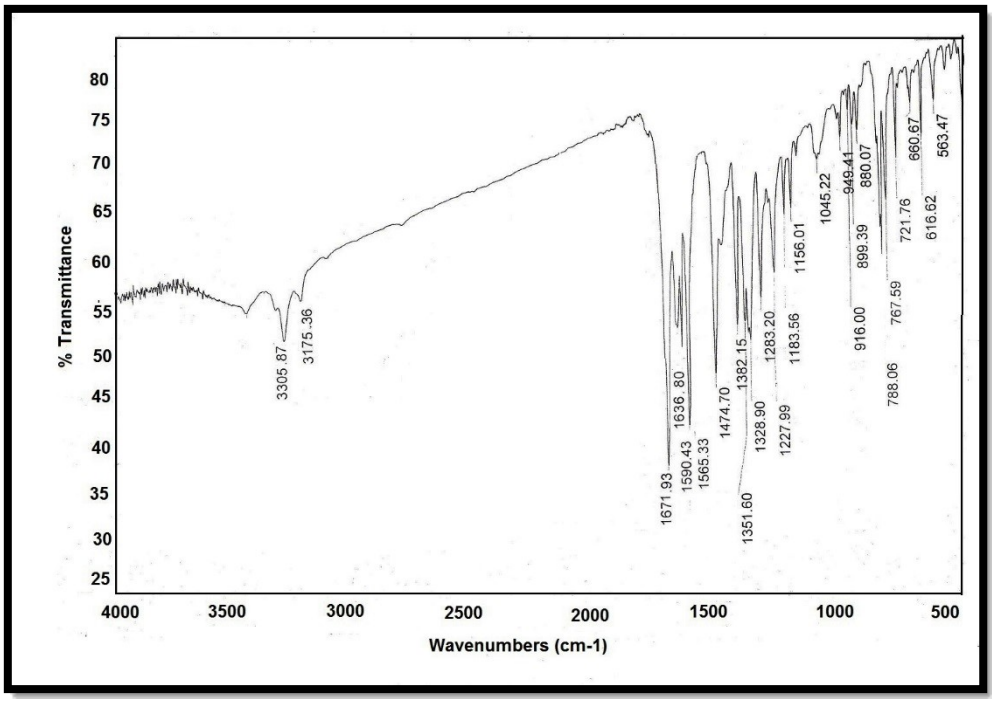
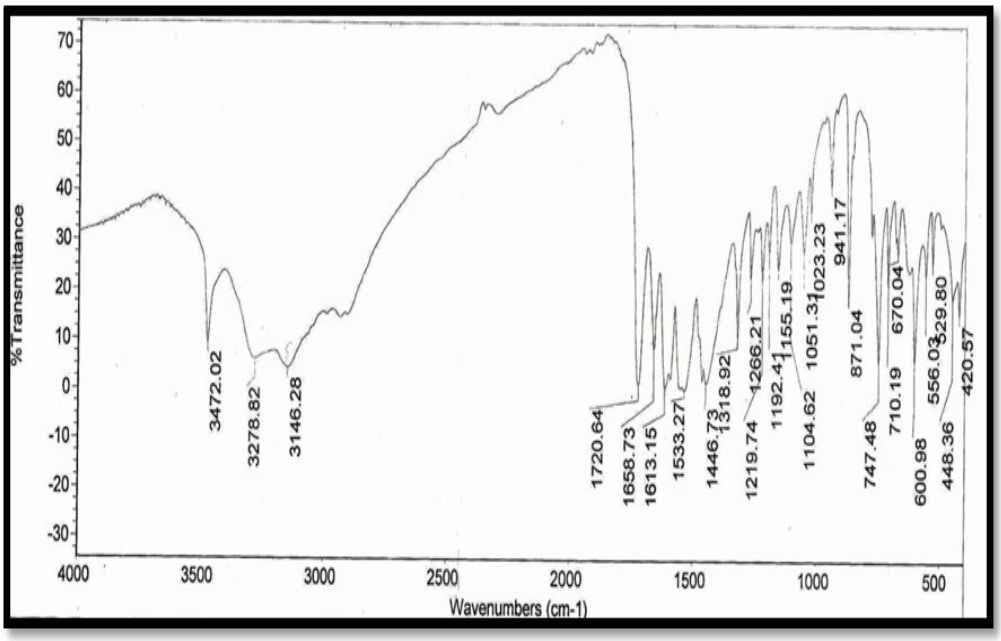
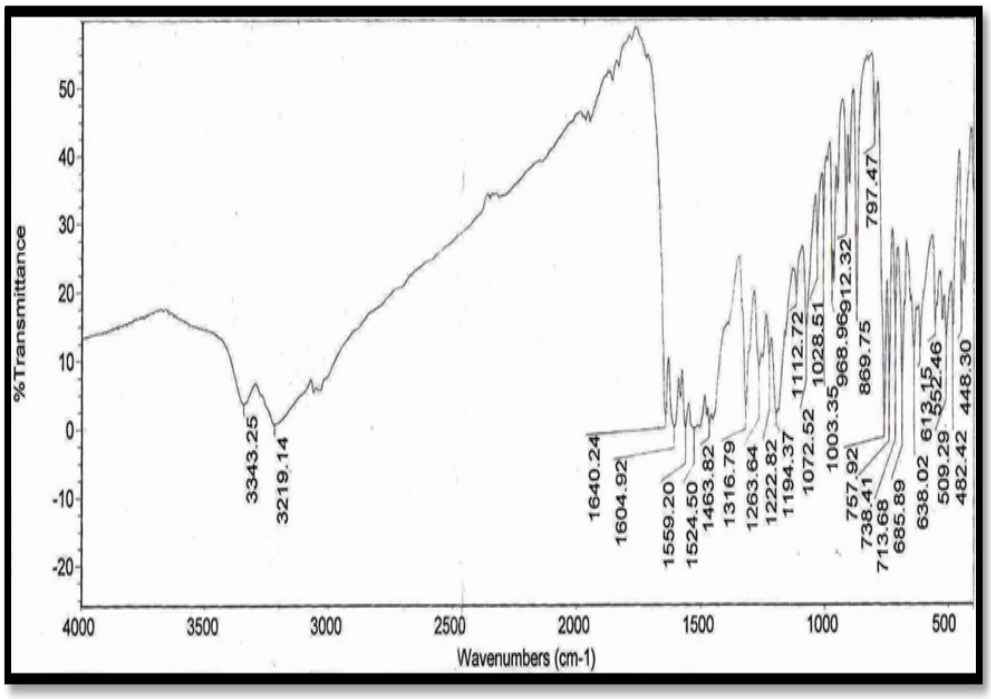


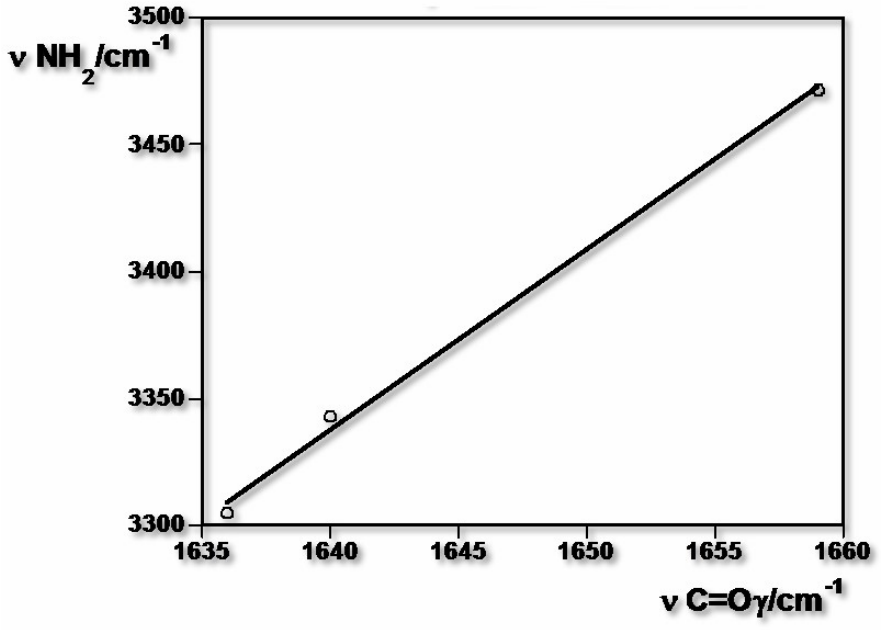
Supplementary Fig 1. Infrared spectrum of **ACC**.



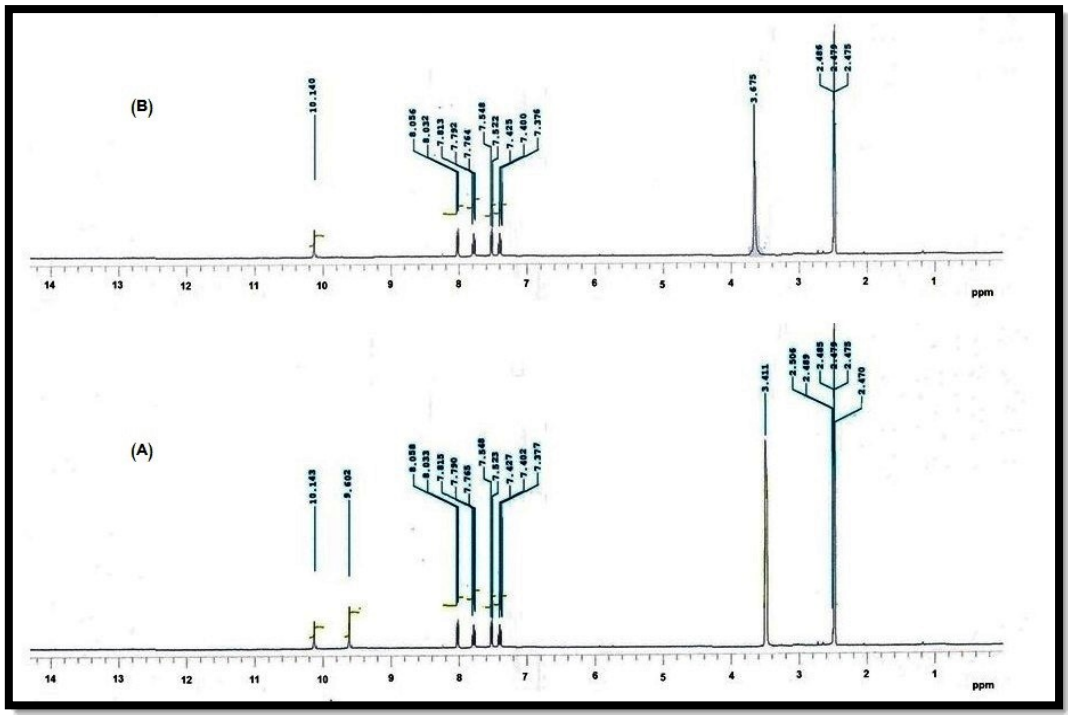
Supplementary Fig 2. Infrared spectrum of **ACMHCA**.



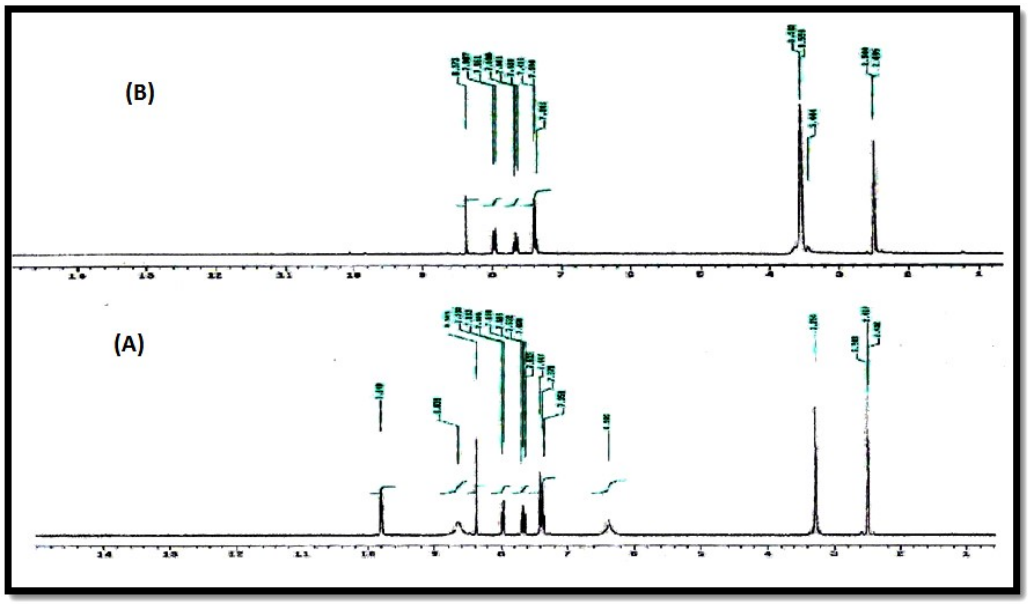
Supplementary Fig 3. Infrared spectrum of **ACMNPHTCA**.



Supplementary Fig. 4. The relation between $\nu NH_2/cm^{-1}$ and $\nu C{=}O_{\gamma\text{–pyrone}}$

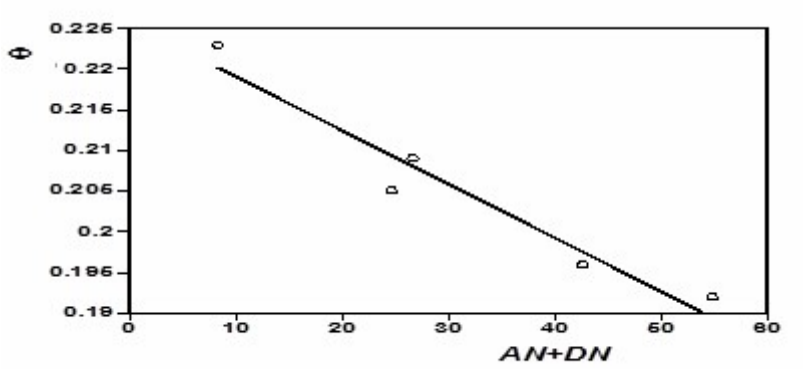


Supplementary Fig. 5.^{1}H-NMR spectra of **ACC** in (DMSO-d_6) (A) in absence of D_2O and (B) in presence of D_2O.

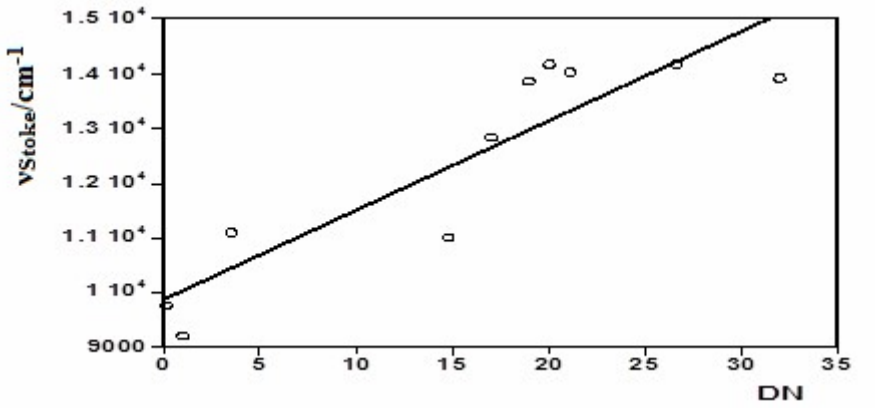


Supplementary Fig. 6.^{1}H-NMR spectra of **ACMHCA** in (DMSO-d_6) (A) in absence of D_2O and (B) in presence of D_2O.

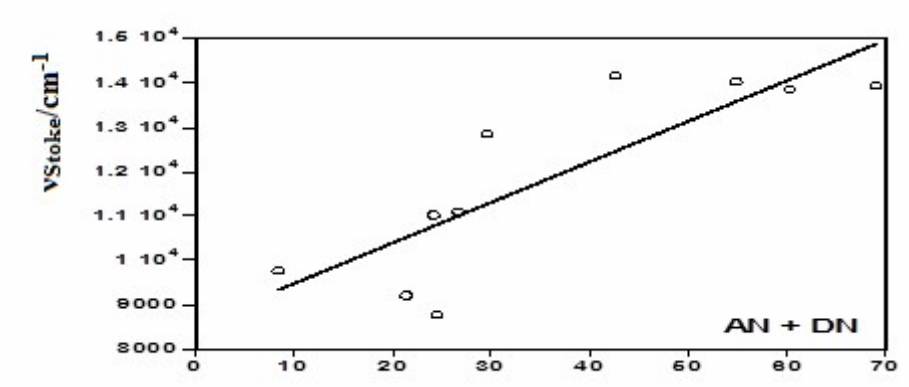
Supplementary Fig. 7. ^{1}H-NMR spectra of **ACMNPHTCA** in (DMSO-d_6) (A) in absent of D_2O and (B) in presence with D_2O.



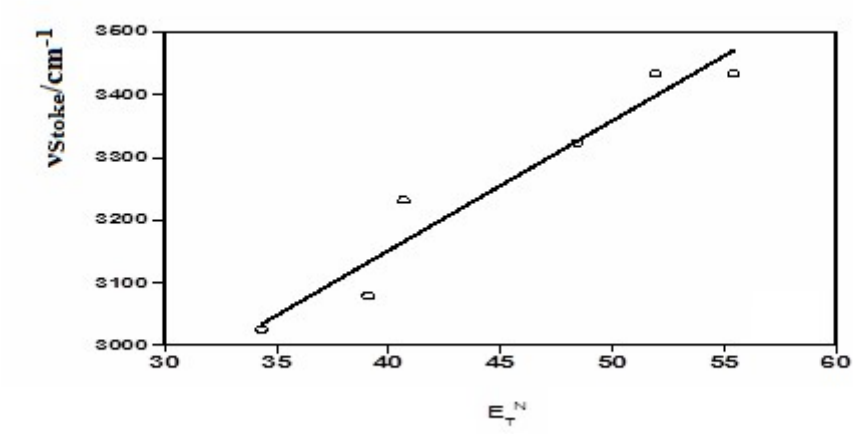
Supplementary Fig. 8. The relation between ϕ_L *vs* (AN +DN)



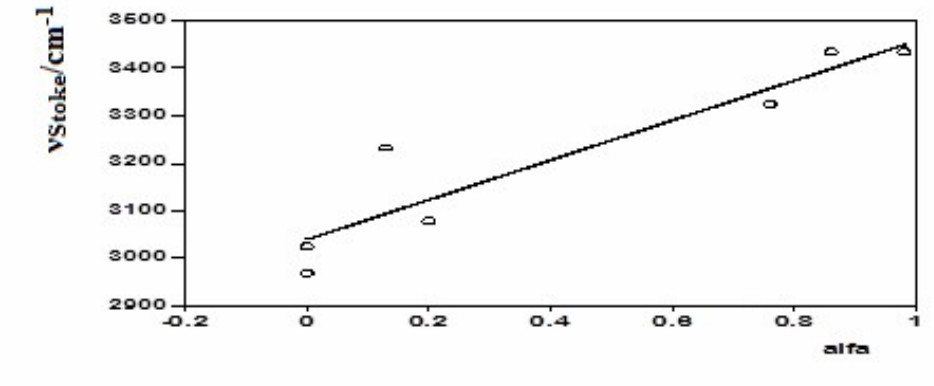
Supplementary Fig. 9. The relation between DN *vs* $\nu_{\text{Stoke shift}}$ of **ACC**.



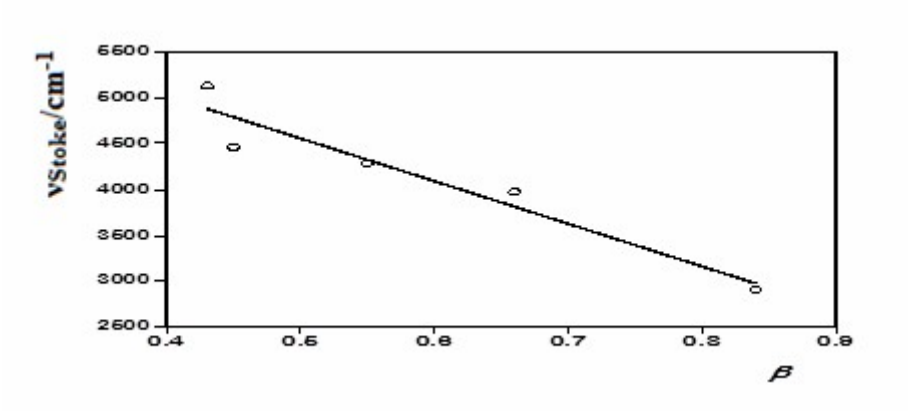
Supplementary Fig. 10. The relation between $\nu_{Stokes\ shift}$ *vs* (AN+DN) of **ACC**.



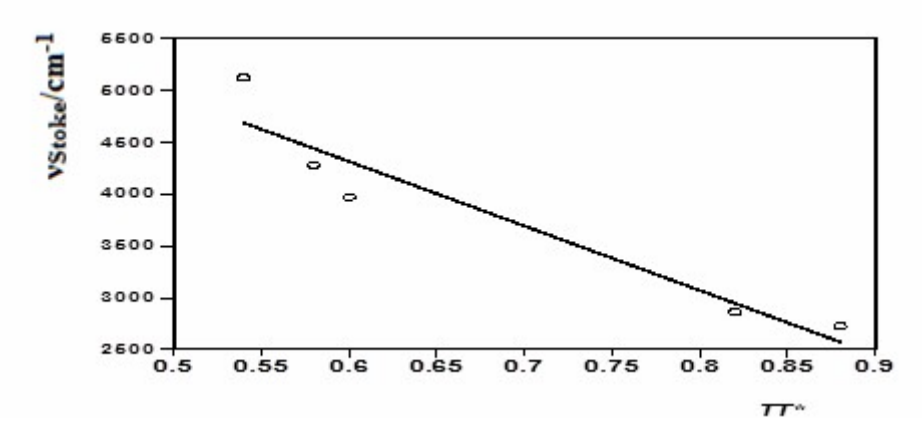
Supplementary Fig. 11. The relation between $\nu_{Stoke\ shift}$ *vs* E_T^n of **ACMHCA**



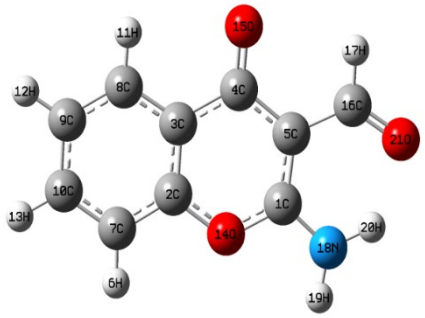
Supplementary Fig. 12. The relation between $\nu_{Stoke\ shift}$ *vs* α of **ACMHCA**



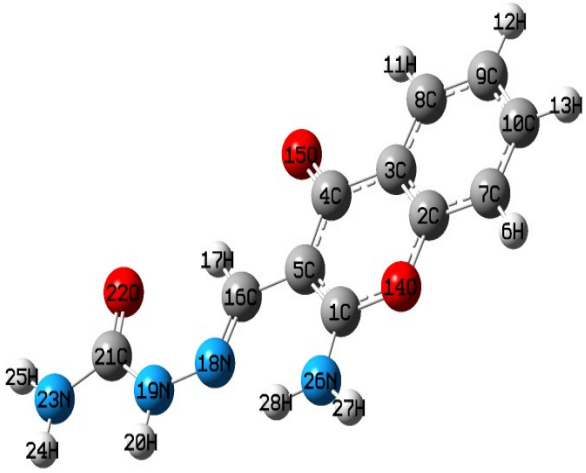
Supplementary Fig. 13. The relation between $\nu_{\text{Stoke shift}}$ *vs* β of **ACMHCA**



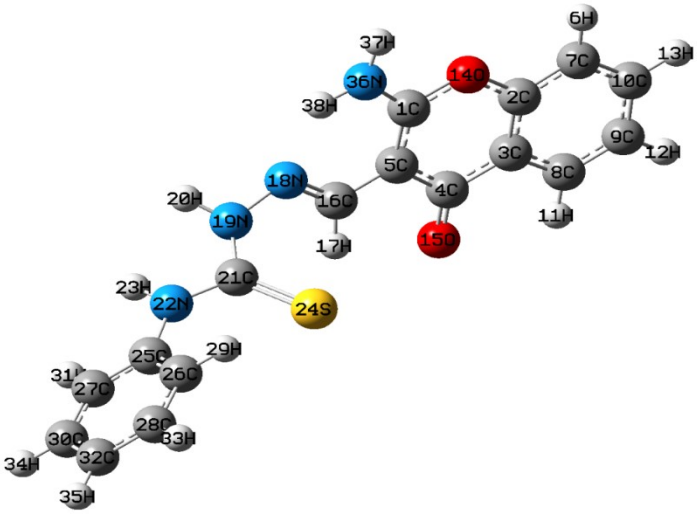
Supplementary Fig. 14. The relation between $\nu_{\text{Stoke shift}}$ *vs* π* of **ACMNPHTCA.**



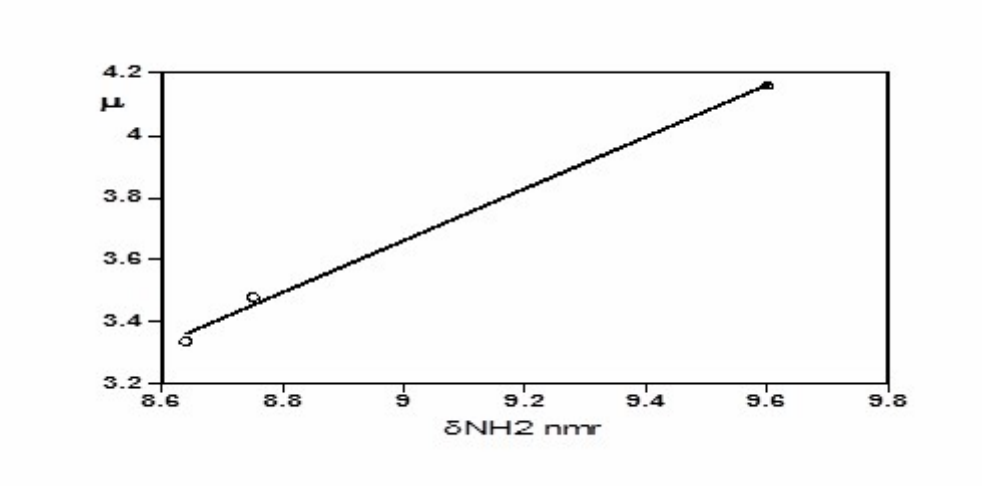
Supplementary Fig. 15. Molecular modeling of **ACC**.



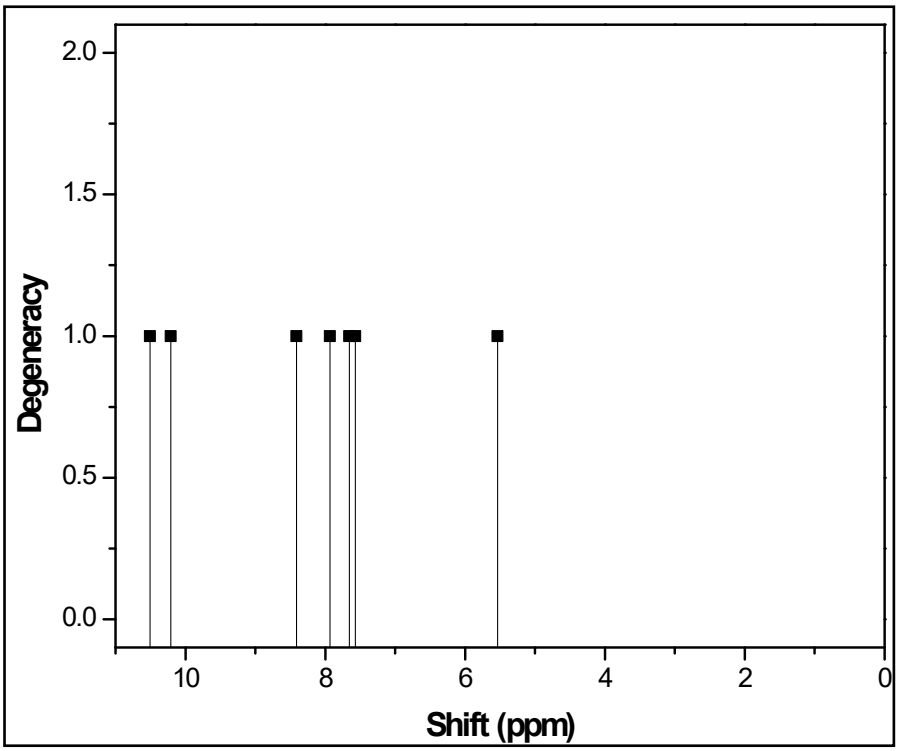
Supplementary Fig.16. Molecular modeling of **ACMHCA**.



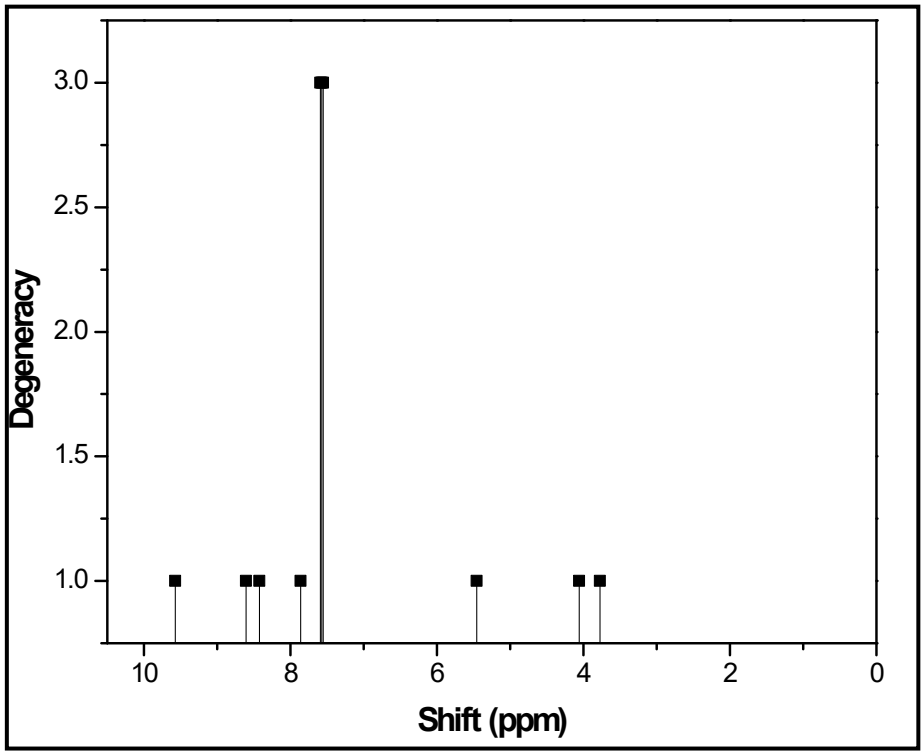
Supplementary Fig.17. Molecular modeling of **ACMNPHTCA**.



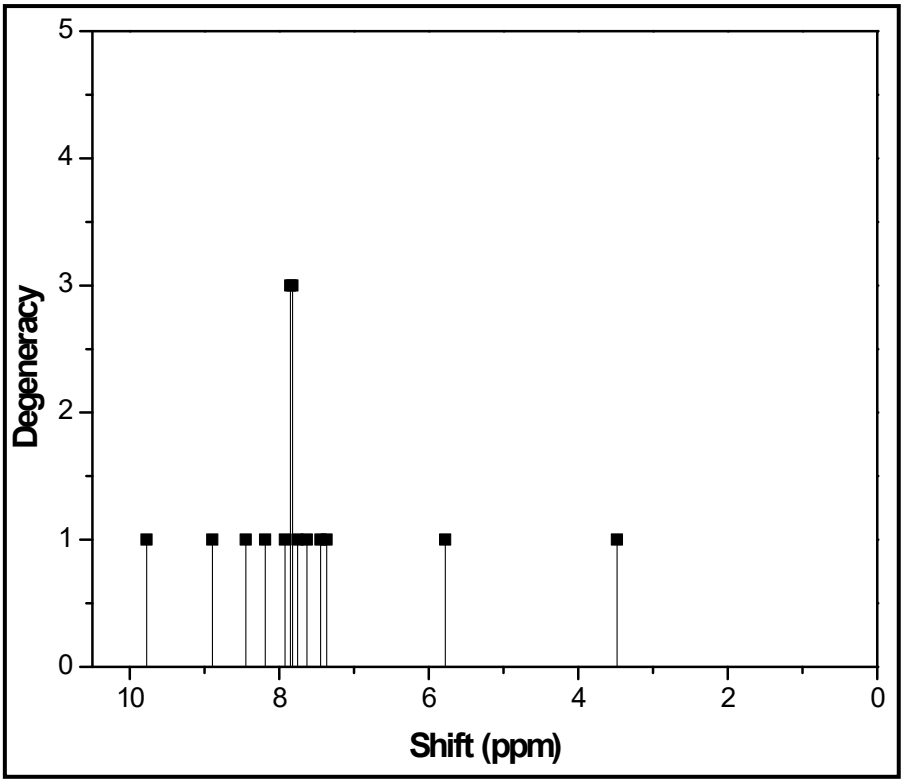
Supplementary Fig.18 The relation between chemical potential (μ) *vs* δ/ppmNH_2



Supplementary Fig.19. Calculated ^{1}H NMR spectrum of compound **ACC** at B3LYP/6-311++ G(d,p).



Supplementary Fig. 20. Calculated ^{1}H NMR spectrum of compound **ACMHCA** at B3LYP/6-311++ G(d,p).



Supplementary Fig. 21. Calculated ^{1}H NMR spectrum of compound **ACMNPHTCA** at B3LYP/6-311++ G(d,p).

Supplementary Table 1. Linear regression analysis of the stokes shift *versus* solvent parameters of **ACC** and its hydrazones **ACMHCA** and **ACMNPHTCA**

Compound	Eqn	intercept	slope	*r*	n
ACC	ν stoke *vs* DN	9887.3	+162.5	0.90059	10
	νstoke *vs* AN	6339.6	+197.95	0.94793	6
	ν stoke vs AN	5682.6	544.81	0.98245	4
	ν stoke *vs* DN+AN	8579.7	+91.014	0.83312	10
	ν stoke *vs* E_T	782.77	+256.82	0.81205	9
	ν stoke *vs* α	10965	+3391	0.8572	7
	ν stoke *vs* β	9854.8	+5266.9	0.90558	7
	ν stoke *vs* β	9492.9	+6241.4	0.90355	10
	νstoke vs π*	1446	+14930	0.92537	5
	ν stoke *vs* π*	21620	-13859	0.89093	6

Continued Supplementary Table 1.

ACMHCA	ν stoke *vs* DN	3039.5	+27.706	0.90494	8
	ν stoke *vs* (DN+AN)	2989.1	+6.6181	0.92913	6
	ν stoke *vs* E_T^n	2325.8	+20.654	0.9673	6
	ν stoke *vs* alfa	3038.3	+418.81	0.93359	7
	ν emission *vs* β	23732	-333.9	0.80	8
	νstoke vs π*	1434.6	+2849.7	0.9134	6
	ν emission /La *vs* β,π*α	24107	-382 π* +412 α, -1168 β	0.912	
	ν emission /La *vs* β,π*α	24756	-1423 π* -24 α, -641 β	0.60	

Continued Supplementary Table 1.

ACMNPHTCA	ν stoke *vs* π*	5911.5	-6299.9	0.99584	5
	ν stoke *vs* π*	8056	-6226.1	0.95496	5
	ν stoke *vs* β	6860.5	-4618.5	0.96233	5
	ν stoke *vs* β	1629.9	+4149.1	0.9259	6
	ν stoke *vs* α	2307.7	+3155	0.95189	6
	ν stoke *vs* E_T	-542.52	+77.803	0.94004	7
	ν stoke *vs* (DN+AN)	1452.6	+45.122	0.91674	7
	ν stoke *vs* AN	1156.1	+102.58	0.98023	5
	ν stoke *vs* DN	1877.7	+91.318	0.8636	7
	ν emission /L_b *vs* β,π*α	23105	+187 π* +736 α, -4451 β	0.8500	8

Supplementary Table 2: Solvent parameters dielectric constant (ε), refractive index (n) and microscopic solvent polarities.

No.	Solvent	ε	n	φ	E_T^{Ne}	$F_{L\text{-}M}$	F_B	$F_{K\text{-}C\text{-}W}$
1	1,4-diox	2.21	1.420	0.619	0.164	0.021	0.042	0.369
2	Benzene	2.30	1.501	-	0.111	0.003	0.004	0.300
3	$CHCl_3$	4.81	1.445	0.9753	0.259	0.148	0.371	0.547
4	Etac	6.02	1.372	0.996	0.228	0.199	0.489	0.564
5	THF	7.58	1.407	1.102	0.209	0.549	0.614	0.207
6	CH_2Cl_2	8.93	1.424	-	0.321	0.219	0.596	0.586
7	2-PrOH	18.00	1.377	1.292	0.540	0.276	0.779	0.712
8	Me_2CO	20.7	1.360	-	0.355	0.285	0.792	0.654
9	EtOH	23.40	1.359	1.305	0.654	0.289	0.813	0.719
10	MeOH	32.63	1.326	1.302	0.762	0.309	0.855	0.722
11	DMF	36.71	1.431	1.419	0.404	0.274	0.836	0.771

Supplementary Table 3: The slope (m), Intercept (C), Correlation coefficient (*r*) and number of data points (n) corresponding to statistical treatment of spectral shifts

Compound	Eqn	intercept	Slope	*r*	n
ACC	ν stoke *vs* FB	8627.9	+17352	0.95238	9
	ν stoke *vs* F2	9166.4	+5478.4	0.95262	9
	(νa+νf) *vs* F3	34840	-6274.1	0.78065	11
	(νa+νf) *vs* F3	34943	-6532.7	0.95264	9
	ν stoke *vs* E_T^n	9139.6	+7758.3	0.85647	9
	ν stoke vs E_T^n	8930.9	+7684.5	0.91198	8
ACMHCA	ν stoke *vs* FB	2922	+ 1562.9	0.954	7
	ν stoke *vs* F2	2985	+480.97	0.96765	6
	(νa+νf) /2 *vs* F3	2558	-574.2	0.84141	7
	(νa+νf)/2 *vs* F3	26799	-2571.6	0.95162	7
	ν stoke *vs* E_T^n	2453.7	+2490.7	0.9913	4
	ν stoke *vs* E_T^n	2983.1	+633.5	0.9736	5

Continued Supplementary Table 3.

ACMNPHTCA	ν stoke vs F1	1976.4	+11375	0.98833	5
	ν stoke *vs* F1	1643.5	+6695.2	0.94061	4
	1^{st}gp F2 vs νstoke	2245.3	+3712.7	0.98212	5
	2^{nd} gp F2 *vs* νstoke	1904.5	+2145	0.954	4
	(νa+νf)/2 *vs* F3	25627	-4468.8	0.98586	5
	(νa+νf)/2 *vs* F3	24692	-1206.3	0.91497	4
	ν stoke *vs* E_T^n	2453.7	+2490.7	0.9913	4
	ν stoke *vs* E_T^n	2983.1	+633.5	0.9736	5

Supplementary Table 4. Total energy (au), energy of HOMO, of LUMO, energy gap, , Hardness(η/ev), Electrophilicity (ω/eV), Softness(S/ eV^{-1}), chemical potential (μ/eV) and dipole moment (Debye) for **ACC** and its hydrazones in gaseous phase using B3LYP/ 6-311G(d,p) level.

Compound	E_T,au kcal/mol	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{gap} (eV)	V_{OC}/TiO_2 **eV**	V_{OC}/PCM eV	S/eV^{-1}	η/eV	ω/eV	μ/eV	μ/D
ACC (keto form)	-665.53	-6.576	-1.740	4.836	2.576(2.26)[#]	2.876 (1.96)	0.413	2.418	3.575	5.911	5.9136
ACC (enol form)	-665.475	-6.338	-2.706	3.632	2.338 (1.294)	2.638 (0.994)	0.275	3.63	2.817	4.158	6.3383
ACMHCA (keto form)	-5456.83	-5.485	-1.192	4.295	1.485 (2.808)	1.785 (2.508)	0.465	2.146	2.596	4.522	7.134
ACMHCA (enol form)	-5456.63	-5.326	-1.186	4.139	1.326 (2.814)	1.626 (2.514)	0.483	2.070	2.561	3.338	5.842
ACMNPHTCA (thione form)	-1423.563	-5.469	-1.493	3.976	1.469 (2.507)	1.769 (2.207)	0.503	1.988	3.049	3.256	6.146
ACMNPHTCA (thiol form)	-1423.546	-5.411	-1.444	3.967	1.411(2.556)	1.711 (2.256)	0.504	1.983	2.961	3.482	4.264

[#]In parenthesis using LUMO instead HOMO