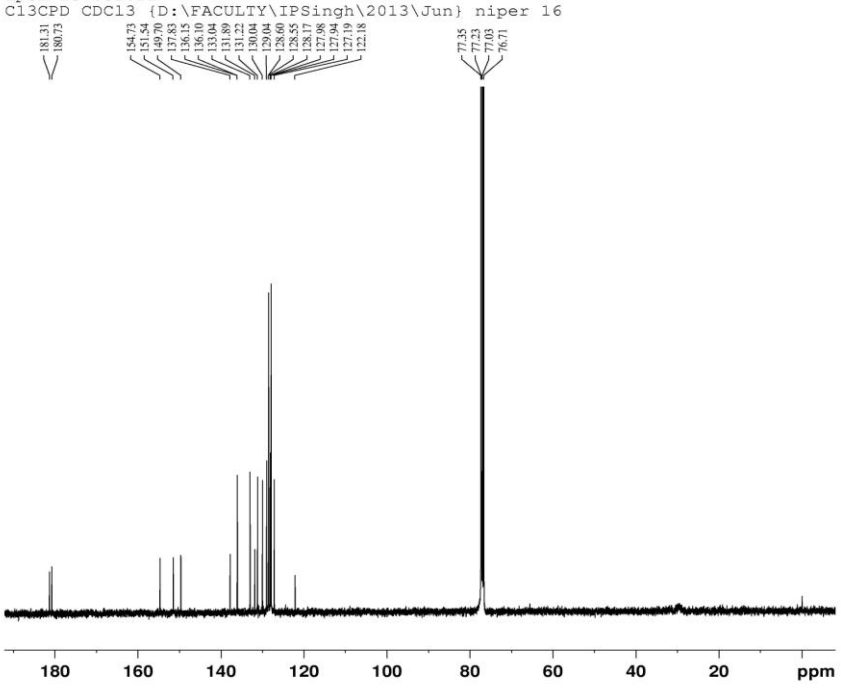
GB	0
PC	1.40

ipsm−237.32.r2
C13CPD CDCl3 {D:\FACULTY\IPSingh\2013\Jun} niper 16



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PULPROG	zgpg30
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SOLVENT	CDCl3
NS	2048
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
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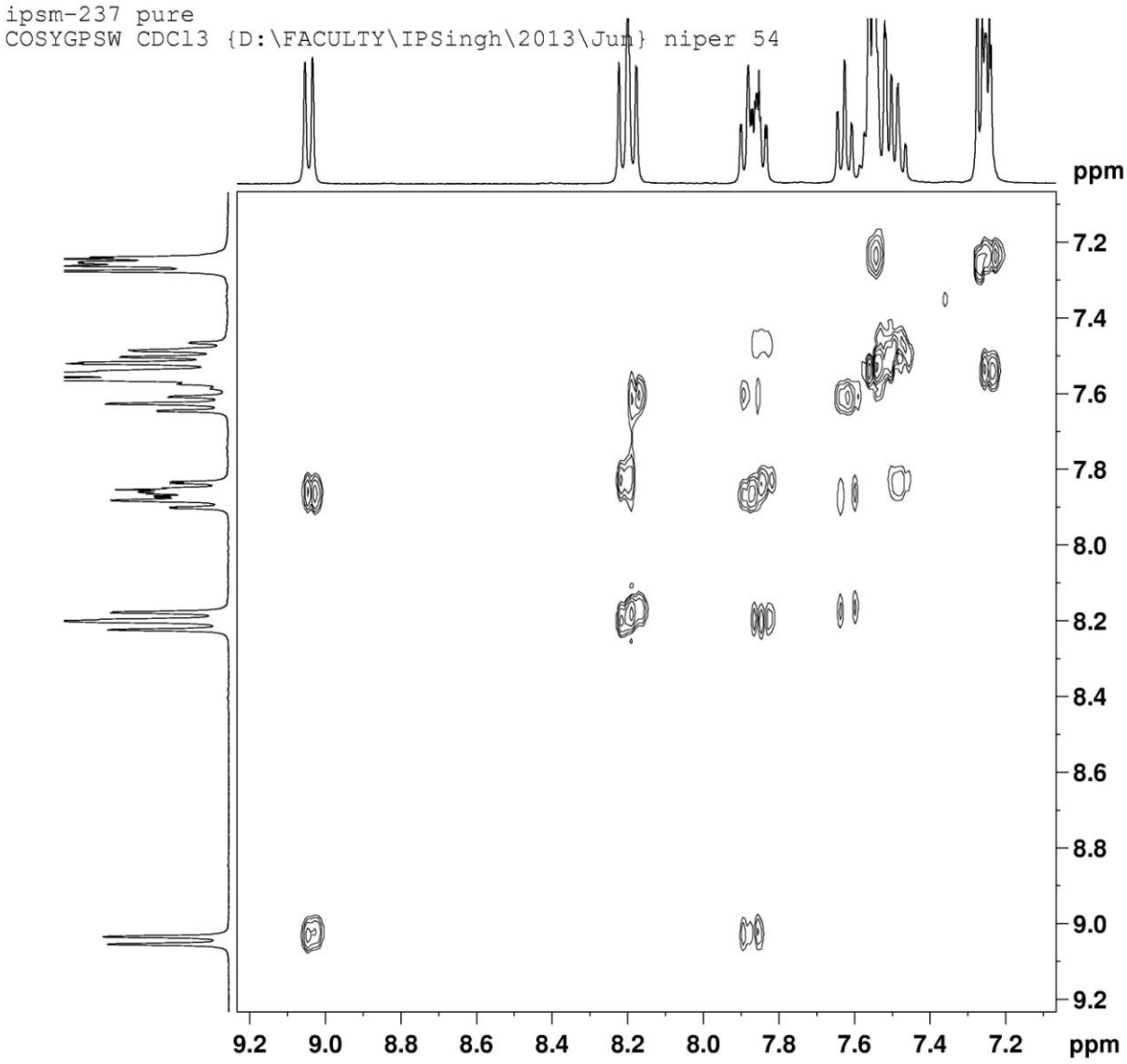
NUC1	13C
P1	9.50 usec
PL1	−1.00 dB
PL1W	44.90434265 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	−2.00 dB
PL12	14.33 dB
PL13	18.33 dB
PL2W	14.80958652 W
PL12W	0.34478071 W
PL13W	0.13725966 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	2.00



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PROCNO	1
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INSTRUM	spect
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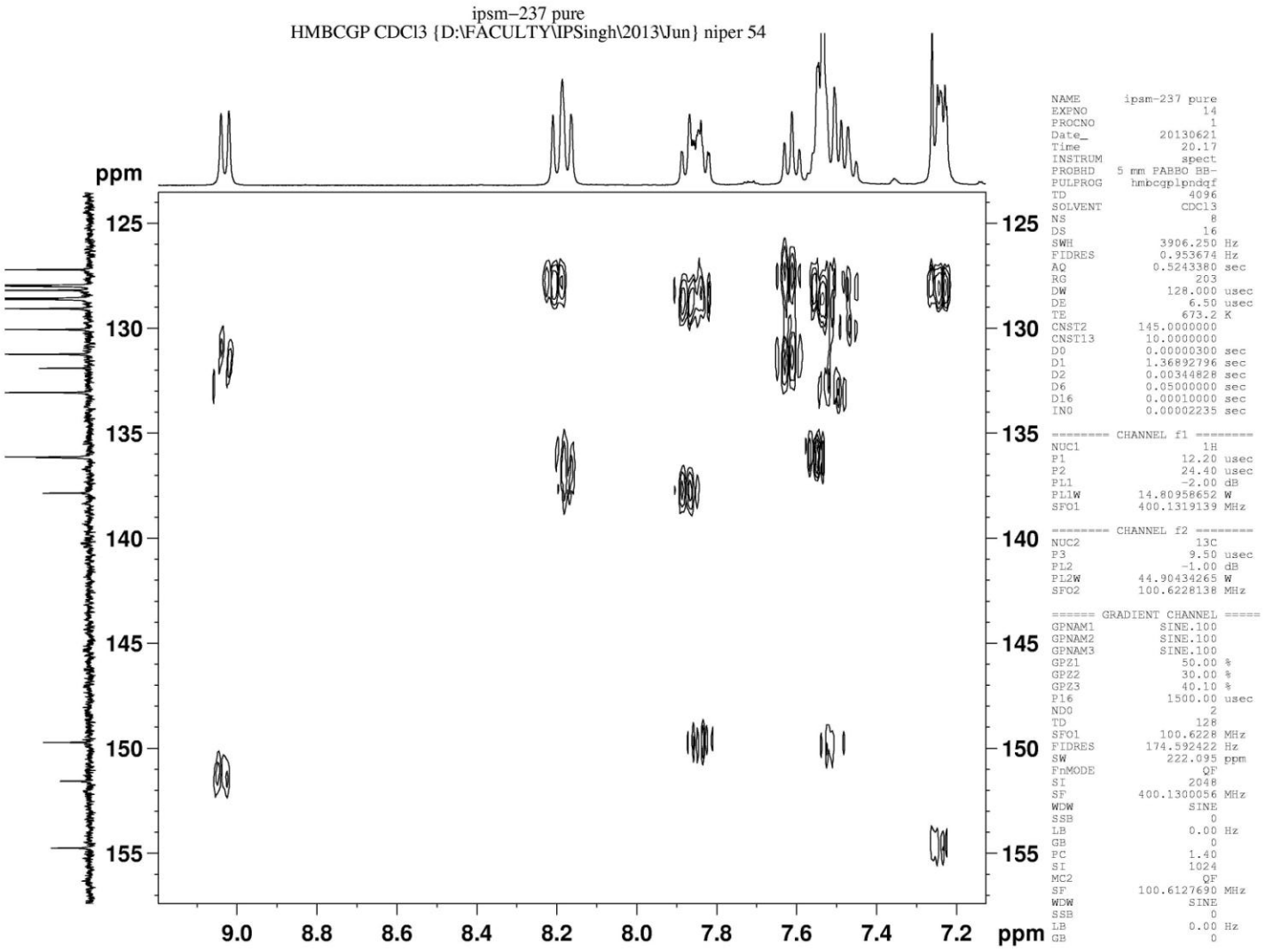
PULPROG	cosygpqf
TD	2048
SOLVENT	CDCl3
NS	8
DS	8
SWH	3906.250 Hz
FIDRES	1.907349 Hz
AQ	0.2621940 sec
RG	144
DW	128.000 usec
DE	6.50 usec
TE	673.2 K
D0	0.00000300 sec
D1	1.41644096 sec
D13	0.00000400 sec
D16	0.00010000 sec
IN0	0.00025600 sec
======== CHANNEL f1 ========	
NUC1	1H
P0	12.20 usec
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1319139 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPZ1	10.00 %
P16	1500.00 usec
ND0	1
TD	128
SFO1	400.1319 MHz
FIDRES	30.517578 Hz
SW	9.762 ppm
FnMODE	QF
SI	1024
SF	400.1300056 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	400.1300056 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

SC33



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PROCNO	1
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INSTRUM	spect
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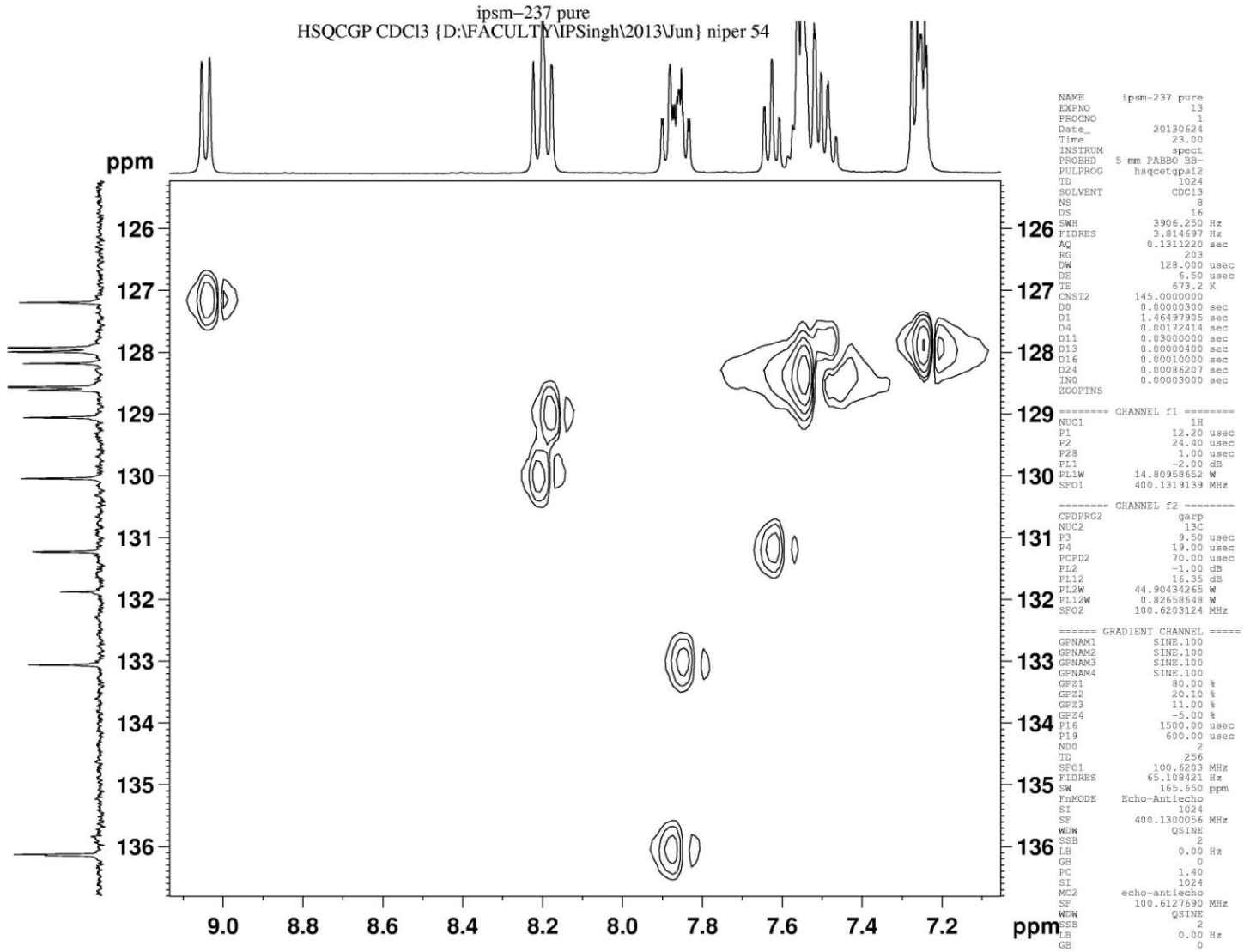
TD	4096
SOLVENT	CDCl3
NS	8
DS	16
SWH	3906.250 Hz
FIDRES	0.953674 Hz
AQ	0.5243380 sec
RG	203
DW	128.000 usec
DE	6.50 usec
TE	673.2 K
CNST2	145.0000000
CNST13	10.0000000
D0	0.00000300 sec
D1	1.36892796 sec
D2	0.00344828 sec
D6	0.05000000 sec
D16	0.00010000 sec
IN0	0.00002235 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
P2	24.40 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1319139 MHz
======== CHANNEL f2 ========	
NUC2	13C
P3	9.50 usec
PL2	-1.00 dB
PL2W	44.90434265 W
SFO2	100.6228138 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPNAM3	SINE.100
GPZ1	50.00 %
GPZ2	30.00 %
GPZ3	40.10 %
P16	1500.00 usec
ND0	2
TD	128
SFO1	100.6228 MHz
FIDRES	174.592422 Hz
SW	222.095 ppm
FnMODE	QF
SI	2048
SF	400.1300056 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	100.6127690 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

SC34

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EXPNO                    13
PROCNO                    1
Date_               20130624
Time                   23.00
INSTRUM                spect
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PULPROG       hsqcetgps12
TD                     1024
SOLVENT             CDCl3
NS                         8
DS                        16
SWH                3906.250 Hz
FIDRES             3.814697 Hz
AQ                 0.1311220 sec
RG                       203
DW                   128.000 usec
DE                     6.50 usec
TE                    673.2 K
CNST2             145.00000000
D0                 0.00000300 sec
D1                 1.46497905 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00010000 sec
D24                0.00086207 sec
IN0                0.00003000 sec
ZGOPTNS

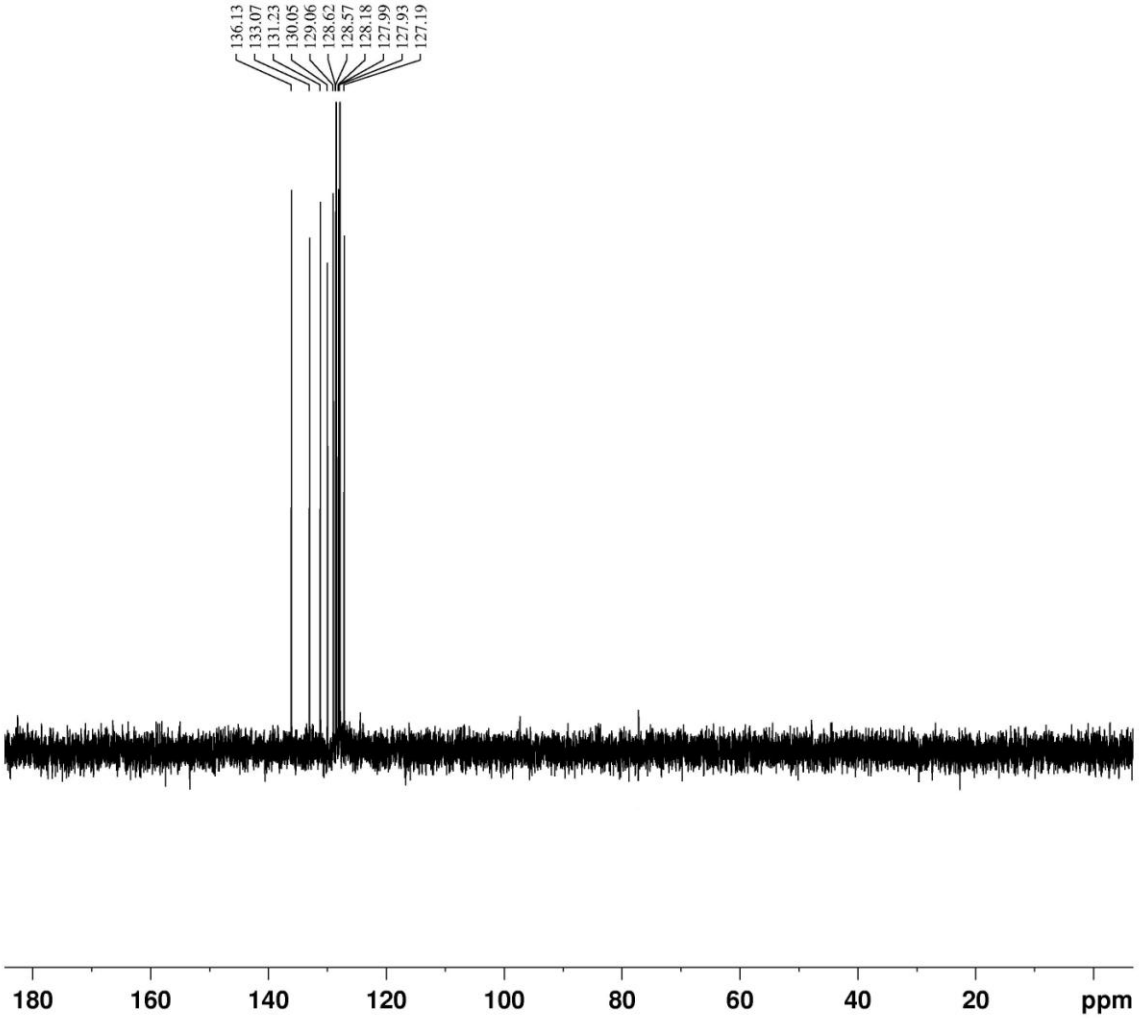
======== CHANNEL f1 ========
NUC1                       1H
P1                      12.20 usec
P2                      24.40 usec
P28                      1.00 usec
PL1                     -2.00 dB
PL1W              14.80958652 W
SFO1              400.1319139 MHz

======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                     13C
P3                       9.50 usec
P4                      19.00 usec
PCPD2                   70.00 usec
PL2                     -1.00 dB
PL12                    16.35 dB
PL2W              44.90434265 W
PL12W              0.82658648 W
SFO2              100.6203124 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPNAM3               SINE.100
GPNAM4               SINE.100
GPZ1                    80.00 %
GPZ2                    20.10 %
GPZ3                    11.00 %
GPZ4                    -5.00 %
P16                   1500.00 usec
P19                    600.00 usec
ND0                         2
TD                        256
SFO1              100.6203 MHz
FIDRES             65.108421 Hz
SW                   165.650 ppm
FnMODE        Echo-Antiecho
SI                       1024
SF                400.1300056 MHz
WDW                     QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
PC                       1.40
SI                       1024
MC2              echo-antiecho
SF                100.6127690 MHz
WDW                     QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
```

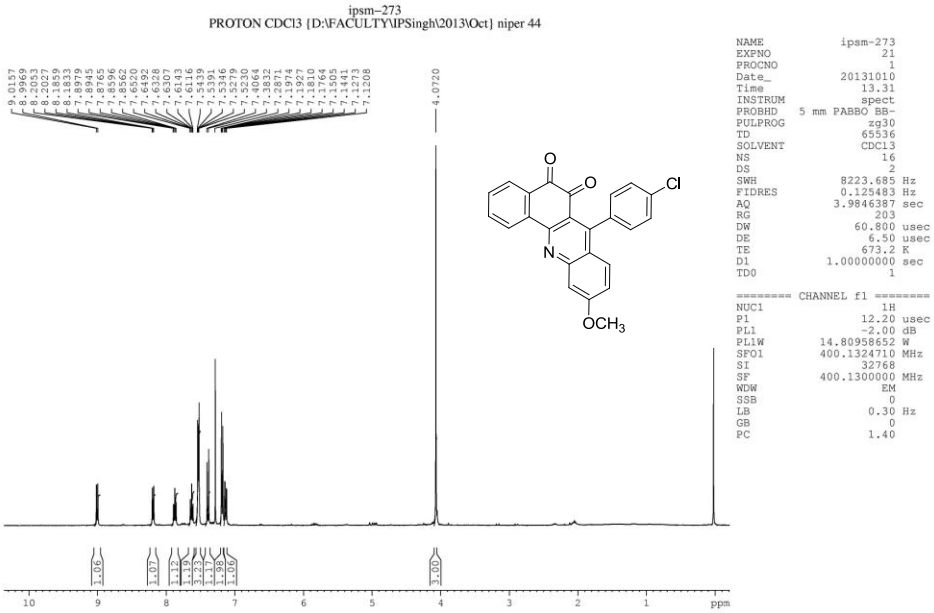
SC35

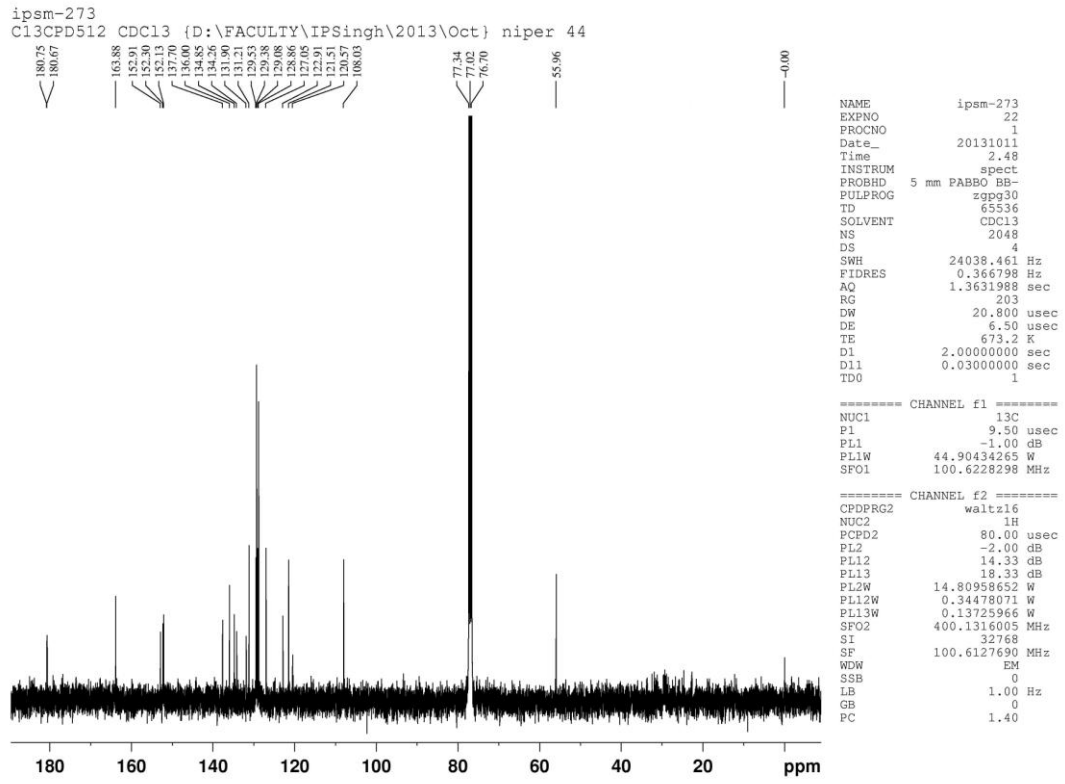
ipsm-237 pure
C13DEPT90 CDCl3 {D:\FACULTY\IPSingh\2013\Jun} niper 54

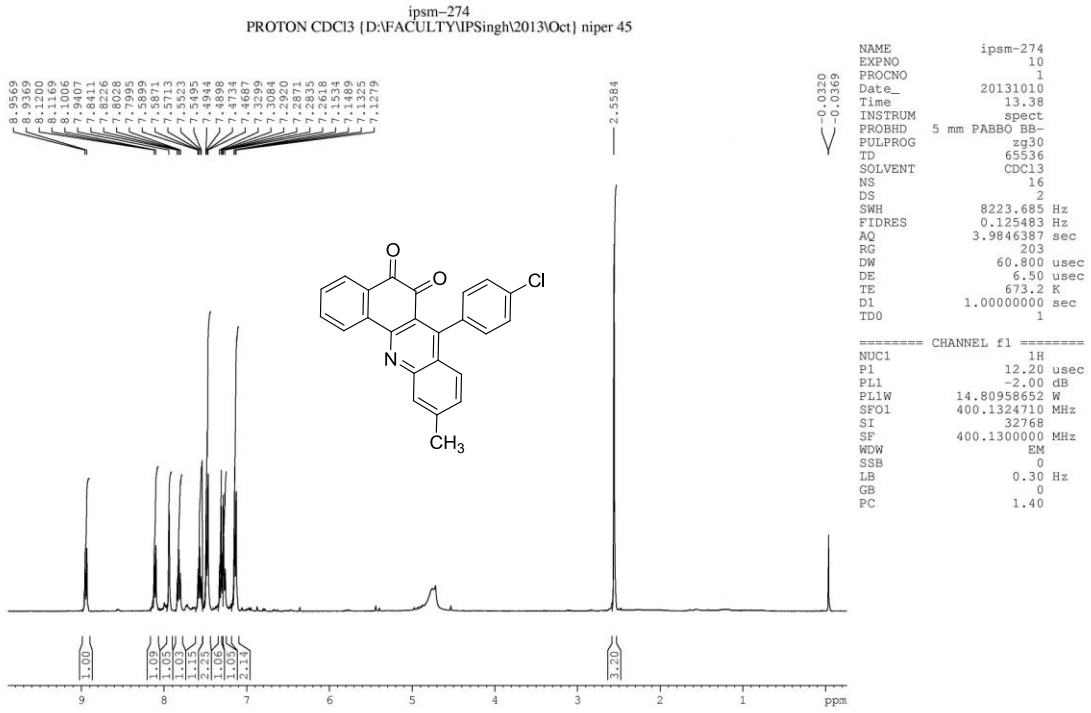


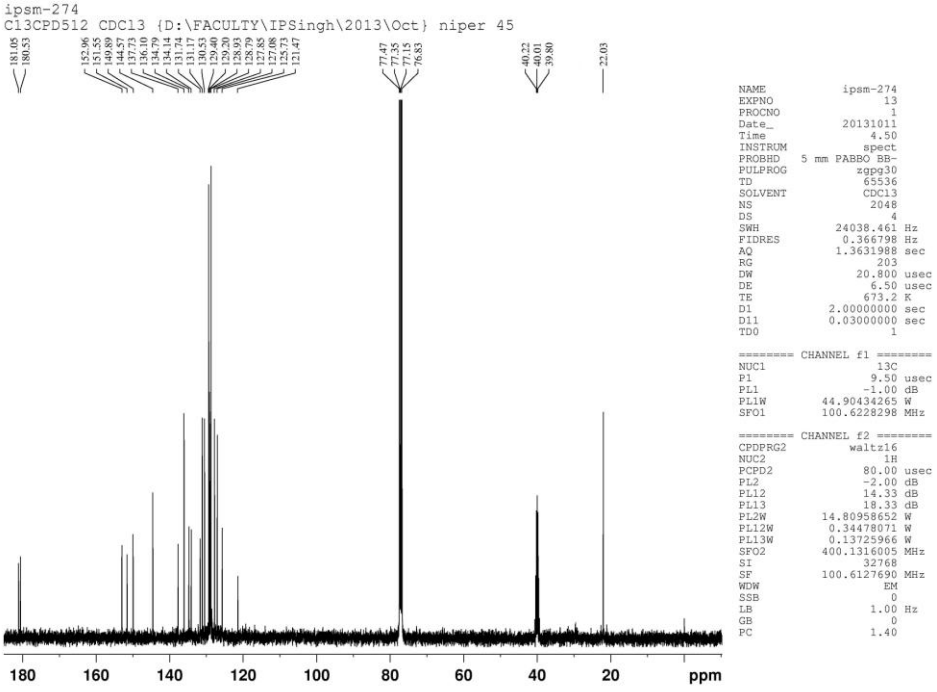
NAME	ipsm-237 pure	
EXPNO	15	
PROCNO	1	
Date_	20130621	
Time	21.06	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	dept90	
TD	65536	
SOLVENT	CDCl3	
NS	256	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	673.2	K
CNST2	145.0000000	
D1	2.00000000	sec
D2	0.00344828	sec
D12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.50	usec
P2	19.00	usec
PL1	-1.00	dB
PL1W	44.90434265	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
P3	12.20	usec
P4	24.40	usec
PCPD2	80.00	usec
PL2	-2.00	dB
PL12	14.33	dB
PL2W	14.80958652	W
PL12W	0.34478071	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

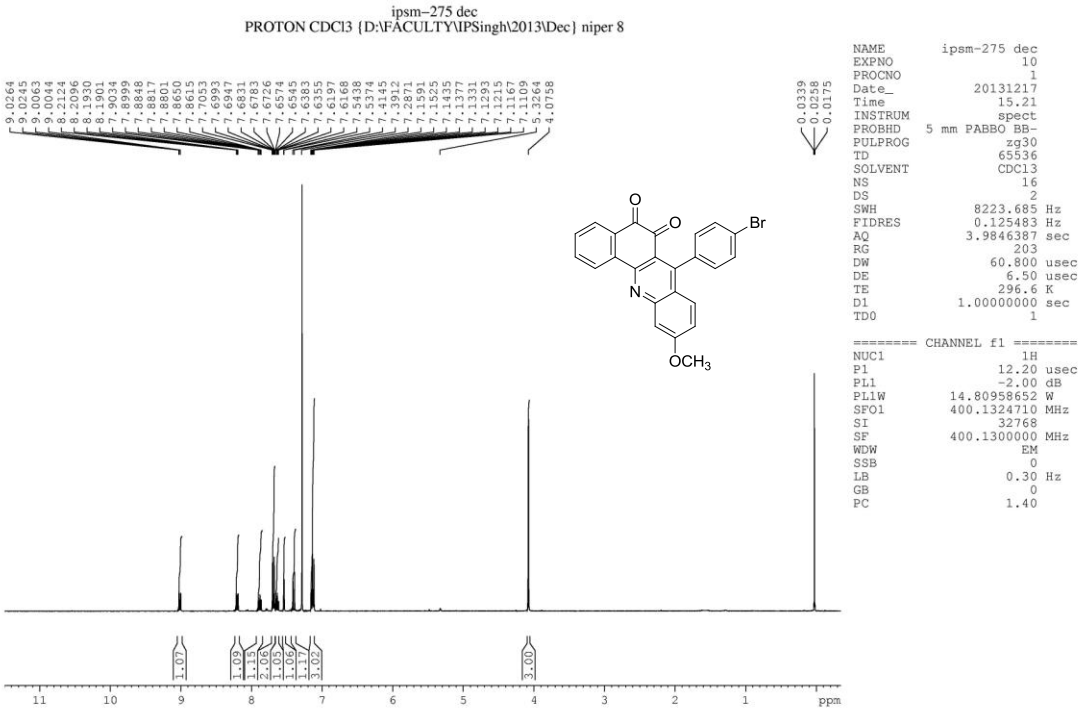
SC36

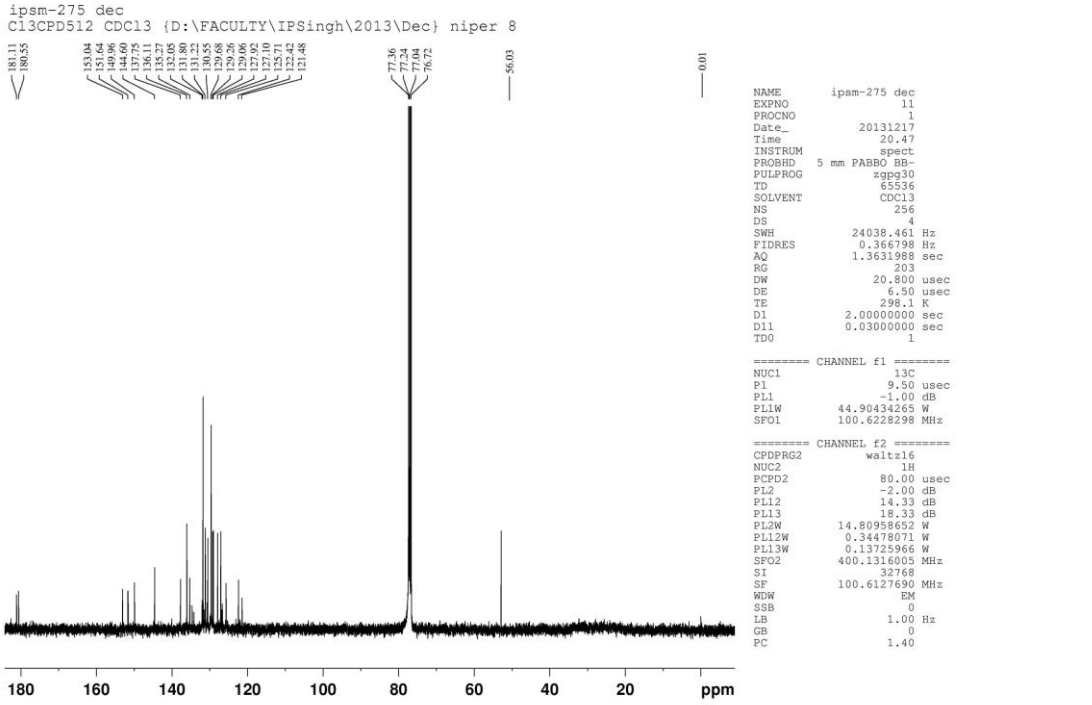

ipsm-273
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 44
9.0157
8.3959
8.2693
8.2027
8.1859
8.1833
8.1679
7.8945
7.8765
7.8596
7.8562
7.8530
7.6492
7.6328
7.6307
7.6143
7.5916
7.5439
7.5391
7.5346
7.5279
7.5230
7.4064
7.3832
7.2871
7.2774
7.1977
7.1810
7.1764
7.1505
7.1491
7.1273
7.1208
4.0720
O
O
Cl
N
OCH3
1.06
1.07
1.12
1.16
3.23
1.17
1.08
1.09
3.00
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-273
EXPNO 21
PROCNO 1
Date_ 20131010
Time 13.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

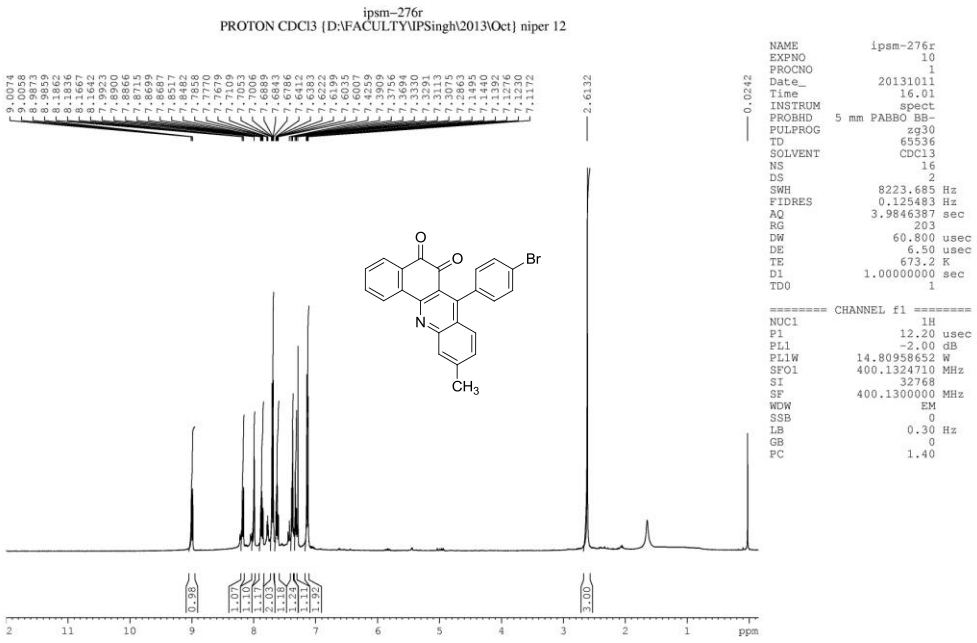

ipsm-273
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 44
180.75
180.67
163.88
153.91
152.30
152.13
137.70
136.00
134.85
134.26
131.90
131.21
129.53
129.38
129.08
128.86
127.05
122.91
121.51
120.57
108.03
77.34
77.02
76.70
55.96
0.00
180
160
140
120
100
80
60
40
20
ppm
NAME ipsm-273
EXPNO 22
PROCNO 1
Date_ 20131011
Time 2.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


ipsm–274
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 45
8.9569
8.9369
8.1200
8.1169
8.1006
7.9407
7.8411
7.8226
7.8028
7.7995
7.7899
7.5871
7.5713
7.5523
7.5495
7.4944
7.4898
7.4734
7.4687
7.3299
7.3084
7.2920
7.2871
7.2835
7.2618
7.1534
7.1489
7.1325
7.1279
2.5584
-0.0320
-0.0369
O
O
Cl
N
CH3
1.00
1.09
1.05
1.03
1.15
2.25
1.06
1.05
2.14
3.20
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-274
EXPNO 10
PROCNO 1
Date_ 20131010
Time 13.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40


ipsm-274
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 45
181.05
180.53
152.96
151.55
149.89
144.57
137.25
136.10
134.79
134.14
131.74
131.17
130.57
129.40
129.20
128.93
128.79
127.68
127.08
125.73
121.47
77.47
77.35
77.15
76.83
40.22
40.01
39.80
23.03
180
160
140
120
100
80
60
40
20
ppm
NAME ipsm-274
EXPNO 13
PROCNO 1
Date_ 20131011
Time 4.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

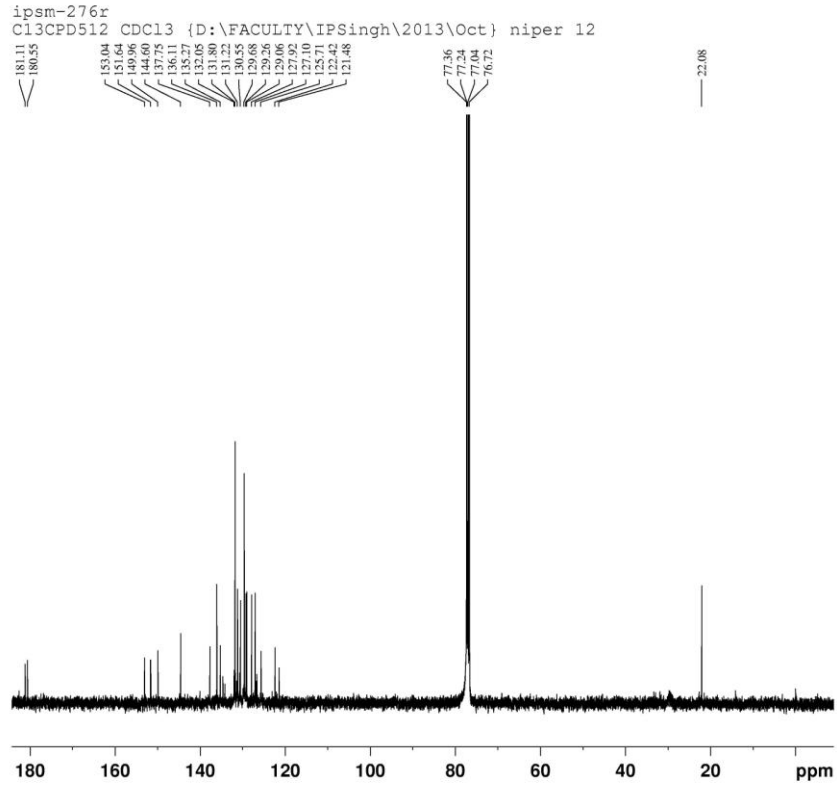

ipsm–275 dec
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Dec} niper 8
NAME ipsm-275 dec
EXPNO 10
PROCNO 1
Date_ 20131217
Time 15.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40
O
O
Br
N
OCH3
ppm


ipsm–275 dec
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Dec} niper 8
NAME ipsm-275 dec
EXPNO 11
PROCNO 1
Date_ 20131217
Time 20.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm




```
NAME           ipsm-276r
EXPNO                 10
PROCNO                 1
Date_           20131011
Time               16.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                    1

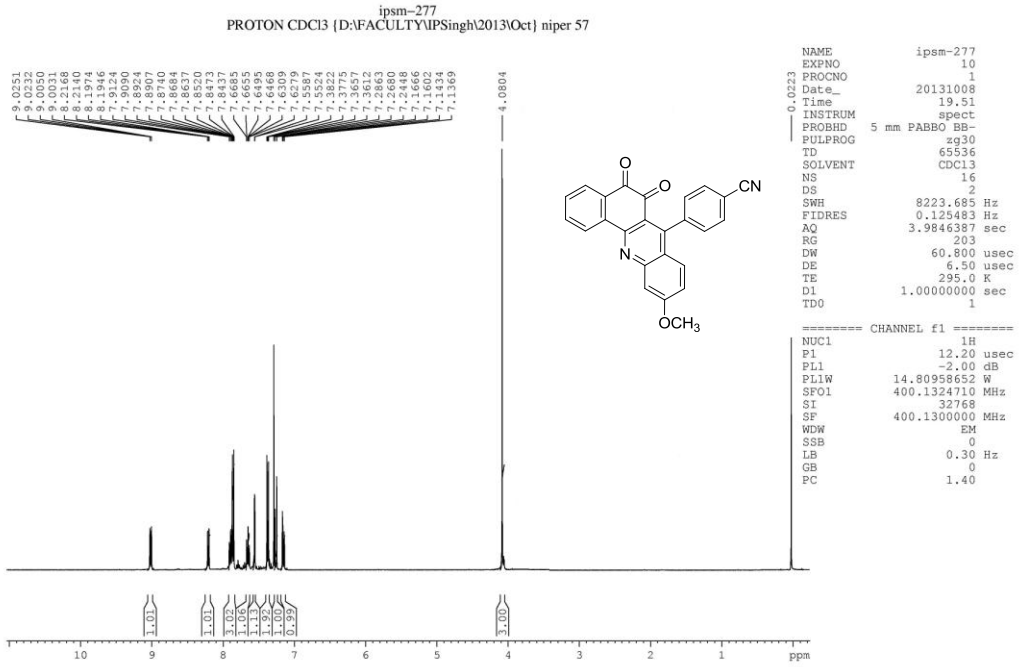
======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1                -2.00 dB
PL1W          14.80958652 W
SFO1          400.1324710 MHz
SI                 32768
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

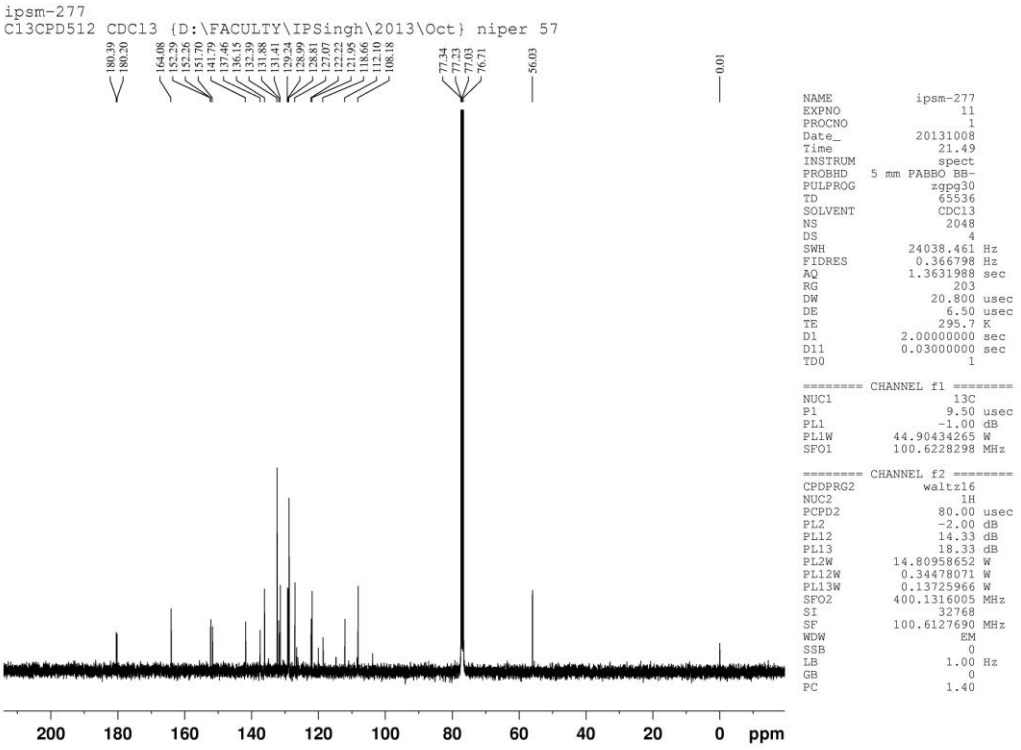


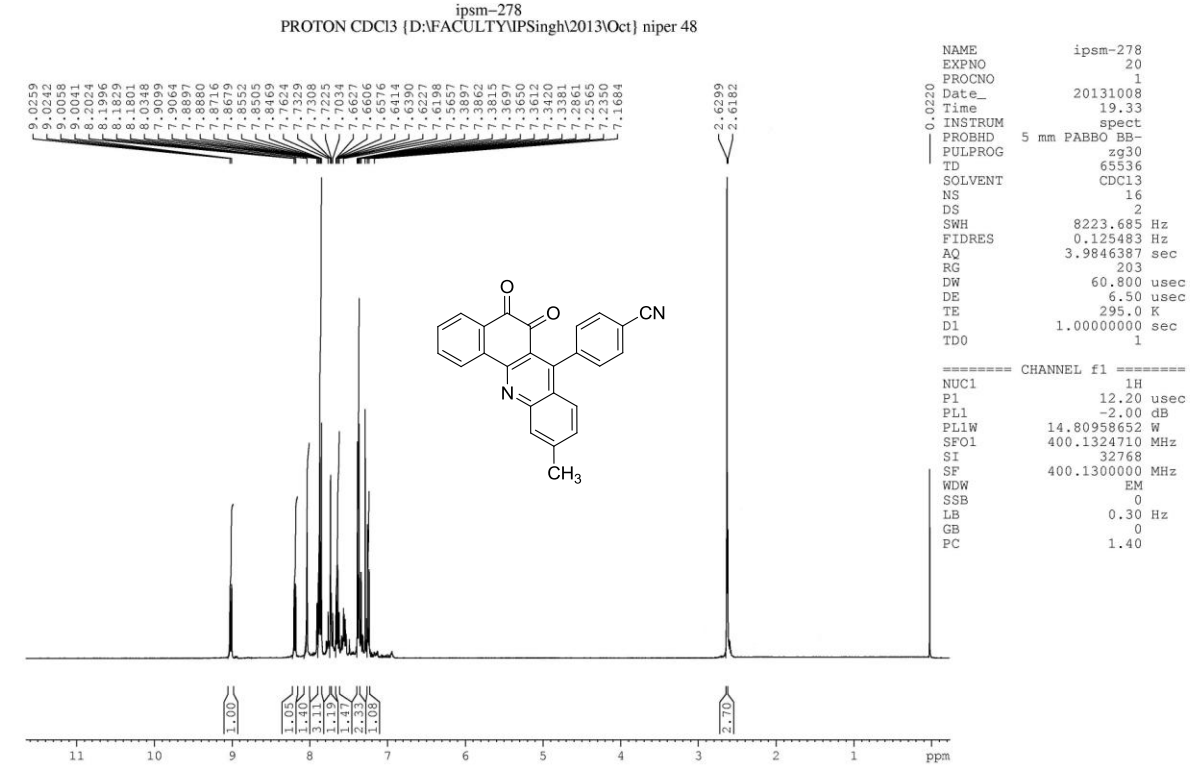

```
NAME           ipsm-276r
EXPNO                 11
PROCNO                 1
Date_           20131012
Time               13.57
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1487
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                673.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

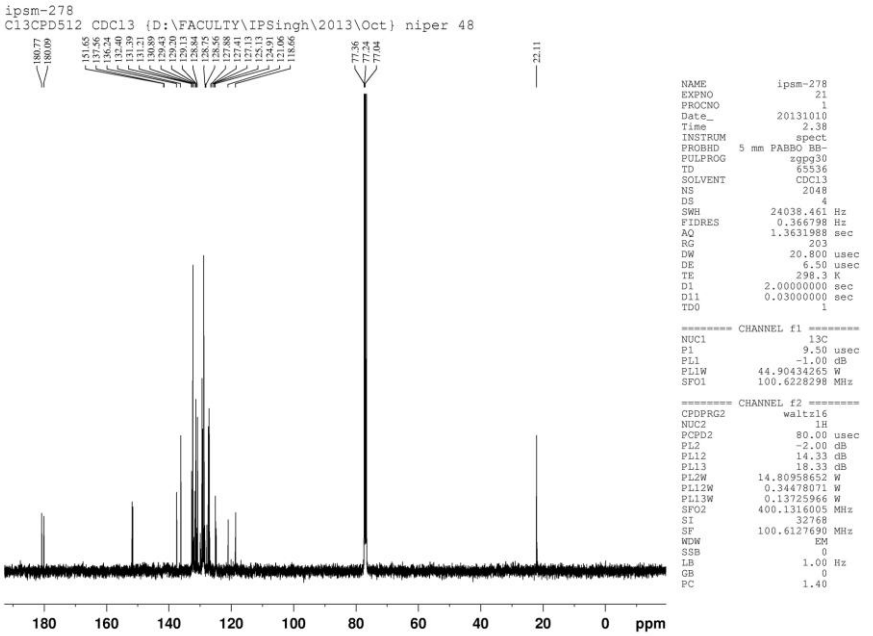
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.50 usec
PL1                -1.00 dB
PL1W          44.90434265 W
SFO1         100.6228298 MHz

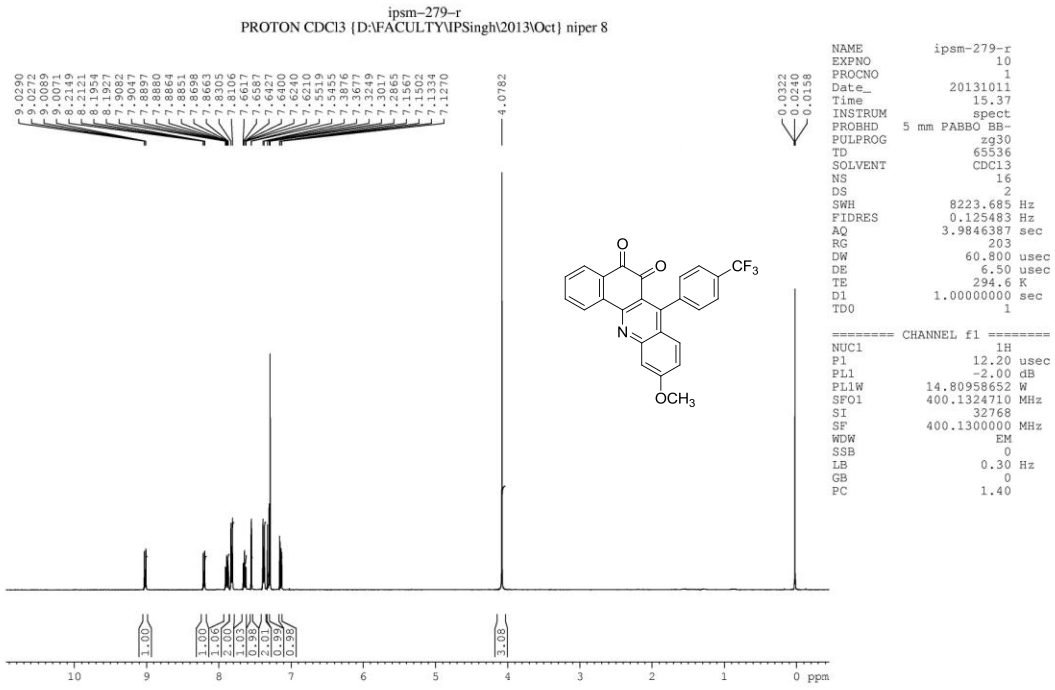
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               14.33 dB
PL13               18.33 dB
PL2W          14.80958652 W
PL12W          0.34478071 W
PL13W          0.13725966 W
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

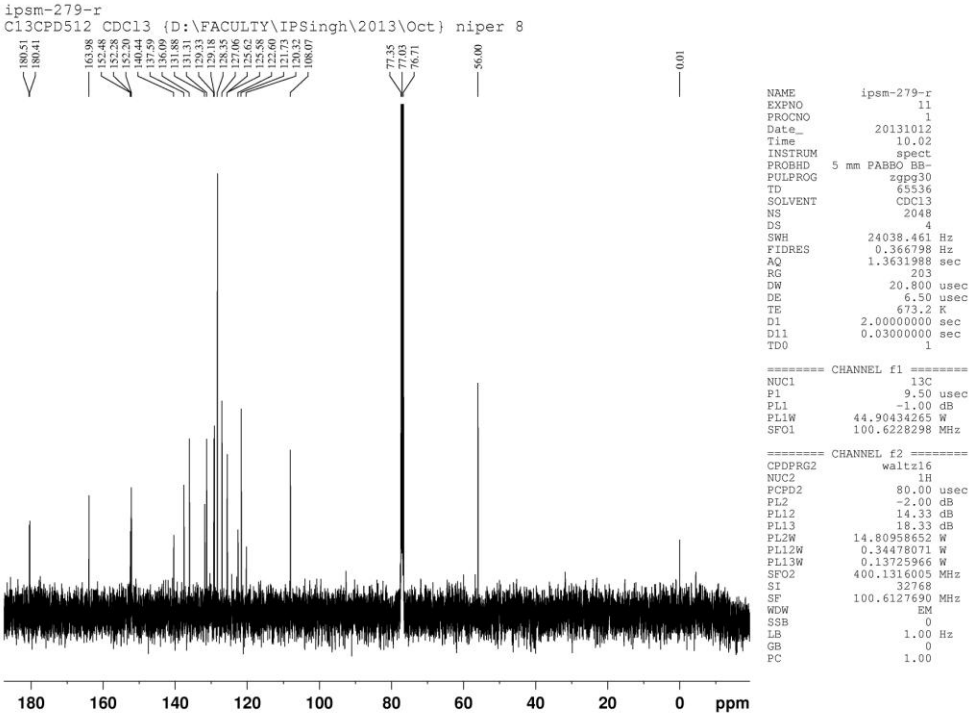

ipsm-277
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 57
9.0251
9.0232
9.0050
9.0031
8.2168
8.2140
8.1974
8.1946
8.1924
7.9090
7.8924
7.8907
7.8740
7.8684
7.8637
7.8550
7.8473
7.8437
7.6685
7.6655
7.6495
7.6468
7.6309
7.6279
7.5587
7.5524
7.3822
7.3775
7.3657
7.3612
7.2643
7.2680
7.2448
7.1666
7.1602
7.1434
7.1369
4.0804
0.0223
O
O
CN
N
OCH3
1.01
1.01
3.02
1.06
1.93
1.00
0.99
3.00
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-277
EXPNO 10
PROCNO 1
Date_ 20131008
Time 19.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

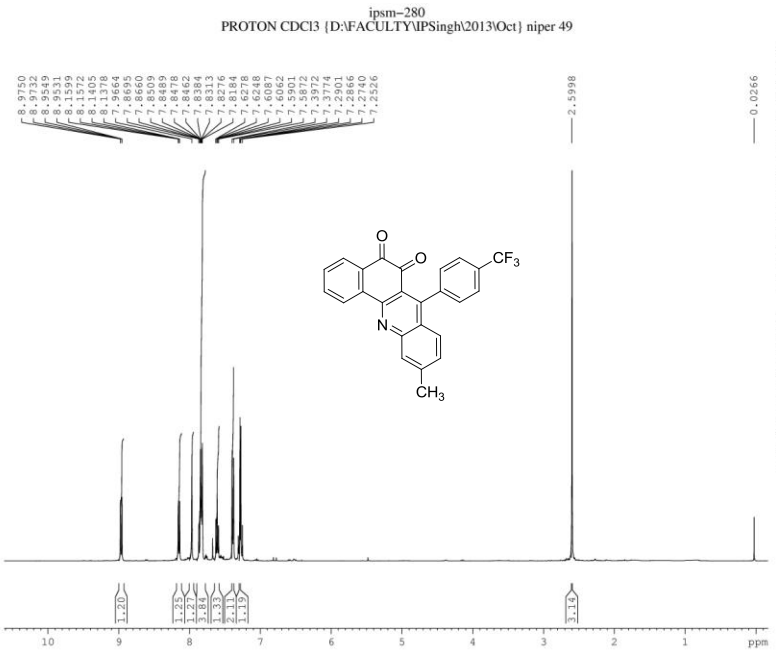

ipsm-277
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 57
180.39
180.20
164.08
152.29
152.26
151.79
141.79
137.46
136.15
132.39
131.88
131.41
129.24
128.99
128.81
127.07
127.02
121.95
118.66
112.10
108.18
77.34
77.23
77.03
76.71
56.03
0.01
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME ipsm-277
EXPNO 11
PROCNO 1
Date_ 20131008
Time 21.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

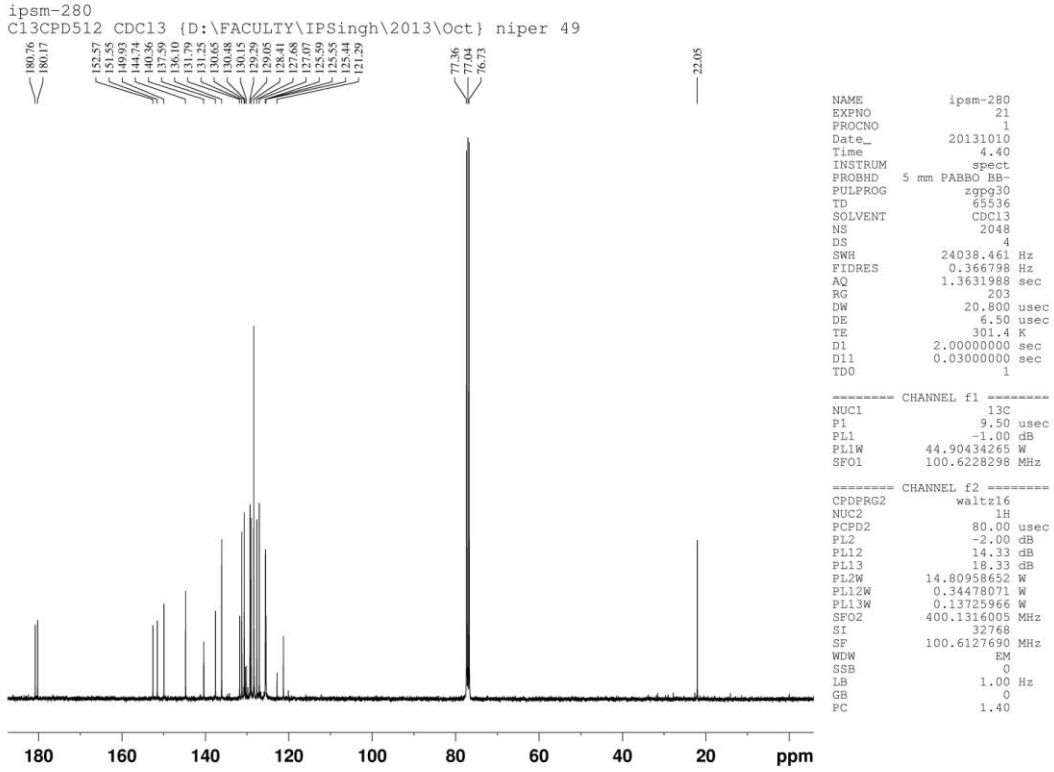

ipsm–278
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 48
9.0259
9.0242
9.0058
9.0041
8.2024
8.1996
8.1829
8.1801
8.0348
7.9099
7.9064
7.8897
7.8880
7.8716
7.8679
7.8552
7.8505
7.8469
7.7624
7.7329
7.7308
7.7225
7.7034
7.6627
7.6606
7.6576
7.6414
7.6390
7.6227
7.6198
7.5657
7.3897
7.3862
7.3815
7.3697
7.3650
7.3612
7.3420
7.3381
7.2861
7.2565
7.2350
7.1684
2.6299
2.6182
0.0220
O
O
CN
N
CH3
1.00
1.05
1.40
3.11
1.19
1.47
2.33
1.08
2.70
11
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-278
EXPNO 20
PROCNO 1
Date_ 20131008
Time 19.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40


ipsm-278
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 48
180.77
180.09
151.45
137.56
136.24
132.40
131.39
131.21
130.90
129.43
129.20
129.13
128.94
128.75
128.56
127.88
127.41
127.11
125.13
124.91
121.06
118.66
77.36
77.24
77.04
22.11
180
160
140
120
100
80
60
40
20
0
ppm
NAME ipsm-278
EXPNO 21
PROCNO 1
Date_ 20131010
Time 2.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

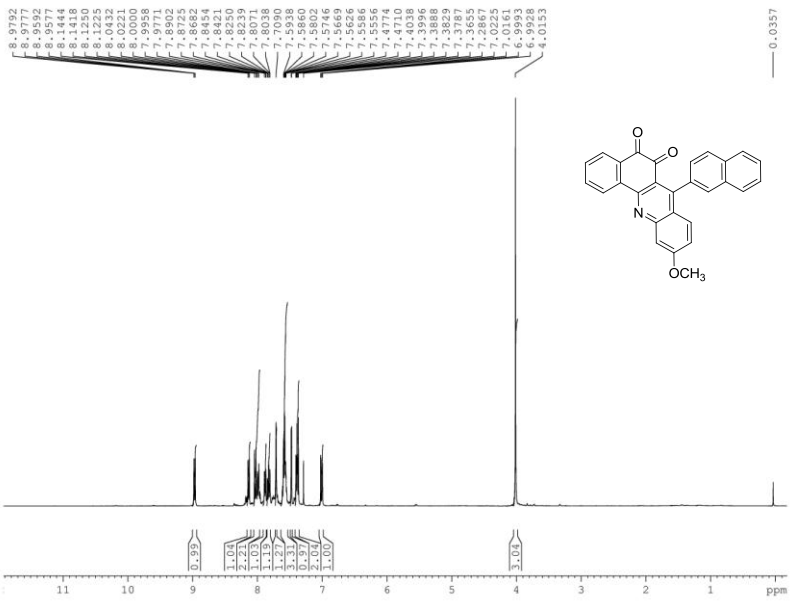

ipsm-279-r
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 8
9.0290
9.0272
9.0089
9.0071
8.2149
8.2121
8.1954
8.1927
7.9082
7.9047
7.8897
7.8880
7.8864
7.8851
7.8698
7.8663
7.8305
7.8106
7.6617
7.6587
7.6427
7.6400
7.6240
7.6210
7.5519
7.5455
7.3876
7.3677
7.3249
7.3017
7.2865
7.1567
7.1502
7.1334
7.1270
4.0782
0.0322
0.0240
0.0158
O
O
CF3
N
OCH3
1.00
1.00
1.06
2.00
2.03
0.98
2.01
0.99
0.98
3.08
10
9
8
7
6
5
4
3
2
1
0 ppm
NAME ipsm-279-r
EXPNO 10
PROCNO 1
Date_ 20131011
Time 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40


ipsm-279-r
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 8
180.51
180.41
163.98
152.48
152.28
152.20
140.44
137.59
136.09
131.88
131.31
129.33
129.18
128.35
127.06
125.62
125.58
125.54
121.73
120.32
108.07
77.35
77.03
76.71
56.00
0.01
180
160
140
120
100
80
60
40
20
0
ppm
NAME ipsm-279-r
EXPNO 11
PROCNO 1
Date_ 20131012
Time 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


ipsm-280
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 49
8.9730
8.8732
8.8549
8.8531
8.1599
8.1572
8.1405
8.1378
8.0564
7.8695
7.8660
7.8509
7.8489
7.8478
7.8462
7.8384
7.8313
7.8276
7.8184
7.6278
7.6248
7.6087
7.6062
7.5901
7.5872
7.3972
7.3774
7.2901
7.2866
7.2740
7.2526
2.5998
0.0266
O
O
CF3
N
CH3
1.20
1.25
1.27
3.84
1.03
2.10
1.19
3.14
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-280
EXPNO 20
PROCNO 1
Date_ 20131008
Time 19.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

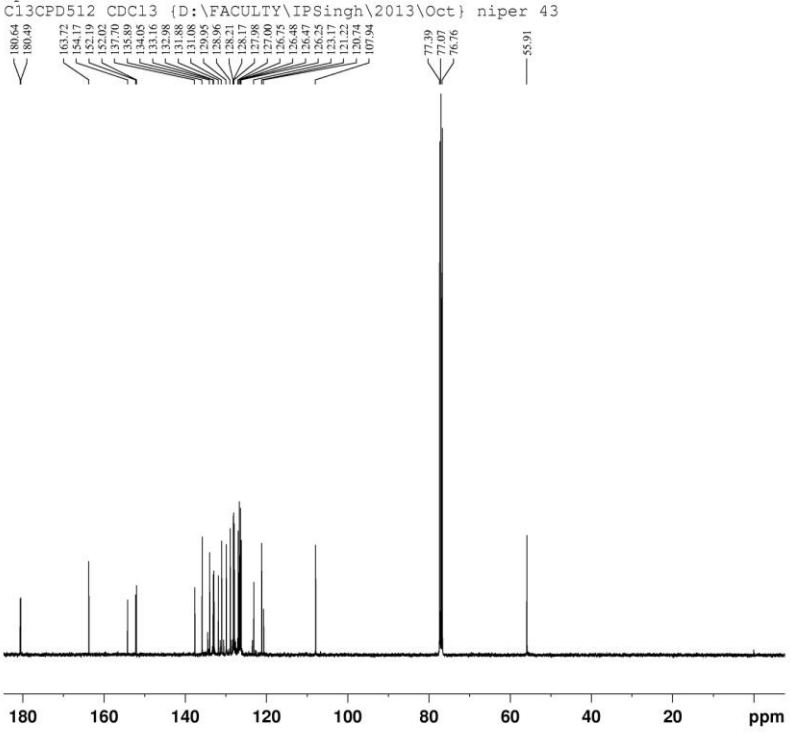

ipsm-280
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 49
180.76
180.17
152.57
151.55
149.93
144.74
140.36
137.59
136.10
131.79
131.25
130.65
130.48
130.15
129.29
129.05
128.41
127.68
127.07
125.59
125.55
125.44
121.29
77.36
77.04
76.73
22.05
180
160
140
120
100
80
60
40
20
ppm
NAME ipsm-280
EXPNO 21
PROCNO 1
Date_ 20131010
Time 4.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 301.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ipsm-281
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 43

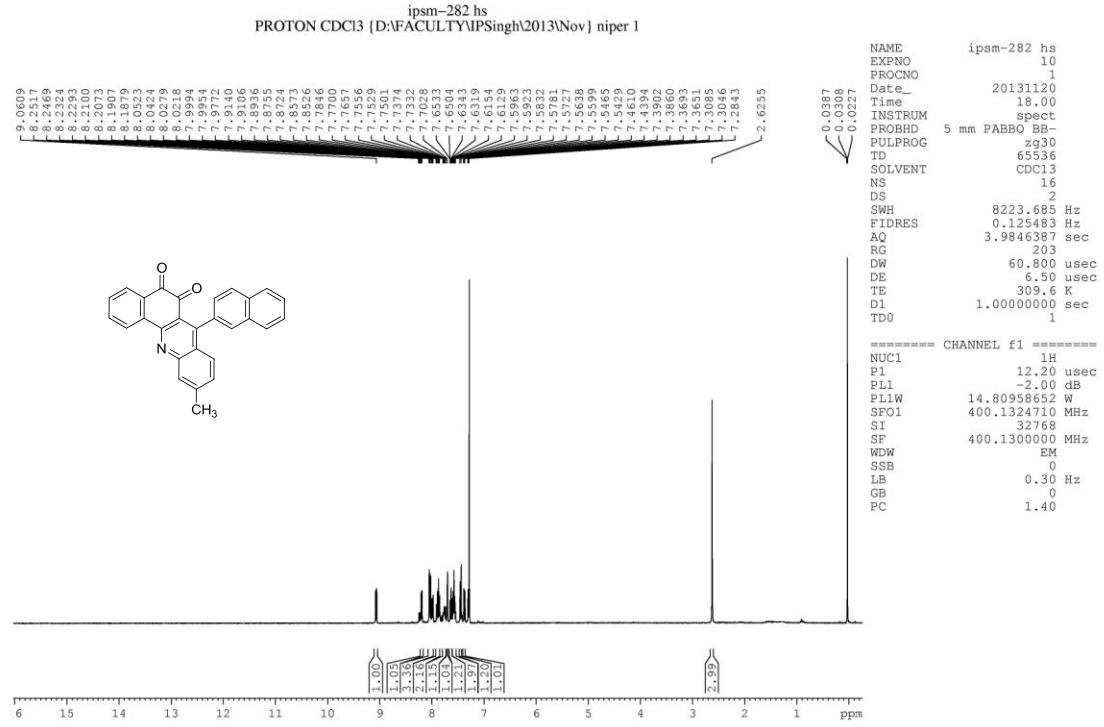


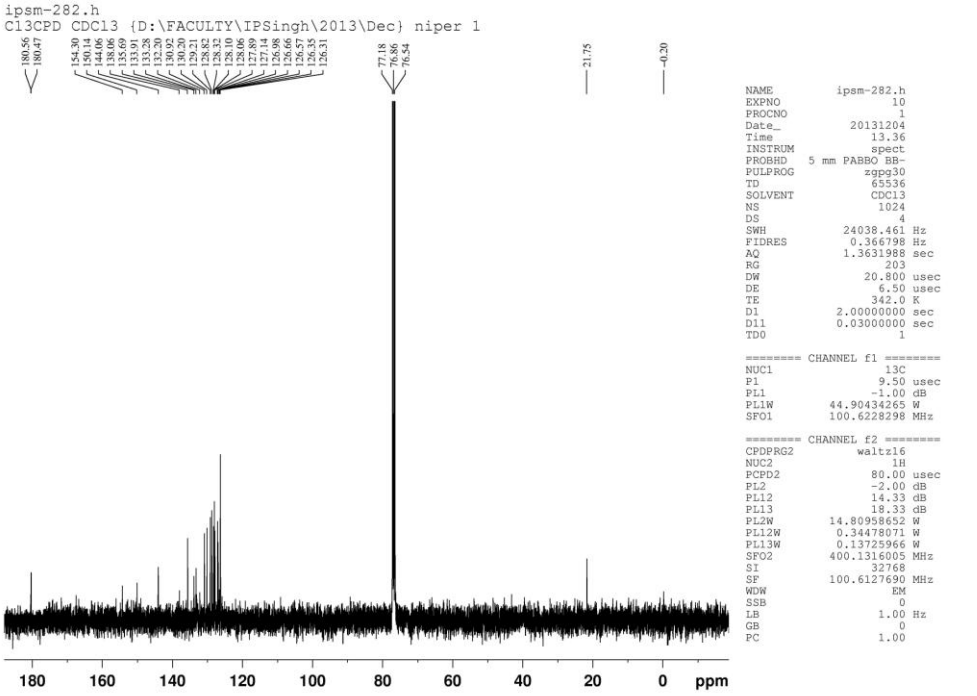
NAME	ipsm-281
EXPNO	10
PROCNO	1
Date_	20131010
Time	13.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

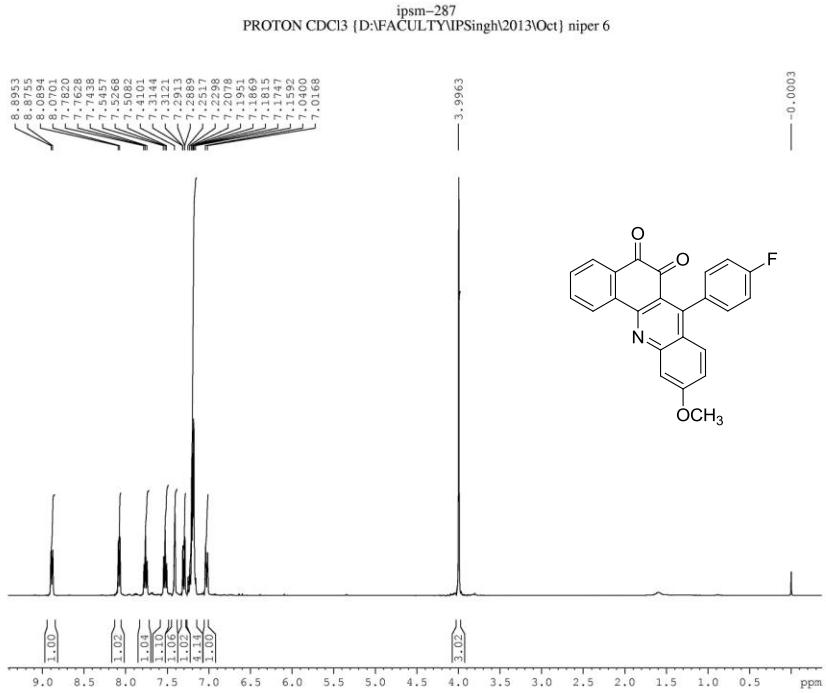
ipsm-281
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 43



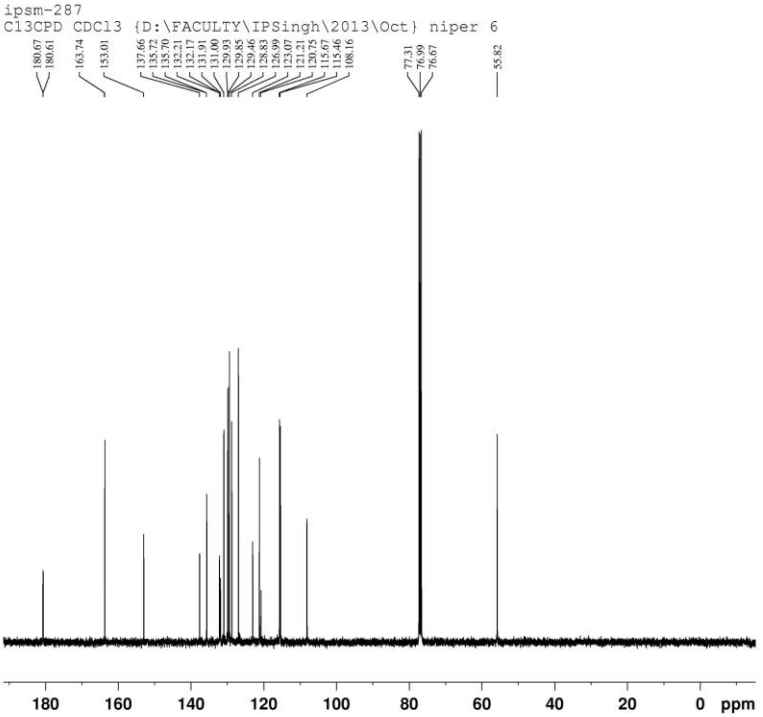
NAME	ipsm-281
EXPNO	11
PROCNO	1
Date_	20131011
Time	0.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-1.00 dB
PL1W	44.90434265 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	14.33 dB
PL13	18.33 dB
PL2W	14.80958652 W
PL12W	0.34478071 W
PL13W	0.13725966 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


ipsm−282 hs
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Nov} niper 1
9.0609
8.2517
8.2469
8.2324
8.2293
8.2100
8.2073
8.1907
8.1879
8.0523
8.0424
8.0279
8.0218
8.0044
7.9954
7.9772
7.9140
7.9106
7.8936
7.8755
7.8724
7.8573
7.8526
7.7846
7.7700
7.7657
7.7556
7.7509
7.7501
7.7374
7.7332
7.7028
7.6533
7.6504
7.6343
7.6319
7.6154
7.6129
7.5963
7.5923
7.5882
7.5781
7.5727
7.5638
7.5599
7.5465
7.5429
7.4610
7.4394
7.3902
7.3860
7.3693
7.3651
7.3085
7.2946
7.2843
2.6255
0.0387
0.0308
0.0227
O
O
N
CH3
1.00
1.05
3.36
2.16
1.15
1.04
1.21
1.97
1.20
1.10
2.99
6
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm−282 hs
EXPNO 10
PROCNO 1
Date_ 20131120
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 309.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 −2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

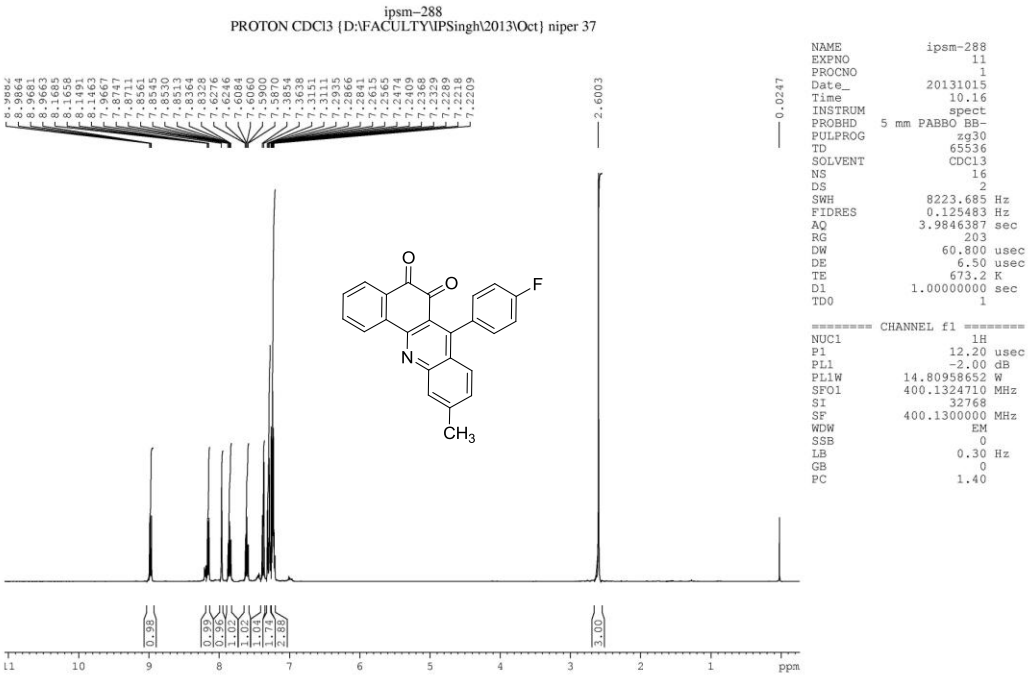

ipsm−282.h
C13CPD CDCl3 {D:\FACULTY\IPSingh\2013\Dec} niper 1
180.56
180.47
154.30
150.14
144.06
138.06
135.69
133.10
133.28
132.20
130.92
130.20
129.21
128.82
128.32
128.10
128.06
127.89
127.14
126.98
126.46
126.57
126.35
126.31
77.18
76.86
76.54
21.75
−0.20
180
160
140
120
100
80
60
40
20
0
ppm
NAME ipsm−282.h
EXPNO 10
PROCNO 1
Date_ 20131204
Time 13.36
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 342.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 −1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 −2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



NAME	ipsm-287
EXPNO	10
PROCNO	1
Date_	20131030
Time	12.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	317.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300129 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

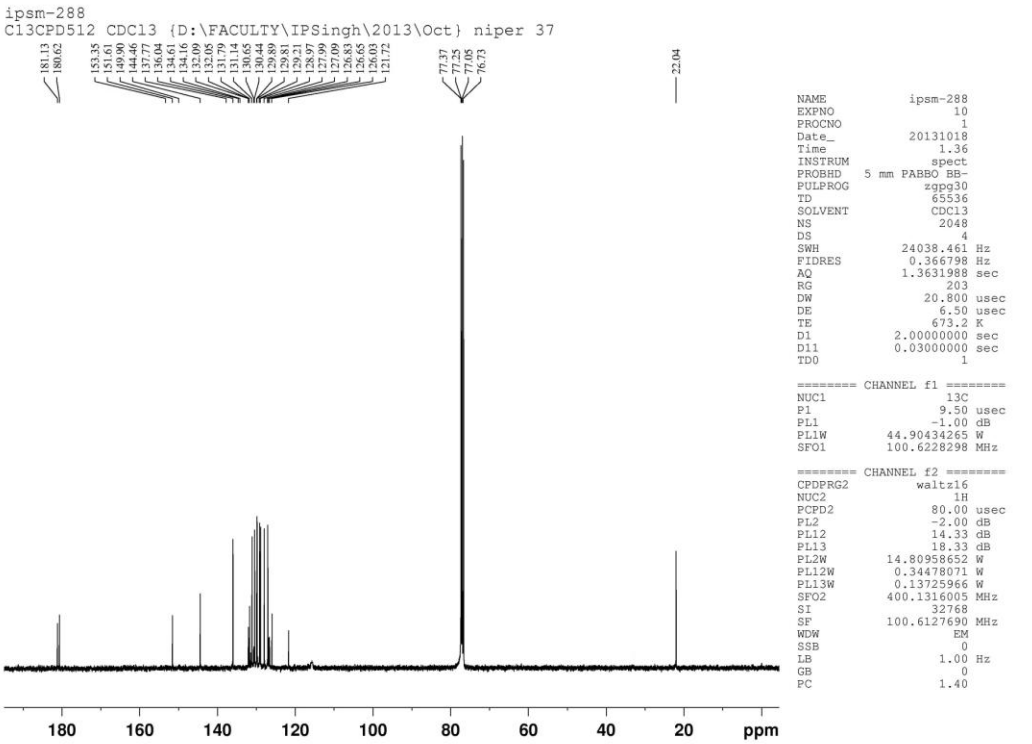


NAME	ipsm-287
EXPNO	11
PROCNO	1
Date_	20131030
Time	13.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1090
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	323.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-1.00 dB
PL1W	44.90434265 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	14.33 dB
PL13	18.33 dB
PL2W	14.80958652 W
PL12W	0.34478071 W
PL13W	0.13725966 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40




```
NAME            ipsm-288
EXPNO                 11
PROCNO                 1
Date_           20131015
Time               10.16
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                    1

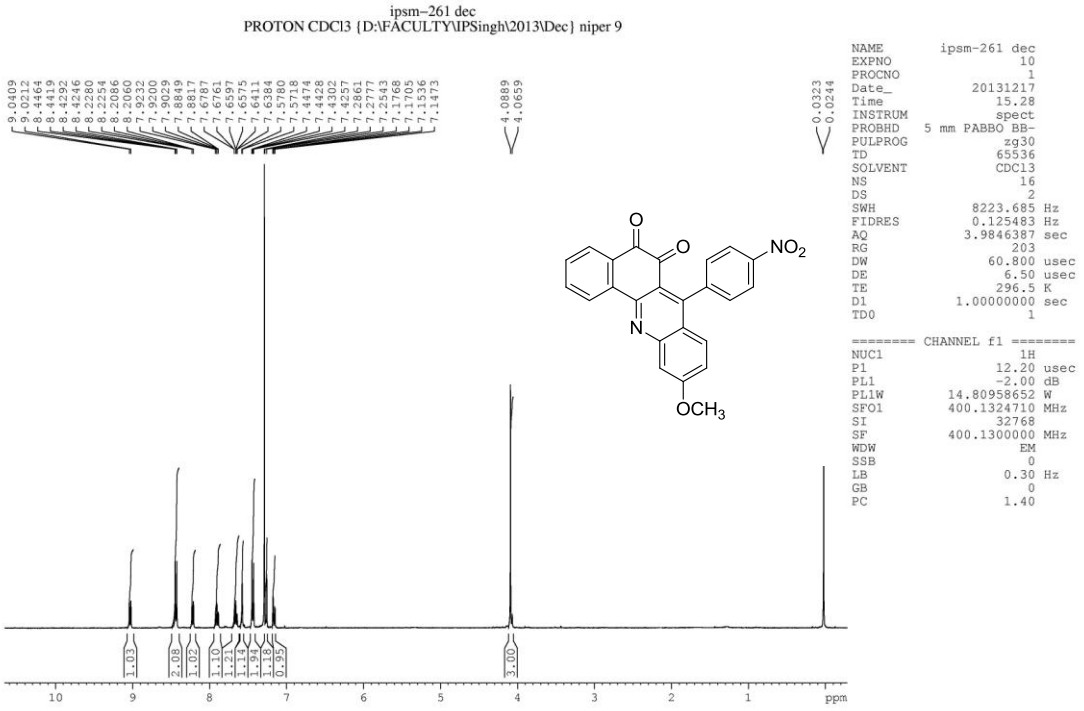
======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1                -2.00 dB
PL1W          14.80958652 W
SFO1          400.1324710 MHz
SI                 32768
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

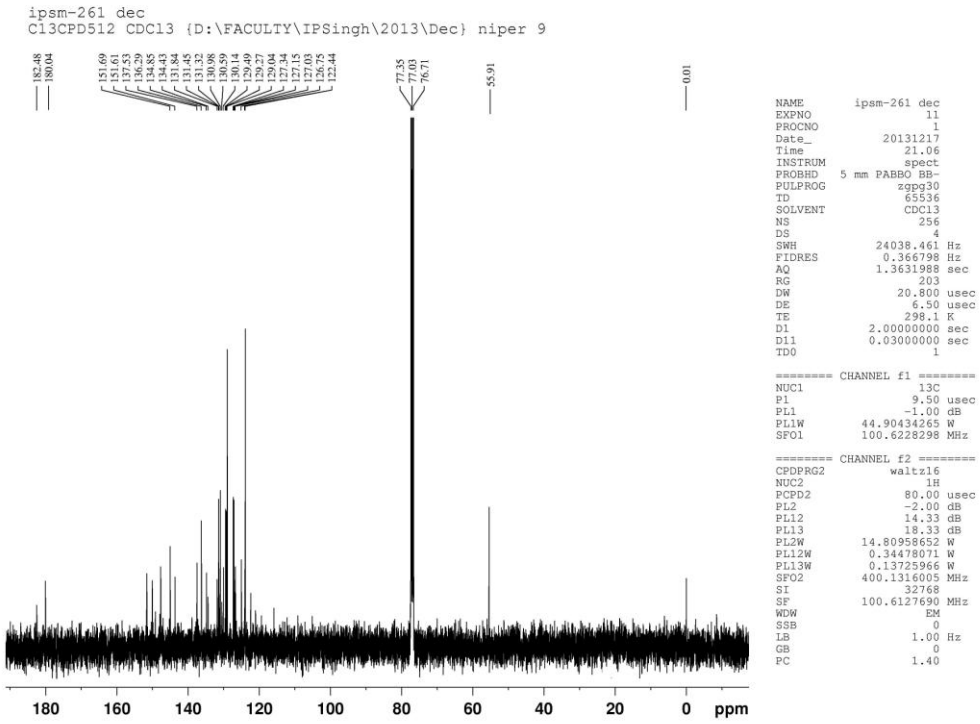


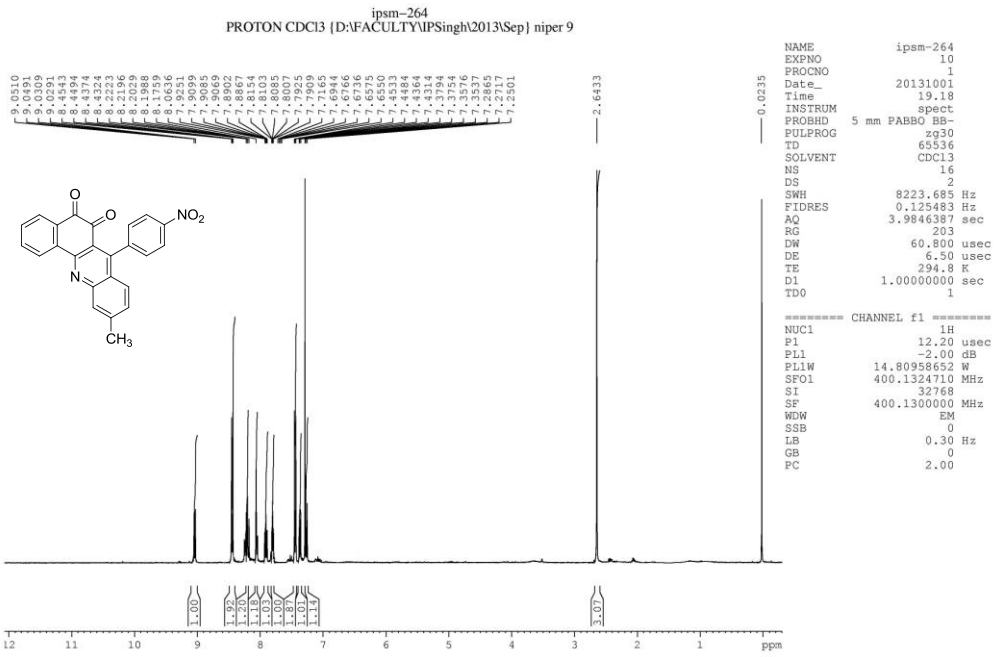

```
NAME            ipsm-288
EXPNO                 10
PROCNO                 1
Date_           20131018
Time               1.36
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2048
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                673.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

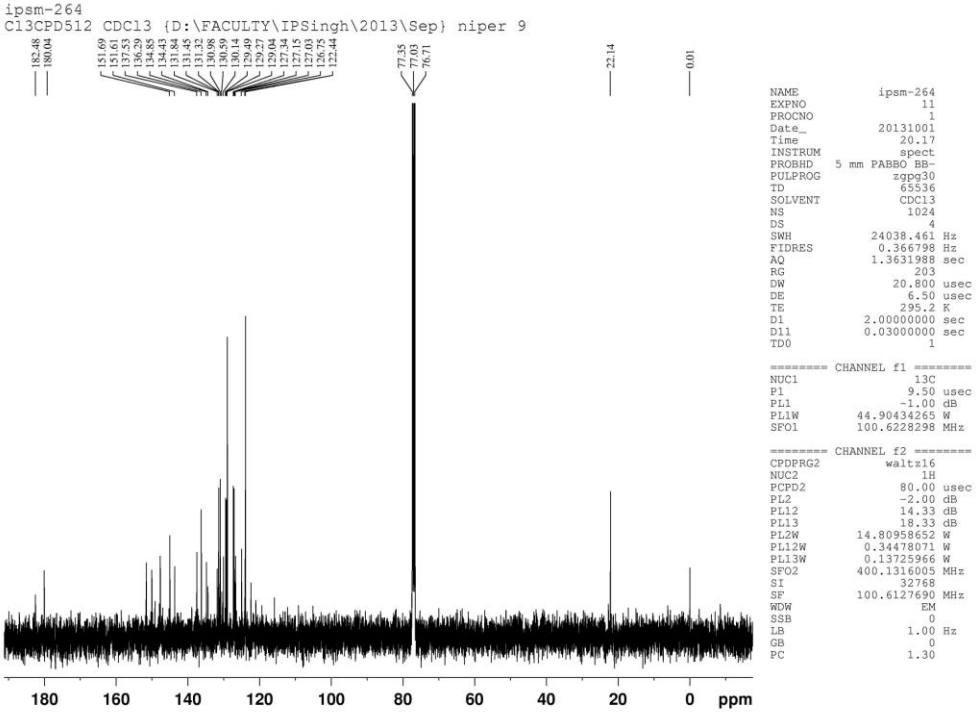
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.50 usec
PL1               -1.00 dB
PL1W          44.90434265 W
SFO1          100.6228298 MHz

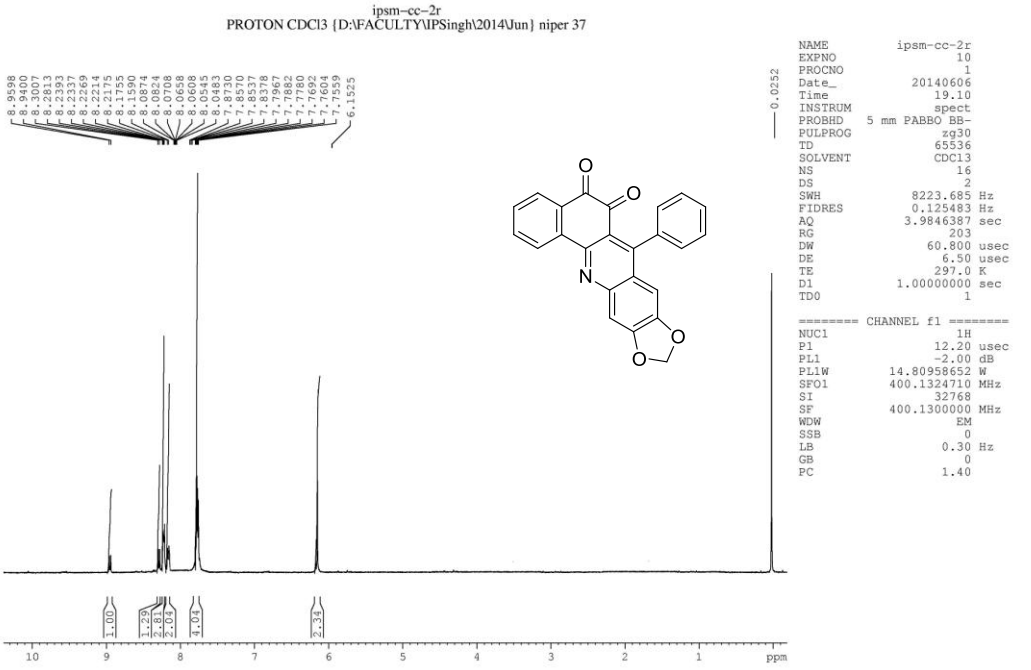
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               14.33 dB
PL13               18.33 dB
PL2W          14.80958652 W
PL12W          0.34478071 W
PL13W          0.13725966 W
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

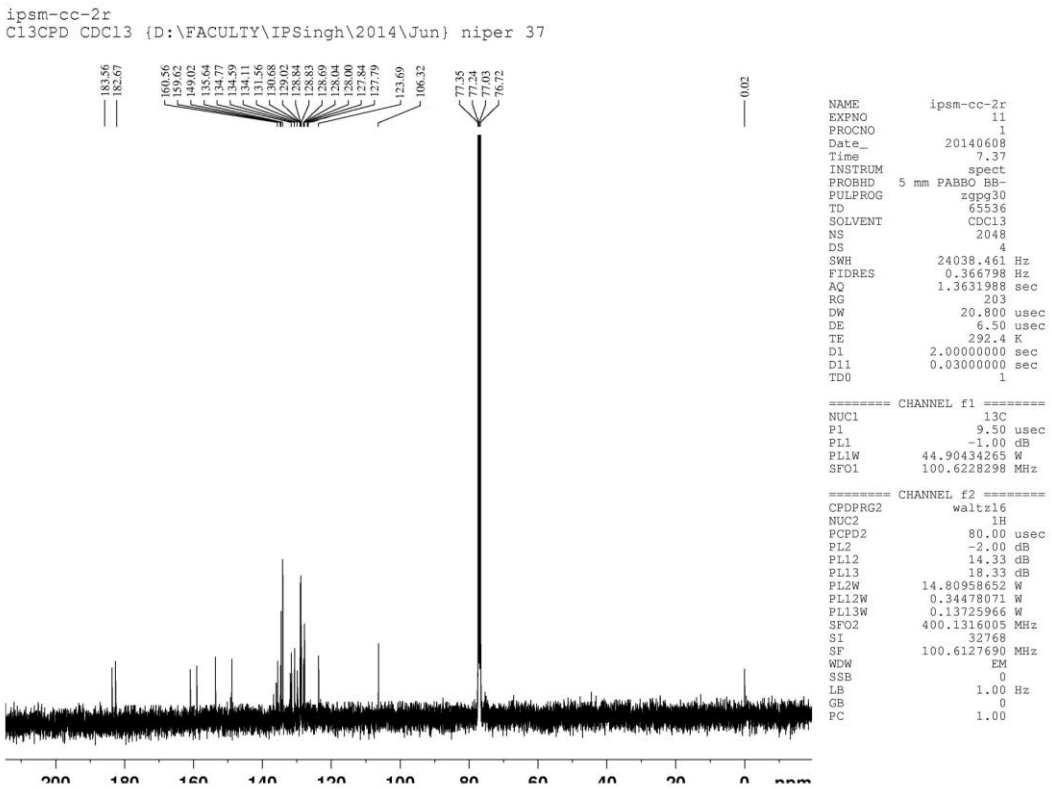

ipsm−261 dec
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Dec} niper 9
9.0409
9.0212
8.4464
8.4419
8.4292
8.4246
8.2280
8.2254
8.2086
8.2060
7.9232
7.9200
7.9029
7.8849
7.8817
7.6787
7.6761
7.6597
7.6575
7.6411
7.6384
7.5760
7.5734
7.4478
7.4428
7.4302
7.4257
7.2861
7.2777
7.2543
7.1768
7.1705
7.1536
7.1473
4.0889
4.0659
0.0323
0.0244
O
O
NO2
N
OCH3
1.03
2.08
1.02
1.10
1.21
1.14
1.94
1.18
0.99
3.00
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-261 dec
EXPNO 10
PROCNO 1
Date_ 20131217
Time 15.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40


ipsm-261 dec
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Dec} niper 9
182.48
180.04
151.69
151.61
137.53
136.29
134.85
134.43
131.84
131.45
131.32
130.98
130.59
130.14
129.49
129.37
129.04
127.34
127.15
127.03
126.75
122.44
77.35
77.03
76.71
55.91
0.01
180
160
140
120
100
80
60
40
20
0
ppm
NAME ipsm-261 dec
EXPNO 11
PROCNO 1
Date_ 20131217
Time 21.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

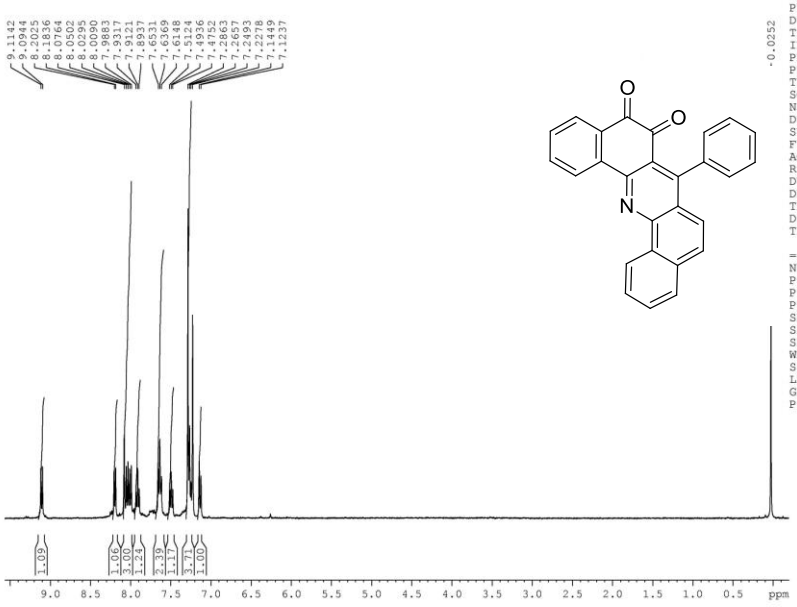

ipsm-264
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Sep} niper 9
9.0510
9.0491
9.0309
9.0291
8.4543
8.4494
8.4474
8.4324
8.2223
8.2196
8.2029
8.1988
8.1759
8.0636
7.9251
7.9099
7.9085
7.9069
7.8902
7.8867
7.8154
7.8103
7.8085
7.8007
7.7925
7.7909
7.7165
7.6944
7.6766
7.6736
7.6575
7.6550
7.4533
7.4484
7.4364
7.4314
7.3794
7.3754
7.3576
7.3537
7.2865
7.2717
7.2501
2.6433
0.0235
O
O
NO2
N
CH3
1.00
1.92
1.18
1.03
1.00
1.87
1.01
1.14
3.07
12
11
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-264
EXPNO 10
PROCNO 1
Date_ 20131001
Time 19.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00


ipsm-264
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2013\Sep} niper 9
182.48
180.04
151.69
151.61
137.53
136.29
134.85
134.43
131.84
131.45
131.32
130.98
130.59
130.14
129.49
129.27
129.04
127.34
127.15
127.03
126.75
122.44
77.35
77.03
76.71
22.14
0.01
180
160
140
120
100
80
60
40
20
0
ppm
NAME ipsm-264
EXPNO 11
PROCNO 1
Date_ 20131001
Time 20.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.30


ipsm-cc-2r
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 37
8.9598
8.9400
8.3007
8.2813
8.2393
8.2337
8.2269
8.2214
8.2175
8.1755
8.1590
8.0874
8.0824
8.0708
8.0658
8.0608
8.0545
8.0483
7.8730
7.8570
7.8537
7.8378
7.7967
7.7882
7.7780
7.7692
7.7604
7.7559
6.1525
0.0252
O
O
N
O
O
1.00
1.25
2.81
2.04
4.04
2.34
10
9
8
7
6
5
4
3
2
1
ppm
NAME ipsm-cc-2r
EXPNO 10
PROCNO 1
Date_ 20140606
Time 19.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -2.00 dB
PL1W 14.80958652 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

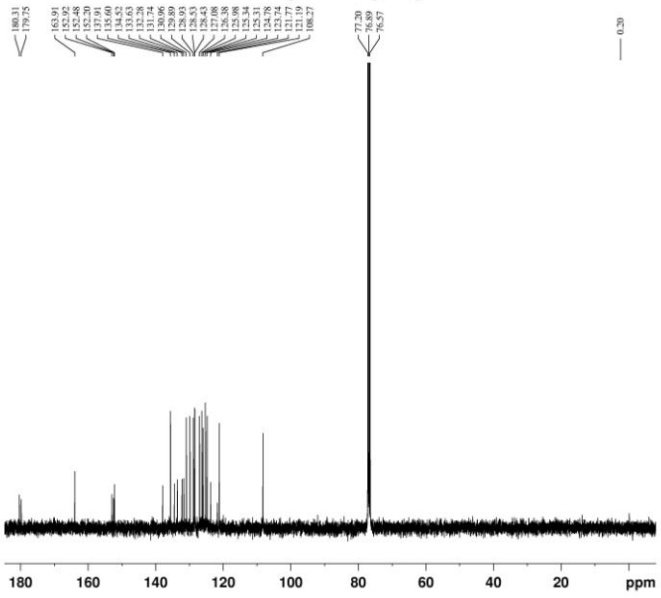

ipsm-cc-2r
C13CPD CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 37
183.56
182.67
160.56
159.62
149.02
135.64
134.77
134.59
134.11
131.56
130.68
129.02
128.91
128.83
126.69
126.04
126.00
127.84
127.79
123.69
106.32
77.35
77.24
77.03
76.72
0.02
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME ipsm-cc-2r
EXPNO 11
PROCNO 1
Date_ 20140608
Time 7.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 292.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -1.00 dB
PL1W 44.90434265 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.33 dB
PL13 18.33 dB
PL2W 14.80958652 W
PL12W 0.34478071 W
PL13W 0.13725966 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

ipsm–cc–nap
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 3



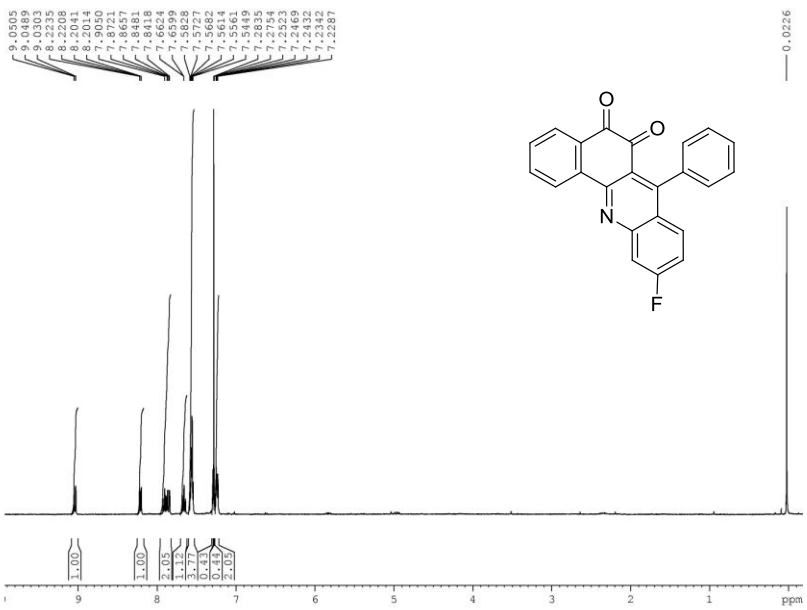
NAME	ipsm-cc-nap
EXPNO	10
PROCNO	1
Date_	20140616
Time	21.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm-cc-4r
C13CPD512 CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 57



NAME	ipsm-cc-4r
EXPNO	10
PROCNO	1
Date_	20140619
Time	20.23
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-1.00 dB
PL1W	44.90434265 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	14.33 dB
PL13	18.33 dB
PL2W	14.80958652 W
PL12W	0.34478071 W
PL13W	0.13725966 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

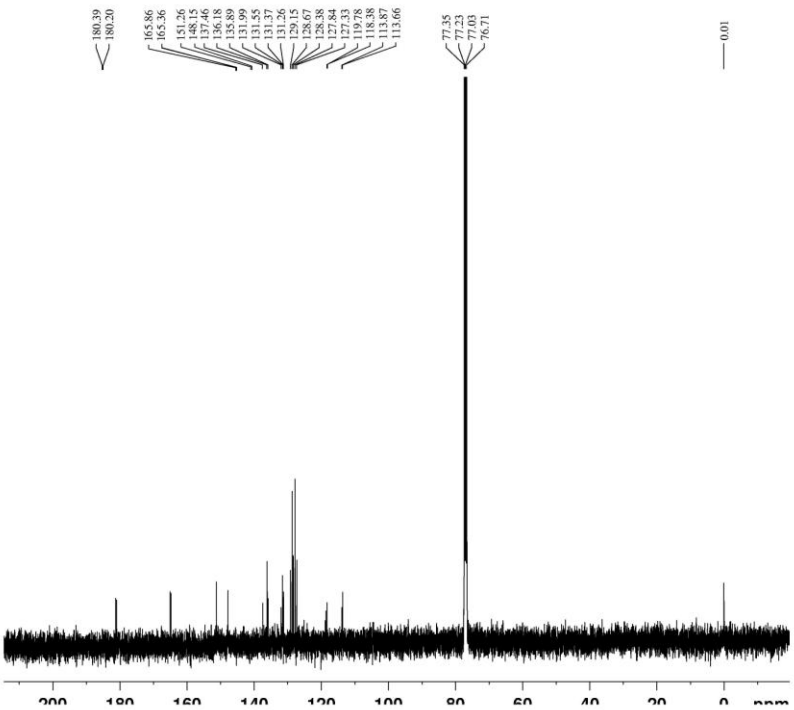
ipsm–cc–12
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 35




```
NAME          ipsm-cc-12
EXPNO                 10
PROCNO                 1
Date_           20140606
Time               18.59
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                    203
DW                 60.800 usec
DE                  6.50 usec
TE                 296.9 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1                -2.00 dB
PL1W          14.80958652 W
SFO1          400.1324710 MHz
SI                 32768
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

ipsm-cc-12
C13CPD CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 35

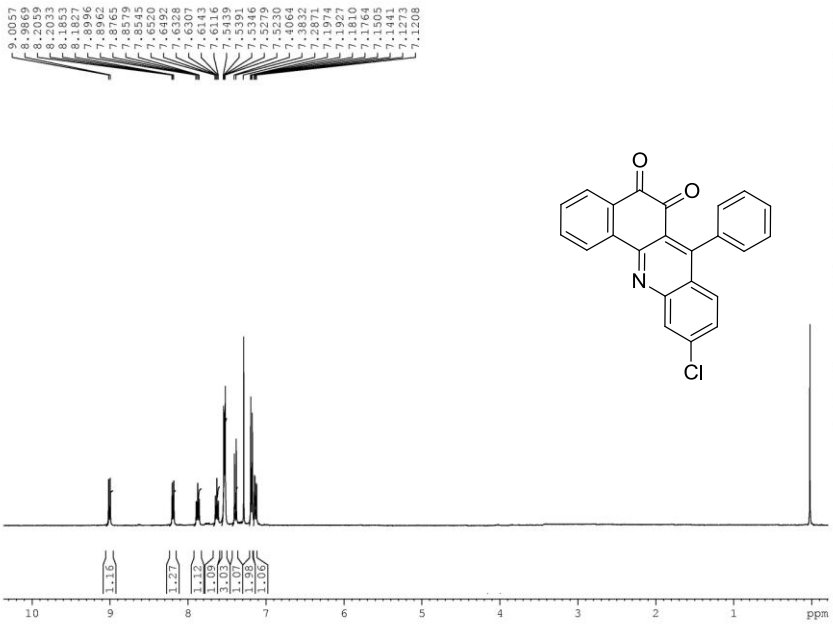



```
NAME          ipsm-cc-12
EXPNO                 11
PROCNO                 1
Date_           20140608
Time                5.35
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2048
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                    203
DW                 20.800 usec
DE                  6.50 usec
TE                 293.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.50 usec
PL1                -1.00 dB
PL1W          44.90434265 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               14.33 dB
PL13               18.33 dB
PL2W          14.80958652 W
PL12W          0.34478071 W
PL13W          0.13725966 W
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

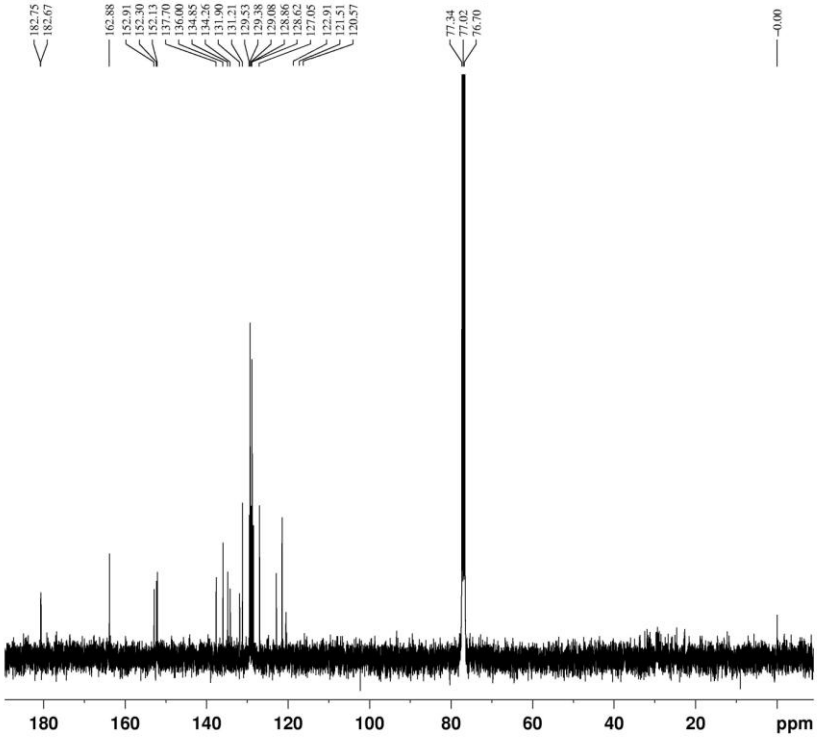
ipsm-chloro-3
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 54




```
NAME        ipsm-chloro-3
EXPNO               10
PROCNO               1
Date_          20140619
Time              18.08
INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  203
DW               60.800 usec
DE                6.50 usec
TE               297.3 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               12.20 usec
PL1               -2.00 dB
PL1W        14.80958652 W
SFO1        400.1324710 MHz
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.40
```

ipsm-chloro-3
C13CPD CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 54

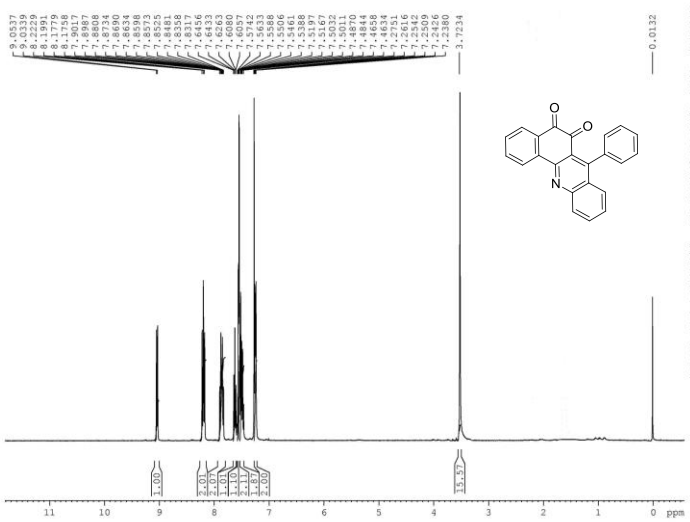



```
NAME        ipsm-chloro-3
EXPNO               11
PROCNO               1
Date_          20140619
Time              20.05
INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               298.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                9.50 usec
PL1              -1.00 dB
PL1W        44.90434265 W
SFO1        100.6228298 MHz

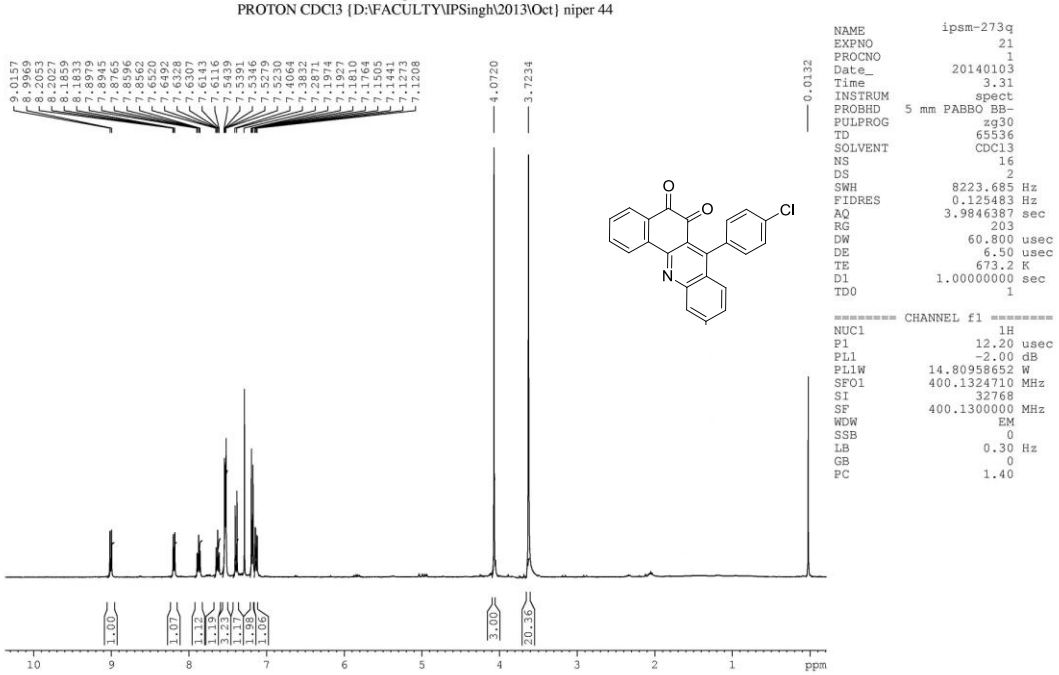
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               -2.00 dB
PL12              14.33 dB
PL13              18.33 dB
PL2W        14.80958652 W
PL12W        0.34478071 W
PL13W        0.13725966 W
SFO2        400.1316005 MHz
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

ipsm-q5.237
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 95



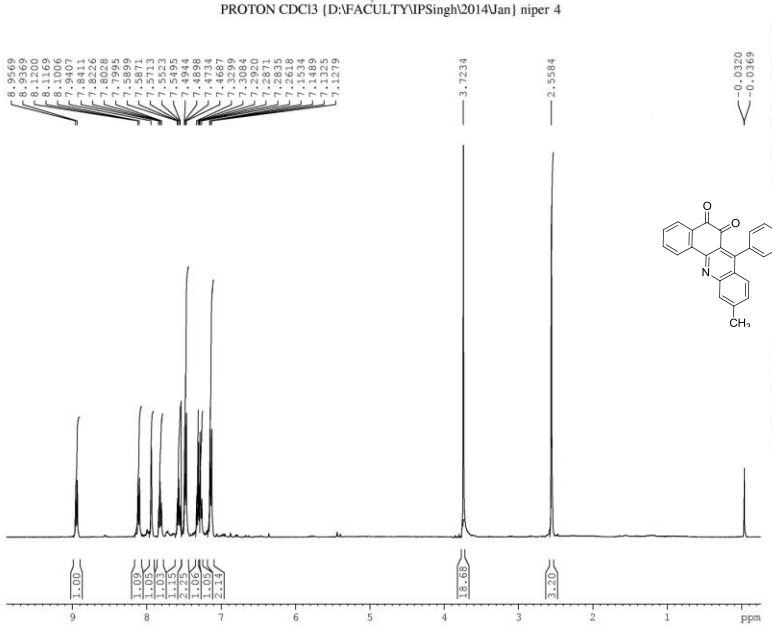
NAME	ipsm-q5.237
EXPNO	10
PROCNO	1
Date_	20140103
Time	11.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300107 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm-273q
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Oct} niper 44



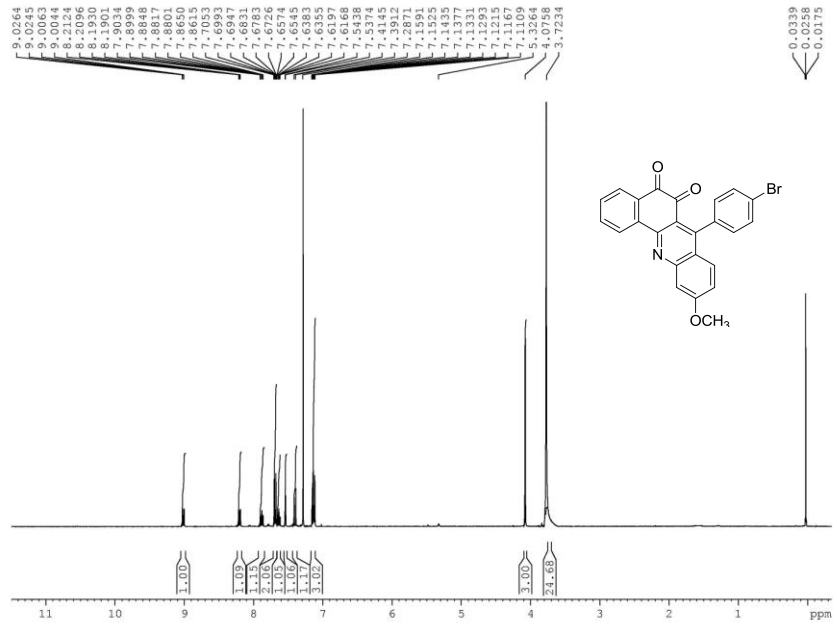
NAME	ipsm-273q
EXPNO	21
PROCNO	1
Date_	20140103
Time	3.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm-274 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 4



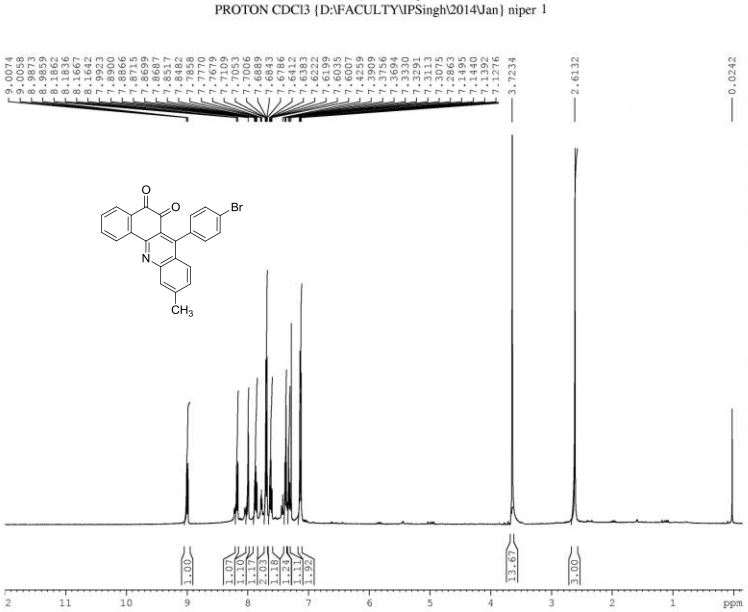
NAME	ipsm-274 q
EXPNO	10
PROCNO	1
Date_	20140103
Time	3.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
	203
	60.800 usec
	6.50 usec
	673.2 K
	1.00000000 sec
	1
=== CHANNEL f1 ========	
	1H
	12.20 usec
	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm-275 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Dec} niper 8



NAME	ipsm-275 q
EXPNO	10
PROCNO	1
Date_	20140107
Time	5.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

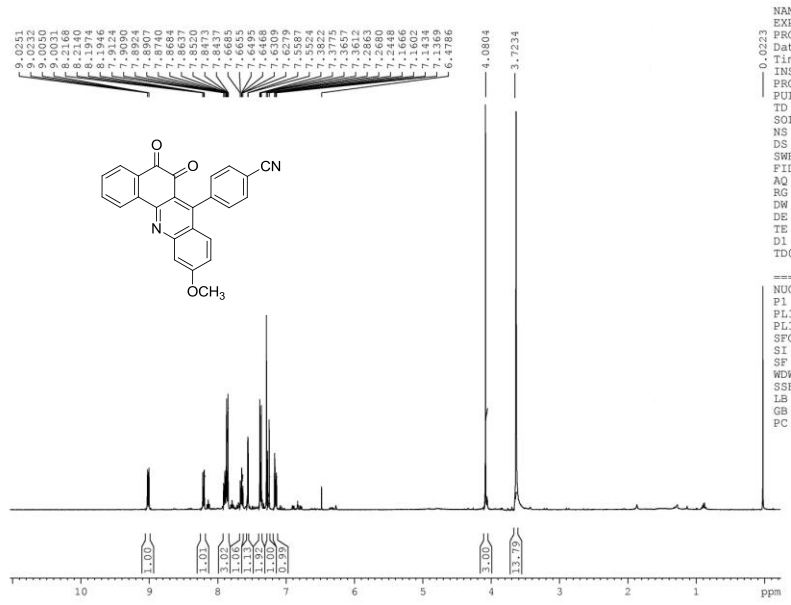
ipsm–276 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 1




```
NAME            ipsm-276 q
EXPNO                   10
PROCNO                   1
Date_             20140103
Time                 6.01
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     203
DW                  60.800 usec
DE                   6.50 usec
TE                  673.2 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.20 usec
PL1                  -2.00 dB
PL1W            14.80958652 W
SFO1            400.1324710 MHz
SI                    32768
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.40
```

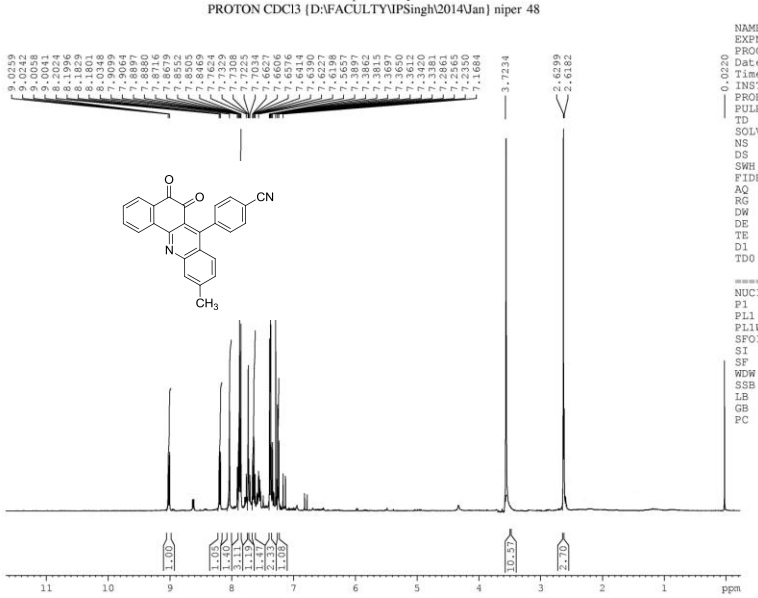
ipsm–277q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 9




```
NAME            ipsm-277q
EXPNO                   10
PROCNO                   1
Date_             20140108
Time                 9.51
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     203
DW                  60.800 usec
DE                   6.50 usec
TE                  295.0 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.20 usec
PL1                  -2.00 dB
PL1W            14.80958652 W
SFO1            400.1324710 MHz
SI                    32768
SF              400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.40
```

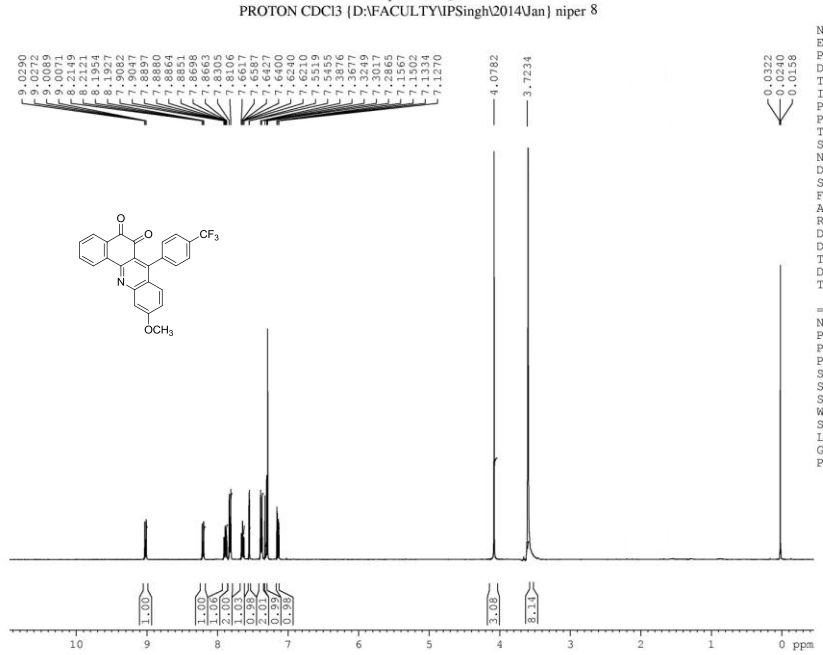
ipsm–278 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 48



```
NAME          ipsm-278 q
EXPNO                 20
PROCNO                 1
Date_           20140108
Time                9.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                   203
DW              60.800 usec
DE               6.50 usec
TE              295.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1              12.20 usec
PL1             -2.00 dB
PL1W        14.80958652 W
SFO1        400.1324710 MHz
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB              0.30 Hz
GB                     0
PC                  1.40
```

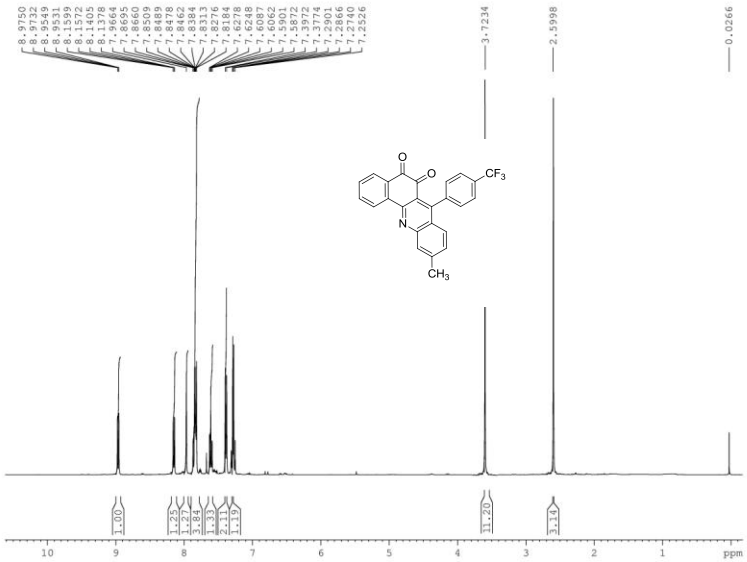
ipsm–279 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 8



```
NAME          ipsm-279 q
EXPNO                 10
PROCNO                 1
Date_           20140101
Time                5.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                   203
DW              60.800 usec
DE               6.50 usec
TE              294.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1              12.20 usec
PL1             -2.00 dB
PL1W        14.80958652 W
SFO1        400.1324710 MHz
SI                 32768
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB              0.30 Hz
GB                     0
PC                  1.40
```

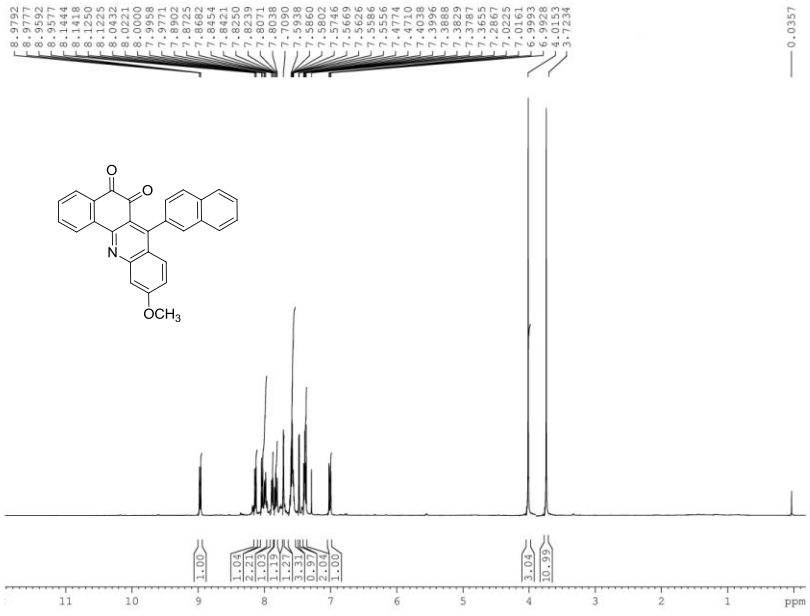
ipsm-280
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan } niper 41




```
NAME            ipsm-280
EXPNO                 10
PROCNO                 1
Date_           20141008
Time               19.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                295.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1                -2.00 dB
PL1W         14.80958652 W
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

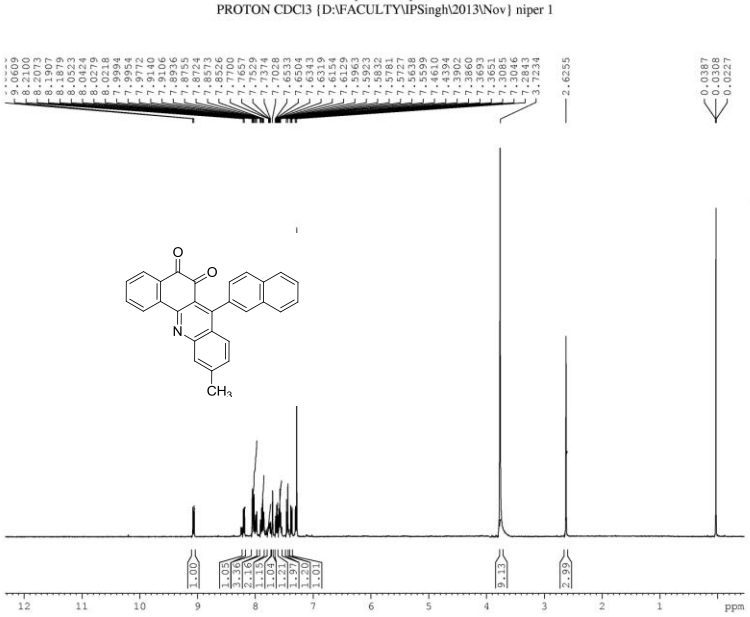
ipsm-281
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan } niper 4




```
NAME            ipsm-281
EXPNO                 10
PROCNO                 1
Date_           20141001
Time                3.24
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                    1

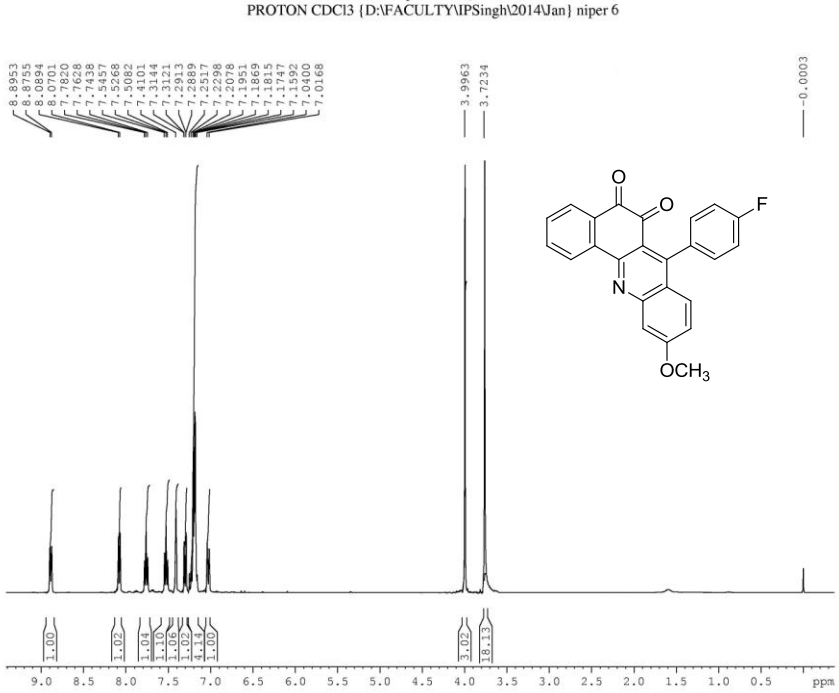
======== CHANNEL f1 ========
NUC1                  1H
P1                 12.20 usec
PL1                -2.00 dB
PL1W         14.80958652 W
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

ipsm–282q
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Nov} niper 1



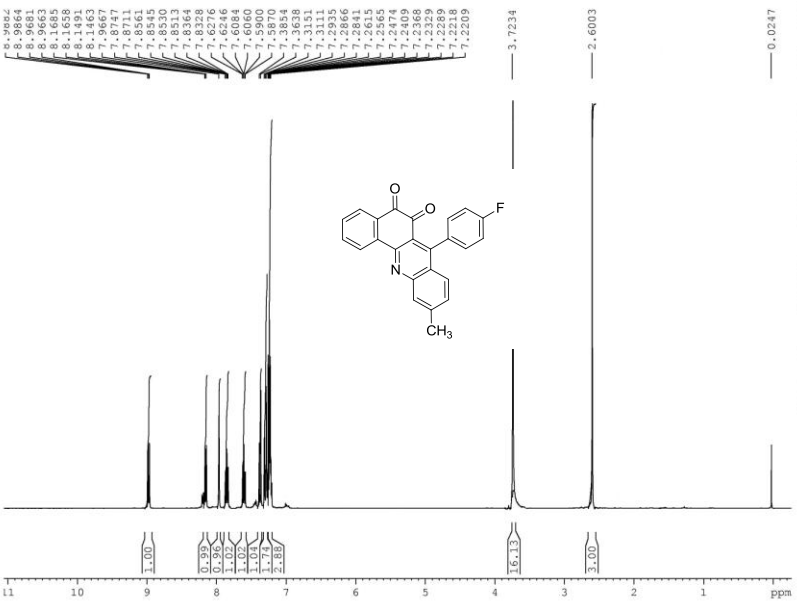
NAME	ipsm-282q
EXPNO	10
PROCNO	1
Date_	20131128
Time	18.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	309.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm–287q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 6



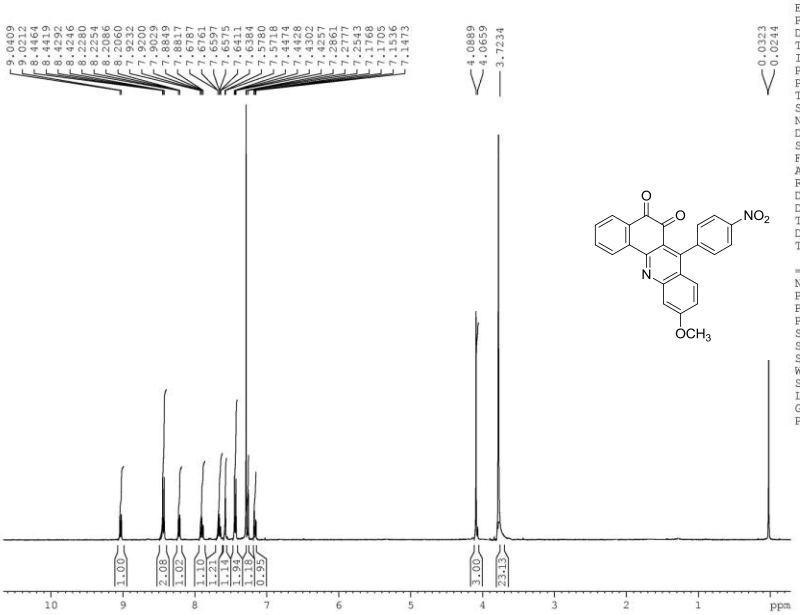
NAME	ipsm-287q
EXPNO	10
PROCNO	1
Date_	201401003
Time	1.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	317.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300129 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm–288 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 3



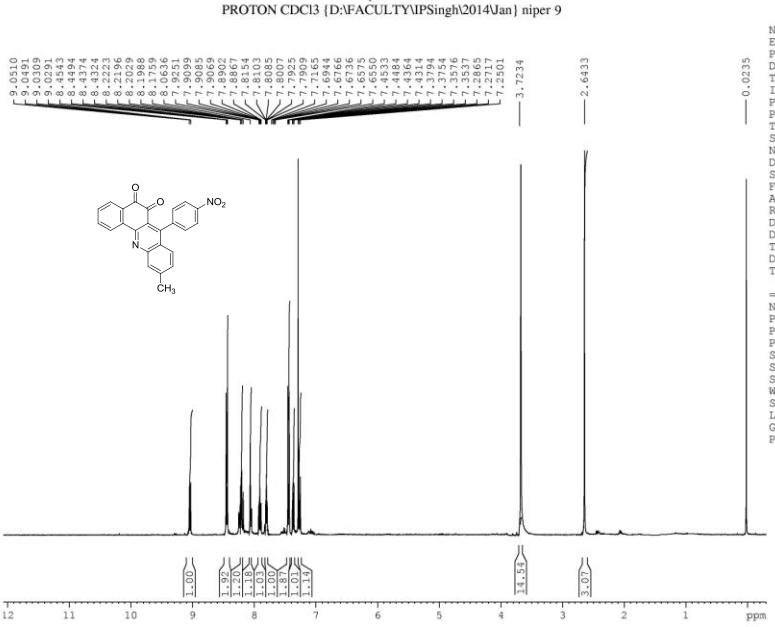
NAME	ipsm-288 q
EXPNO	11
PROCNO	1
Date_	20140105
Time	1.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm–261q
PROTON CDCl3 {D:\FACULTY\IPSingh\2013\Dec} niper 9



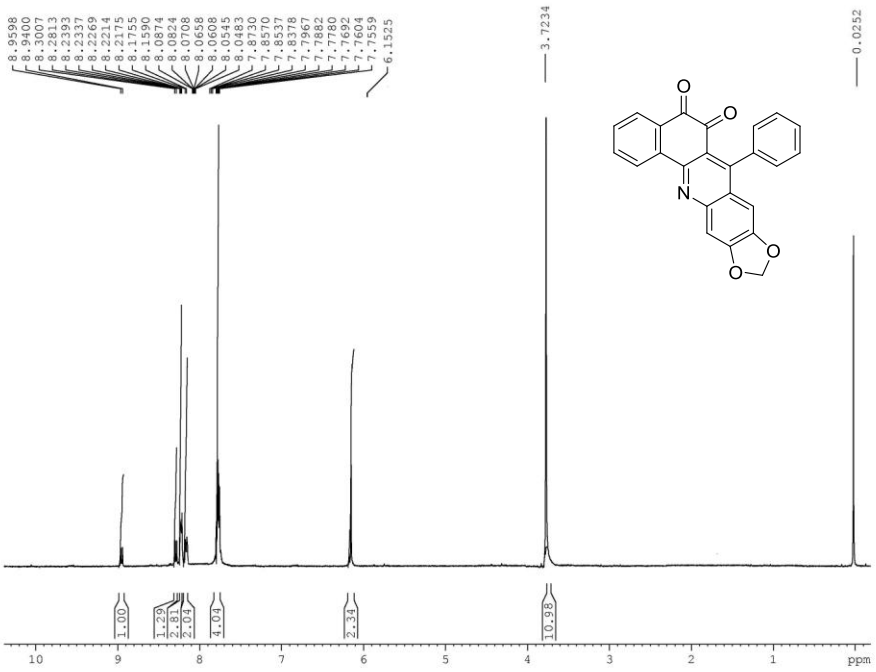
NAME	ipsm-261q
EXPNO	10
PROCNO	1
Date_	20131217
Time	15.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm–264 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jan} niper 9



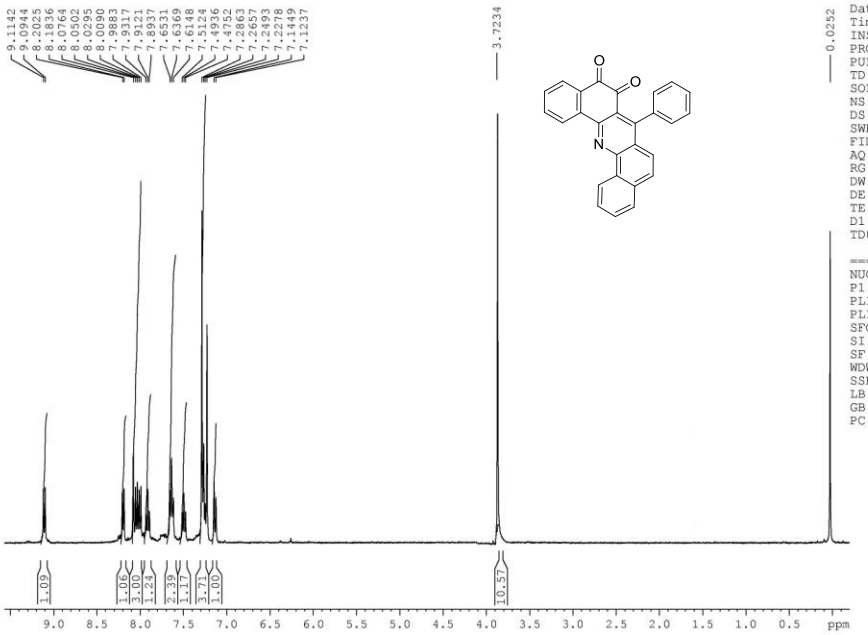
NAME	ipsm-264 q
EXPNO	10
PROCNO	1
Date_	20140101
Time	9.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	294.8 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

ipsm–cc–2r
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 37



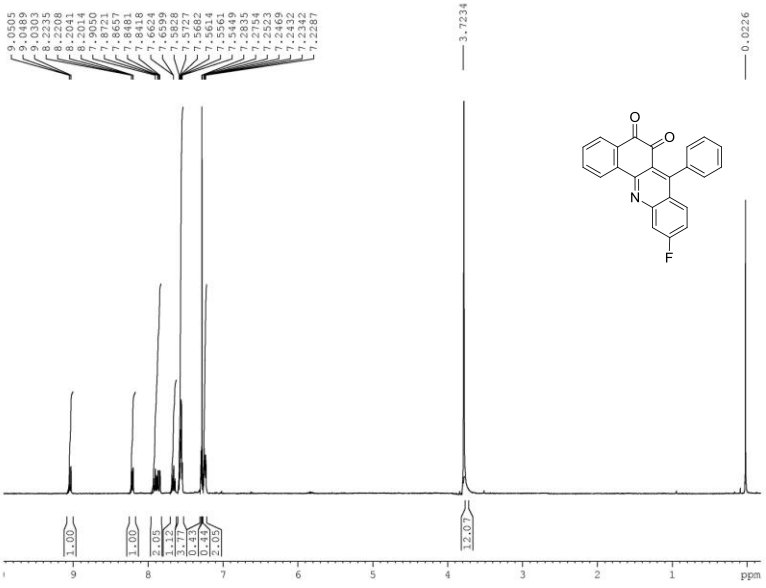
NAME	ipsm-cc-2r
EXPNO	10
PROCNO	1
Date_	20140606
Time	19.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm–cc–napq
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 34

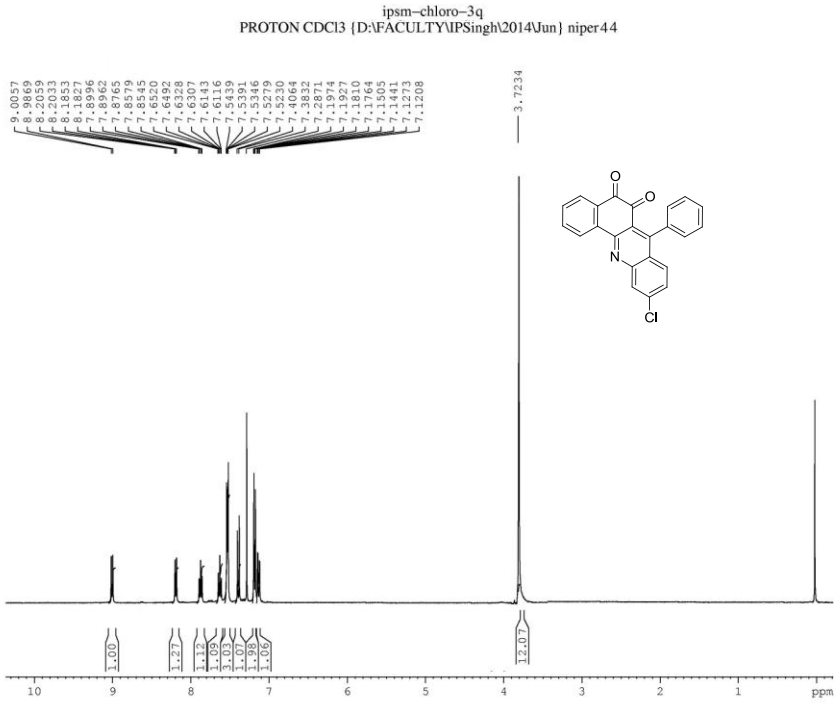


NAME	ipsm-cc-napq
EXPNO	10
PROCNO	1
Date_	20140620
Time	20.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

ipsm–cc–12 q
PROTON CDCl3 {D:\FACULTY\IPSingh\2014\Jun} niper 25



NAME	ipsm-cc-12q
EXPNO	10
PROCNO	1
Date_	20140620
Time	10.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40



NAME	ipsm-chloro-3q
EXPNO	10
PROCNO	1
Date_	20140620
Time	18.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	297.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.20 usec
PL1	-2.00 dB
PL1W	14.80958652 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.40