Electronic Supplementary information

Designing symmetrically folded scaffolds of pyridazinone and triazinone derivatives linked Via N, N-diethyl-4-nitro-benzenesulfonamide: to explore luminescent materials

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Experimental Section

General information

All the reagents were purchased from Sigma Aldrich and were used without further purification. Reactions were conducted at an ambient temperature and monitored by thin-layer chromatography (TLC) over silica gel G UV active plates. The melting points of compounds were checked by the Buchi melting apparatus and uncorrected.

Characterization

^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on JEOL Resonance ECZ500R NMR spectrometer. Mass spectra were recorded on a SCIEX X500R QTOF mass spectrometry.
Raman study was done by Horiba LabRam HR evolution spectrometer. The sample was irradiated with the 633 nm output from a He\Ne laser (30 mW, 1800 groves/mm grating, slit width 200 µm) and Peltier cooled (-60 °C) CCD detector (model: Syncerity 356399, manufactured by Horiba Instrument Inc.) was used.

Photophysical properties

Steady-state UV-visible absorption spectra were measured by Cary 100 Bio, Agilent in the 200–800 nm range. The instrument has photometric linearity till absorbance 3.5 and has a wavelength resolution of 0.2 nm. Fluorescence spectrophotometry (Fluorolog 3-21, Horiba Scientific) was used for fluorescence measurements in solution states.

X-ray Diffraction measurement

SCXRD data was collected on a Rigaku: XtaLAB Synergy-i diffractometer Cu-Kα radiation (Kα = 1.54184 Å) for all compounds. All the atoms were refined with anisotropic thermal parameters except the hydrogen atoms. Hydrogen atoms were set to ride on the parent atoms after placing them

in idealized positions around the respective parent atoms. The absence of additional symmetry and voids was confirmed using PLATON (ADDSYM).[1] The structures were solved by direct methods and refined by full-matrix least-squares on F2 using the latest version of SHELX-2019.[2] The packing diagrams were generated using Mercury version 3.1.[3] The refinement converged to the final values of R1 & wR2 and the crystallographic parameter of compound DP, DT, DPM, and DTM are depicted in Table S1. PLATON analyzed the bond lengths, angles, and other geometrical parameters.

Computational methods: The theoretical calculations to obtain possible conformational structures of the compounds in the gas phase were performed with a well-known method DFT/B3LYP level of theory available in Gaussian09 software. The 6-31G++(d,p) basis set was used during complete computations. The self-consistent field (SCF) equation was solved iteratively to get the optimized geometries whose energies were found minimal on the potential energy surface.

Synthetic procedures

5,6-bis(4-methoxyphenyl)-3-oxo-2,3-dihydropyridazine-4-carbonitrile (PYZ-OMe): Synthesis of methoxy substituted pyridazinone, a mixture of cyanoacetohydrazide (1 mmol, synthesized by mixing of hydrazine hydrate and cyanoethyl acetate at 0°C), potassium carbonate (1 mmol), and p-Anisil (1 mmol) was added in the 100 ml round bottom flask. The reaction mixture was heated at 110°C for 10-15 minutes. The completion of the reaction was monitored via TLC. The reaction mixture was poured into ice-cold water neutralized by HCl and filtered. The residue was washed with water, dried, and recrystallization from ethyl acetate to obtain a pure product. ^{1}H-NMR (500 MHz, $CDCl_3$ δ, ppm): δ 12.72 (s, 1H), 7.16 (d, *J* = 9.3 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.88 (d, *J* = 8.0 Hz, 2H), 6.75 (d, *J* = 8.0 Hz, 2H), 3.82 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$ δ, ppm) δ 160.94, 159.77, 157.80, 151.34, 145.86, 131.94, 130.44, 130.29, 126.84, 124.88, 114.09, 113.94, 113.38, 55.05, 54.94. (Fig. S1, a and b)

5,6-bis(4-methoxyphenyl)-1,2,4-triazin-3(2H)-one **(TYZ-OMe)**: Synthesis of methoxy substituted triazinone, a mixture of semicarbazide (1 mmol), p-Anisil (1 mmol) and ethanol was added in a 100-round bottom flask. The mixture was heated at 110°C for 2h. The completion of the reaction was monitored via TLC. The reaction mixture was poured into ice-cold water. The residue was washed with water, dried, and recrystallized ethyl acetate to obtain a pure product. ^{1}H-NMR (500 MHz, $CDCl_3$ δ, ppm): δ 13.07 (s, 1H), 7.36 (d, *J* = 125.4 Hz, 4H), 6.80 (d, *J* = 9.3 Hz, 4H), 3.82 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$ δ, ppm) δ 166.45, 162.19, 160.08, 154.30, 142.25, 131.81, 130.10, 127.68, 127.03, 113.77, 113.49, 55.31, 55.21. (Fig. S2, a and b)

N, N-bis(2-chloroethyl)-4-nitro benzenesulfonamide **(BPN)*:*** In 100 ml round bottom flask, p-nitro sulphonyl chloride and Bis(2-Chloroethyl) amine hydrochloride were dissolved in TEA/DCM for 5h at room temperature and completion of reaction monitored via TLC. The reaction mixture was poured into the ice-cold water to obtain the precipitate. The residue was filtered, washed with water, and dried at room temperature. Pyridazinone and triazinone were synthesized using a previously described method.[4,5] ^{1}H-NMR (500 MHz, $CDCl_3$ δ, ppm): δ 8.39 (d, J = 8.8 Hz, 1H), 8.05 (d, J = 8.9 Hz, 1H), 3.71 (t, J = 6.7 Hz, 2H), 3.58 (t, J = 6.6 Hz, 2H). ^{13}C-NMR (125 MHz, $CDCl_3$ δ, ppm) δ 150.47, 144.81, 128.62, 124.71, 51.32, 41.96 (ESI Fig. S3, a and b).

N, N-bis(2-(5-cyano-6-oxo-3,4-diphenylpyridazin-1(6H)-yl)ethyl)-4-nitrobenzenesulfonamide **(DP):** In a 200 ml round bottom flask, anhydrous potassium carbonate (1 mmol) and hetero-aromatic compounds (1 mmol) were added to a small amount of dry DMF, and the mixture was agitated for 30 minutes. After that, compound BPN (0.5 mmol) was added to the mixture, and agitated was maintained for the next 15-20 hours. After completion, the reaction was

monitored via TLC, and DMF was removed in vacuo after the reaction was finished. Column chromatography was applied to isolate the desired products. All the compounds DT, DPM, and DTM were synthesized in a similar fashion presented in Scheme 1. Yield: 85%, M.P.: 142(±1)°C, White solid, ^{1}H-NMR (500 MHz, $CDCl_3$ δ, ppm): δ 8.25 (d, J = 8.8 Hz, 1H), 7.98 (d, J = 8.3 Hz, 1H), 7.42 (t, J = 7.2 Hz, 1H), 7.37 – 7.31 (m, 3H), 7.24 (d, J = 7.8 Hz, 2H), 7.17 (d, J = 7.3 Hz, 2H), 7.10 (d, J = 7.4 Hz, 2H), 4.58 (t, J = 5.7 Hz, 2H), 3.92 (t, J = 5.6 Hz, 2H). ^{13}C-NMR (125 MHz, $CDCl_3$ δ, ppm) δ 157.15, 151.74, 150.25, 146.74, 145.31, 134.20, 132.41, 130.72, 129.40, 129.34, 129.07, 128.94, 128.48, 128.43, 124.67, 113.89, 113.20, 50.89, 46.18. (Fig. S4, a and b).
HRMS(ESI): *m/z*: $[M + H]^+$ calculated for $C_{44}H_{32}N_8O_6S$: 801.2244; found: 801.2260.
Elemental Analysis for $C_{44}H_{32}N_8O_6S$: C, 65.99; H, 4.03; N, 13.99%; found C, 65.43; H, 4.16; N, 14.24%.

4-nitro-N, N-bis(2-(3-oxo-5,6-diphenyl-1,2,4-triazin-2(3H)-yl)ethyl)benzenesulfonamid (DT): Yield: 72%, M.P.: 155(±1)°C, White solid, ^{1}H-NMR (500 MHz, $CDCl_3$ δ, ppm): δ 8.13 (d, J = 8.5 Hz, 1H), 7.91 (d, J = 8.3 Hz, 1H), 7.43-7.39 (dd, J = 15.3, 7.4 Hz, 4H), 7.34 (t, J = 7.4 Hz, 2H), 7.31 – 7.26 (m, 4H), 4.51 (t, J = 5.1 Hz, 2H), 4.00 (t, J = 5.1 Hz, 2H). ^{13}C-NMR (125 MHz, $CDCl_3$ δ, ppm) δ 167.10, 153.31, 149.90, 145.41, 143.14, 134.74, 133.92, 131.76, 129.97, 129.58, 128.94, 128.67, 128.32, 128.28, 124.48, 50.82, 45.37. (Fig. S5, a and b)
HRMS(ESI): *m/z*: $[M + H]^+$ calculated for $C_{40}H_{32}N_8O_6S$**:** 753.2244; Found: 753.2231.
Elemental Analysis $C_{40}H_{32}N_8O_6S$: C, 63.82; H, 4.28; N, 14.89%; found: c, 63.59; H, 4.51; N, 14.81%.

N,N-bis(2-(5-cyano-3,4-bis (4-methoxy phenyl) – 6 -oxo pyridazin- 1(6 H)-yl) ethyl)-4-nitrobenzene sulfonamide (DPM): Yield: 78%, M.P.: 151(±1)°C, Pale yellow solid, ^{1}H-NMR (500 MHz, $CDCl_3$ δ, ppm): δ 8.18 (d, J = 7.8 Hz, 1H), 7.94 (d, J = 8.5 Hz, 1H), 7.09 (d, J = 8.6 Hz, 2H), 7.01 (d, J = 8.4 Hz, 2H), 6.83 (d, J = 8.7 Hz, 2H), 6.75 (d, J = 7.9 Hz, 2H), 4.51 (t, J = 5.9 Hz, 2H), 3.89 (t, J = 5.9 Hz, 2H), 3.80 (s, 3H), 3.77 (s, 3H). ^{13}C-NMR (125 MHz, $CDCl_3$ δ, ppm) δ 161.46, 160.38, 157.23, 151.41, 150.11, 146.53, 145.40, 130.98, 130.75, 128.45, 126.73, 124.56, 124.53, 114.36, 113.87, 113.71, 112.99, 55.48, 55.41, 50.60, 46.00. (Fig. S6, a and b)
HRMS(ESI): *m/z*: $[M + H]^+$ calculated for $C_{48}H_{40}N_8O_{10}S$: 921.2666; Found: 921.2715.
Elemental Analysis for $C_{48}H_{40}N_8O_{10}S$: C, 62.60; H, 4.38; N, 12.17%; found: C, 62.71; H, 4.30; N, 12.02%.

N,N-bis(2-(5,6-bis(4-methoxyphenyl)-3-oxo-1,2,4-triazin-2(3H)-yl)ethyl)-4nitrobenzenesulfonamide (DTM): Yield: 80%, M.P.: 150(±1)°C, Yellow solid, ^{1}H-NMR (500 MHz, $CDCl_3$ δ, ppm): δ 8.07 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 9.0 Hz, 1H), 7.43 (d, J = 9.0 Hz, 2H), 7.20 (d, J = 8.8 Hz, 2H), 6.85 (d, J = 8.0 Hz, 2H), 6.76 (d, J = 8.3 Hz, 2H), 4.44 (t, J = 5.7 Hz, 2H), 3.98 (t, J = 5.6 Hz, 2H), 3.82 (s, 3H), 3.80 (s, 3H). ^{13}C-NMR (125 MHz, $CDCl_3$ δ, ppm) δ 166.05, 162.83, 160.66, 153.51, 149.85, 145.64, 142.87, 132.26, 130.35, 128.31, 127.11, 126.73, 124.49, 114.24, 113.85, 55.55, 55.49, 50.53, 45.20. (Fig. S7, a and b)
HRMS(ESI): *m/z*: $[M + H]^+$ calculated for $C_{44}H_{40}N_8O_{10}S$: 873.2666; found: 873.2749.
Elemental Analysis for $C_{44}H_{40}N_8O_{10}S$: C, 60.54; H, 4.62; N, 12.84%; found: C, 60.51; H, 4.69; N, 12.77%.

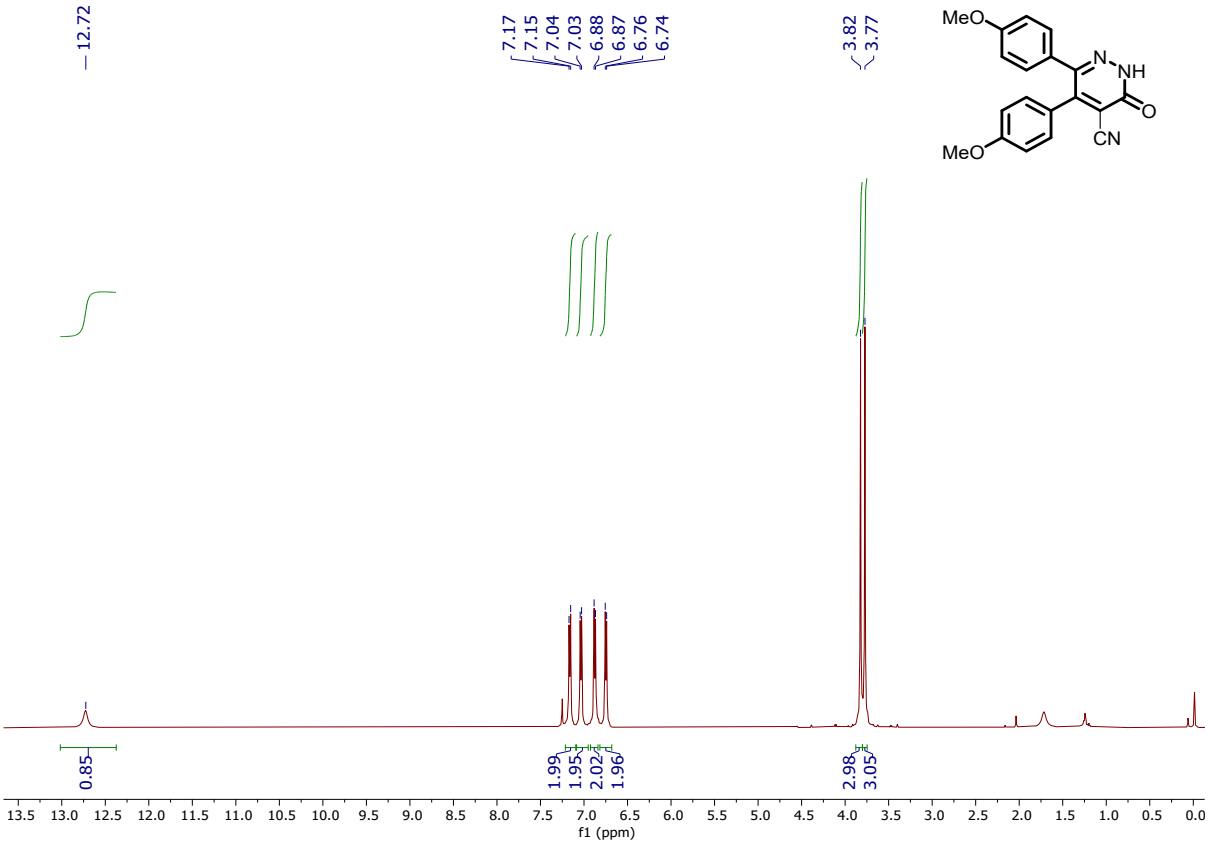

Fig. S1 (a): ^{1}H NMR of 5,6-bis(4-methoxyphenyl)-3-oxo-2,3-dihydropyridazine-4-carbonitrile (Pyz-OMe)

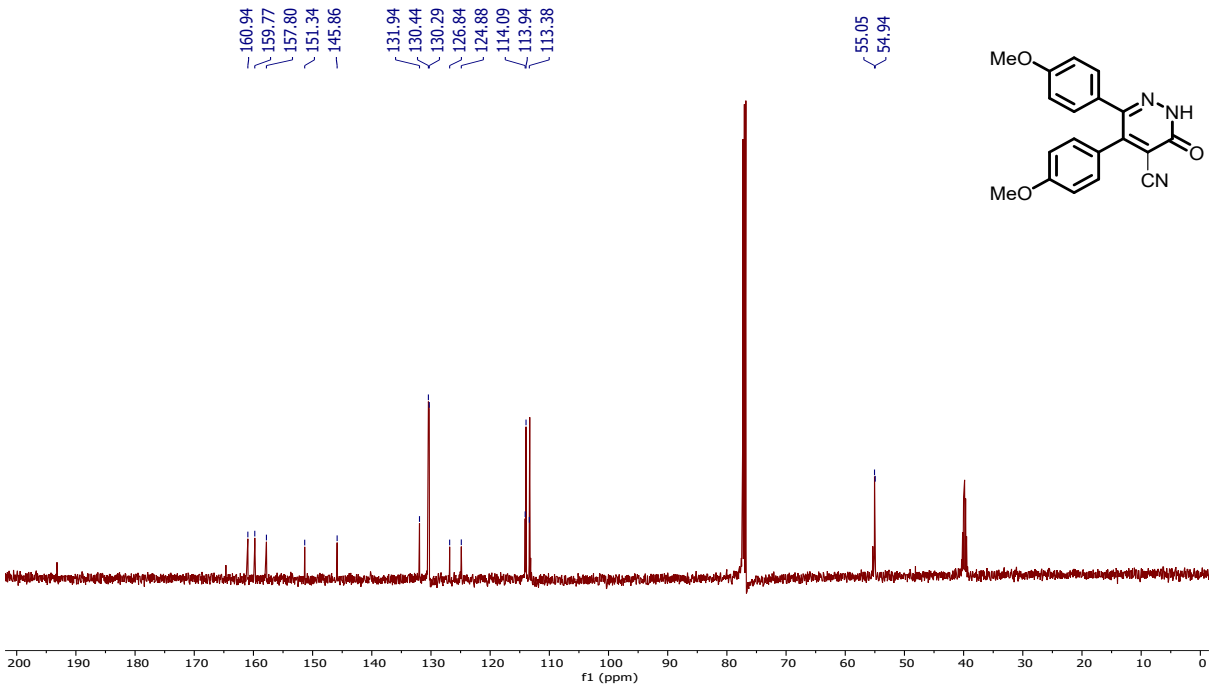

Fig. S1 (b): ^{13}C NMR of 5,6-bis(4-methoxyphenyl)-3-oxo-2,3-dihydropyridazine-4-carbonitrile (Pyz-OMe)

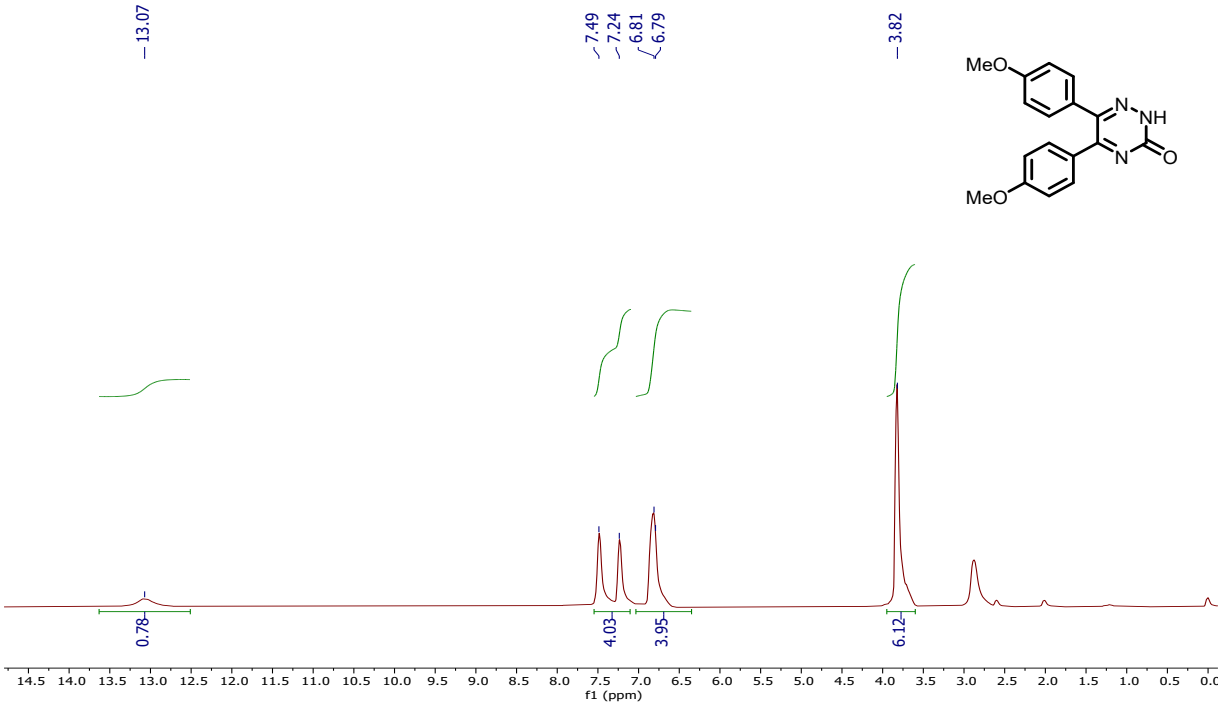

Fig. S2 (a): ^{1}H NMR of 5,6-bis(4-methoxyphenyl)-1,2,4-triazin-3(2H)-one (Tyz-OMe)

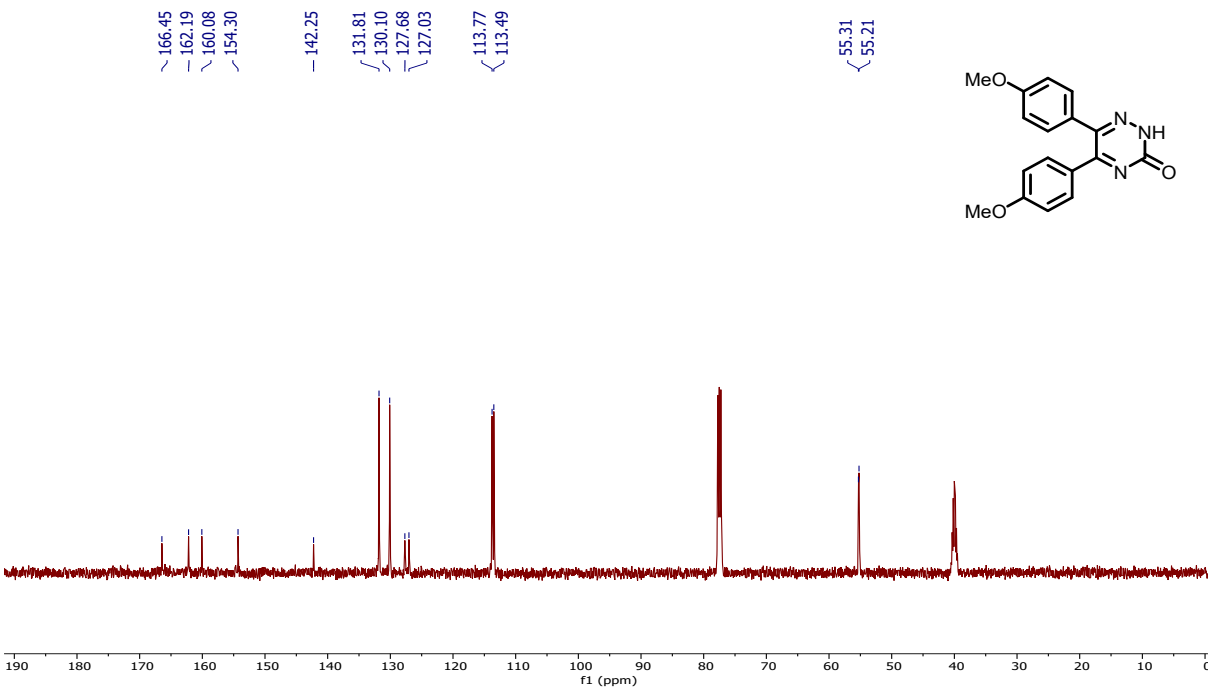

Fig. S2 (b): ^{13}C NMR of 5,6-bis(4-methoxyphenyl)-1,2,4-triazin-3(2H)-one (Tyz-OMe)

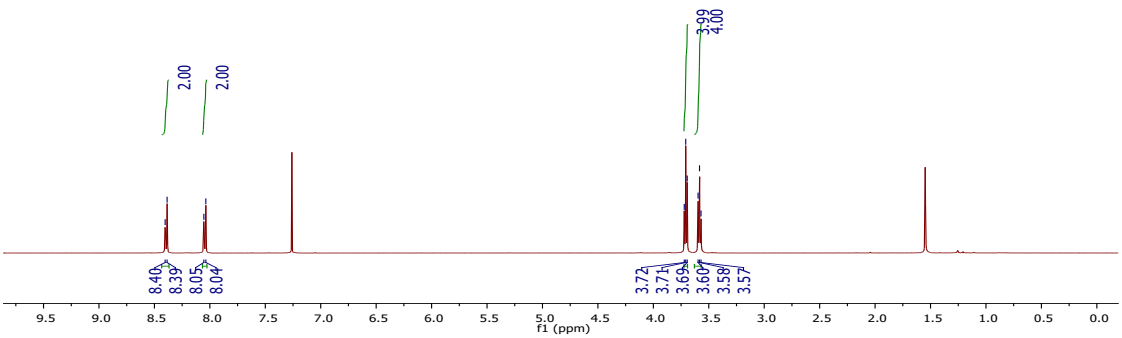

Fig. S3 (a): ^{1}H NMR of N,N-bis(2-chloroethyl)-4-nitrobenzenesulfonamide (BPN)

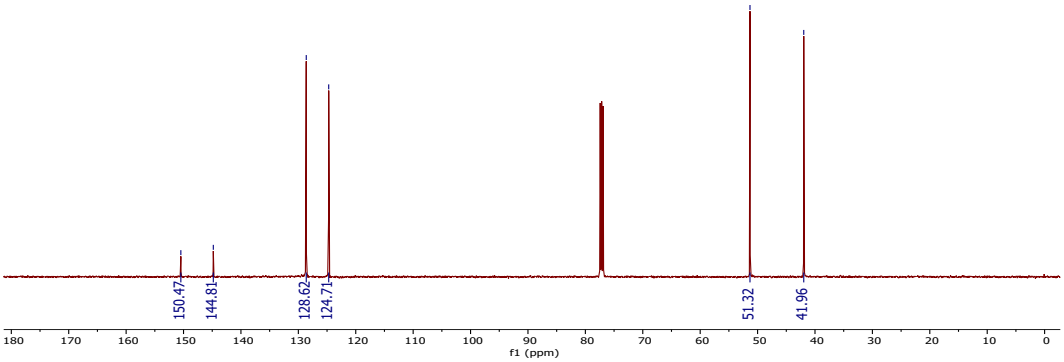

Fig. S3 (b): ^{13}C NMR of N,N-bis(2-chloroethyl)-4-nitrobenzenesulfonamide (BPN)

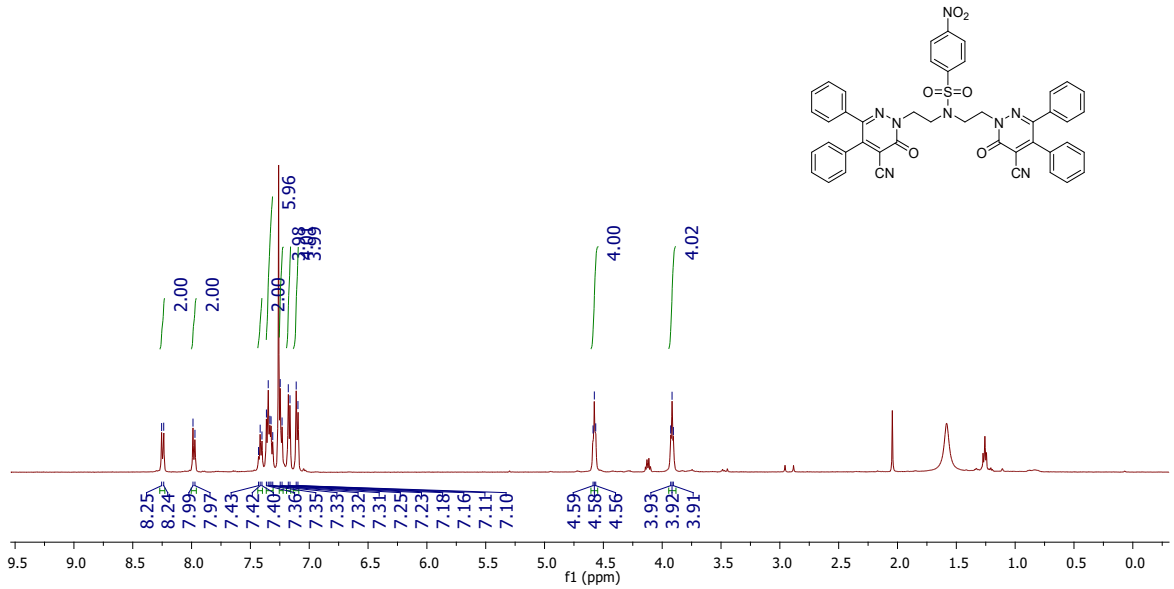

Fig. S4 (a): ^{1}H NMR of N,N-bis(2-(5-cyano-6-oxo-3,4-diphenylpyridazin-1(6H)-yl)ethyl)-4-nitrobenzenesulfonamide (DP)

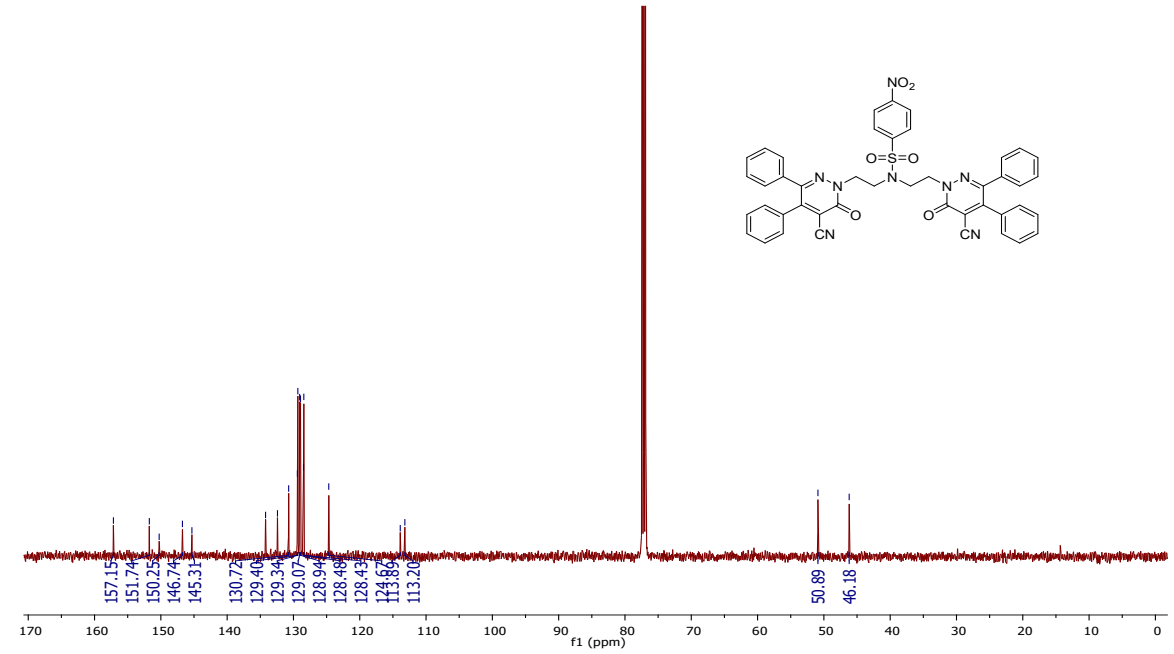

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Fig. S4 (b): ^{13}C NMR of N,N-bis(2-(5-cyano-6-oxo-3,4-diphenylpyridazin-1(6H)-yl)ethyl)-4-nitrobenzenesulfonamide (DP)

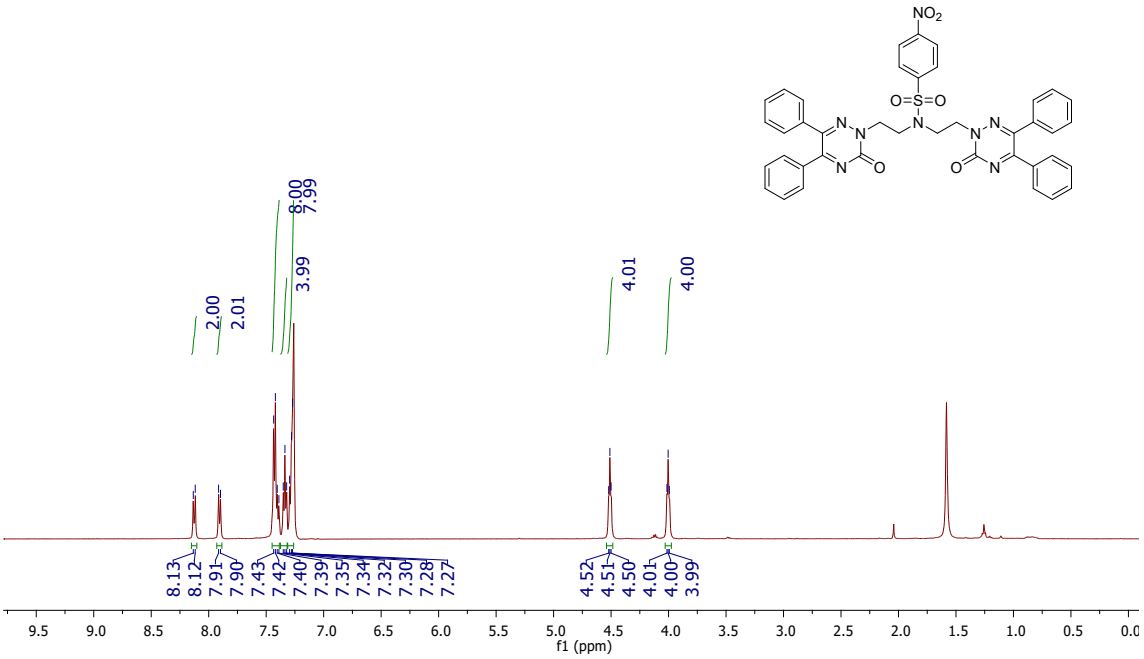


Fig. S5 (a): ^{1}H NMR of 4-nitro-N,N-bis(2-(3-oxo-5,6-diphenyl-1,2,4-triazin-2(3H)-yl)ethyl)benzenesulfonamid (DT).

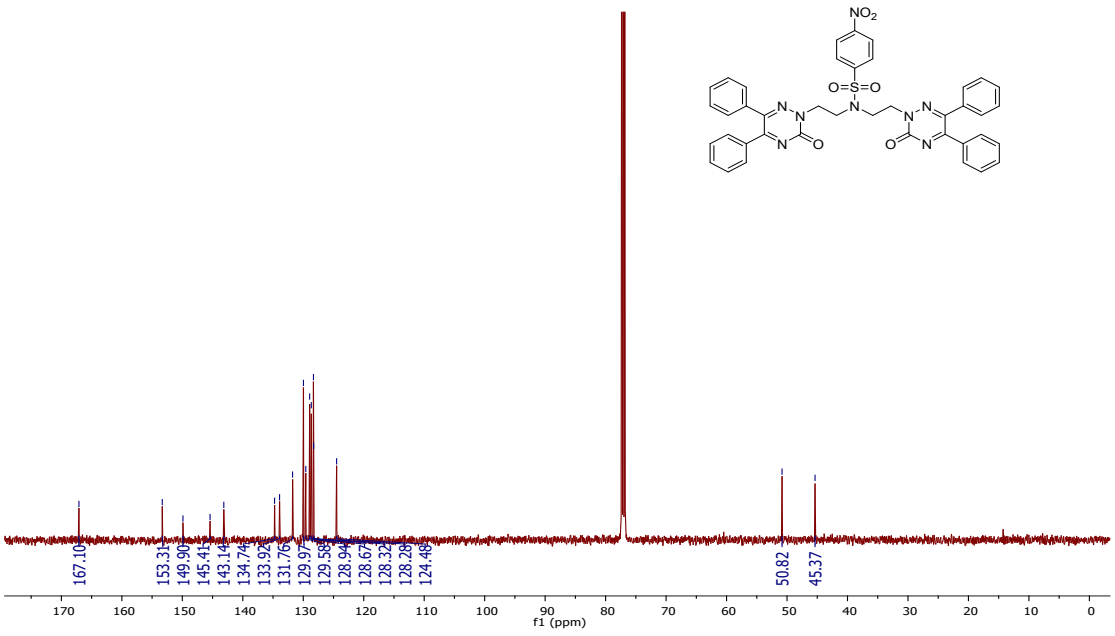


Fig. S5 (b): ^{13}C NMR of 4-nitro-N,N-bis(2-(3-oxo-5,6-diphenyl-1,2,4-triazin-2(3H)-yl)ethyl)benzenesulfonamid (DT).

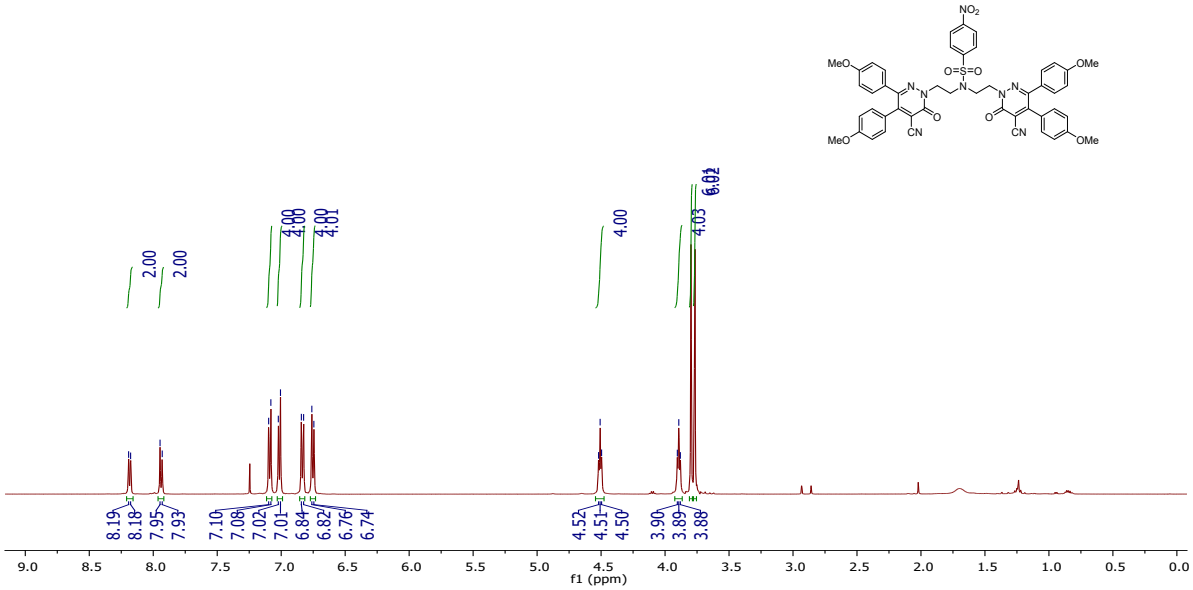


Fig. S6 (a): ^{1}H NMR of N,N-bis(2-(5-cyano-3,4-bis(4-methoxyphenyl)-6-oxopyridazin-1(6H)-yl)ethyl)-4-nitrobenzenesulfonamide (DPM).

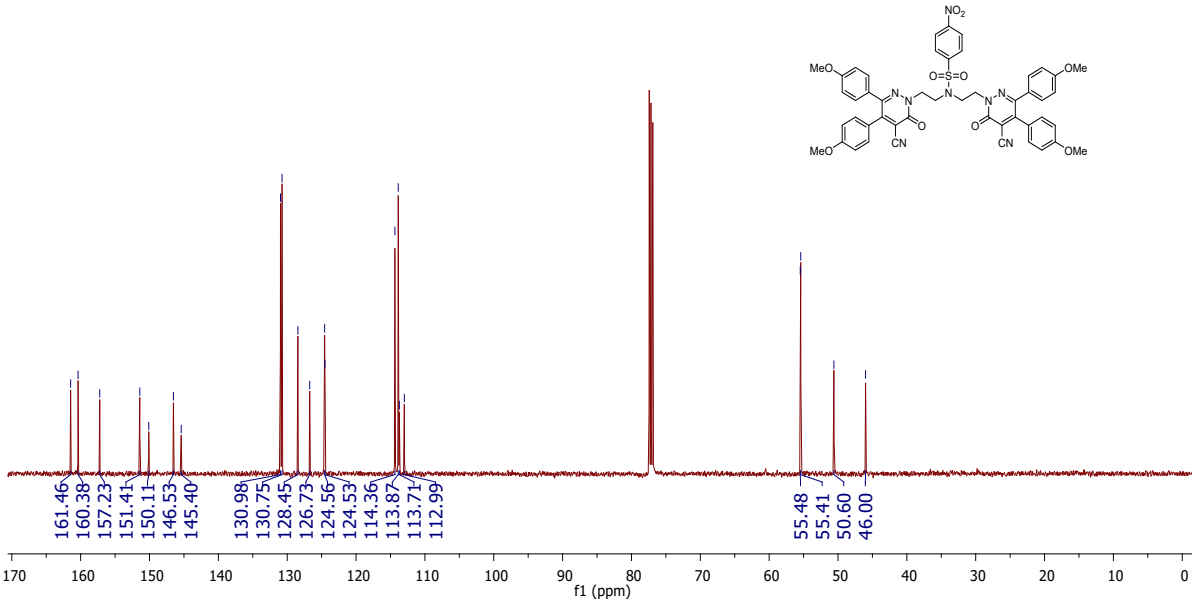


Fig. S6 (b): ^{13}C NMR of N,N-bis(2-(5-cyano-3,4-bis(4-methoxyphenyl)-6-oxopyridazin-1(6H)-yl)ethyl)-4-nitrobenzenesulfonamide (DPM).

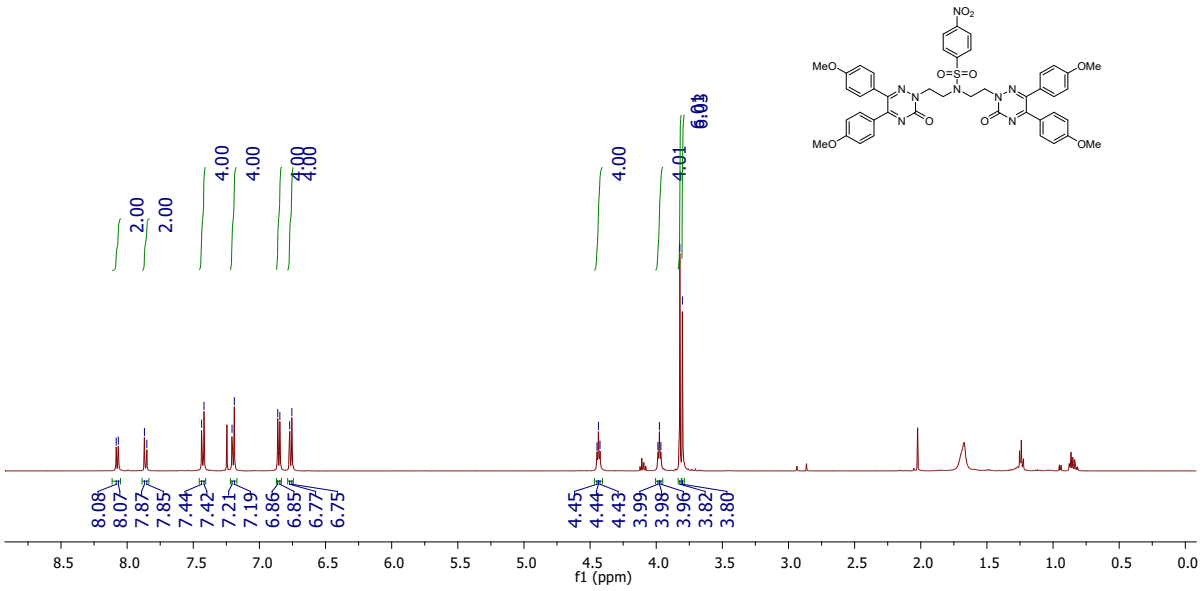


Fig. S7 (a): ^{1}H NMR of N, N-bis(2-(5,6-bis(4-methoxyphenyl)-3-oxo-1,2,4-triazin-2(3H)-yl)ethyl)-4-nitrobenzenesulfonamide (DTM).

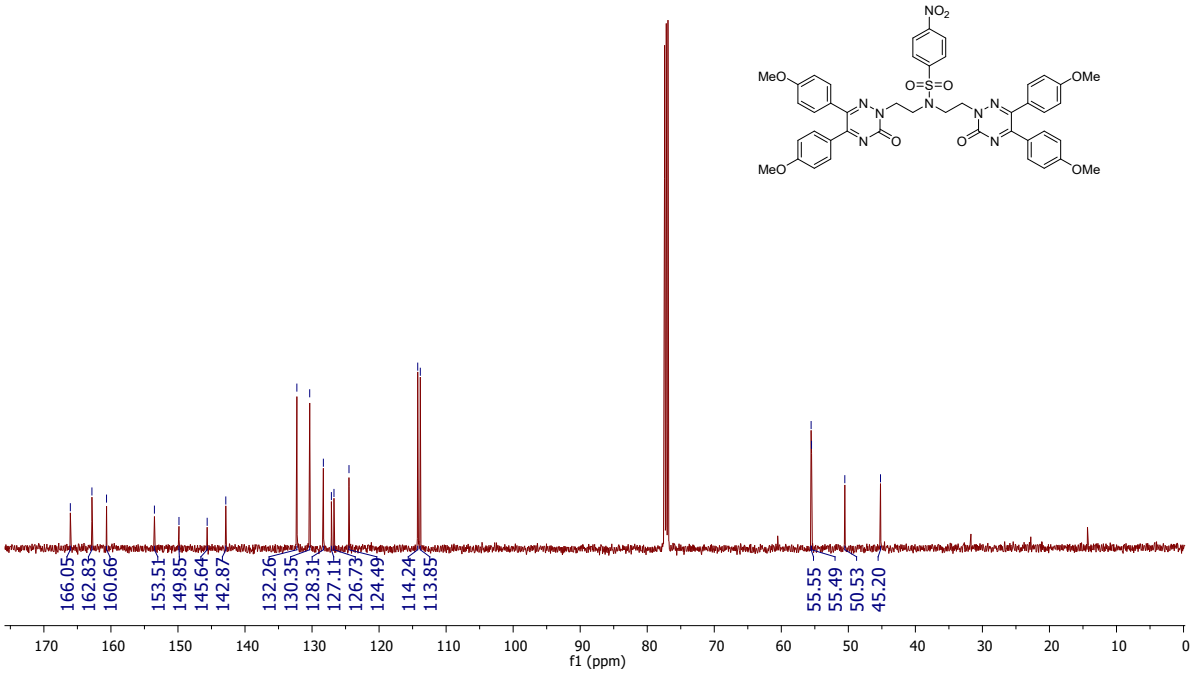


Fig. S7 (b): ^{13}C NMR of N, N-bis(2-(5,6-bis(4-methoxyphenyl)-3-oxo-1,2,4-triazin-2(3H)-yl)ethyl)-4-nitrobenzenesulfonamide (DTM).

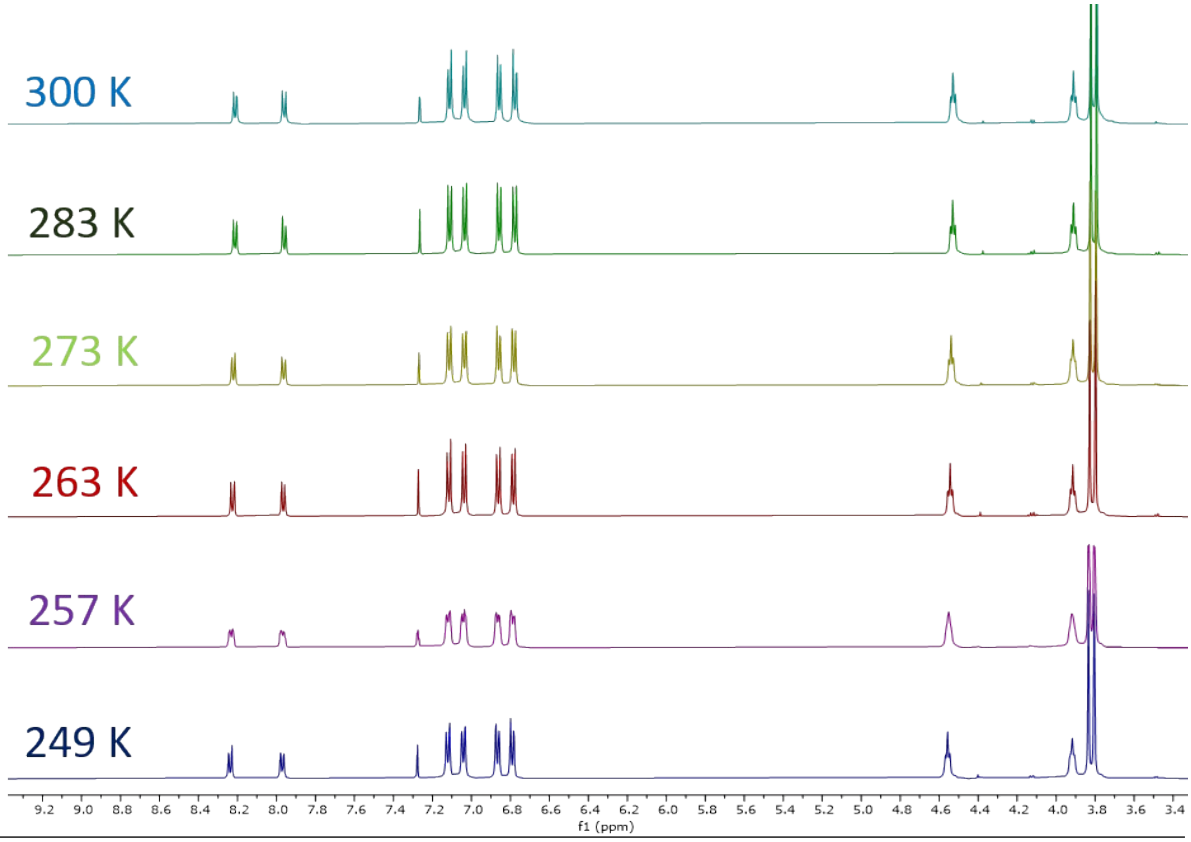


Fig. S8: Temperature-dependent ^{1}H NMR stacked spectra of the compound DPM, recorded at 500MHz in $CDCl_3$ (249-300K).

Table S1. Crystal data and structure refinement for the compounds.				
Crystal data	**DP**	**DT**	**DPM**	**DTM**
Empirical formula	$C_{44}H_{32}N_8O_6S$	$2(C_{40}H_{32}N_8O_6S)$	$C_{48}H_{40}N_8O_{10}S$	$C_{44}H_{40}N_8O_{10}S$
F.W.	800.83	1505.63	920.94	940.44
CCDC No.	2219084	2300044	2300051	2298730
Crystal System	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	P21/c	P21/c	$P\bar{1}$	$P\bar{1}$
T(K)	293	293	293(2)	293
a (Å)	19.1248 (2)	19.8963 (9)	10.4679(3)	11.29667 (11)
b (Å)	9.6274 (10)	23.786 (1)	13.6068(4)	12.50697 (11)
c (Å)	25.5382 (3)	17.7301 (8)	19.0674(7)	16.65629 (15)
α, β, γ (°)	90, 102.5220 (10), 90	90, 105.279 (5), 90	69.406(3), 81.975(3), 67.586(3)	82.1895 (7), 74.1486 (8), 78.7063 (8)
V(Å3)	4590.30 (9)	8094.3 (7)	2350.19(15)	2211.51 (4)
Dcalc (mg m -3)	1.159	1.236	1.301	1.363
Z	4	4	2	2
μ (mm-^{1})	1.06	1.17	1.169	1.24
GOF on F^2	1.075	1.591	1.036	1.889
wR (F^2)	0.035	0.154	0.061	0.094
R_w (F_o^2)[b]	0.109	0.449	0.188	0.324
[a]R1 = $\Sigma\|\|F_o\|-\|F_c\|\|/\Sigma\|F_o\|$; [b]$wR_2 = [\Sigma[w(\|F_o^2\|-\|F_c^2\|)]^2/\Sigma[w(\|F_o^2\|^2]^{1/2}$.				

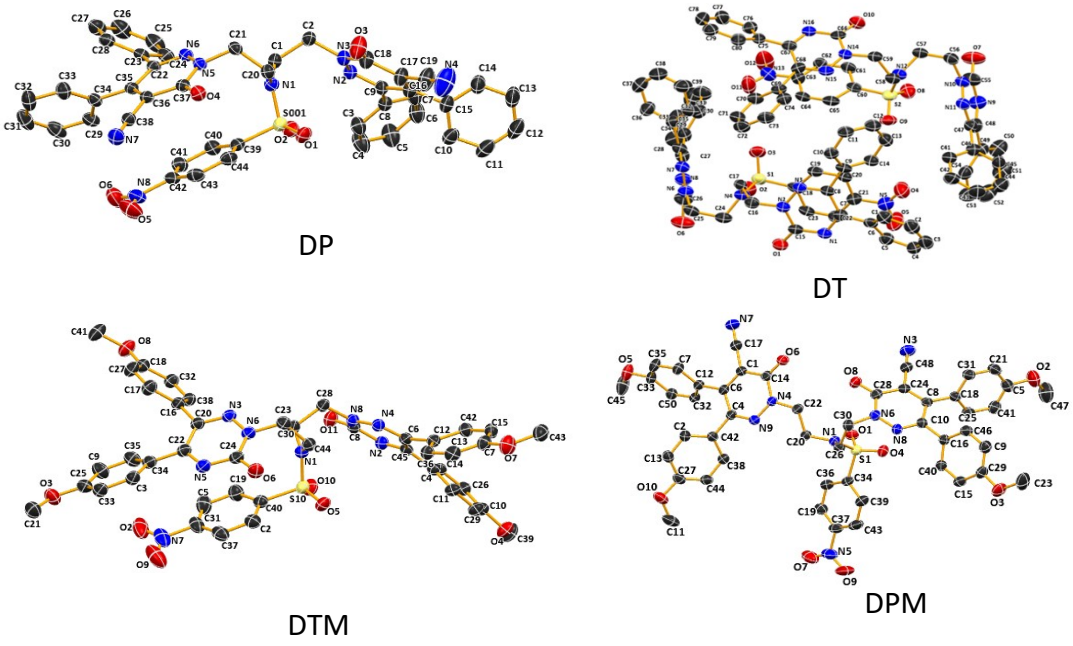


Fig. S9: ORTEP diagram of compounds DP, DT, DPM, and DTM. Thermal ellipsoids are drawn at the probability level of 30%.

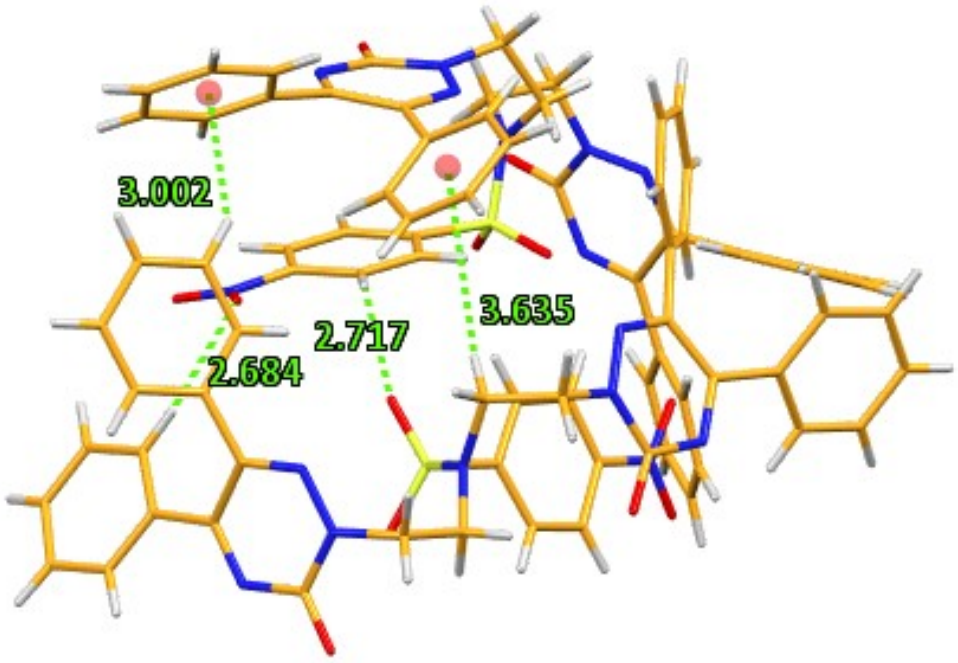


Fig. S10: The asymmetric unit of compound DT stabilized by C-H···π and C-H···O the intermolecular interactions.

Table S2: Representation of key bonds and angles showing intra-molecular interactions in their crystal structure and optimized structures at the DFT/B3LYP level of theory of compounds DP, DT, DPM, and DTM.

S. No.	D-H···A	Crystal structure			Optimized structure		
		H···A	D···A	D-H···A	H···A	D···A	D-H···A
		(Å)	(Å)	(°)	(Å)	(Å)	(°)
Compound DP							
1	(Pyridazinone centroid) π···π (centroid of PNS)	3.717			4.130		
2	(C38N7 centroid) π···π (O5N8O6 centroid)	3.751			5.024		
3	C3H3···O2	2.757	3.652	161.95	2.632	3.630	152.62
4	C20H20B···O1	2.512	2.883	102.59	2.381	2.877	10593
5	C1H1B···O2	2.323	2.816	110.64	2.313	2.865	109.38
6	C43H43··· π (C38N7 centroid)	3.377	3.583	95.17	3.309	3.860	112.81
7	C2H2B···π (C18O3 centroid)	2.358	2.557	90.46	2.300	2.555	90.59
8	C1H1A···N6	2.694	3.407	130.39	2.766	3.585	131.28
9	C1H1B···N2	2.724	3.004	97.20	2.763	3.045	94.31
10	C44H44···O1	2.547	2.900	102.91	2.573	2.962	100.13
11	C40H40···O2	2.639	2.953	100.46	2.548	2.945	100.48
12	C14H14B···O48	2.373	2.781	104.65	2.227	2.774	105.45
13	C2H2B···O3	2.554	2.759	91.7	2.521	2.735	89.27
Compound DT							
1	(Triazinone centroid) π···π (PNS)	3.654			3.745		
2	(Triazinone centroid) π···π (S1O2 centroid)	3.351			3.627		
3	C17H17A···O1	2.429	2.888	108.46	2.426	2.928	106.44
4	C24H24B···O2	2.730	2.800	106.27	2.328	2.830	106.07
5	C40H···N7	2.795	2.940	90.20	2.769	2.930	87.51
6	C34H···N8	2.592	2.866	97.55	2.610	2.856	94.34
7	C25H25···AO6	2.460	2.741	96.26	2.444	2.750	94.34
8	C24H24B···O6	2.886	3.335	109.39	2.793	3.304	108.54
9	C24H24A···O1	2.705	3.314	121.27	2.670	3.387	122.62
10	C16H16A···O1	2.422	2.773	100.77	2.773	2.414	98.75
11	C5H ···π (O5N5O4)	3.094	3.560	112.88	2.838	3.392	111.71
12	C40H ···π (S1O3)	3.436	4.229	144.73	3.146	4.140	152.52
Compound DPM							
1	(S1O4 centroid) π···π (Pyridazinone centroid)	3.444			3.825		
2	(O2N7O9) π···π (phenyl ring)	3.468					
3	C26H26A···N8	2.770	3.034	96.90	2.777	3.050	94.01
4	C26H26A···O4	2.505	2.872	102.44	2.426	2.917	105.70
5	C20H20B···O1	2.489	2.908	105.83	2.361	2.942	111.56

6	C22H22B···O6	2.479	2.744	95.29	2.407	2.743	95.96
7	C26H26A···π (S1O4 centroid)	2.686	2.483	91.25	2.432	2.715	98.87
8	C2H2···π (Phenyl centroid)	3.269	3.653	107.21	3.208	3.737	110.95
9	C32H32 ···π (Phenyl centroid)	3.609	3.842	97.40	3.510	2.892	102.50
10	C46H46···π (Phenyl centroid)	3.471	3.839	106.47	3.366	3.794	104.97
11	C7H7···π (C17N7 centroid)	2.940	3.268	102.33	2.882	3.210	97.54
12	C31H31···π (C48N3 centroid)	3.285	3.420	90.39	2.907	3.225	97.02
Compound DTM							
1	(Triazinone centroid) π···π (PNS)	3.767			4.414		
2	C5H···O2	2.404	2.707	98.83	2.398	2.721	95.29
3	C37H···O9	2.438	2.724	97.75	2.407	2.724	95.06
4	C19H···O10	2.729	2.993	97.29	2.497	2.924	102.15
5	C2H···O5	2.511	2.884	104.22	2.658	2.997	97.47
6	C30H30B···O10	2.396	2.855	108.49	2.421	2.871	103.05
7	C44H44B···O5	2.735	2.833	108.31	2.361	2.833	104.28
8	C28H28B···O11	2.514	2.737	92.75	2.372	2.735	97.33
9	C14H···N2	2.505	2,783	97.46	2.512	2.808	94.19
10	C36H···N4	2.746	2.904	90.29	2.799	2.942	86.63
11	C38H···N3	2.802	2.945	89.51	2.654	2.879	90.69
12	C3H···N5	2.558	2.828	97.11	2.462	2.770	94.66
13	C11H··· π (phenyl centroid)	3.026	3.718	132.54	3.096	3.766	120.72
14	C42H··· π (phenyl centroid)	3.783	4.109	104.01	3.638	4.083	103.87
15	C35H··· π (phenyl centroid)	2.899	3.579	131.08	3.109	3.855	126.58
16	C17H··· π (phenyl centroid)	3.805	4.054	98.80	3.768	4.137	107.56

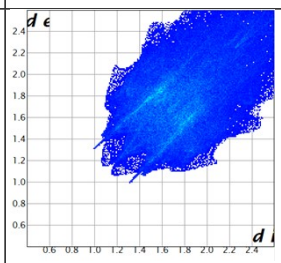
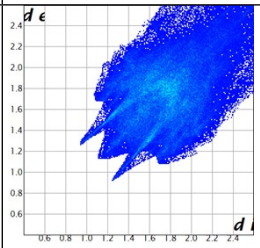
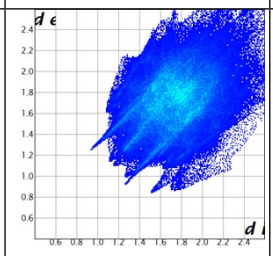
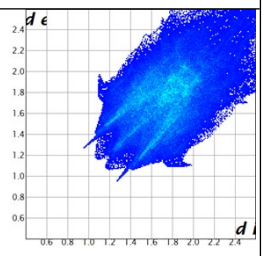
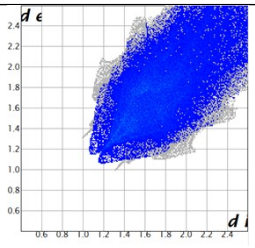
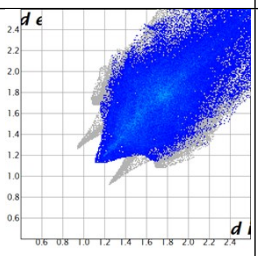
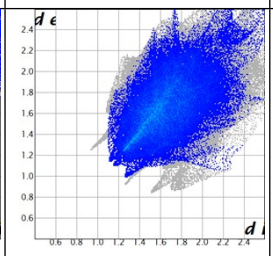
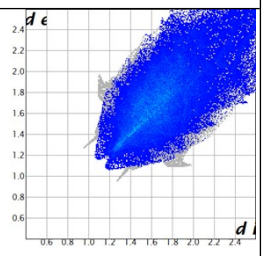
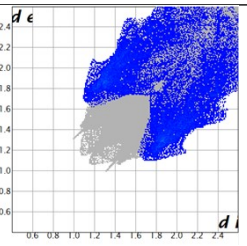
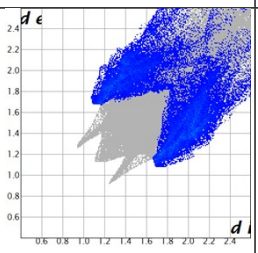
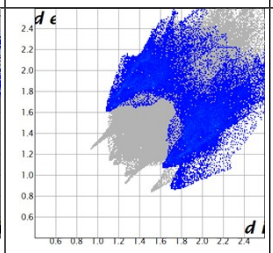
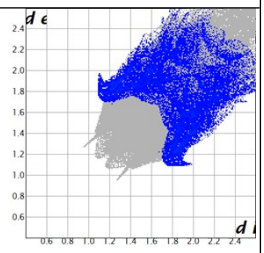
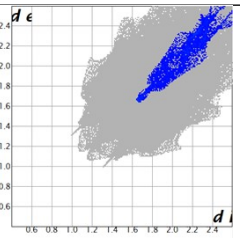
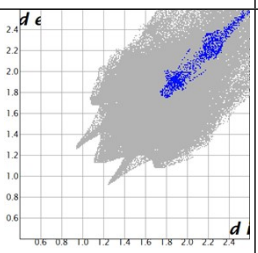
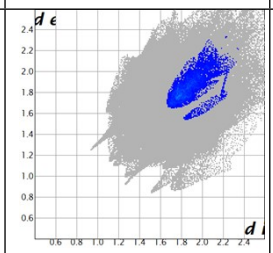
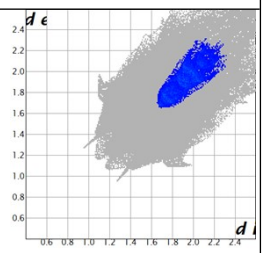
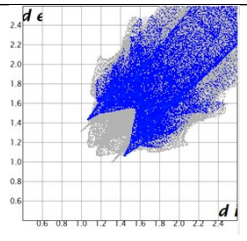
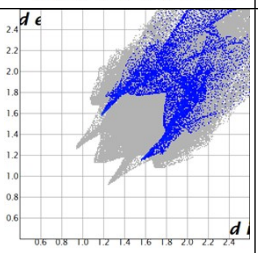
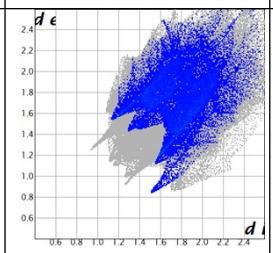
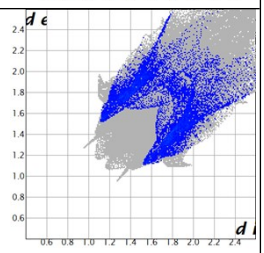
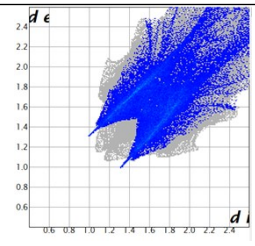
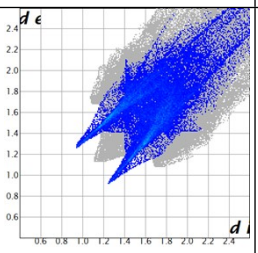
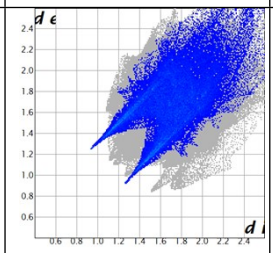
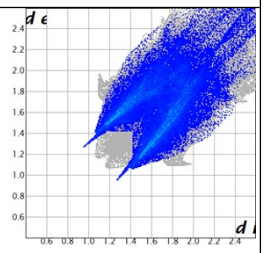
Table S3: Intermolecular H-bond geometry parameters of compounds DP, DP, DPM, and DTM.

S. No.	D-H···A	Crystal Structure			Symmetry code
		H···A	D···A	D-H···A	
		(Å)	(Å)	(°)	
Compound DP					
1	C11H···O1	2.633	3.296	128.78	2-x, -1/2+y, 1.5-z
2	C6H6···π (Phenyl centroid)	2.885	3.770	159.26	
3	C43H43···N2	2.626	3.358	136.01	x, -1+y, z
4	C26H726···π (Phenyl centroid)	3.715	4.254	199.80	
5	C1H1···N7	2.783	3.335	116.86	
6	C28H28···(C18O2 centroid)	3.472	3.986	117.39	
7	C27H27···π (C18O3 centroid)	3.573	4.045	114.24	
8	C20H20A···π (Phenyl centroid)	3.628	4.148	116.16	
9	C12H12···O2	2.645	3.502	153.69	2-x, -1/2+y, 1.5-z
10	C10H10···π (Phenyl centroid)	3.529	4.275	137.01	
11	C25H25···π (O6N6O5 centroid)	3.475	4.310	150.73	
12	C33H33···O4	2.483	3.392	165.59	1-x, 2-y, 1-z
13	(C28N7 centroid) π···π (C37O4 centroid)	3.296			

14	(C38N7 centroid) π···π (Pyridazinone centroid)	3.794			
Compound DT					
1	C2H···O7	2.336	3.260	161.11	x, 1/2-y, 1/2+z
2	C10H···π (PNS)	3.079	3.794	134.92	
3	C13H···π (Phenyl centroid)	3.364	3.935	124.51	
4	C12H···π (Phenyl centroid)	4.451	4.004	120.45	
5	C54H··· O4	2.682	3.492	145.98	x, y, z
6	C20H ···O9	2.691	3.498	145.82	x, y, z
7	C42H ···π (Phenyl centroid)	3.036	3.788	138.45	
8	C43H···π (Phenyl centroid)	3.856	4.217	106.03	
9	C17H17A···π (Phenyl centroid)	3.639	4.458	148.57	
10	C10H···π (Phenyl centroid)	3.481	4.173	104.54	
11	C77H ···O6	2.367	3.268	169.27	x, 1/2-y, -1/2+z
12	C71H ···π (Phenyl centroid)	3.366	3.969	124.66	
13	C72H ···π (Phenyl centroid)	3.430	3.991	121.17	
14	C72H ···π (Phenyl centroid)	3.620	3.715	132.93	
15	C56H56A ···O6	2.313	3.238	157.82	1-x, -1/2+y, 1/2-z
16	C25H25A ···O7	2.265	3.154	151.89	1-x, -1/2+y, 1/2-z
17	C23H ···O10	2.469	3.217	137.59	1-x, -1/2+y, 1/2-z
18	C61H··· O1	2.445	3.219	140.89	1-x, -1/2+y, 1/2-z
19	C80H··· O5	2.695	3.132	109.75	1-x, -1/2+y, 1/2-z
20	C79H··· O5	2.812	3.198	105.78	
21	C5H ···O12	2.679	3.111	109.21	1-x, -1/2+y, 1/2-z
22	C16H16A···π (Phenyl centroid)	2.789	2.625	144.62	
23	C24H24A···π (Phenyl centroid)	3.648	4.500	147.92	
24	C58H58B···π (Phenyl centroid)	3.624	4.453	145.05	
Compound DPM					
1	(O9N5O7 centroid) π···π(PNS)	3.472			
2	(C28O8 centroid) π···π (C48N3 centroid)	3.403			
3	(Pyridazinone centroid) π···π(PNS)	3.858			
4	C45H45A ···π (phenyl centroid)	3.478	4.085	123.35	
5	C45H45C ···π (phenyl centroid)	3.775	4.085	102.08	
6	C50H ···π (phenyl centroid)	3.386	4.272	159.97	
7	C11H11A ···π (phenyl centroid)	3.039	3.721	129.16	
8	C20H20B ···O1	2.526	3.478	167.17	1-x, 1-y, 1-z
9	C36H···O1	2.430	3.265	173.02	1-x, 1-y, 1-z
10	C38H···O1	2.726	3.567	150.83	
11	C32H···O4	2.729	3.610	158.39	
12	C11H11B ···π (phenyl centroid)	3.138	3.553	108.27	
13	C43H43 ···π (C48N3 centroid)	3.725	4.288	121.47	
14	C11H11C ···π (C17N7 centroid)	3.599	4.357	137.65	
15	C2H···O5	2.506	3.261	138.58	1-x, 1-y, 2-z
14	C11H11C ···π (phenyl centroid)	3.169	3.535	105.88	
15	C20H20A···O9	2.544	3.349	140.44	-x, 1-y, 1-z

16	C20H20A ···π (O7N5O9 centroid)	2.818	3.585	135.59	
17	C26H26B ···π (phenyl centroid)	2.912	3.811	154.58	
18	C20H20A ···π (phenyl centroid)	3.780	4.476	130.96	
19	C23H23C ···π (phenyl centroid)	3.483	4.244	137.87	
20	C23H23B ···π (Pyridazinone centroid)	3.704	4.031	1-3.08	
21	C23H23A ···π (Pyridazinone centroid)	3.707	4.031	102.85	
22	C31H ···O6	2.738	3.184	110.45	2-x, -y, 1-z
23	C46H ···O6	2.665	3.577	166.73	2-x, -y, 1-z
24	C26H26B ···π (O9N5O7 centroid)	3.370	3.955	120.72	
25	C20H20A···π (O9N5O7 centroid)	2.818	3.585	136.59	
Compound DTM					
1	(Phenyl centroid) π···π (phenyl centroid)	3.733			
2	(Phenyl centroid) π···π (PNS)	3.860			
3	(Phenyl centroid) π···π (phenyl centroid)	3.730			
4	C32H ···π (phenyl centroid)	3.868	4.652	143.85	
6	C28H28A···O4	2.605	3.388	137.84	x, -1+y, z
7	C41H41AA···N2	2.725	3.533	142.23	
8	C41H41A··· π (Triazinone centroid)	3.547	4.472	162.64	
9	C41H41A···O10	2.703	3.379	127.96	x, -1+y, z
10	C42H···O11	2.643	3.544	163.30	-x, 1-y, 1-z
11	C28H28A ···π (phenyl centroid)	3.748	4.394	126.47	
12	C14H··· π (Triazinone centroid)	2.910	3.440	117.46	
13	C28H28B···O2	2.339	3.526	157.32	-1+x, y, z
14	C28H28B ···π (O2N7O9 centroid)	3.328	4.201	150.69	
15	C43H43B···O5	2.750	3.467	155.80	
16	C36H ···π (O2N7O9 centroid)	3.548	3.716	93.09	
17	C44H44B ···π (O2N7O9 centroid)	2.851	3.750	152.82	
18	C21H21A···O6	2.653	3.116	110.13	2-x, 2-y, -z
19	C21H21B···O6	2.807	3.116	99.72	2-x, 2-y, -z
20	C28H28A···O4	2.609	3.389	137.64	
21	C39H39B···O11	2.750	3.666	157.92	
22	C41H41A···N2	2.733	3.529	140.71	x, -1+y, z
23	C41H41A···O10	2.695	3.380	128.79	x, -1+y, z
24	C41H41C···O10	2.560	3.359	145.45	1-x, 2-y, 1-z
25	C19H19···O8	2.614	3.471	153.43	1-x, 2-y, 1-z
26	C41H41B···O11	2.826	3.462	139.71	

Table S4: Fingerprint plots and decomposed fingerprints showing various interactions of compounds

DP, DT, DPM, and DTM.				
Interaction	DP	DT	DPM	DTM
Fingerprint				
H···H				
C···H				
C···C				
N···H				
O···H				

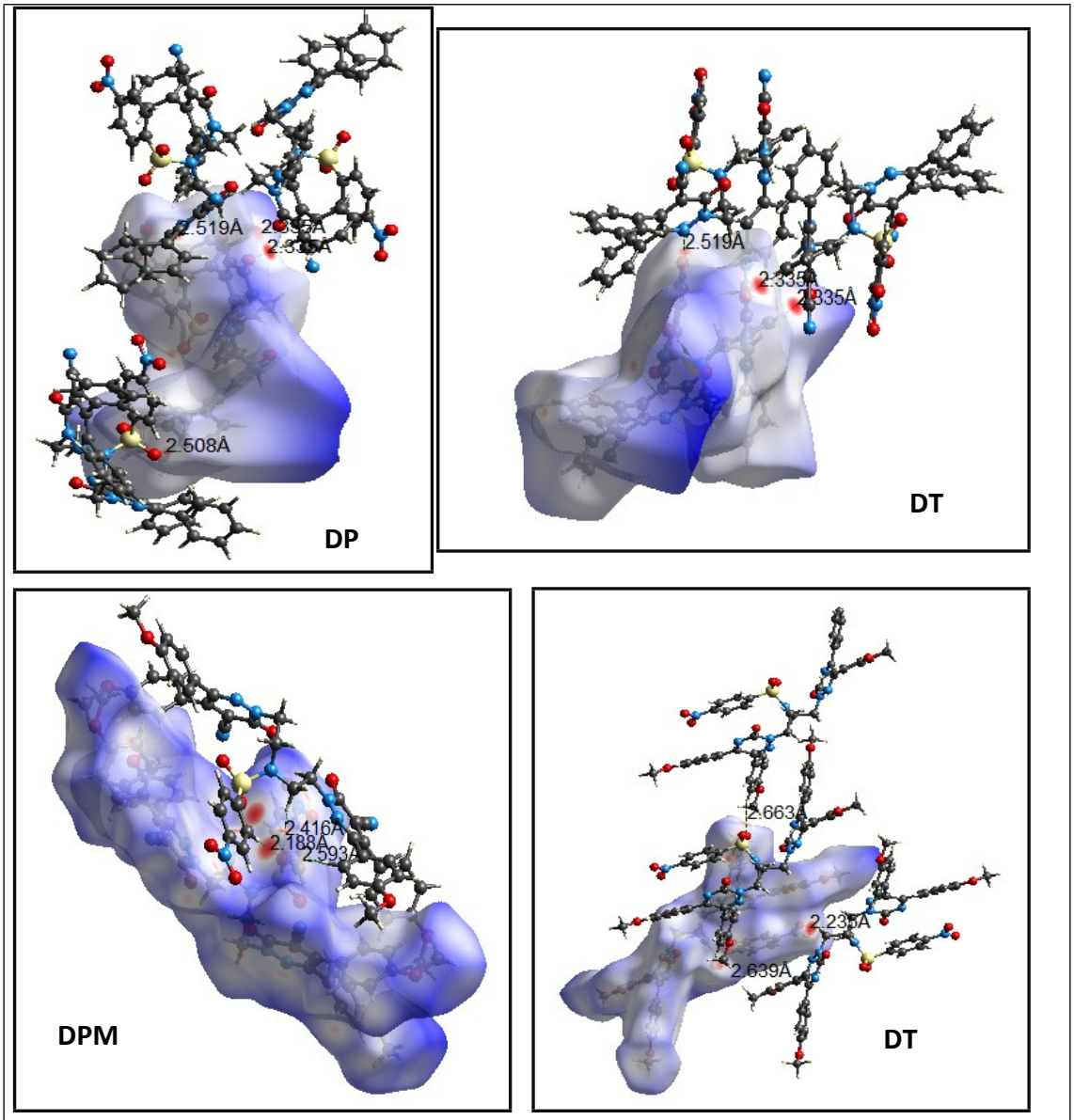


Fig. S11: Hirshfeld surfaces of DP, DT, DPM, and DTM mapped with d_{norm} surrounded with neighboring molecules associated with close contacts are shown along with distances between the atoms involved.

Table S5: Energy E(eV), Wavelength λ(nm), and Oscillator Strength (f) of the **s**elected UV-vis absorption energy transitions at the TD-DFT/B3LYP level for compounds in the gaseous phase acetonitrile.

DP				
Excited state	**λ/nm**	**E/eV**	**f**	**Major contribution**
S1	401	3.091	0.002	H-1 → L (76%), H → L (23%)
S2	381	3.244	0.190	H-1 → L+1(41%), H → L+2(31%)

S3	380	2.258	0.010	H-1 → L+1 (21%), H → L (37%)
S4	378	3.372	0.017	H → L 9(39%)
S5	360	3.441	0.004	H-3 → L (91%)
S7	355	3.486	0.003	H-1 → L+2(71%)
S8	346	3.575	0.016	H-2 → L+2(83%)
S9	346	3.576	0.009	H-3 → L+1(80%)
S12	338	3.667	0.021	H-5 → L+2(49%)
S13	337	3.703	0.066	H-2 → L (71%)
S18	325	3.805	0.020	H-7 → L+2(68)
DT				
S3	367	3.374	0.165	H-1 → L+2(51%)
S2	401	3.085	0.235	H → L (57%)
S4	362	3.418	0.023	H-3 → L (88%)
S5	360	3.438	0.119	H-1 → L+2(21%), H → L+2(59%)
S10	342	3.624	0.035	H-2 → L (52%)
S13	334	3.712	0.005	H-9 → L (94%)
S14	331	3.743	0.0004	H-4 → L (88%)
S19	318	3.894	0.007	H-7 → L (71%)
S20	315	3.935	0.003	H-8 → L (80%)
DPM				
S1	456	2.717	0.009	H-1 → L (26%), H → L (71%)
S2	454	2.730	0.003	H-1 → L (73%), H → L (25%)
S3	446	2.777	0.161	H → L+1 (78%)
S4	442	2.802	0.078	H-1 → L+2(83%)
S5	410	3.016	0.0004	H → L+2(92%)
S6	403	3.047	0.0004	H-1 → L+2(93%)
S7	398	3.112	0.051	H-2 → L+1(62%)
S8	396	3.129	0.008	H-3 → L (81%)
S10	392	3.149	0.057	H-3 → L+2(80%)
S11	360	3.438	0.001	H-3 → L+1(96%)
S13	338	6.658	0.035	H-4 → L (95%)
DTM				
S1	497	2.493	0.003	H-3 → L (9%), H → L (90%)
S2	461	2.685	0.006	H-1 → L (98%)
S3	439	2.820	0.001	H-3 → L (88%)
S4	410	3.023	0.156	H → L+1(91%)
S5	403	3.075	0.197	H-1 → L+1 (83%)
S6	397	3.118	0.001	H-2 → L (98%)
S7	380	3.262	0.0002	H-1 → L+1(90%)
S8	374	3.309	0.0002	H → L+2(95%)
S16	332	3.723	0.097	H-2 → L+1(90%)
S18	329	3.768	0.002	H-3 → L+2(96%)
S20	325	3.805	0.001	H-6 → L (79%)

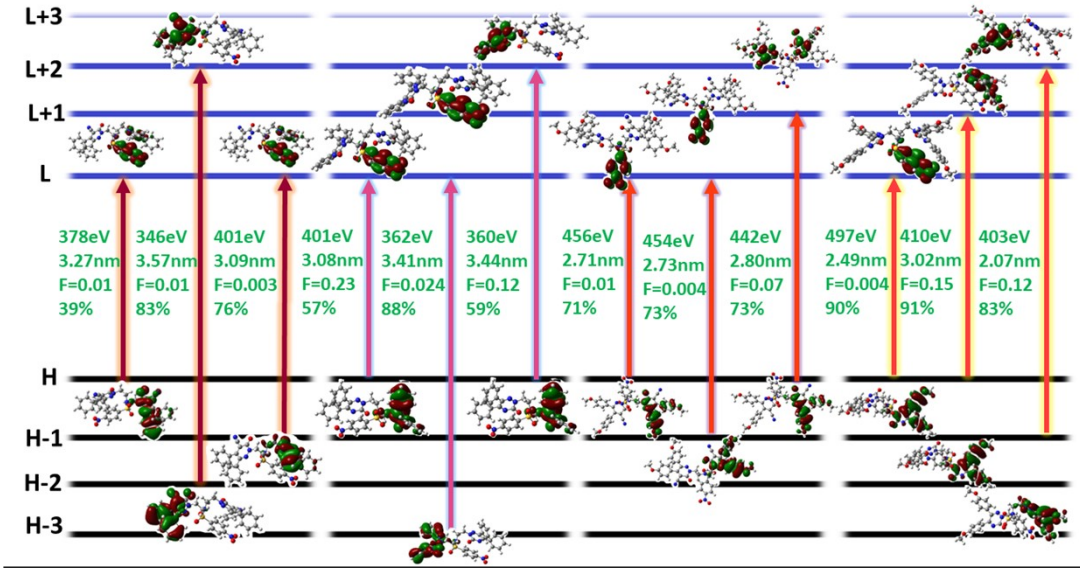
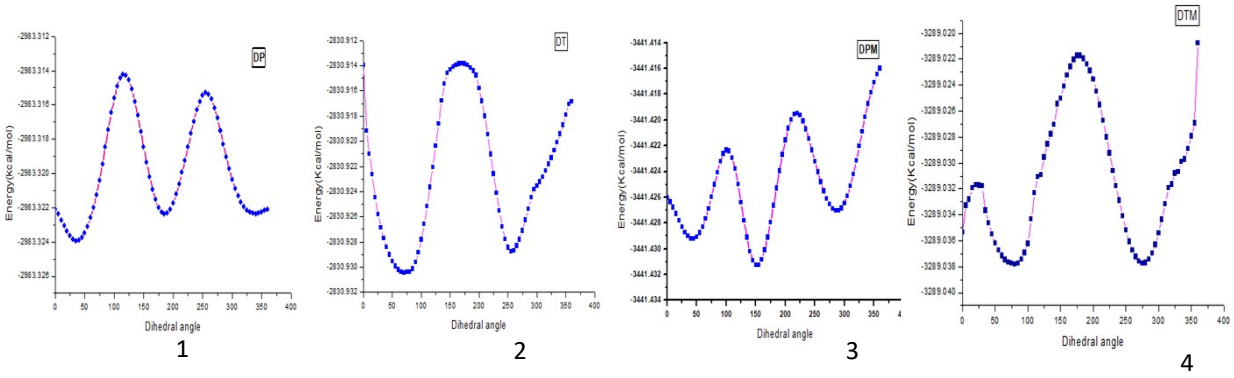
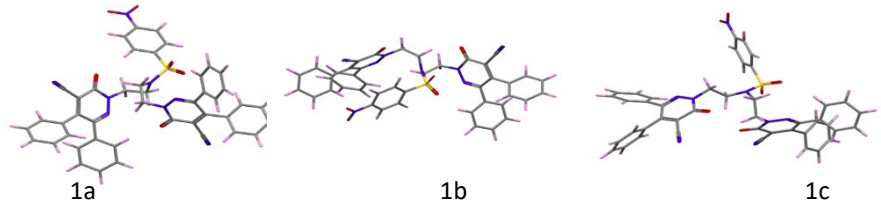


Fig.: S12: Energy level diagram representing the dominant transitions and molecular orbitals calculated through TD-DFT calculations performed in acetonitrile via the CPCM model.



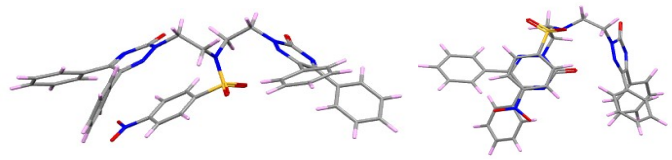
1 2 3 4



1a
0 Kcal/mol

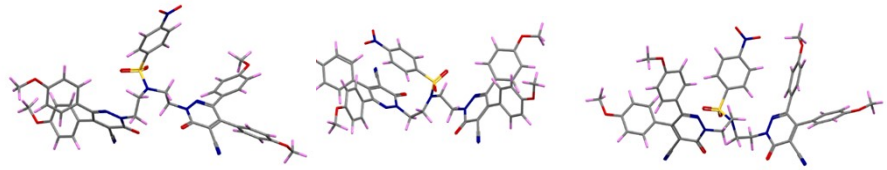
1b
0.93 Kcal/mol

1c
1.10 Kcal/mol



2a
0 Kcal/mol

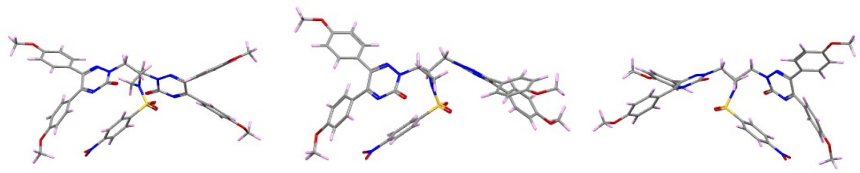
2b
1.36 Kcal/mol



3a
1.35 Kcal/mol

3b
0 Kcal/mol

3c
4.82 Kcal/mol



4a
2.18 Kcal/mol

4b
0 Kcal/mol

4c
0.05 Kcal/mol

Fig. S13: Representation of potential energy surface scans through the linker dihedrals (scans 1, 2, 3, and 4). Different possible conformers of compounds DP, DT, DPM, and DTM were obtained by performing 1-D potential energy scanning.

Table S6: Photophysical Properties of DP, DT, DPM, and DTM in several solvents.								
Compounds	**DP**		**DT**		**DPM**		**DTM**	
Solvents	λ_{abs} **(max/nm)**	λ_{em} **(max/ nm)**	λ_{abs} **(max/ nm)**	λ_{em} **(max/ nm)**	λ_{abs} **(max/ nm)**	λ_{em} **(max/ nm)**	λ_{abs} **(max/ nm)**	λ_{em} **(max/ nm)**
Toluene	358	440	353	457	368	486	360	492
$CHCl_3$	358	440	353	453	372	501	365	502
EtOAc	358	440	352	451	365	507	360	513
ACN	358	445	352	453	368	542	362	526
MeOH	355	450	354	462	368	555	365	550

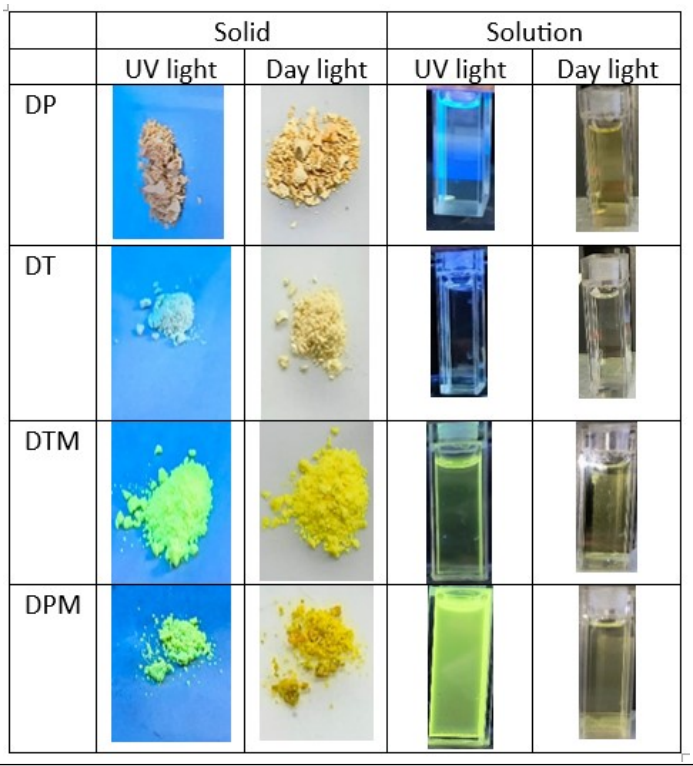


Fig. S14: Photos of the compounds in UV light and Daylight.

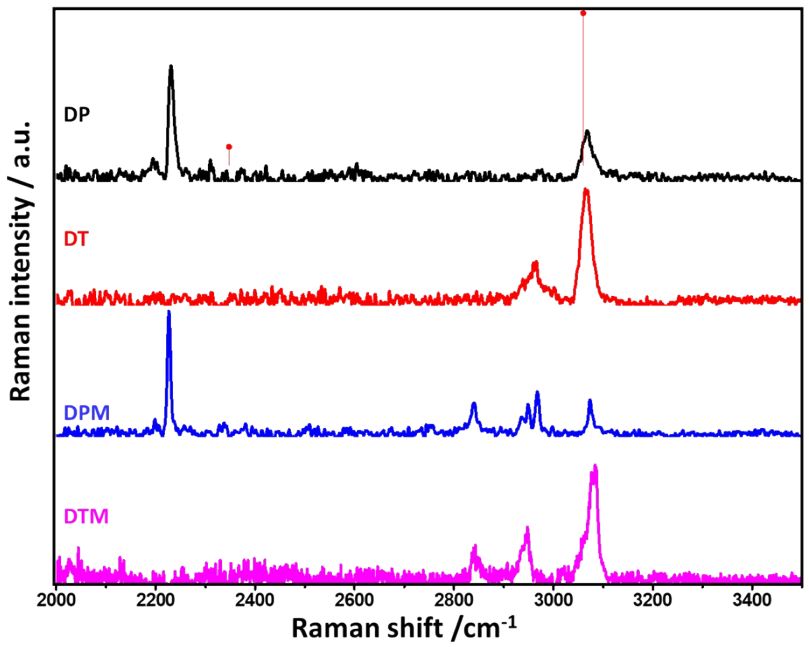


Fig. S15: Experimental and theoretical Raman spectra of DP, DT, DPM, and DTM.

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3 a) A Spek, J. Appl. Cryst., 2003, 36, 7-13. (b) Spek, A.; Utrecht University, Utrecht, The Netherlands 2008.

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