Electronic Supplementary Information for

Unprecedented transformation from cyclized zwitterionic oxazolidine derivatives to corresponding non-zwitterionic aromatic amides *via* Vilsmeier reagent in a one-pot reaction: optical property and crystallography

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Contents **Page No.**

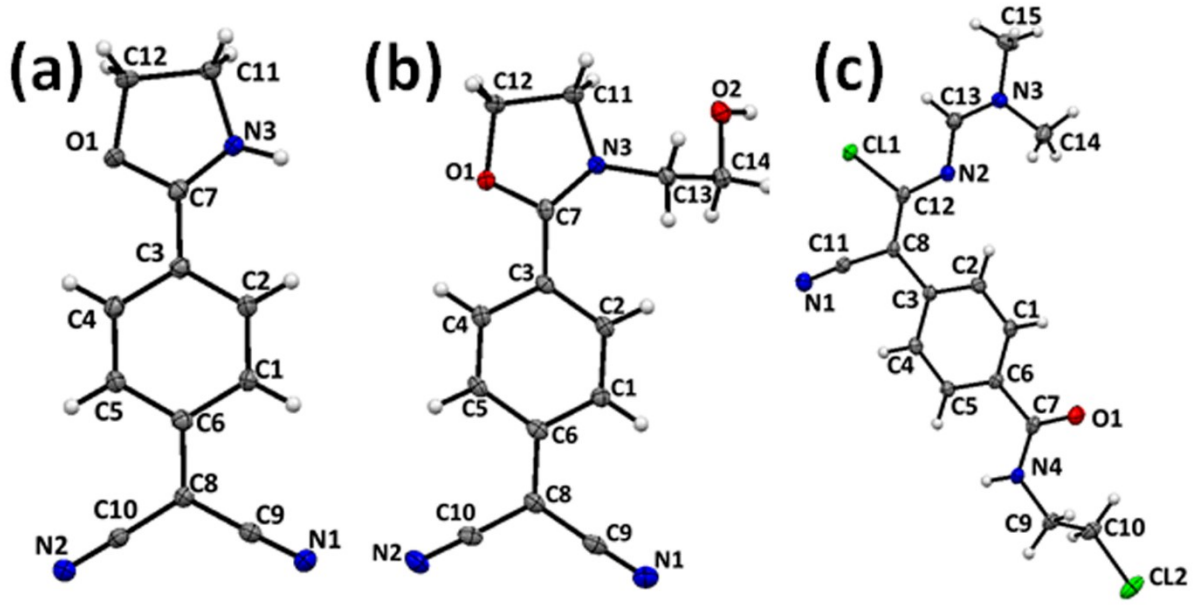

Fig. S1 Molecular Ortep diagrams of obtained compounds (a) **[1],** (b) **[2]** and (c) **[3]** indicating 50% thermal ellipsoids.

Table S1 Basic crystallographic data of obtained compounds **[1]**, **[2]** and **[3]**.

Compound	**[1]**	**[2]**	**[3]**
CCDC No.	**1914412**	**1901738**	**1935036**
Empirical formula	$C_{12}H_9N_3O$	$C_{14}H_{13}N_3O_2$	$C_{15}H_{16}N_4Cl_2O$
Formula weight	172.20	255.27	177.26
Temperature/K	293(2)	293(2)	293(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	P21/n	P21/c
a, b, c (Å)	6.3852(3),7.1557(6),11.6848(3)	6.15037(8),15.2072(2),13.27838(19)	12.5950(7),16.6928(8),7.6628(5)
α, β, γ (°)	93.970(5),93.665(3),111.132(6)	90.00,101.9346(13), 90.00	90.00,99.088(5),90.00
Volume/Å^3	494.52(5)	1215.08(3)	1590.85(15)
Z	2	4	4
Density (ρ) calculated (g/cm^3)	1.156	1.395	1.295
Absorption coefficient (μ, mm^{-1})	0.596	0.788	0.124
F(000)	182.0	536.0	654.0
Crystal size/mm^3	0.08 × 0.05 × 0.03	0.4 × 0.1 × 0.05	0.5 × 0.05 × 0.03
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.618 to 159.09	8.952 to 148.188	6.334 to 61.994
Index ranges	-8 ≤ h ≤ 8, -8 ≤ k ≤ 9, -14 ≤ l ≤ 8	-7 ≤ h ≤ 7, -18 ≤ k ≤ 13, -16 ≤ l ≤ 14	-16 ≤ h ≤ 16, -24 ≤ k ≤ 23, -10 ≤ l ≤ 11
Reflections collected	5730	6120	17497
Independent reflections	2078 [R_{int} = 0.0271,R_{sigma}= 0.0269]	2399 [R_{int} = 0.0107, R_{sigma} = 0.0090]	4485 [R_{int} = 0.0428, R_{sigma} = 0.0408]
Data/restraints/parameters	2078/0/65	2399/0/173	4485/0/201
Goodness-of-fit on F2	1.171	1.045	1.155
Final R indexes [I>=2σ (I)]	R1 = 0.1276, wR2 = 0.3834	R1 = 0.0332, wR2 = 0.0851	R1 = 0.0527, wR2 = 0.1460
Final R indexes [all data]	R1 = 0.1314, wR2 = 0.3849	R1 = 0.0337, wR2 = 0.0855	R1 = 0.0717, wR2 = 0.1547
Largest diff. peak/hole /e Å^{-3}	1.04/-0.64	0.19/-0.29	0.58/-0.62

Table S2a Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **[1]**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
O1	9769(6)	8995(6)	1218(3)	18.6(8)
N3	10934(7)	9024(7)	3026(4)	16.6(9)
N2	-2938(7)	2624(7)	1045(4)	21.0(10)
N1	-1027(8)	2225(7)	4686(4)	22.3(11)
C7	9226(8)	8426(7)	2244(4)	14.4(10)
C4	5274(9)	6662(8)	1432(4)	16.9(11)
C9	-556(9)	2896(8)	3822(5)	17.7(11)
C3	6922(8)	7283(7)	2389(4)	15.4(10)
C8	64(9)	3684(8)	2774(4)	16.4(10)
C6	2358(8)	4952(8)	2644(4)	15.4(10)
C10	-1599(9)	3092(8)	1826(4)	17.0(11)
C2	6212(9)	6769(8)	3484(4)	17.6(11)
C5	3064(9)	5542(8)	1561(4)	17.1(11)
C1	4000(9)	5640(8)	3603(4)	16.3(10)
C11	13040(8)	10223(8)	2561(4)	16.4(10)
C12	12204(8)	10191(8)	1296(4)	17.4(11)

Table S2b Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **[1]**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
O1	13.4(18)	26(2)	13.9(18)	6.1(15)	1.2(13)	3.9(15)
N3	15(2)	21(2)	13(2)	3.4(16)	1.5(16)	5.2(17)
N2	14(2)	30(3)	16(2)	3.3(18)	-0.2(17)	4.5(18)
N1	17(2)	32(3)	15(2)	6.2(19)	3.2(17)	4.6(19)
C7	17(2)	15(2)	13(2)	4.5(18)	4.6(18)	8.1(19)
C4	20(3)	18(2)	13(2)	3.5(19)	2.0(19)	7(2)
C9	14(2)	18(2)	19(3)	1(2)	-2.4(19)	3.6(19)
C3	16(2)	14(2)	17(2)	3.0(18)	2.1(19)	6.2(19)
C8	15(2)	20(2)	14(2)	4.4(19)	1.8(18)	5(2)
C6	14(2)	16(2)	17(2)	2.3(19)	1.0(19)	6.2(19)
C10	16(2)	19(2)	16(3)	6.4(19)	6(2)	4(2)
C2	16(2)	20(3)	15(2)	2.3(19)	0.2(19)	5(2)
C5	16(2)	21(3)	14(2)	2.6(19)	-0.5(19)	7(2)
C1	17(2)	21(3)	11(2)	5.0(19)	3.2(18)	7(2)
C11	14(2)	16(2)	19(3)	2.9(19)	3.8(19)	5.0(19)
C12	12(2)	21(3)	18(3)	4(2)	3.8(19)	3.5(19)

Table S2c Bond Lengths for Compound **[1]**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C7	1.320(6)	C9	C8	1.404(7)
O1	C12	1.473(6)	C3	C2	1.414(7)
N3	C7	1.300(7)	C8	C6	1.443(7)
N3	C11	1.472(6)	C8	C10	1.412(7)
N2	C10	1.152(7)	C6	C5	1.412(7)
N1	C9	1.158(7)	C6	C1	1.414(7)
C7	C3	1.430(7)	C2	C1	1.373(7)
C4	C3	1.413(7)	C11	C12	1.535(7)
C4	C5	1.373(7)			

Table S2d Bond Angles for compound **[1]**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	O1	C12	108.9(4)	C9	C8	C10	117.8(5)
C7	N3	C11	111.9(4)	C10	C8	C6	120.8(5)
O1	C7	C3	119.0(4)	C5	C6	C8	121.8(5)
N3	C7	O1	113.5(4)	C5	C6	C1	117.3(5)
N3	C7	C3	127.5(5)	C1	C6	C8	121.0(5)
C5	C4	C3	120.8(5)	N2	C10	C8	179.2(6)
N1	C9	C8	178.3(6)	C1	C2	C3	120.7(5)
C4	C3	C7	120.5(5)	C4	C5	C6	121.5(5)
C4	C3	C2	118.0(5)	C2	C1	C6	121.6(5)
C2	C3	C7	121.5(5)	N3	C11	C12	101.2(4)
C9	C8	C6	121.3(5)	O1	C12	C11	104.5(4)

Table S2e Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Compound **[1]**.

Atom	x	y	z	U(eq)
H3	10844.24	8751.89	3730.74	20
H4	5692.59	7017.16	706.28	20
H2	7254.14	7199.99	4131.13	21
H5	2008.35	5162.42	919.57	20
H1	3570.71	5320.82	4332.36	20
H11A	14156.92	9600.3	2630.74	20
H11B	13667.46	11583.6	2939.61	20
H12A	12472.01	11545.19	1094.01	21
H12B	12957.75	9566.26	786.25	21

Table S3a Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **[2]**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
O1	706.9(12)	5716.7(5)	1053.3(6)	16.31(18)
O2	-1523.0(13)	5797.5(5)	4264.4(6)	18.64(19)
N3	1045.6(14)	5535.4(6)	2720.9(7)	13.5(2)
N2	11171.2(17)	8282.4(7)	580.0(8)	22.4(2)
N1	10930.7(17)	9053.9(7)	3779.1(8)	24.9(2)
C6	7444.1(17)	7603.8(7)	2112.5(8)	14.5(2)
C3	3702.8(17)	6504.4(7)	2057.3(8)	14.0(2)
C2	4508.8(17)	7041.9(7)	2916.2(8)	14.6(2)
C1	6325.1(18)	7575.3(7)	2942.9(8)	15.0(2)
C5	6586.1(18)	7076.8(7)	1242.6(8)	15.3(2)
C7	1830.6(17)	5921.1(7)	1987.9(8)	13.6(2)
C4	4760.8(18)	6549.2(7)	1212.9(8)	15.4(2)
C13	1969.8(18)	5517.6(7)	3832.4(8)	14.8(2)
C8	9363.2(18)	8153.2(7)	2151.4(9)	15.8(2)
C11	-962.5(18)	5018.5(8)	2284.4(8)	17.5(2)
C14	701.2(19)	6105.6(8)	4428.7(8)	17.5(2)
C10	10384.8(18)	8227.8(7)	1298.3(9)	17.2(2)
C12	-882.6(18)	5013.8(8)	1145.9(8)	17.5(2)
C9	10256.8(18)	8651.2(8)	3039.3(9)	18.1(2)

Table S3b Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **[2]**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
O1	16.4(4)	20.3(4)	12.6(4)	-0.7(3)	3.6(3)	-3.3(3)
O2	17.2(4)	21.6(4)	19.2(4)	-1.7(3)	8.7(3)	1.0(3)
N3	13.5(4)	14.7(4)	13.2(4)	-0.5(3)	4.3(3)	-1.8(3)
N2	19.6(5)	26.1(5)	23.5(5)	4.7(4)	8.7(4)	-1.8(4)
N1	21.7(5)	28.9(6)	24.2(5)	-1.4(4)	4.9(4)	-6.2(4)
C6	13.8(5)	12.8(5)	17.4(5)	4.3(4)	4.4(4)	3.1(4)
C3	13.5(5)	14.0(5)	15.0(5)	2.4(4)	4.3(4)	1.5(4)
C2	15.6(5)	16.0(5)	13.6(5)	2.1(4)	6.3(4)	1.7(4)
C1	16.0(5)	14.8(5)	14.5(5)	0.1(4)	3.6(4)	0.6(4)
C5	16.7(5)	16.4(5)	14.8(5)	2.6(4)	7.7(4)	2.1(4)
C7	14.1(5)	14.2(5)	13.2(5)	-0.4(4)	4.2(4)	3.6(4)
C4	17.2(5)	15.5(5)	13.9(5)	0.7(4)	4.3(4)	1.9(4)
C13	15.8(5)	16.7(5)	12.3(5)	2.2(4)	3.9(4)	-0.4(4)
C8	14.3(5)	16.7(5)	17.3(5)	2.6(4)	5.1(4)	0.3(4)
C11	16.4(5)	19.6(5)	17.0(5)	-2.1(4)	4.8(4)	-5.7(4)
C14	20.0(6)	18.6(5)	15.3(5)	-1.4(4)	6.5(4)	-2.3(4)
C10	13.6(5)	15.7(5)	22.0(6)	3.9(4)	3.1(4)	0.0(4)
C12	16.5(5)	18.8(5)	17.7(6)	-2.3(4)	4.9(4)	-4.6(4)
C9	13.4(5)	18.8(6)	23.0(6)	4.9(5)	5.6(4)	-0.5(4)

Table S3c Bond Lengths for Compound **[2]**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C7	1.3265(13)	C6	C8	1.4383(15)
O1	C12	1.4708(13)	C3	C2	1.4074(15)
O2	C14	1.4195(14)	C3	C7	1.4413(15)
N3	C7	1.3111(14)	C3	C4	1.4095(15)
N3	C13	1.4681(13)	C2	C1	1.3751(15)
N3	C11	1.4775(13)	C5	C4	1.3737(15)
N2	C10	1.1583(16)	C13	C14	1.5135(15)
N1	C9	1.1590(16)	C8	C10	1.4089(16)
C6	C1	1.4160(15)	C8	C9	1.4134(16)
C6	C5	1.4153(16)	C11	C12	1.5226(15)

Table S3d Bond Angles for compound **[2]**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	O1	C12	108.59(8)	O1	C7	C3	117.31(9)
C7	N3	C13	128.99(9)	N3	C7	O1	112.90(9)
C7	N3	C11	110.67(9)	N3	C7	C3	129.78(10)
C13	N3	C11	120.20(9)	C5	C4	C3	120.95(10)
C1	C6	C8	121.14(10)	N3	C13	C14	112.38(9)
C5	C6	C1	117.32(10)	C10	C8	C6	121.13(10)
C5	C6	C8	121.53(10)	C10	C8	C9	117.80(10)
C2	C3	C7	123.51(10)	C9	C8	C6	121.05(10)
C2	C3	C4	118.25(10)	N3	C11	C12	101.31(8)
C4	C3	C7	118.23(10)	O2	C14	C13	108.02(9)
C1	C2	C3	120.77(10)	N2	C10	C8	178.16(12)
C2	C1	C6	121.40(10)	O1	C12	C11	103.77(8)
C4	C5	C6	121.24(10)	N1	C9	C8	177.87(12)

Table S3e Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Compound **[2]**.

Atom	x	y	z	U(eq)
H2	-2241.01	6110.75	4578.79	28
H2A	3804.61	7036.24	3472.15	18
H1	6829.41	7924.74	3518.63	18
H5	7270.82	7087.86	680.4	18
H4	4215.28	6216.85	627.24	18
H13A	3509.59	5705.27	3957.19	18
H13B	1936.42	4918.82	4080.48	18
H11A	-2298.58	5302.58	2403.75	21
H11B	-875.26	4427.68	2565.14	21
H14A	1375.67	6087.27	5156.47	21
H14B	729.98	6708.38	4192.93	21
H12A	-368.96	4450.55	943.54	21
H12B	-2334.76	5138.13	723.43	21

Table S4a Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **[3]**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Cl1	4556.9(4)	1140.4(3)	4484.9(8)	21.31(15)
Cl2	10226.1(6)	7633.1(4)	4155.7(9)	31.61(18)
C3	6664.3(19)	663.2(14)	3599(3)	19.0(4)
N4	6524.5(15)	1444.6(12)	3647(3)	17.1(4)
O5	9114.1(15)	5049.3(11)	2349(3)	27.6(4)
N6	7570.2(16)	349.2(12)	3267(3)	19.1(4)
C7	7728(2)	-515.6(15)	3185(4)	27.0(5)
C8	6526.0(19)	4671.8(14)	3837(3)	19.1(5)
N9	3632.9(18)	3084.4(13)	4984(3)	25.6(5)
C10	8604(2)	6640.8(15)	2821(3)	21.3(5)
C11	4419.1(19)	2830.5(14)	4607(3)	18.4(4)
C12	7143.3(19)	3115.6(14)	3185(3)	20.2(5)
C13	6165.6(18)	3238.4(14)	3821(3)	15.6(4)
C14	5626.9(18)	1773.9(14)	4041(3)	16.8(4)
C15	9412(2)	6783.9(16)	4471(3)	24.2(5)
C16	8246.7(19)	5201.7(14)	2850(3)	18.3(4)
N17	7930.3(16)	5959.3(12)	3077(3)	20.4(4)
C18	7498.3(18)	4546.2(14)	3206(3)	16.2(4)
C19	5878.5(19)	4033.5(14)	4135(3)	19.7(5)
C20	5431.5(18)	2582.1(14)	4142(3)	16.1(4)
C21	7788.2(19)	3758.1(14)	2892(3)	20.2(5)
C22	8465(2)	849.9(17)	2939(4)	30.1(6)

Table S4b Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **[3]**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Cl1	15.9(3)	18.3(3)	31.0(3)	2.1(2)	7.8(2)	-3.1(2)
Cl2	34.3(4)	33.0(4)	28.8(3)	-4.5(3)	8.9(3)	-19.4(3)
C3	18.6(11)	19.6(11)	19.6(11)	0.4(9)	5.2(8)	-1.2(9)
N4	14.6(9)	17.8(9)	19.8(9)	-0.8(7)	5.5(7)	-0.5(7)
O5	20.2(9)	23.5(9)	43.2(11)	-4.0(8)	18.2(8)	-3.0(7)
N6	18.1(10)	15.8(9)	24.3(10)	-1.1(8)	6.3(8)	0.2(7)
C7	32.7(14)	18.9(11)	31.6(14)	0.6(10)	11.7(11)	5.6(10)
C8	15.2(10)	16.4(10)	26.9(12)	-1.1(9)	6.9(9)	0.5(8)
N9	19.1(10)	23.9(11)	36.5(12)	2.8(9)	12.1(9)	1.0(8)
C10	19.2(11)	18.4(11)	26.8(12)	2.2(9)	5.6(9)	-3.8(9)
C11	16.2(11)	16.2(10)	23.4(11)	0.6(9)	4.7(8)	-2.4(8)
C12	17.8(11)	16.2(10)	28.5(12)	-1.1(9)	9.2(9)	0.9(8)
C13	13.2(10)	17.1(10)	16.8(10)	0.8(8)	2.9(8)	-1.0(8)
C14	13.3(10)	20.5(11)	16.7(10)	1.7(8)	2.9(8)	-2.9(8)
C15	26.1(13)	22.2(12)	25.5(12)	-2.3(10)	7.8(10)	-9.5(10)
C16	13.9(10)	21.0(11)	20.2(11)	-0.1(9)	3.7(8)	-3.0(8)
N17	12.5(9)	17.2(9)	33.0(11)	1.3(8)	7.8(8)	-2.0(7)
C18	13.8(10)	16.3(10)	18.8(10)	0.8(8)	3.4(8)	-1.9(8)
C19	15.3(10)	19.6(11)	26.3(12)	-0.7(9)	9.8(9)	1.4(8)
C20	10.6(9)	20.2(11)	17.9(10)	0.5(8)	3.7(8)	-1.1(8)
C21	13.8(10)	20.4(11)	28.4(12)	-1.3(9)	9.8(9)	-0.5(8)
C22	20.2(12)	27.7(13)	45.2(17)	-8.8(12)	13.2(11)	-5.3(10)

Table S4c Bond Lengths for Compound **[3]**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C14	1.788(2)	C10	C15	1.511(4)
Cl2	C15	1.788(3)	C10	N17	1.451(3)
C3	N4	1.317(3)	C11	C20	1.438(3)
C3	N6	1.317(3)	C12	C13	1.409(3)
N4	C14	1.334(3)	C12	C21	1.385(3)
O5	C16	1.240(3)	C13	C19	1.406(3)
N6	C7	1.460(3)	C13	C20	1.479(3)
N6	C22	1.456(3)	C14	C20	1.376(3)
C8	C18	1.402(3)	C16	N17	1.345(3)
C8	C19	1.382(3)	C16	C18	1.497(3)
N9	C11	1.155(3)	C18	C21	1.396(3)

Table S4d Bond Angles for compound **[3]**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N6	C3	N4	121.6(2)	C20	C14	Cl1	114.98(17)
C3	N4	C14	122.4(2)	C10	C15	Cl2	109.67(18)
C3	N6	C7	122.0(2)	O5	C16	N17	121.7(2)
C3	N6	C22	121.5(2)	O5	C16	C18	121.1(2)
C22	N6	C7	116.5(2)	N17	C16	C18	117.1(2)
C19	C8	C18	120.8(2)	C16	N17	C10	121.9(2)
N17	C10	C15	110.0(2)	C8	C18	C16	124.3(2)
N9	C11	C20	175.2(3)	C21	C18	C8	117.8(2)
C21	C12	C13	120.7(2)	C21	C18	C16	117.9(2)
C12	C13	C20	123.6(2)	C8	C19	C13	121.7(2)
C19	C13	C12	117.3(2)	C11	C20	C13	115.4(2)
C19	C13	C20	119.1(2)	C14	C20	C11	118.1(2)
N4	C14	Cl1	119.39(18)	C14	C20	C13	126.5(2)
N4	C14	C20	125.6(2)	C12	C21	C18	121.7(2)

Table S4e Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **[3]**.

Atom	x	y	z	U(eq)
H3	6109.95	325.48	3804.6	23
H7A	7087.89	-785.45	3401.17	41
H7B	8320.98	-671.18	4065.02	41
H7C	7877.26	-658.88	2035.13	41
H8	6313.92	5190.74	4058.84	23
H10A	8160.7	7113.67	2554.81	26
H10B	8978.72	6539.77	1829.94	26
H12	7357.84	2597.66	2960.21	24
H15A	9863.08	6314.37	4728.62	29
H15B	9038.26	6878	5466.61	29
H17	7311.03	6041.98	3381.95	25
H19	5236.88	4132.38	4553.17	24
H21	8431	3662.1	2475.16	24
H22A	8237.83	1184.93	1930.8	45
H22B	9048.92	516.1	2715.51	45
H22C	8696.42	1179	3955.44	45

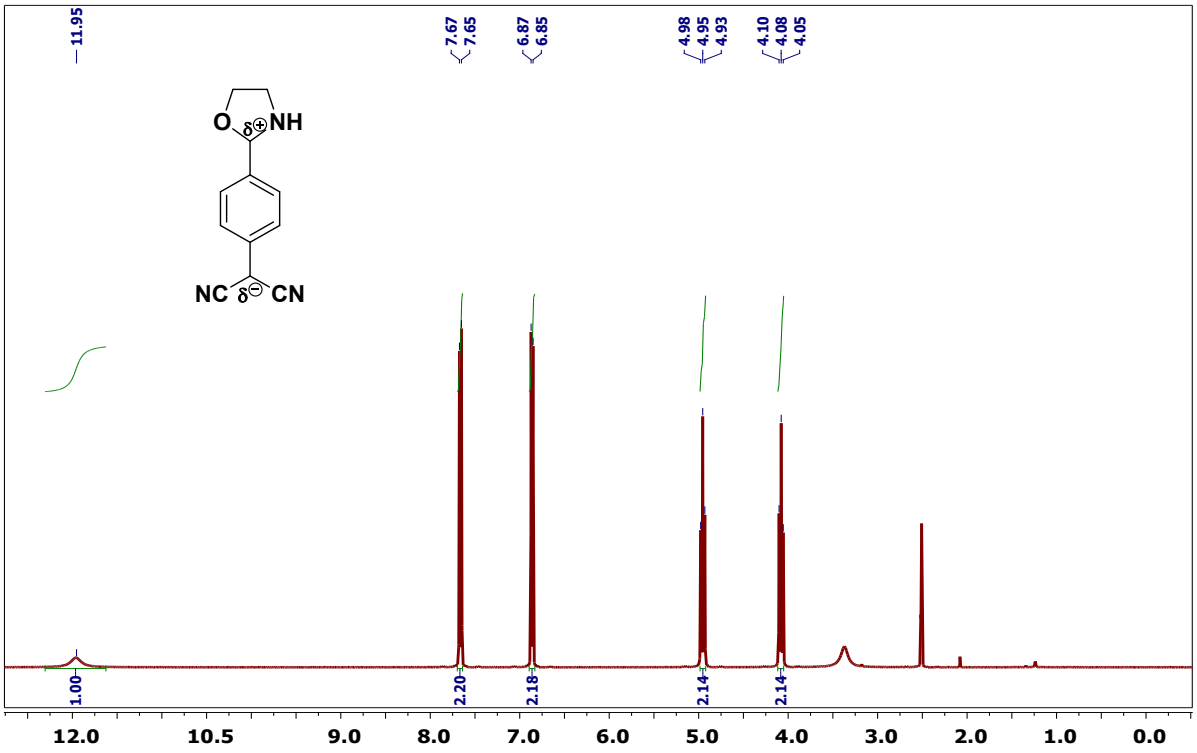

Fig. S2a ^{1}H NMR of compound **[1]**.

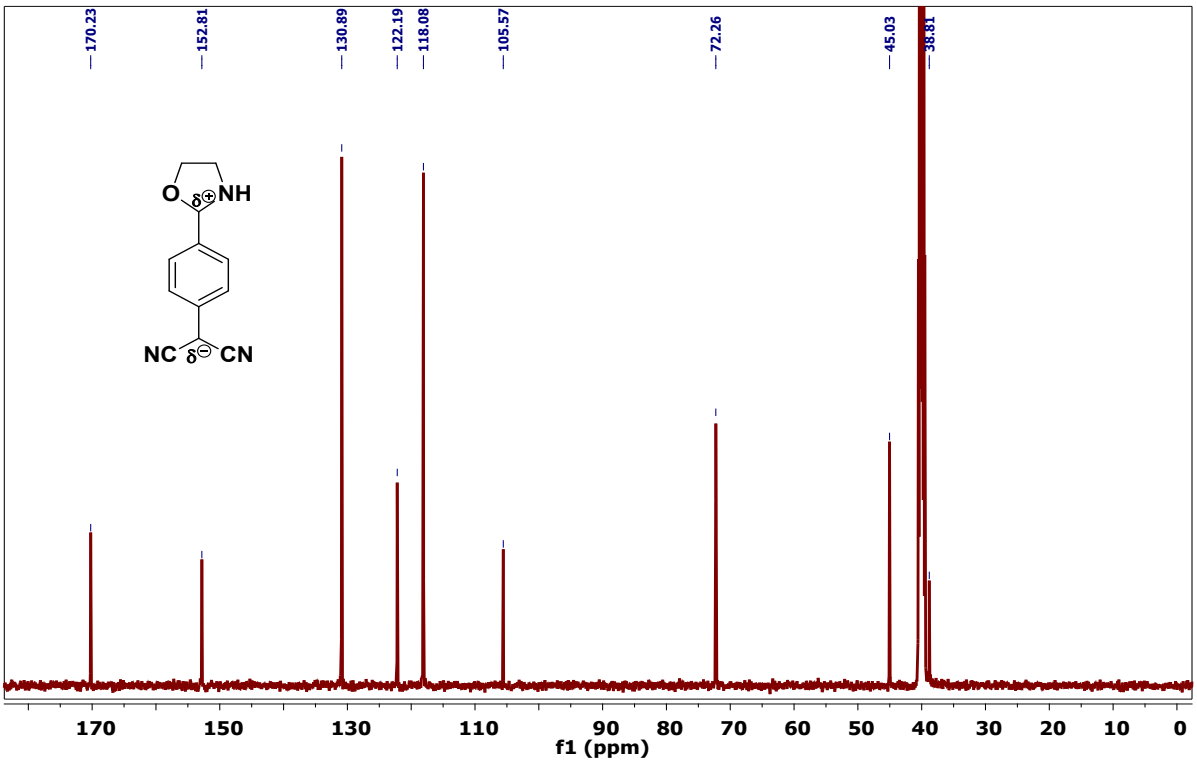

Fig. S2b ^{13}C NMR of compound **[1]**.

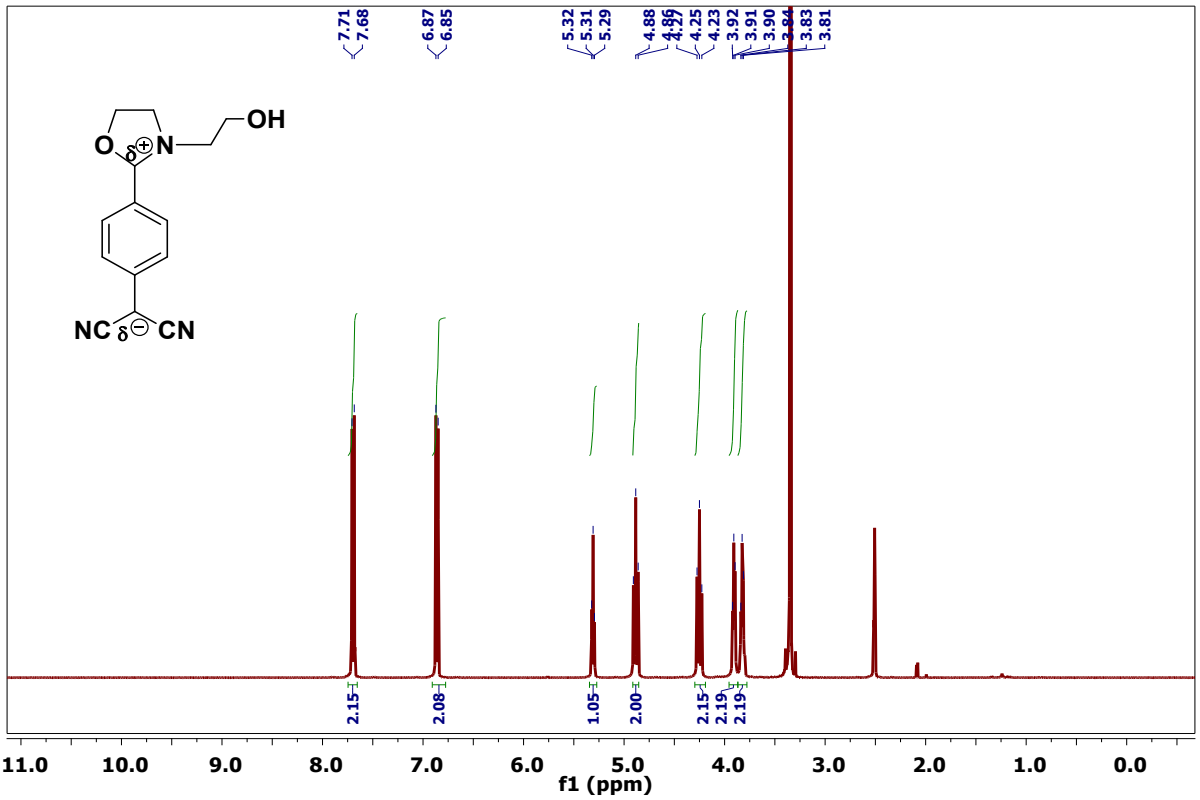

Fig. S3a ^{1}H NMR of compound **[2]**.

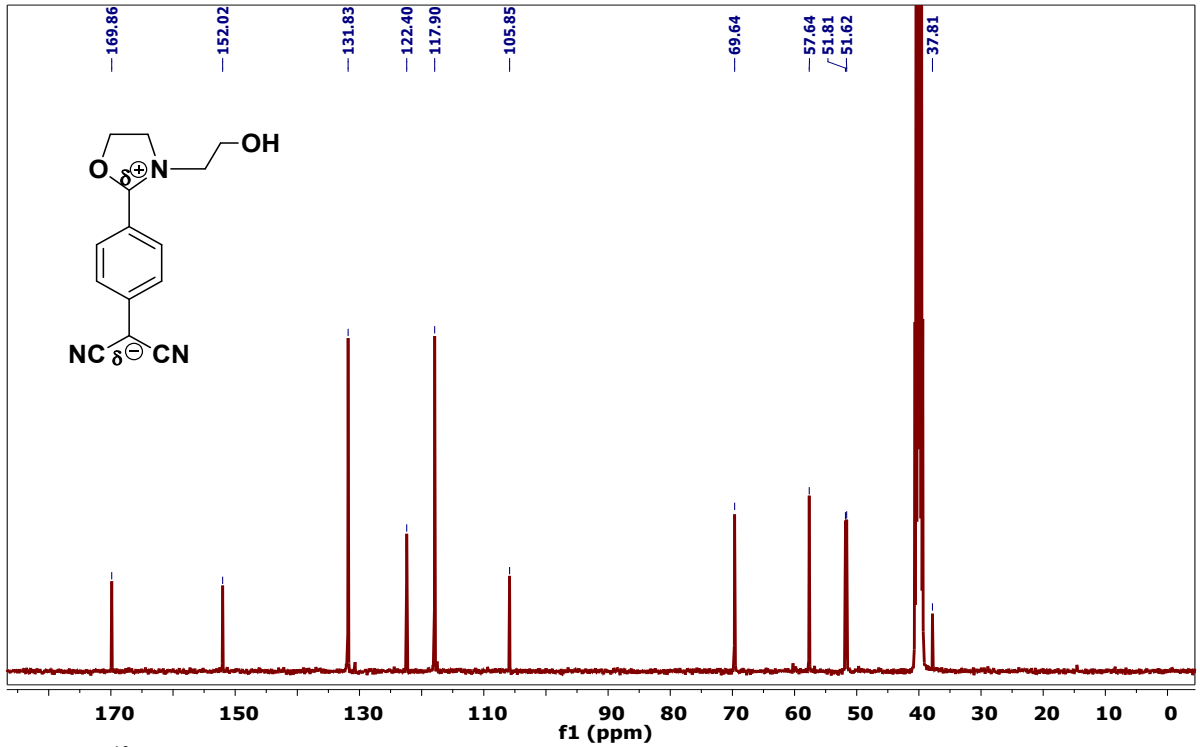

Fig. S3b ^{13}C NMR of compound **[2]**.

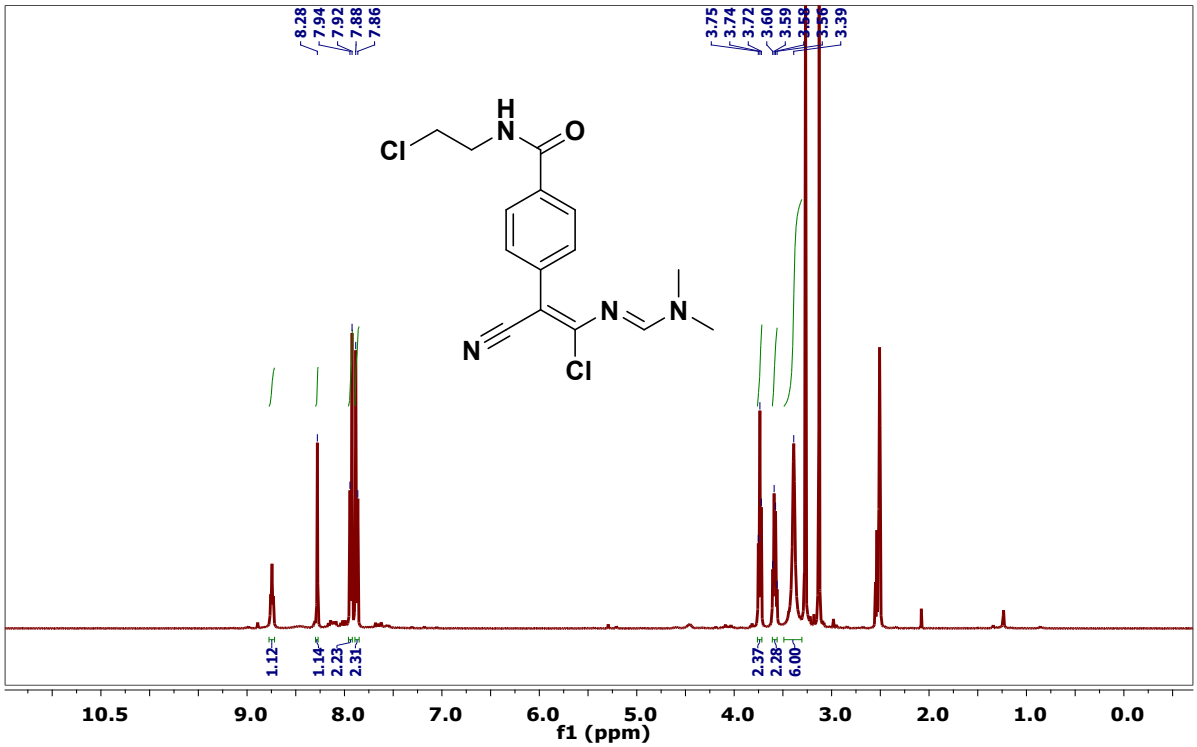

Fig. S4a ^{1}H NMR of compound **[3]**.

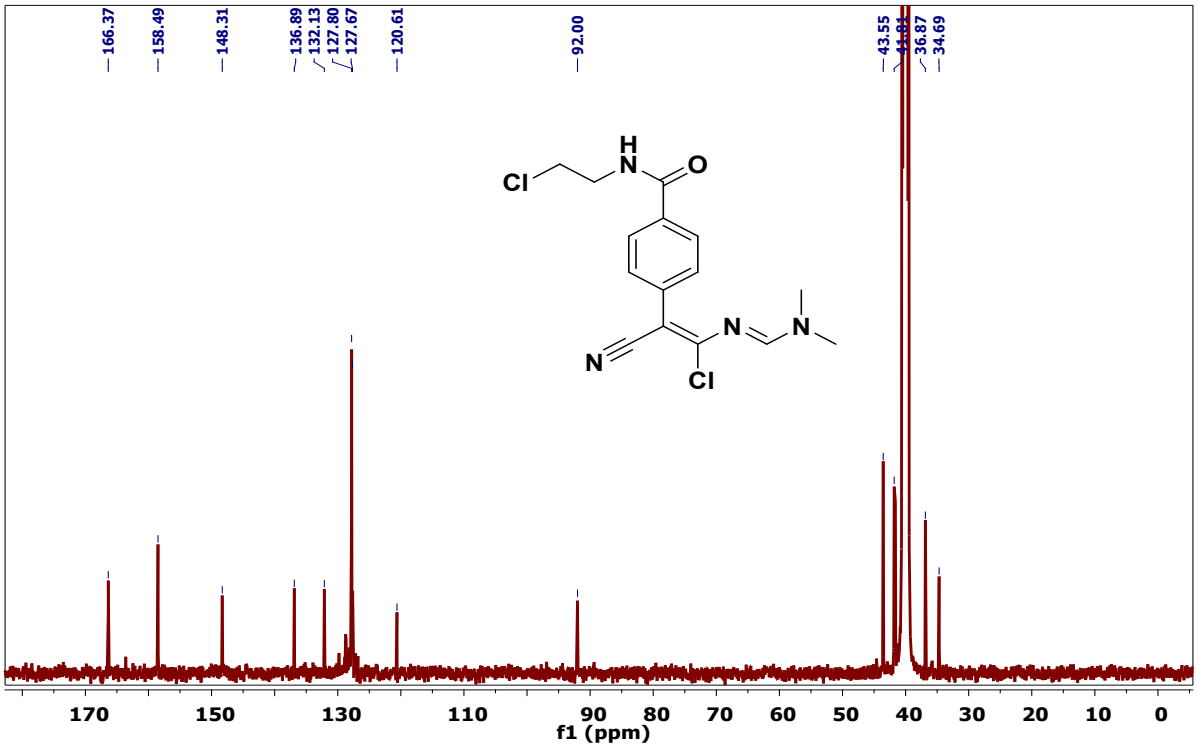

Fig. S4b ^{13}C NMR of compound **[3]**.

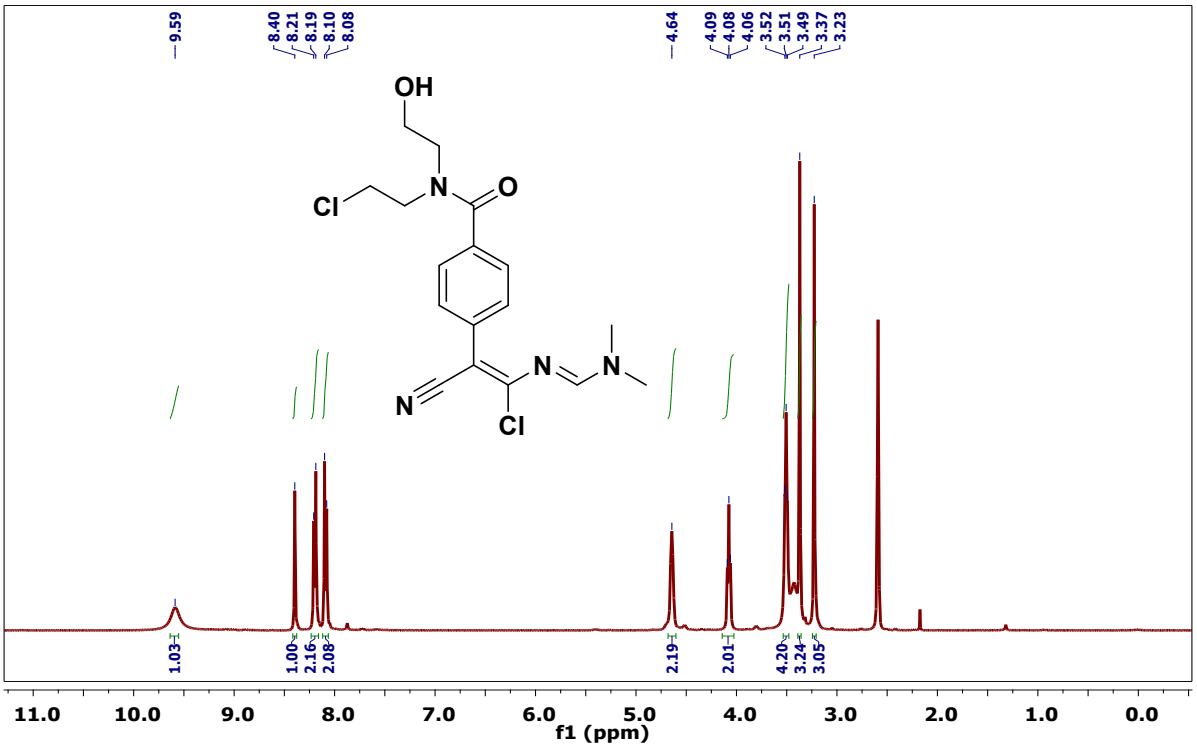

Fig. S5a ^{1}H NMR of compound **[4]**.

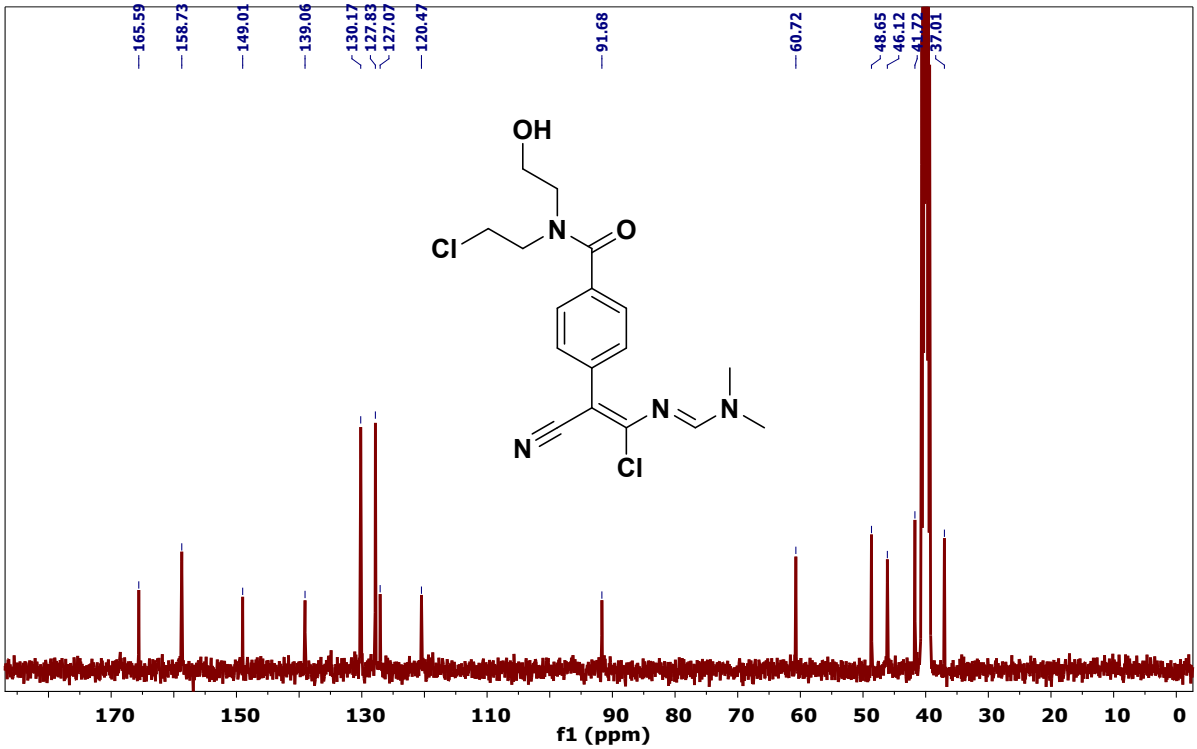

Fig. S5b ^{13}C NMR of compound **[4]**.

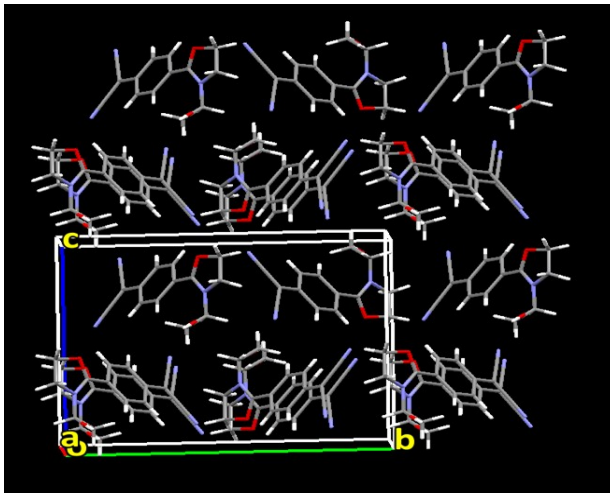

Fig. S6 Molecular dipoles of **[2]** arranged in head-tail fashion, zig-zag orientation along the axis *ob*; as arrays along *oa*.

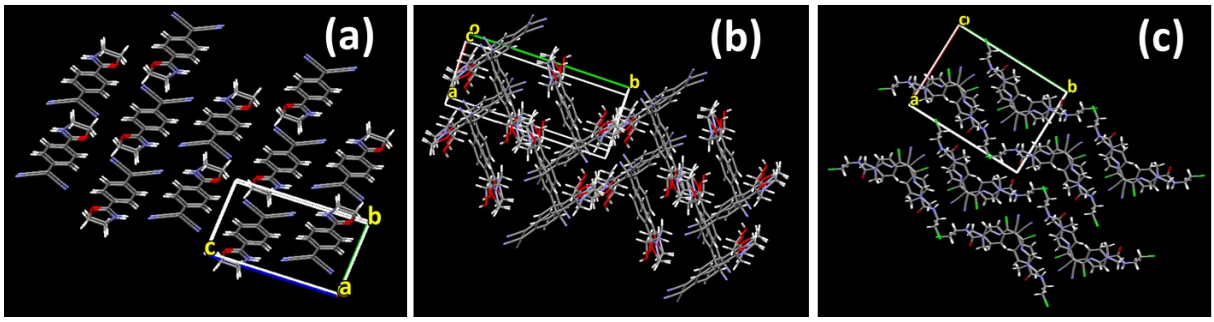

Fig. S7 Supramolecular assemblies in **[1]**, **[2]** and **[3]**.

Table S5 Absorption, emission wavelengths, corresponding stokes shift and quantum yields of compound **[1]** in various solvents.

S.No.	Solvent/State	λ_{abs}	λ_{emi}	Stokes shift (nm)	Quantum yield (%)
1	MeCN	433	480	47	0.04
2	MeOH	427	470	43	0.04
3	EtOH	420	466	46	0.18
4	IPA	435	470	35	0.21
5	THF	455	488	33	0.05
6	DMF	428	468	40	0.20
7	DMSO	429	475	46	0.35
8	Solid	450	498	48	3.8

Table S6 Absorption, emission wavelengths, corresponding stokes shift and quantum yields of compound **[3]** in different solvents.

S.No.	Solvent/State	λ_{abs}	λ_{emi}	Stokes shift (nm)	Quantum yield (%)
1	MeCN	355	425, 403	70, 48	0.2
2	MeOH	354	427, 404	73, 50	0.58
3	EtOH	356	430, 405	74, 49	1.85
4	IPA	355	427, 401	72, 46	0.9
5	THF	355	430, 405	75, 50	0.12
6	DMF	360	430, 409	70, 49	1.53
7	DMSO	363	435, 410	72, 47	0.1
8	Solid	425	508	83	0.5

Table S7 Absorption, emission wavelengths, corresponding stokes shift and quantum yields of compound **[4]** in varied solvents.

S.No.	Solvent/State	λ_{abs}	λ_{emi}	Stokes shift (nm)	Quantum yield (%)
1	MeCN	362	432, 405	70, 43	0.05
2	MeOH	360	427, 405	67, 45	0.25
3	EtOH	360	428, 403	68, 43	1.89
4	IPA	360	428, 403	68, 43	0.9
5	THF	360	430, 405	70, 45	0.09
6	DMF	367	432, 408	65, 41	1.22
7	DMSO	368	437, 415	69, 47	0.88
8	Solid	405	500	95	0.45

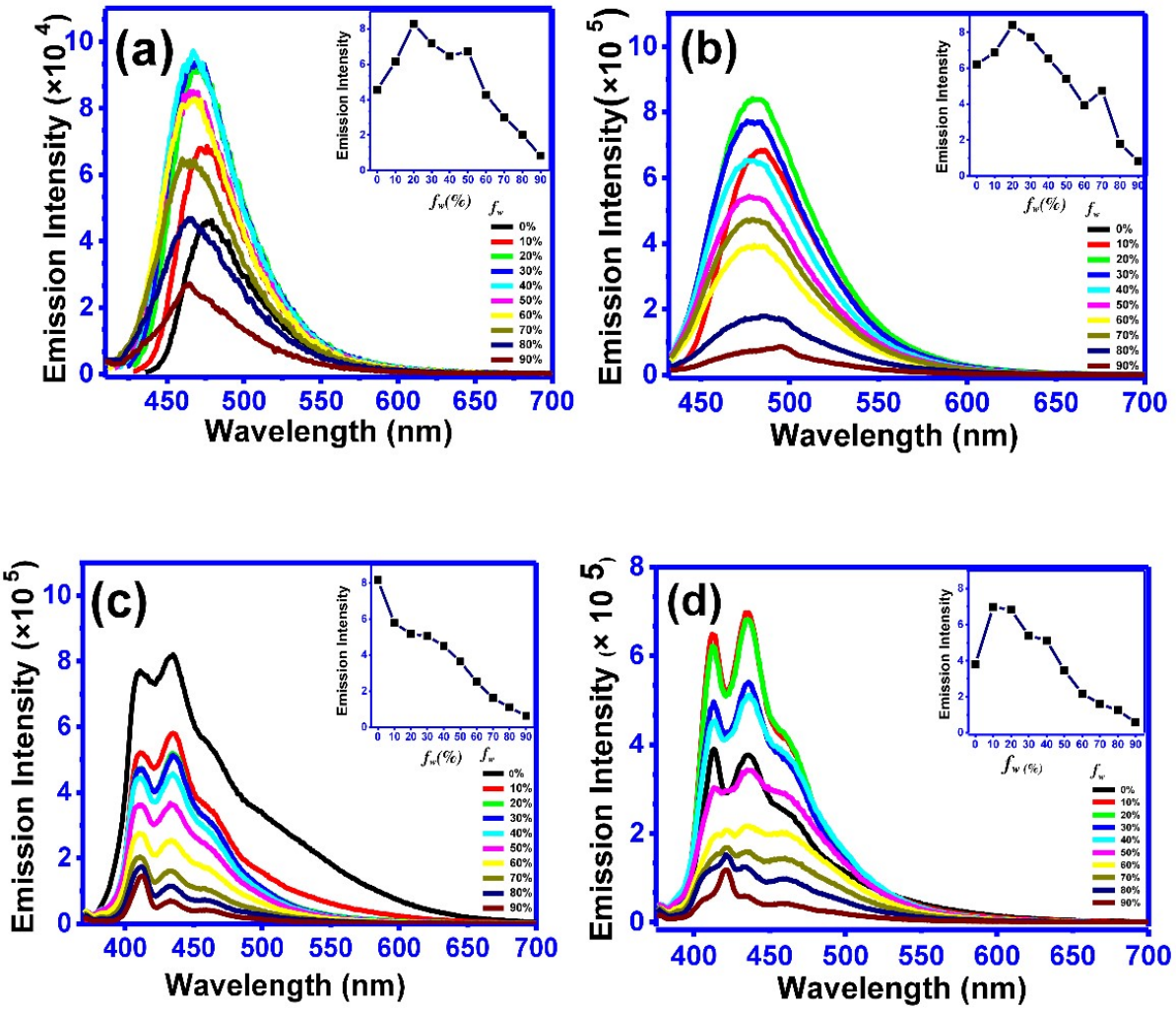

Fig. S8 Decreased emission intensity on the addition of 0 to 90% water fraction to the 10 ppm DMSO solutions of compounds (a) **[1]**, (b) **[2]**, (c) **[3]** and (d) **[4]**; indicate aggregation quenching property.

Table S8 X and Y coordinate values from the chromaticity output diagrams of all the compounds considered in this study.

Compound	X Coordinate	Y Coordinate
[1]	0.06	0.61
[2]	0.37	0.56
[3]	0.35	0.54
[4]	0.34	0.56

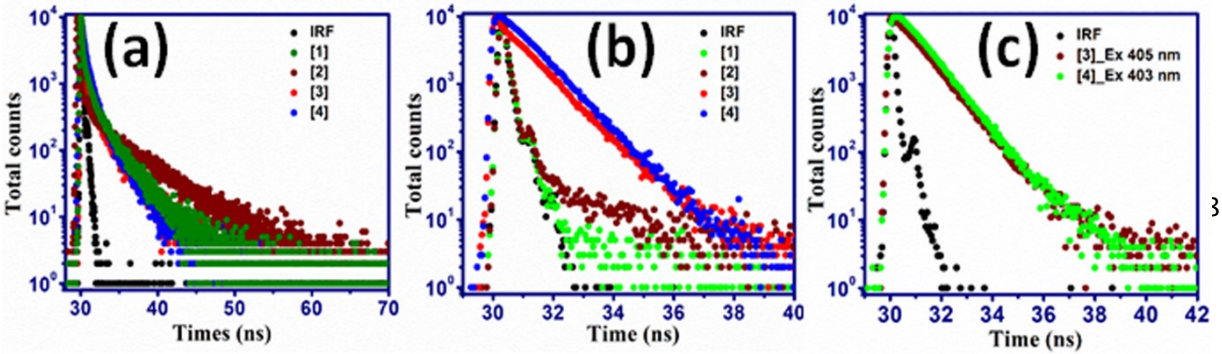

Fig. S9 Fluorescence lifetime decay of compounds **[1]** to **[4]** in (a) solids (b) solutions and (c) represents the decay of **[3]** and **[4]** solutions (in ethanol) with λ_{em} of 405 nm and 403 nm.

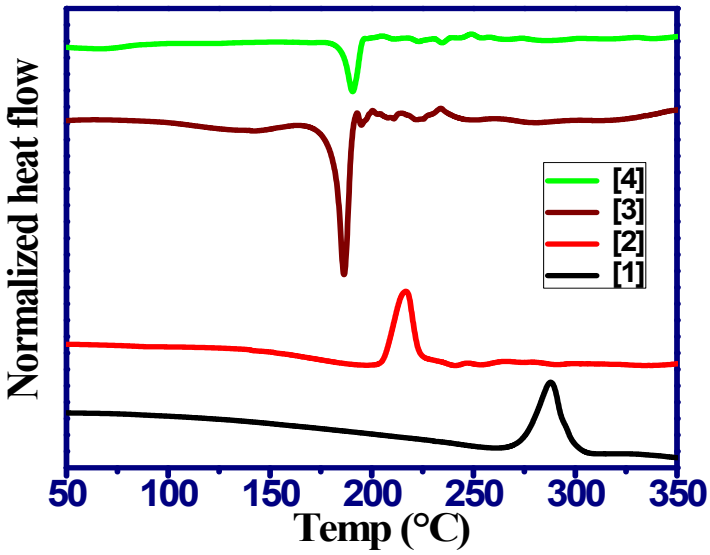

Fig. S10 DSC plots of all four pure solids **[1]**, **[2]**, **[3]** and **[4]**.