Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information for Synthesis, Characterization, DFT, and TD-DFT Studies of the Photovoltaic Properties of Novel Reactive Azonitrobenzaldehyde derivatives

Hitler Louis[a,b*], Izubundu B. Onyebuenyi[a,b], Joseph O. Odey[a,b], Azuaga T. Igbalagh[c*] MaryJane T. Mbonu[a,b], , Ededet A. Eno[a,b], Anthony M.S. Pembere[d], and Ofiong E. Offiong[b].

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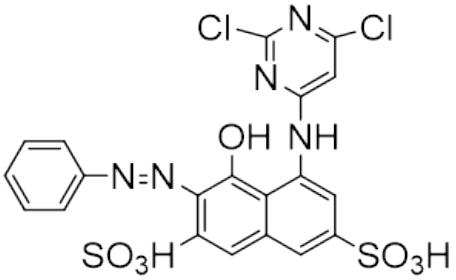
[b]Department of Pure and Applied Chemistry, Faculty of Physical Sciences, University of Calabar, Calabar, Nigeria

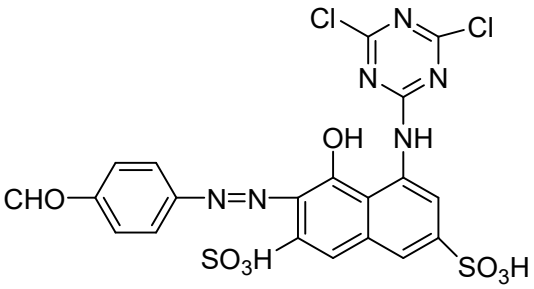
[c]Department of Chemical Sciences, Federal University of Wukari, Wukari, Nigeria

[d]Department of Physical Sciences, Jaramogi Oginga Odinga University of Science and Technology, Bondo, Kenya

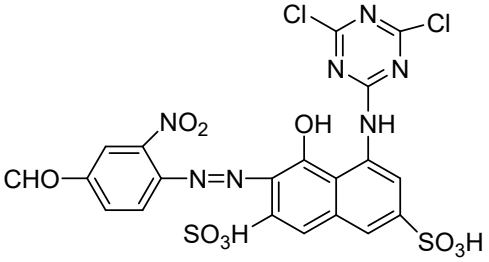
[**]**Corresponding author's email: louismuzong@gmail.com; shies4me@gmail.com**



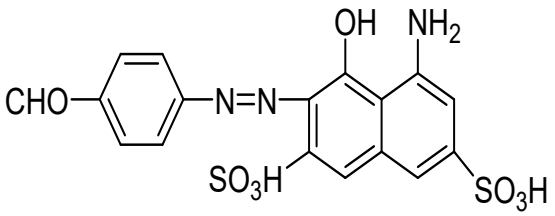
(a) Cyanurated H-acid with aniline



(b) Cyanurated H-acid with p-aminobenzaldehyde



(c) Cyanurated H-acid with 4-amino-3-nitobenzaldehyde nitrobenzaldehye



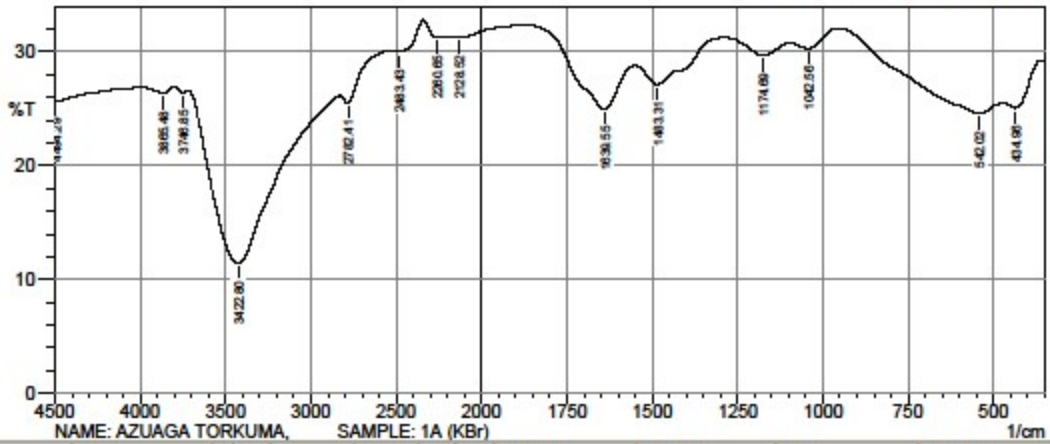
(d) Non-cyanurated H-acid with p-aminobenzaldehyde

Figure S1. The molecular structures of the synthesized dyes A, B, C and D.

SHIMADZU

FTIR ANALYSIS RESULT NARICT,ZARIA

FTIR- 8400S FOURIER TRANSFORM INFRARED SPECTROPHOTOMETER



NAME: AZUAGA TORKUMA, SAMPLE: 1A (KBr)

	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	434.96	25.071	1.68	472.58	359.74	65.075	1.557
2	542.02	24.594	1.829	953.83	473.54	269.745	8.602
3	1042.56	30.267	0.978	1093.67	954.8	70.699	0.872
4	1174.69	29.676	1.3	1287.53	1094.64	99.714	1.647
5	1483.31	27.149	2.26	1551.78	1288.49	141.688	4.074
6	1639.55	24.967	4.758	1874.87	1552.75	175.252	9.363
7	2128.52	31.233	0.305	2201.82	1875.84	162.719	0.661
8	2260.65	31.243	0.686	2340.7	2202.78	68.958	0.778
9	2483.43	29.967	0.867	2536.48	2341.66	99.951	2.019
10	2782.41	25.495	1.326	2831.6	2537.44	161.945	1.286
11	3422.8	11.453	14.957	3716.95	2832.56	642.711	130.413
12	3746.85	26.401	0.275	3798.93	3717.92	46.611	0.191
13	3865.48	26.376	0.554	3994.71	3799.89	111.877	0.867
14	4494.29	25.714	0.014	4500.08	3995.67	291.753	0.04

Comment;

NAME: AZUAGA TORKUMA, SAMPLE: 1A (KBr)

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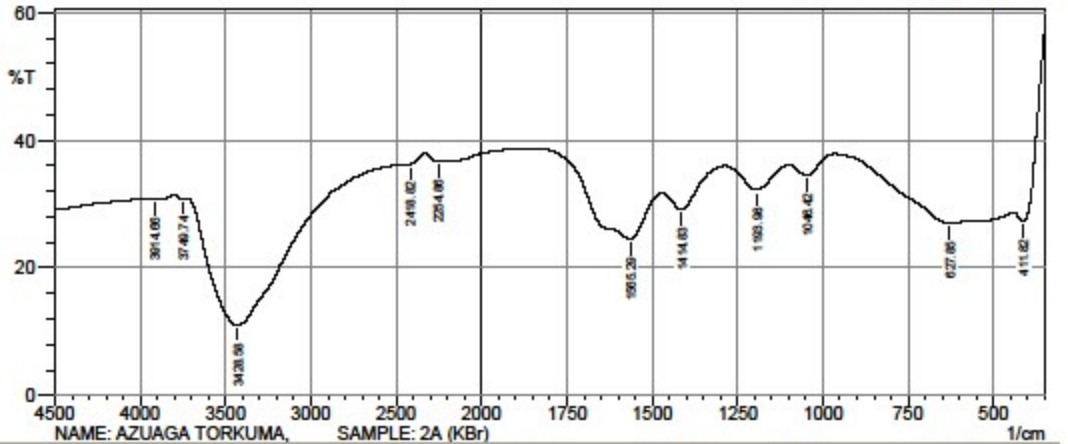
FTIR ANALYSIS RESULT NARICT,ZARIA

FTIR- 8400S FOURIER TRANSFORM INFRARED SPECTROPHOTOMETER



NAME: AZUAGA TORKUMA, SAMPLE: 2A (KBr)

	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	411.82	27.314	11.297	443.64	349.13	43.924	7.319
2	627.85	26.995	4.931	966.37	444.61	267.187	16.119
3	1046.42	34.529	2.264	1099.46	967.33	58.732	1.635
4	1193.98	32.207	3.815	1288.49	1100.43	87.591	4.199
5	1414.83	29.193	3.896	1471.74	1289.46	89.481	3.751
6	1565.29	24.505	8.965	1859.44	1471.74	196.581	20.335
7	2254.86	36.669	1.431	2336.84	1865.23	200.93	4.74
8	2418.82	36.305	0.371	2441	2337.8	44.706	0.325
9	3428.58	11.061	21.096	3726.6	2441.96	800.146	190.15
10	3749.74	30.842	0.199	3805.68	3727.56	39.688	0.116
11	3914.66	30.704	0.37	3992.78	3806.64	95.014	0.65

Comment;

NAME: AZUAGA TORKUMA, SAMPLE: 2A (KBr)

User; Administrator

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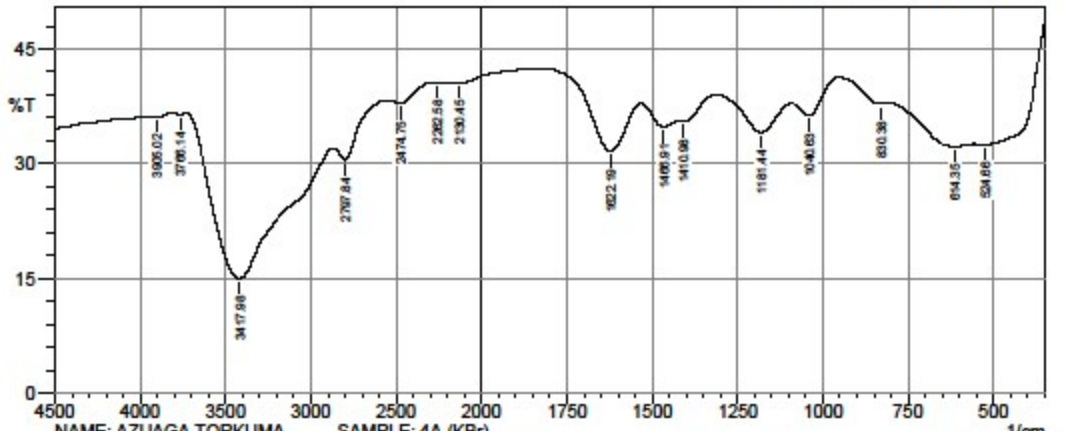
FTIR ANALYSIS RESULT NARICT,ZARIA

FTIR- 8400S FOURIER TRANSFORM INFRARED SPECTROPHOTOMETER



NAME: AZUAGA TORKUMA, SAMPLE: 4A (KBr)

	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	524.66	32.501	2.624	557.45	349.13	94.625	11.434
2	614.35	32.26	1.547	803.38	558.41	113.716	2.565
3	830.38	37.816	0.69	951.9	804.34	59.852	0.533
4	1040.63	36.326	2.791	1091.75	952.87	57.869	1.947
5	1181.44	34.045	4.282	1314.53	1092.71	96.992	4.88
6	1410.98	35.515	0.298	1419.66	1315.5	44.839	0.297
7	1466.91	34.826	1.693	1532.5	1420.62	49.865	1.162
8	1622.19	31.642	7.652	1830.51	1533.46	126.566	9.134
9	2130.45	40.554	0.422	2197.96	1831.47	140.36	0.707
10	2262.58	40.59	0.039	2297.3	2198.92	38.5	0.021
11	2474.75	37.877	1.158	2553.84	2298.26	104.642	1.475
12	2797.84	30.486	3.005	2871.14	2554.8	146.083	3.272
13	3417.98	15.013	19.951	3726.6	2872.1	539.854	142.202
14	3766.14	36.402	0.271	3813.4	3727.56	37.529	0.139
15	3905.02	36.114	0.194	3939.74	3814.36	55.165	0.2

Comment;

NAME: AZUAGA TORKUMA, SAMPLE: 4A (KBr)

User; Administrator

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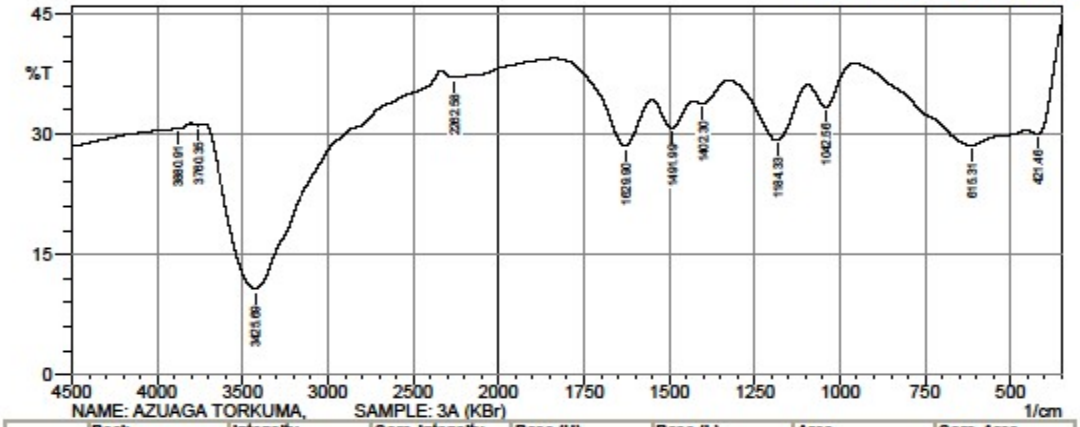
FTIR ANALYSIS RESULT NARICT,ZARIA

FTIR- 8400S FOURIER TRANSFORM INFRARED SPECTROPHOTOMETER



NAME: AZUAGA TORKUMA, SAMPLE: 3A (KBr)

	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	421.46	30.05	4.576	453.29	349.13	49.237	3.919
2	615.31	28.533	4.574	957.69	454.25	246.98	13.464
3	1042.56	33.387	3.758	1093.67	958.65	60.295	2.725
4	1184.33	29.215	7.163	1326.1	1094.64	111.582	10.114
5	1402.3	33.725	1.046	1429.3	1327.07	46.731	0.652
6	1491.99	30.71	3.438	1550.82	1430.26	58.92	2.659
7	1629.9	28.504	7.147	1838.22	1551.78	133.273	8.96
8	2262.58	37.052	1.091	2333.94	1839.19	208.346	4.218
9	3425.69	10.663	22.024	3724.67	2334.91	852.472	208.912
10	3760.35	31.074	0.205	3801.82	3725.63	38.57	0.116
11	3880.91	30.628	0.147	3901.16	3802.79	50.211	0.148

Comment;
NAME: AZUAGA TORKUMA, SAMPLE: 3A (KBr)

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Figure S2: FT-IR of dyes A, B, C and D.

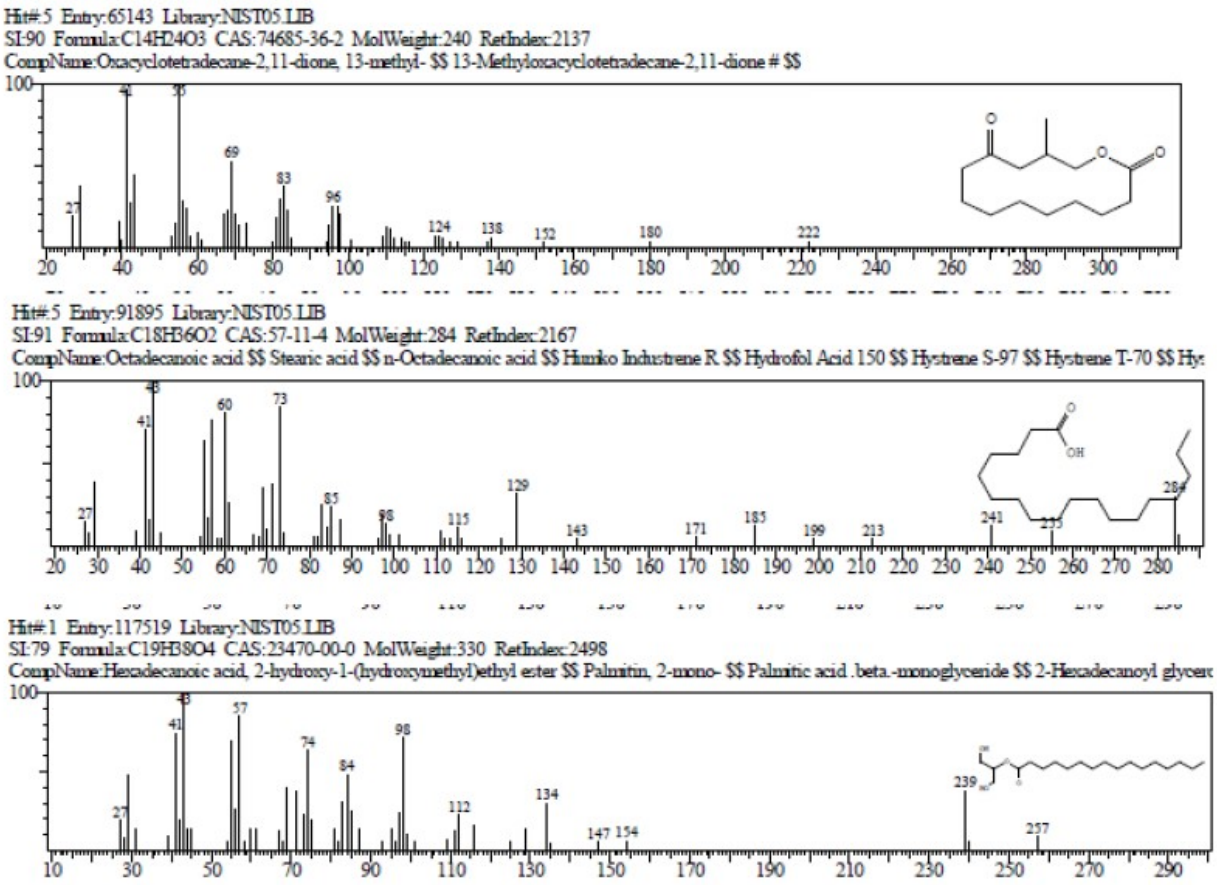

Figure S3: Mass spectra of the dyes.

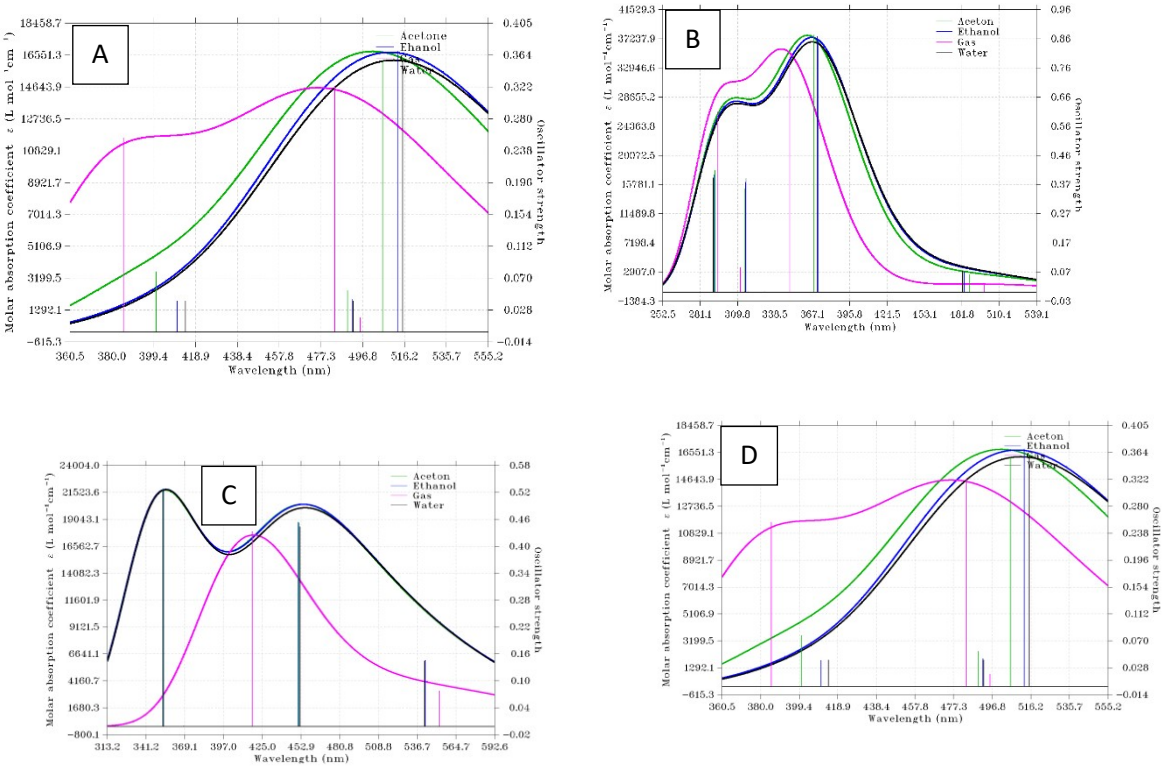

Figure S4: Graphical representation of the Theoritical UV-Vis absorption spectra of the optimized dyes in their different phases.

The Graphical representation of the Experimental UV-Vis absorption spectra of the optimized dyes in thei different phases is as seen in S5 to S11

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Spectrum Version: v2.30

NARICT, ZARIA UV-VISBLE SPECTRAL SCAN RESULT

07/23/2015

01:13:03 PM

RawData - C:\AZUAGA 4D ET.spc

No.	P/V	Wavelength	Abs.	Description
1	P	630.60	0.050	
2	P	591.00	0.056	
3	P	576.20	0.058	
4	P	564.60	0.057	
5	P	359.80	0.127	

Measurement Properties

Wavelength Range (nm.):	350.00 to 700.00
Scan Speed:	Fast
Sampling Interval:	0.2
Auto Sampling Interval:	Enabled
Scan Mode:	Auto

Instrument Properties

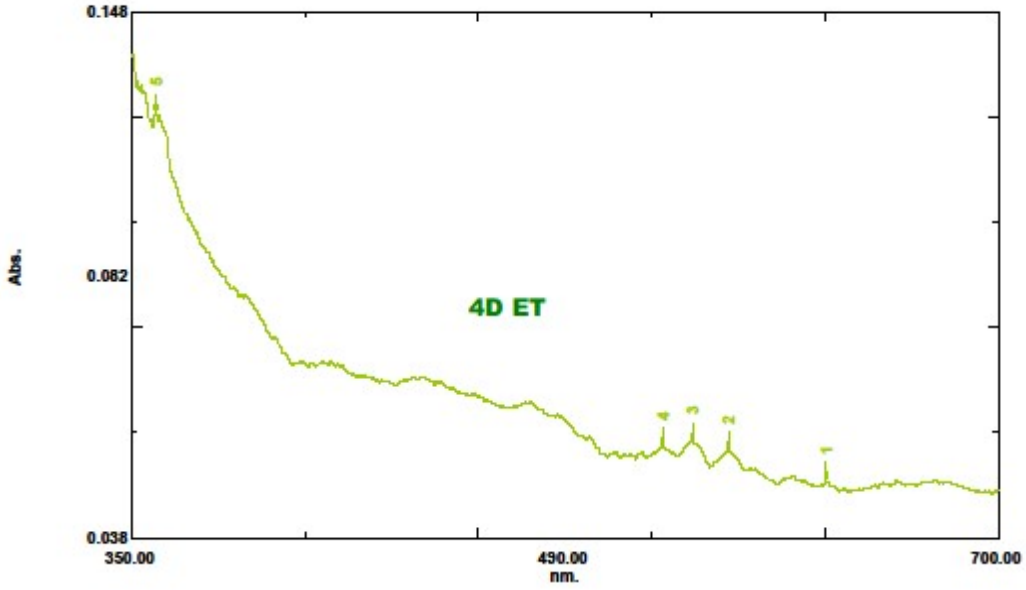
Instrument Type:	UV-2500PC Series
Measuring Mode:	Absorbance
Slit Width:	2.0 nm
Light Source Change Wavelength:	360.0 nm
S/R Exchange:	Normal

Attachment Properties

Attachment:	None

Sample Preparation Properties

Weight:	1g
Volume:	4ml
Dilution:	1
Path Length:	1
Additional Information:	



ANALYSIS VERIFIED BY NAME_____ SIGN_____ DATE_____

Figure S 5

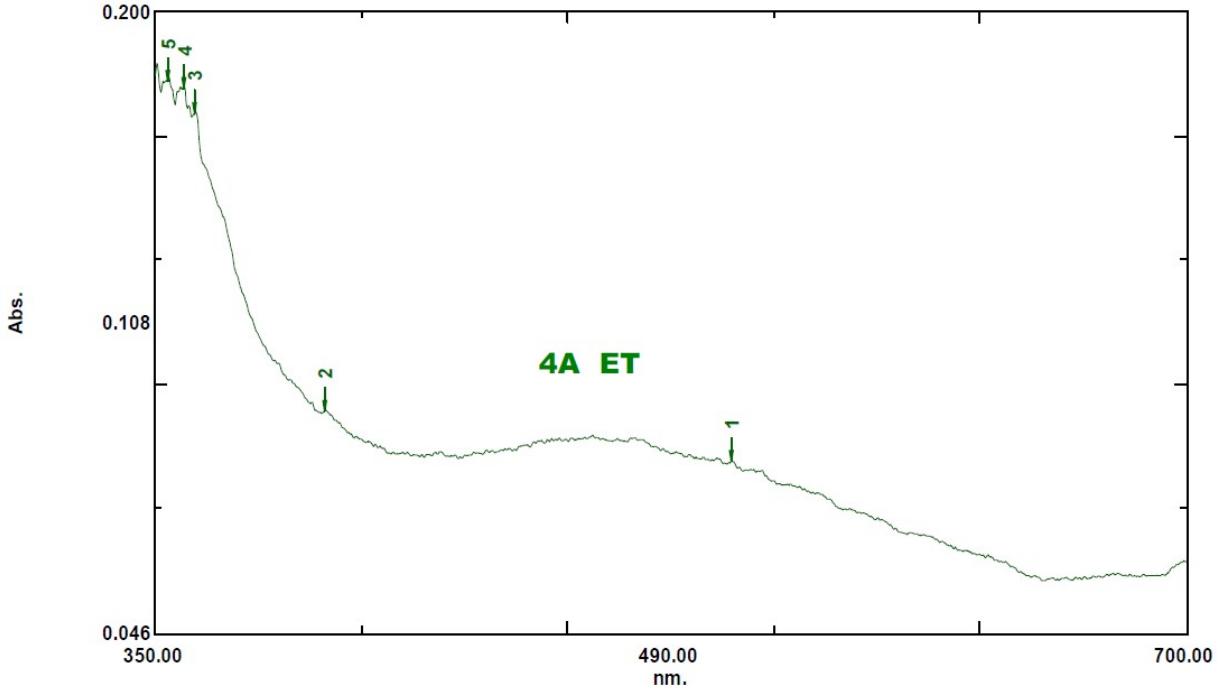


Figure S6:

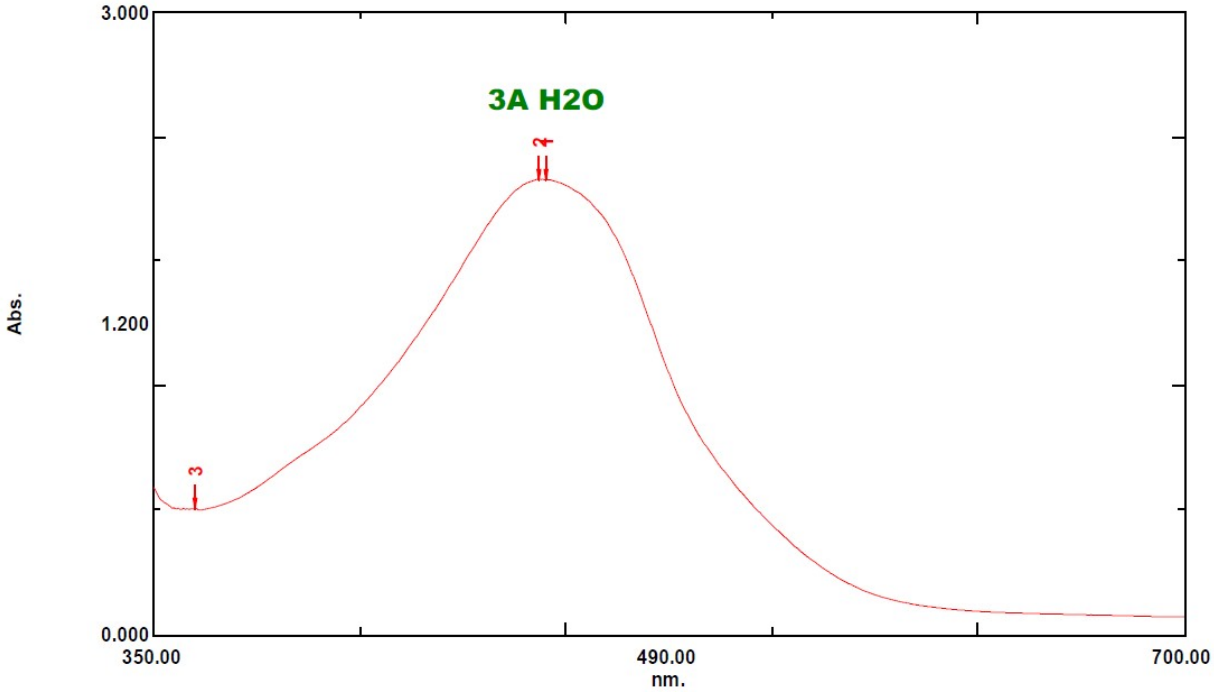


Figure S7

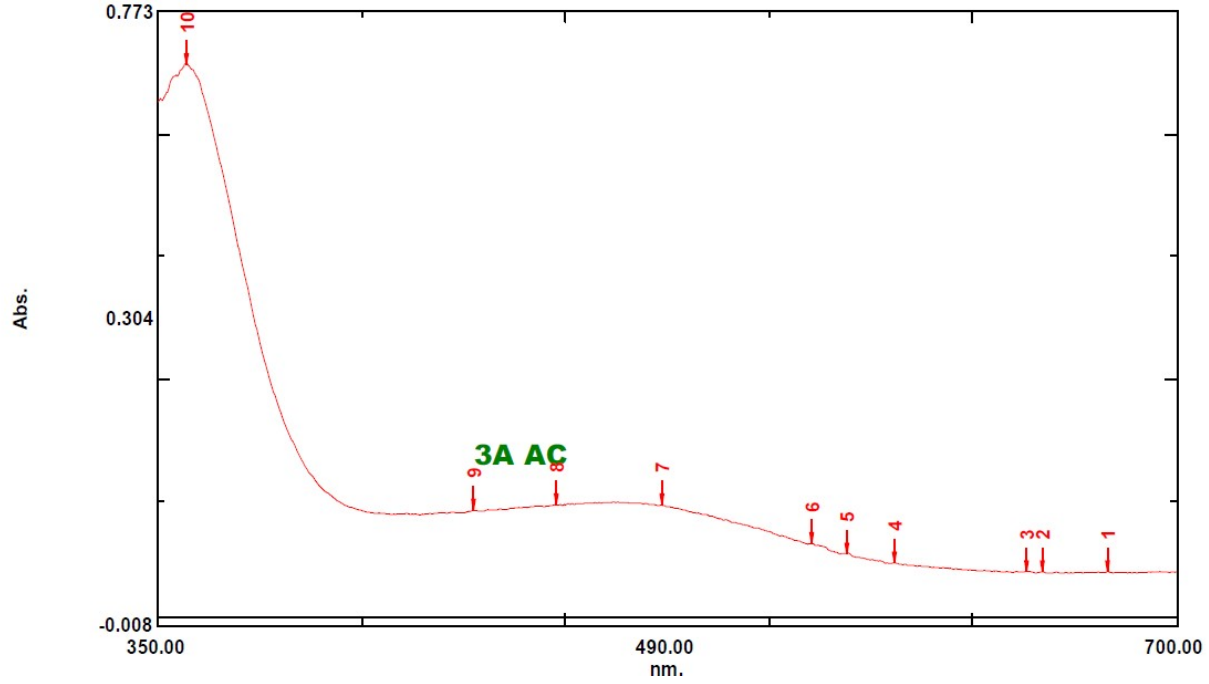


Figure S8

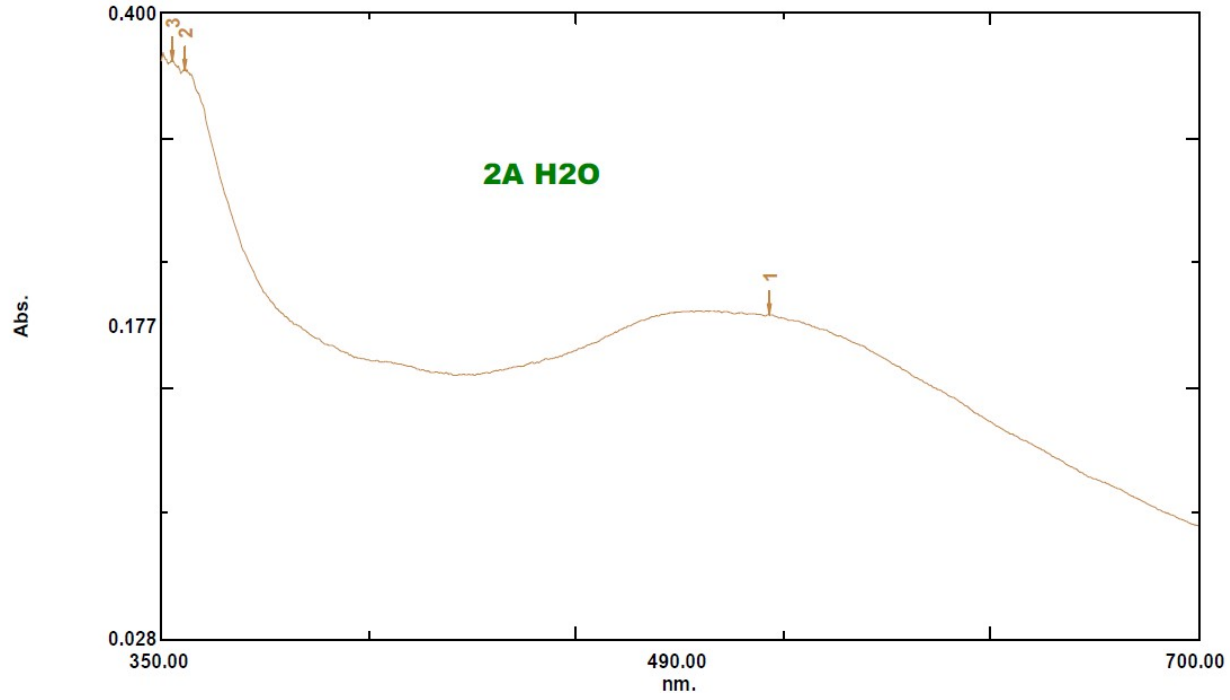


Figure S 9

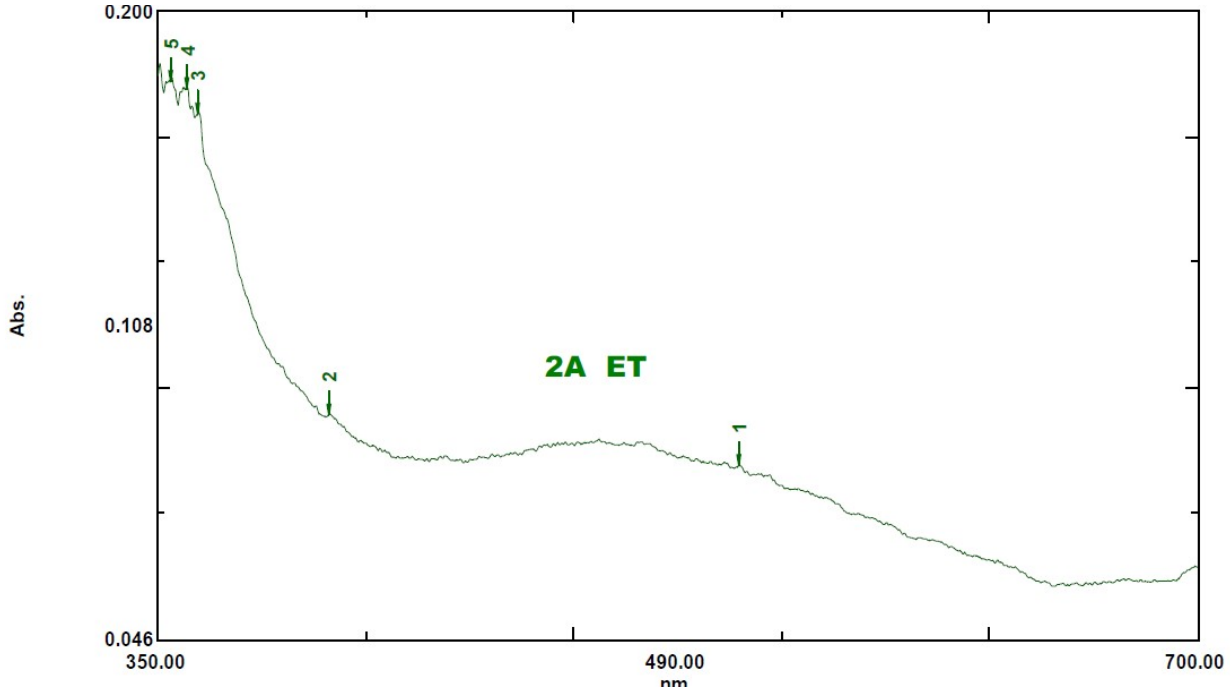


Figure S 10

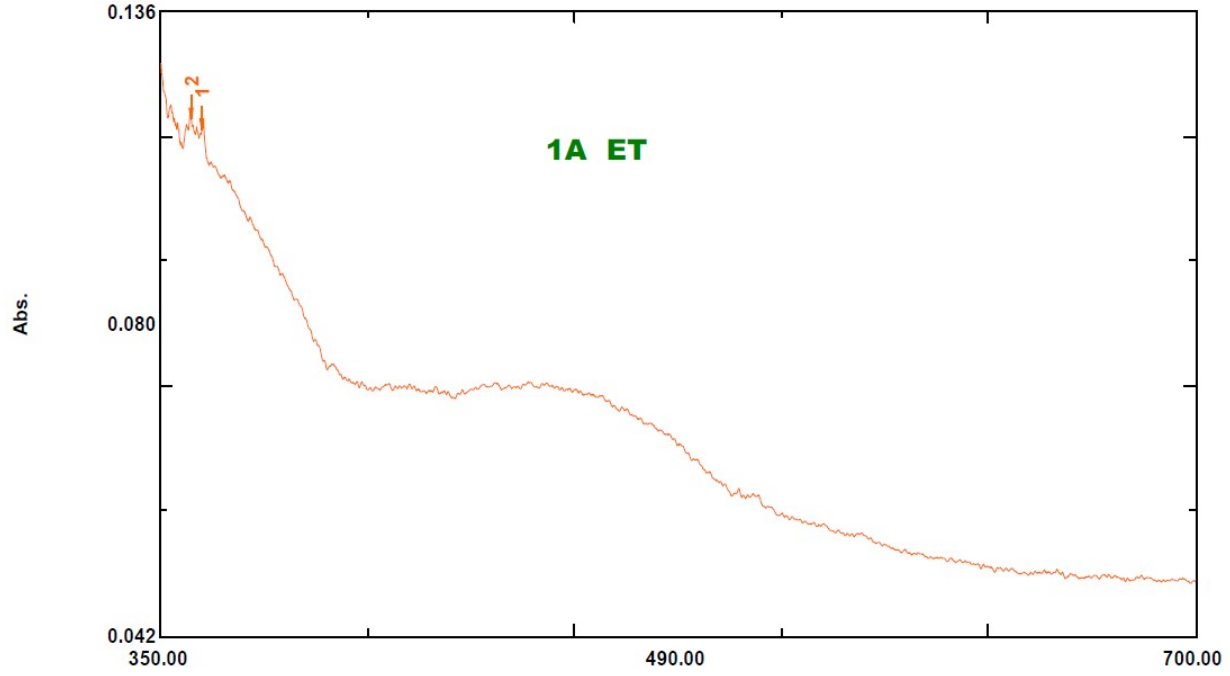


Figure S 11

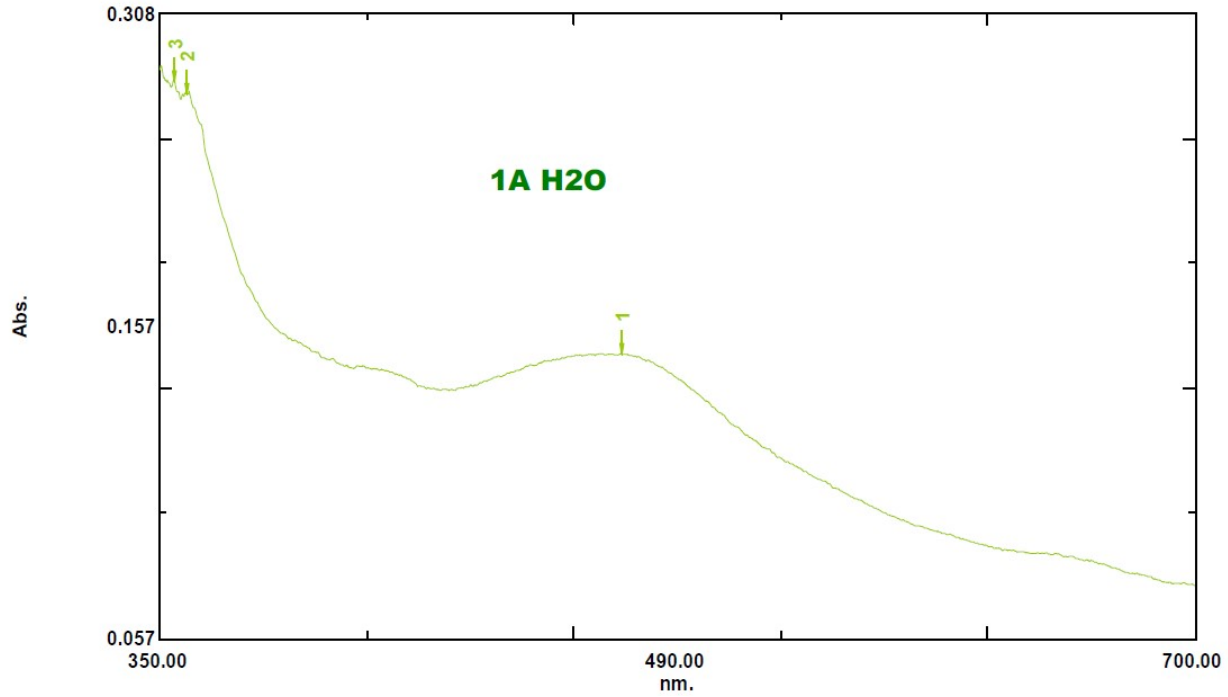


Figure S 12

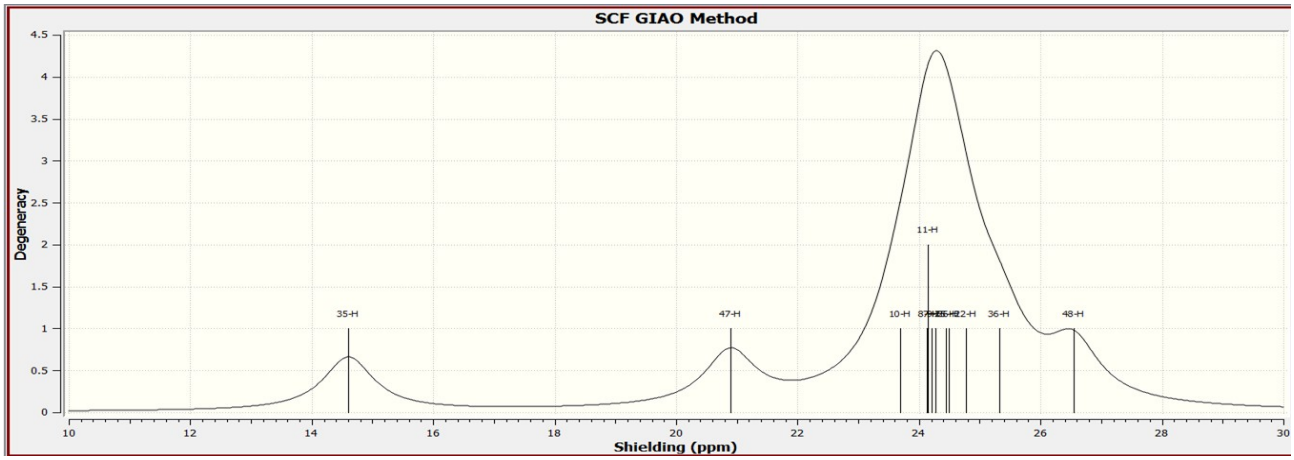


Figure S13: HNMR PLOT FOR DYE A.

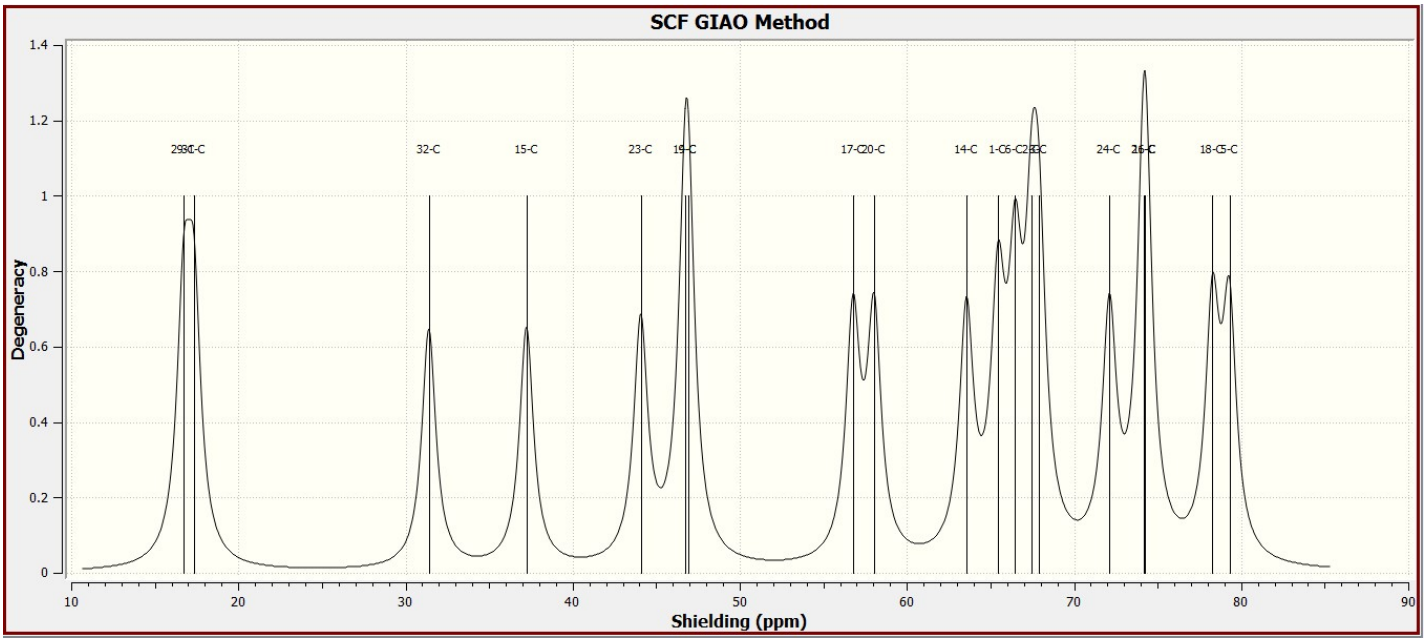


Figure S 14: CNMR PLOT FOR DYE A

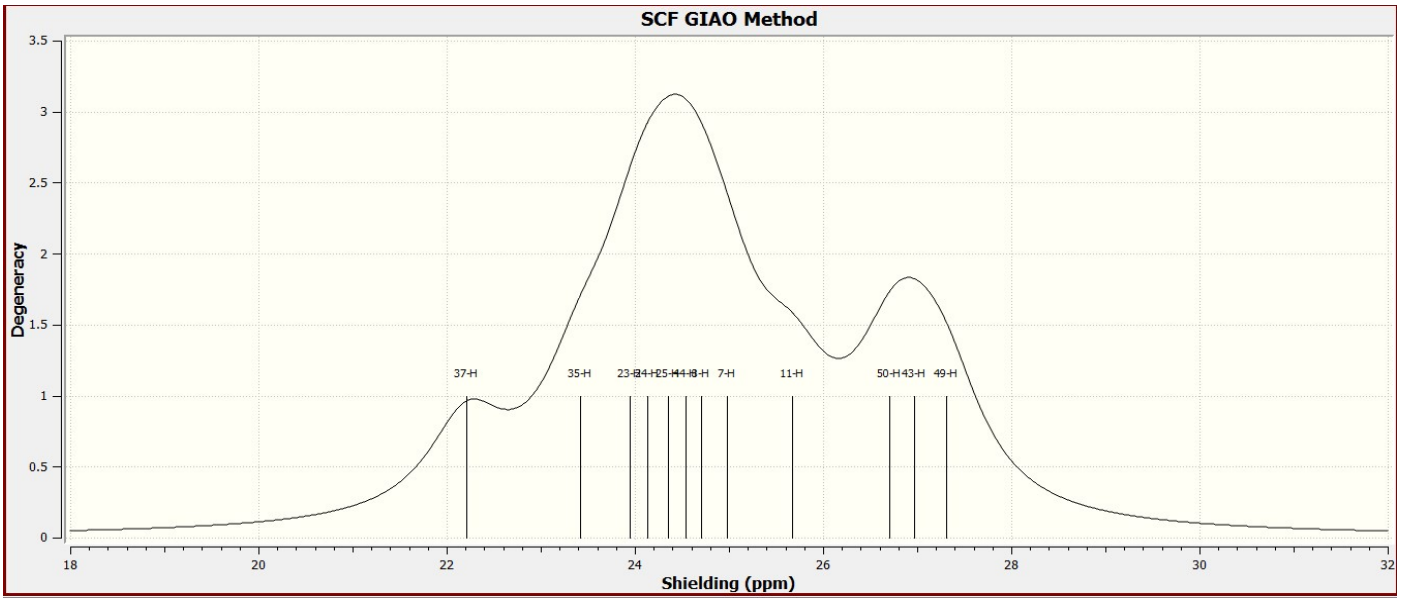


Figure S15 HNMR PLOT FOR DYE B

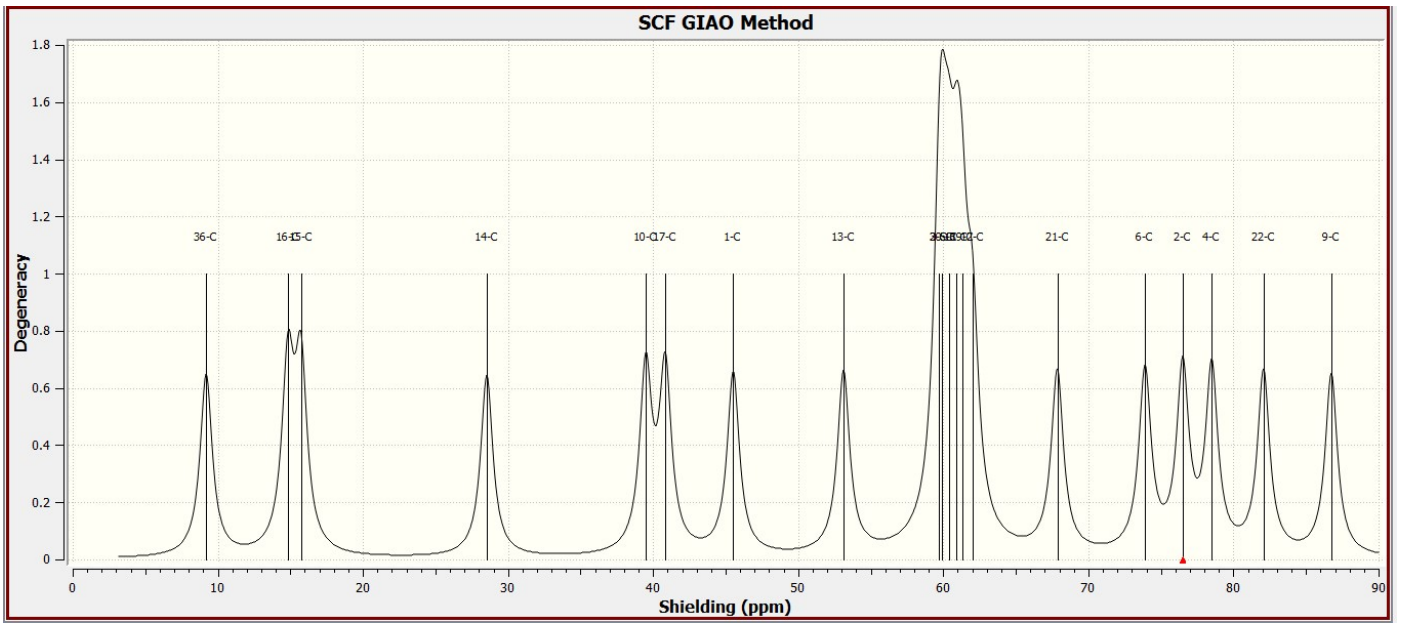


Figure S 16: CNMR PLOT FOR DYE B

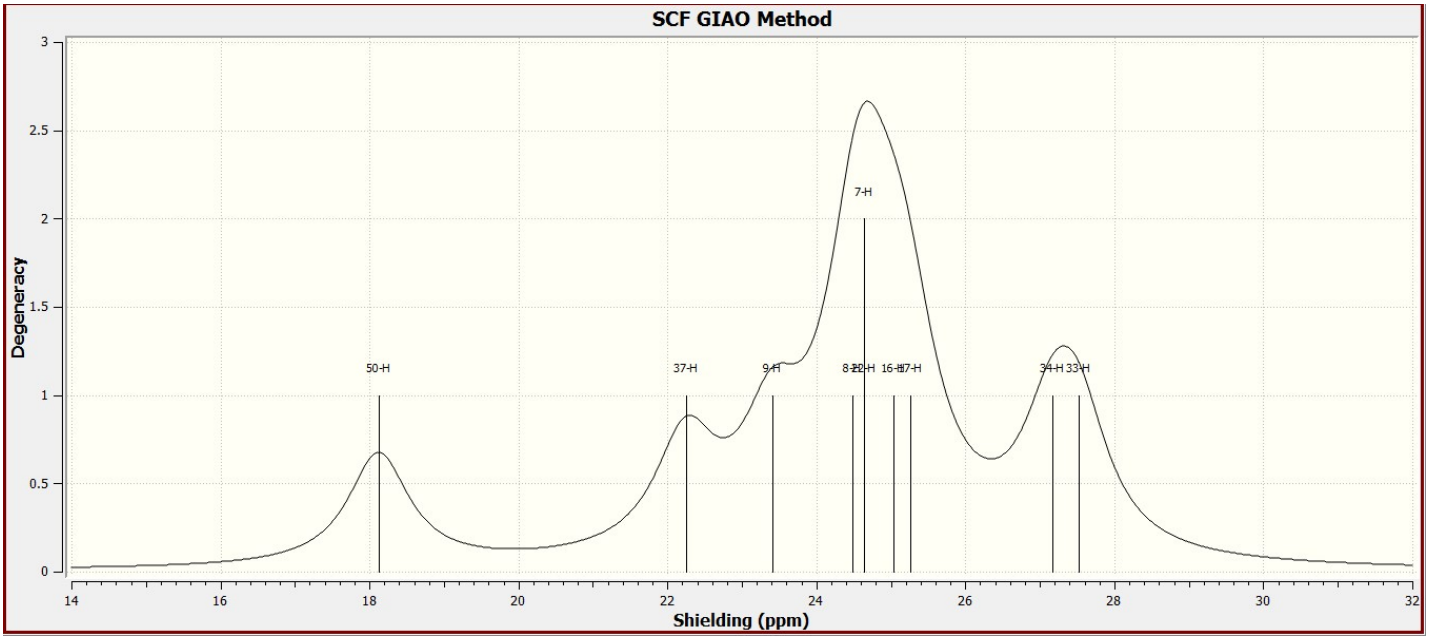


Figure S 17: HNMR PLOT FOR DYE C

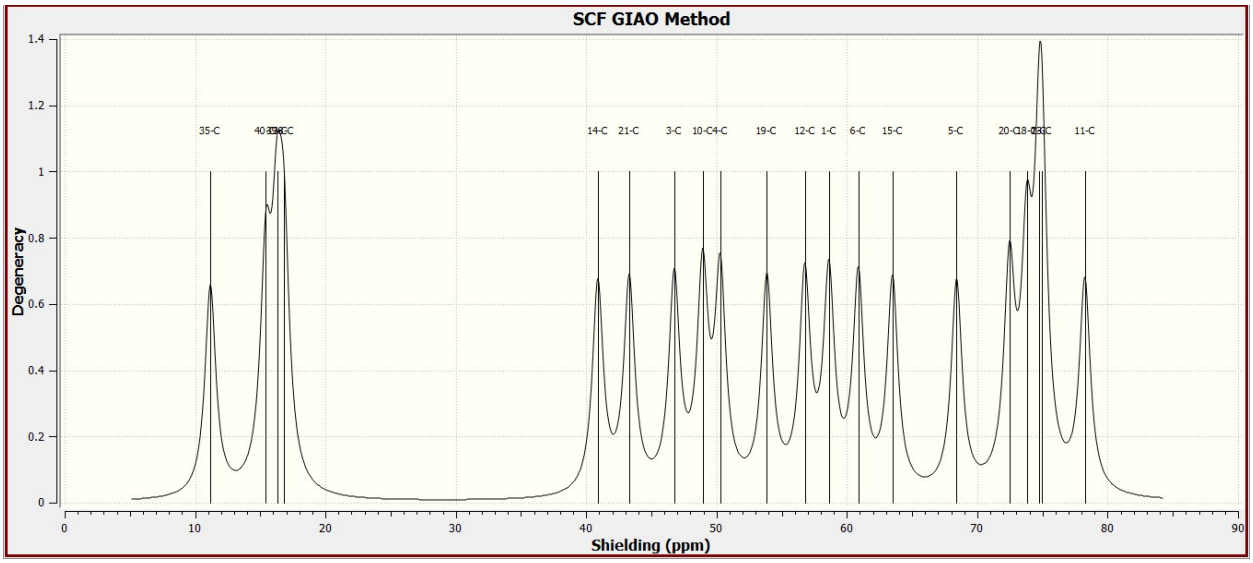


Figure S 18: CNMR PLOT FOR DYE C

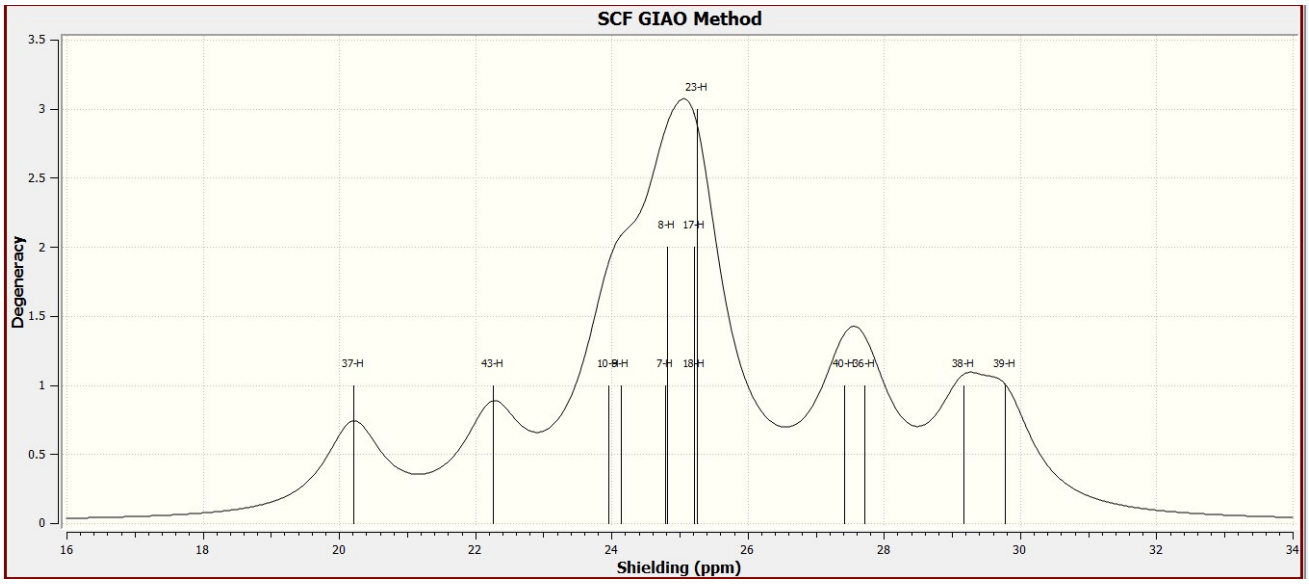


Figure S 19 HNMR PLOT FOR DYE D

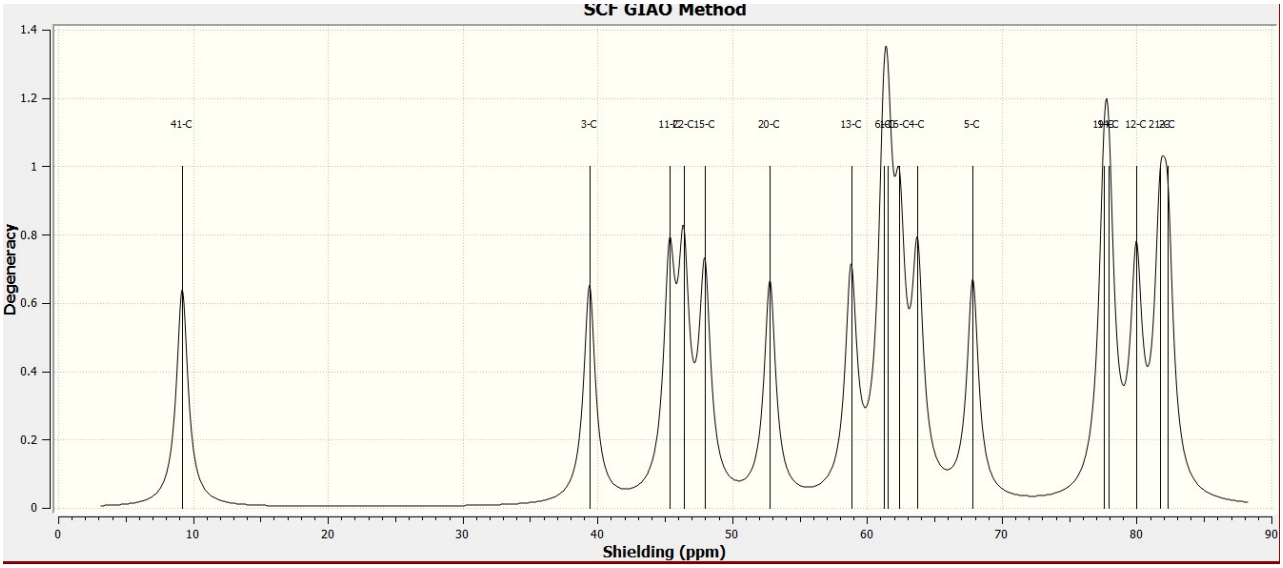


Figure S20: CNMR PLOT FOR DYE

Table S1: Second order perturbation for dye A

S/N	Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
1	LP (1) C 14	BD*(π*) C18 - C19	51.07	0.17	0.100
2	LP*(1) C 17	BD*(π*) C18 - C19	48.83	0.15	0.096
	LP (1) N 28	BD*(π*) C32 - N33	67.53	0.24	0.118
4	LP (1) N12	LP*(1) H35	82.73	0.56	0.209
5	LP (3) O 27	LP*(1) H 35	379.20	0.64	0.451
6	BD (π) C32 - N 33	BD*(π*) C29 - N 30	47.94	0.28	0.107

7	LP (1) C 14	BD*(π*) N12 - N13	127.60	0.07	0.100
8	LP*(1) C 15	LP (1) C16	1726.93	0.01	0.131
9	LP (2) O 27	LP*(1) C15	87.43	0.18	0.136
10	LP*(1) C 17	BD*(π*) C21 - C23	60.95	0.13	0.101

Table S2: Second order Perturbation for dye B

S/N	Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
1	BD*(σ*) O45 - S46	BD*(σ*) O42 - H 43	19062.41	17.91	44.697
2	BD (σ) C19 - C20	BD*(σ*) C18 - C 19	58397.60	0.19	2.966
3	LP (1) O38	BD*(σ*) S 40 - O 41	57407.44	0.30	3.760
4	LP (1) O38	BD*(σ*) O 39 - S 40	28213.86	0.48	3.523
5	LP (1) O38	BD*(σ*) C 17 - C 22	20960.83	0.27	2.150
6	BD (π) C19 - C20	BD*(σ*) C 36 - O 38	53017.61	5.33	16.602
7	LP (1) O42	BD*(σ*) C 21 - C 22	31414.11	2.22	7.470
8	BD (σ*) C19 - C20	BD*(σ*) C 19 - H 44	64601.60	0.22	3.399
9	LP (2) O42	BD*(π*) C 5 - C 6	25673.95	0.01	0.524
10	LP (1) S40	BD*(σ*) C 21 - C 22	19268.56	5.58	9.266

Table S3: Second order perturbation for dye C

S/N	Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
1	LP*(1) C3	LP (1) C2	2127.87	0.01	0.139
2	LP*(1) C14	LP (1) C13	1819.82	0.01	0.131
3	BD*(π*) C39 - N 43	BD*(π*) C38 - N 44	247.03	0.01	0.080
4	LP*(1) C12	BD*(π*) C18 - C 21	60.52	0.13	0.101
5	BD (π)C38 - N44	BD*(π*) C40 - N 45	389.62	0.63	0.452
6	LP (1) C15	BD*(π*) N29 - N 30	110.44	0.09	0.103
7	LP (1) C2	BD*(π*) C1 - C6	75.12	0.14	0.111
S8	LP (3) O48	BD*(π*) N46 - O47	161.96	0.15	0.141
9	BD*(π*) C40 - N45	BD*(π*)C38 - N 44	160.94	0.02	0.077
10	LP (2) O49	LP*(1) C 14	85.91	0.18	0.136

Table S4: Second order perturbation for dye D

S/N	Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
1	LP (1) C 14	LP*(1) C 13	1747.32	0.01	0.132
2	BD*(π*) 15 - C 16	BD*(π*) C 11 - C 12	164.11	0.01	0.075
3	BD*(π*) N31 - N32	BD*(π*) C 15 - C 16	72.67	0.02	0.066
4	LP (1) C 14	BD*(π*) C 20 - C 21	68.86	0.14	0.104
5	LP (1) C 14	BD*(π*) C 15 - C 16	68.69	0.14	0.103
6	LP (1) C 6	BD*(π*) C 1 - C 2	63.69	0.14	0.105
7	LP (1) C6	BD*(π*) C 4 - C 5	60.64	0.15	0.104
8	LP (1) C6	BD*(π*) C 41 - O 42	59.26	0.12	0.101

9	LP*(1) C3	BD*(π*) C 1 - C 2	58.67	0.14	0.103
10	LP*(1) C3	BD*(π*) C 4 - C 5	55.14	0.15	0.102