Supporting Information

$SnCl_2$-Catalyzed synthesis of dihydro-5*H*-benzo[*f*]pyrazolo[3,4-*b*]quinoline and dihydroindeno[2,1-*b*]pyrazolo[4,3-*e*]pyridine with high fluorescence and their Photophysical properties

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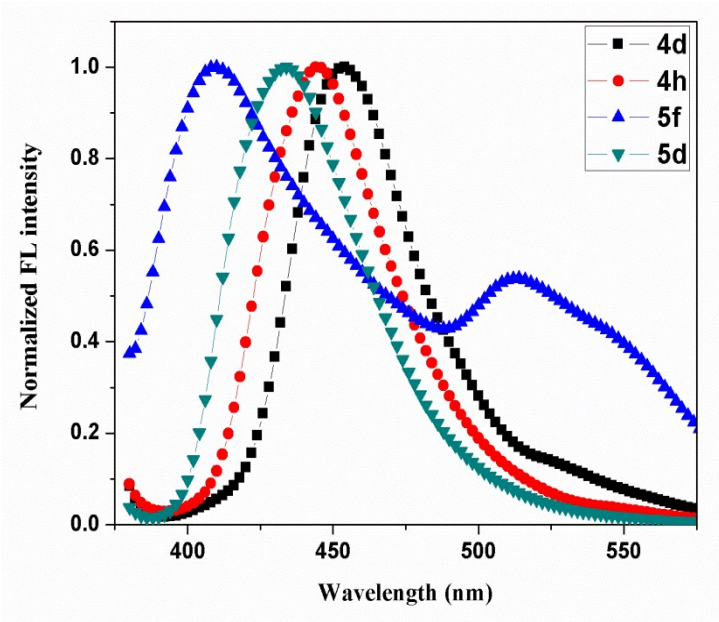
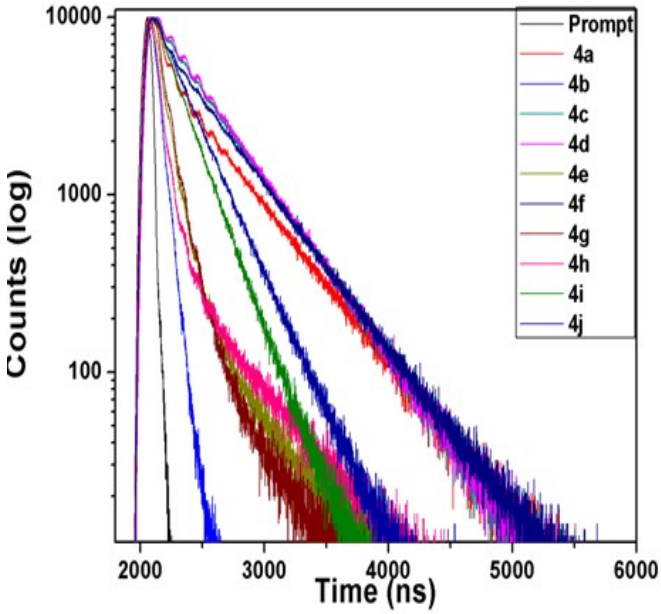
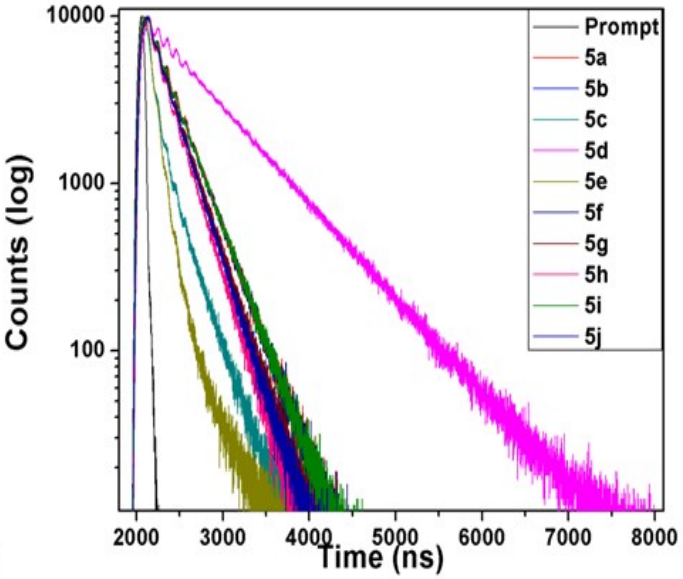
S1 Figure S1 The selected solid state spectra of compounds **4d, 4h, 5d** and **5f.**



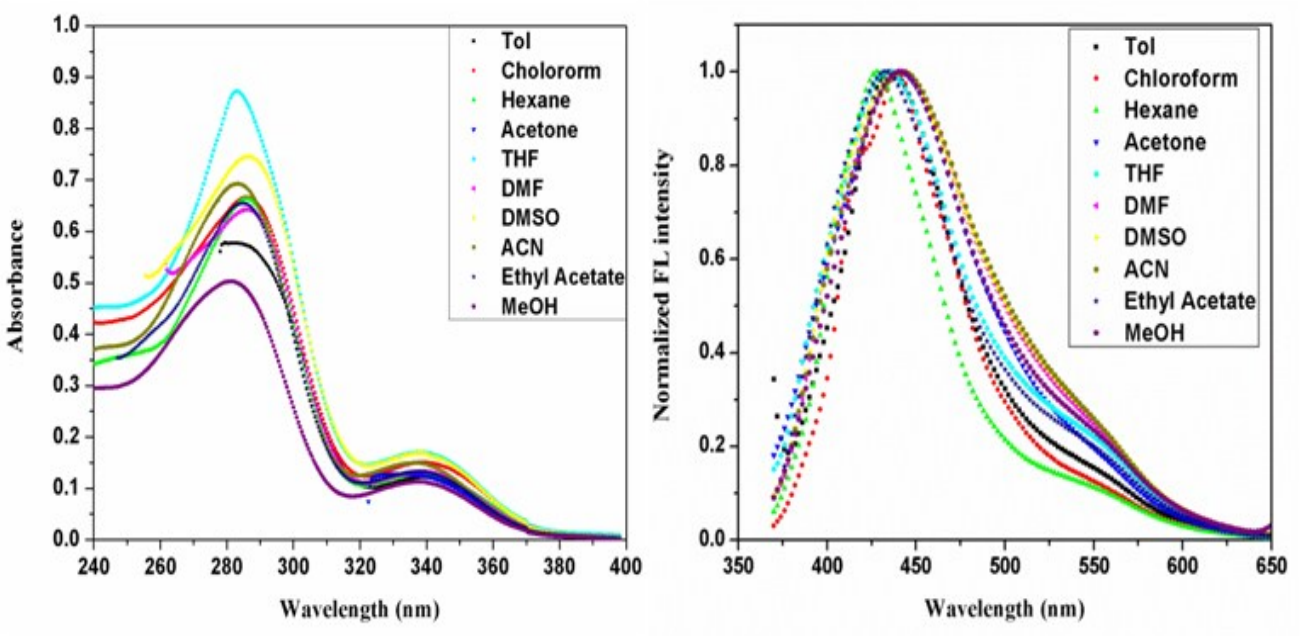
S1 Figure S2 Time-resolved lifetime decay spectra of compound **4a-j (left)** and **5a-j (right)** in chloroform solvents with exciting at 320 nm.





S1 Figure S3 Absorption and Emission spectra of compounds **4a-e, 5a-b** and **5e** in different solvents

4a



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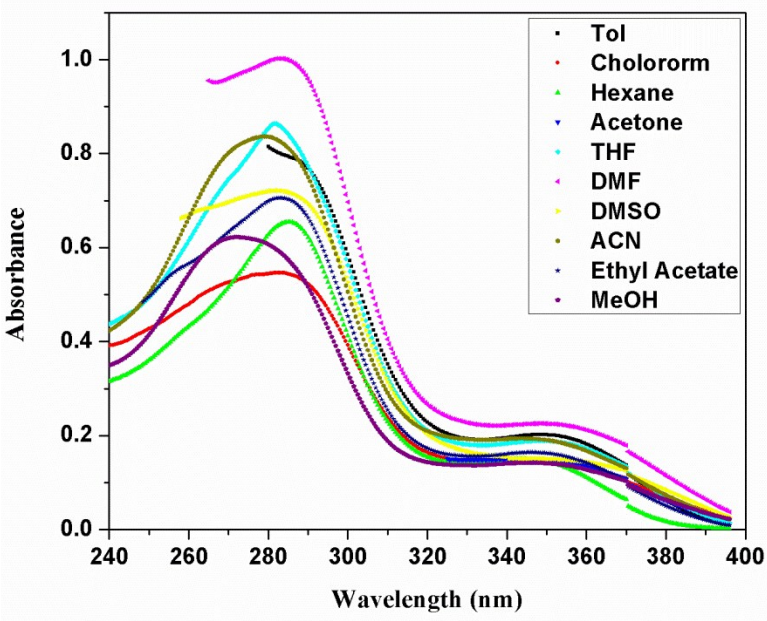

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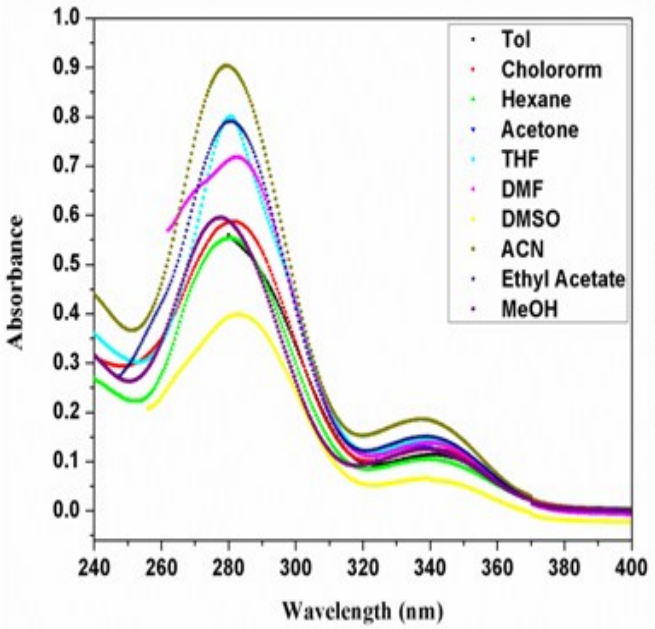
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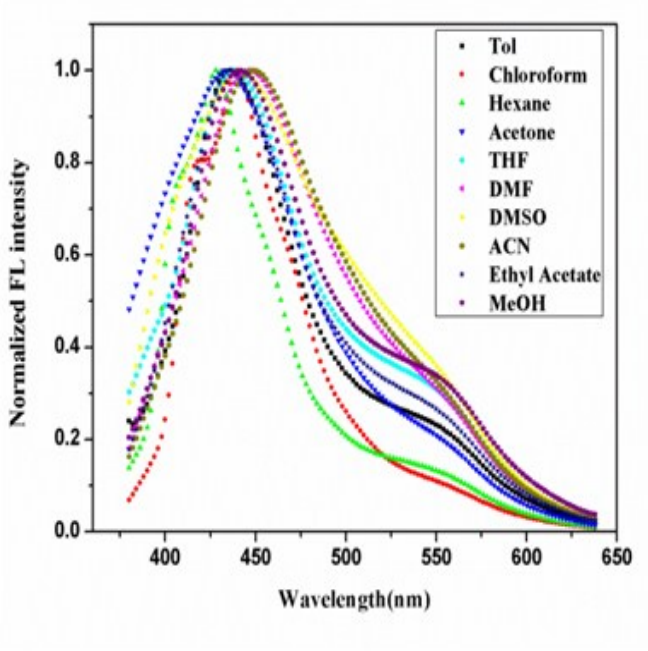
Wavelength (nm)
Tol
Cholororm
Hexane
Acetone
THF
DMF
DMSO
ACN
Ethyl Acetate
MeOH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Wavelength(nm)
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Acetone
THF
DMF
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ACN
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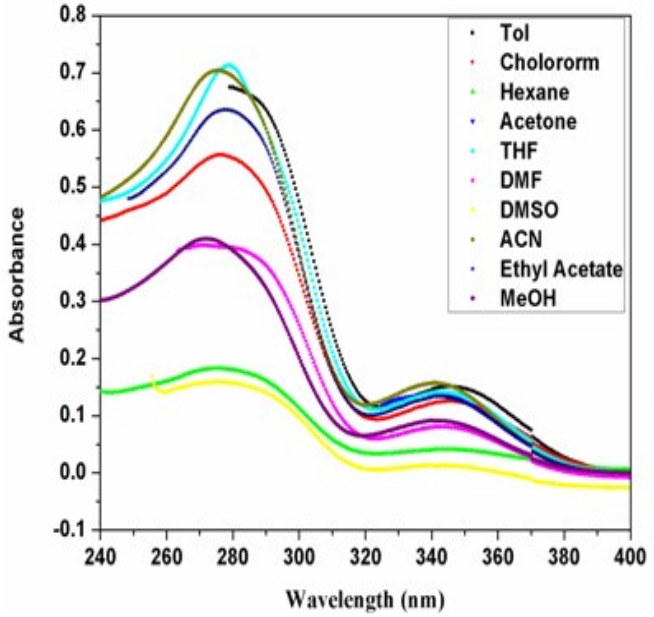
MeOH

4d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Wavelength (nm)
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Cholororm
Hexane
Acetone
THF
DMF
DMSO
ACN
Ethyl Acetate
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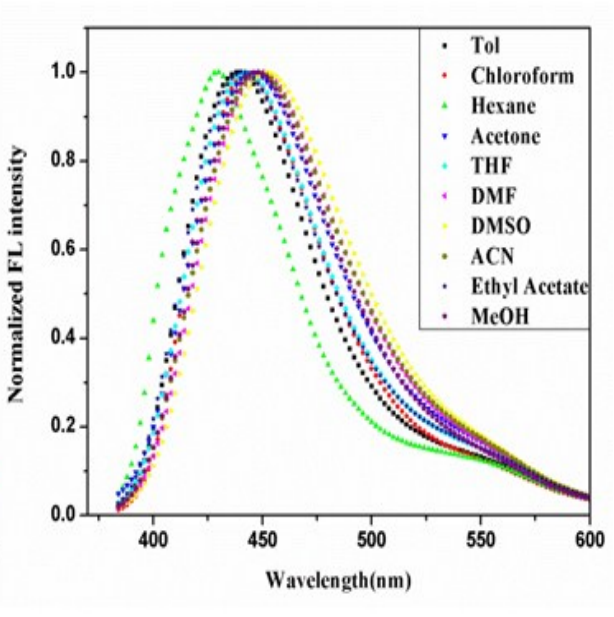
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Wavelength(nm)
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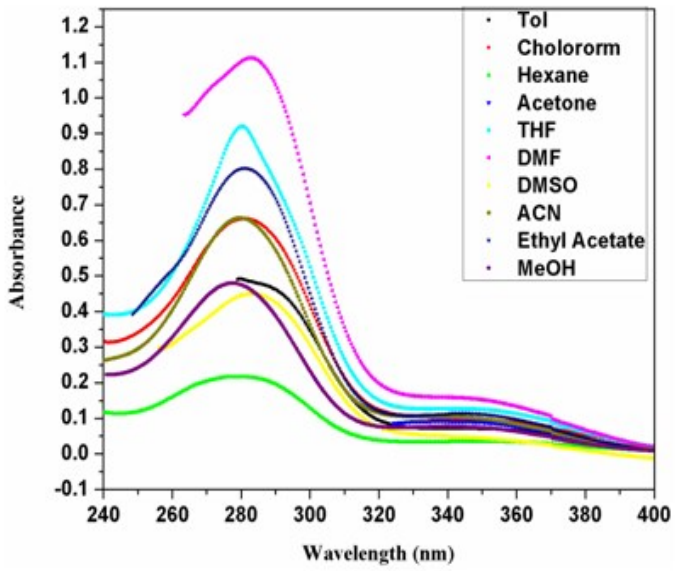
Chloroform
Hexane
Acetone
THF
DMF
DMSO
ACN
Ethyl Acetate
MeOH

4e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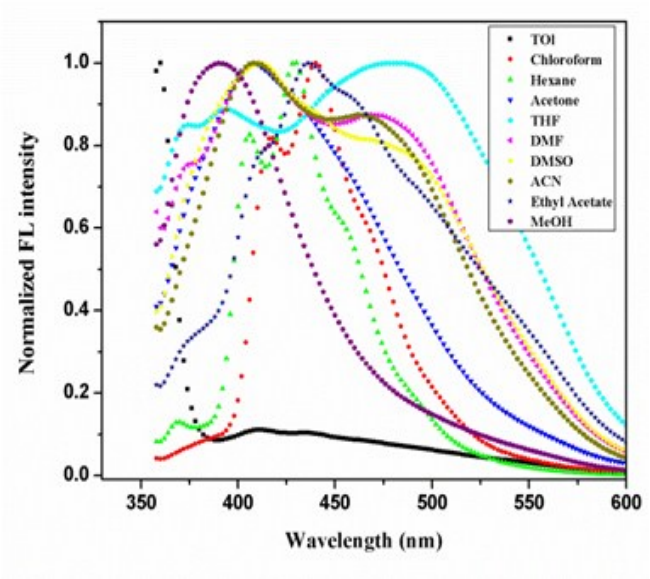
Cholororm
Hexane
Acetone
THF
DMF
DMSO
ACN
Ethyl Acetate
MeOH
Absorbance
Wavelength (nm)


TOl
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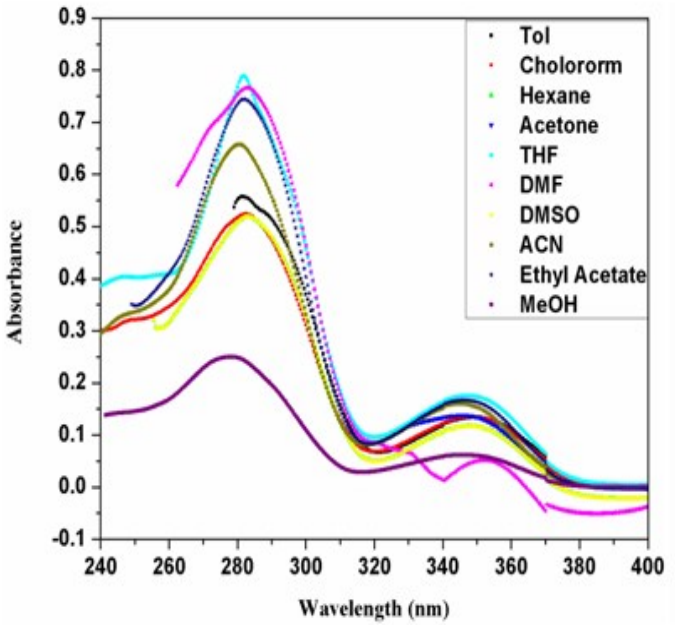
Hexane
Acetone
THF
DMF
DMSO
ACN
Ethyl Acetate
MeOH
Normalized FL intensity
Wavelength (nm)

5a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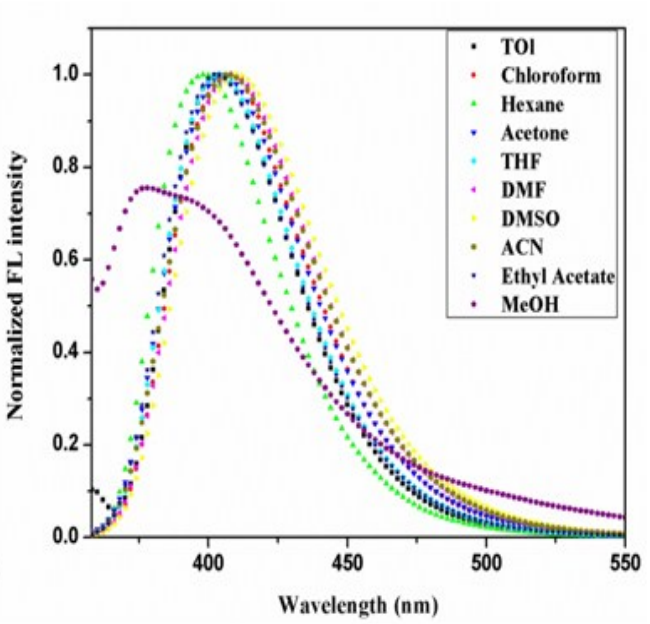
Absorbance
Wavelength (nm)


TOl
Chloroform
Hexane
Acetone
THF
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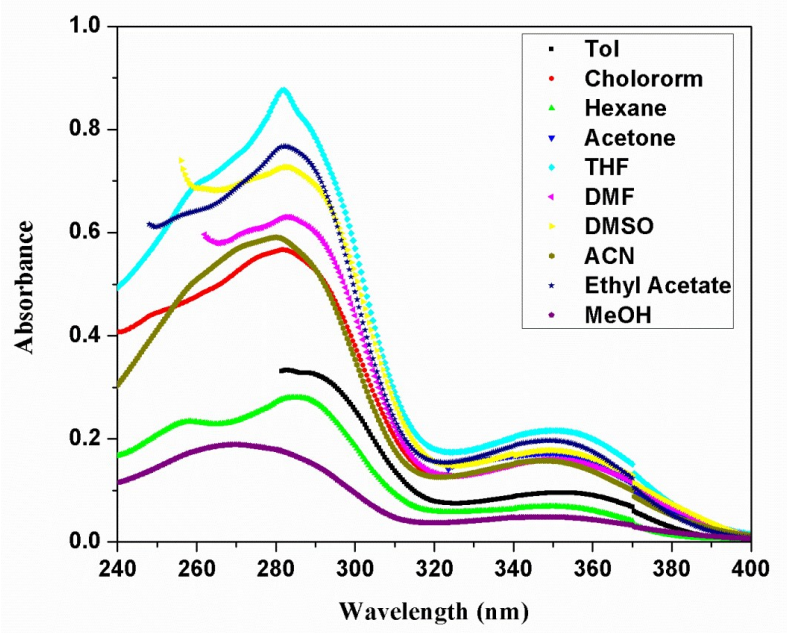
DMSO
ACN
Ethyl Acetate
MeOH
Normalized FL intensity
Wavelength (nm)

5b


Absorbance
Wavelength (nm)
Tol
Cholororm
Hexane
Acetone
THF
DMF
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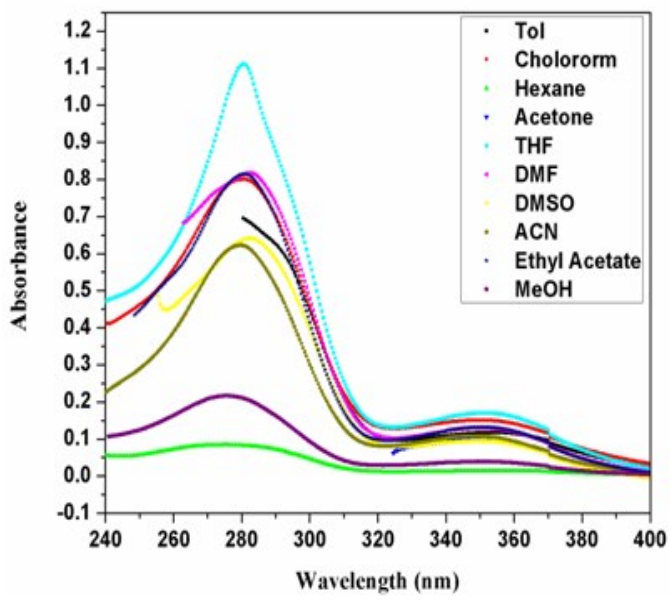
ACN
Ethyl Acetate
MeOH

5e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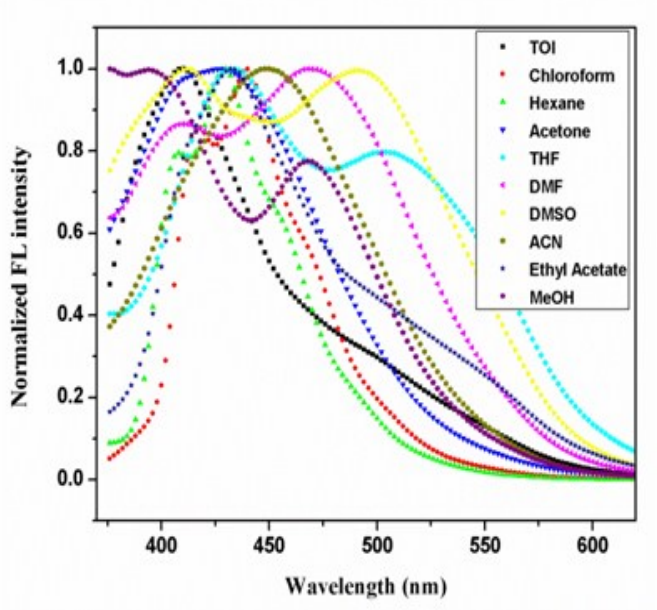
Normalized FL intensity
Wavelength (nm)
TOl
Chloroform
Hexane
Acetone
THF
DMF
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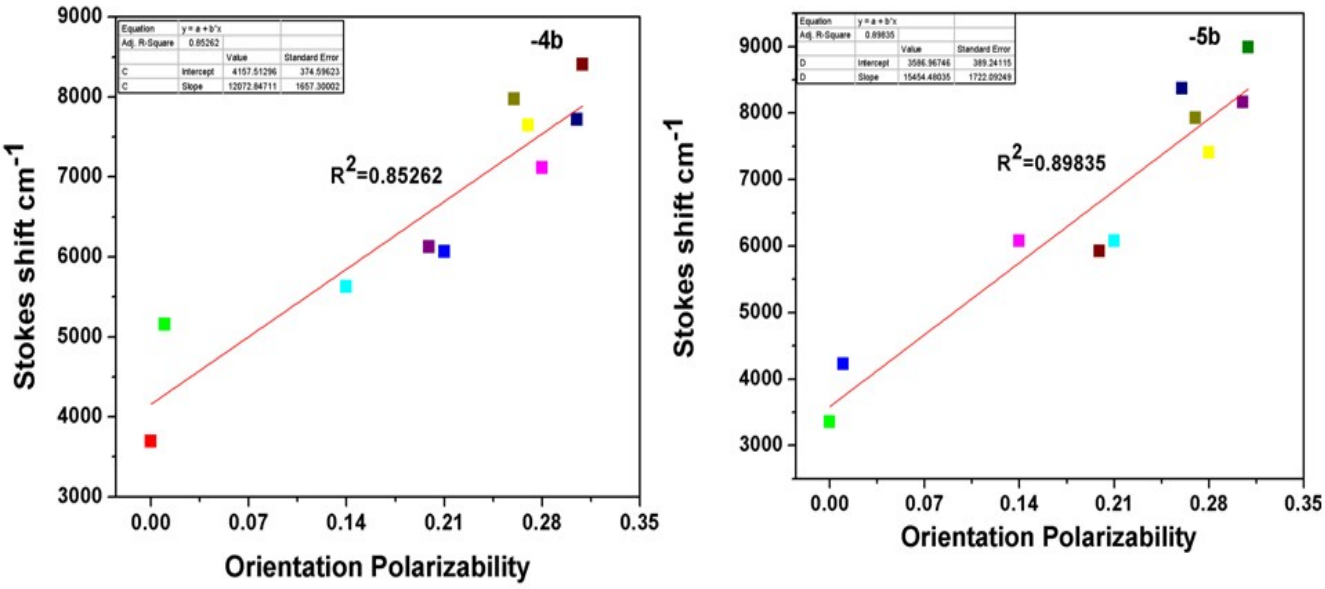
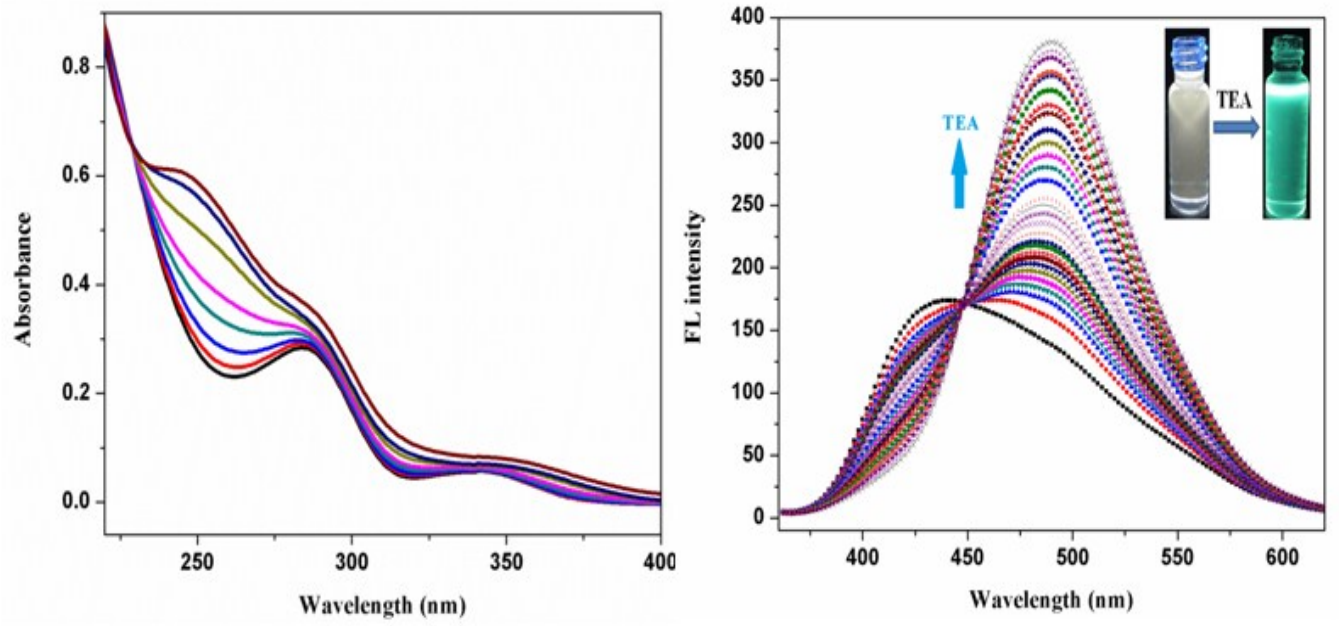
ACN
Ethyl Acetate
MeOH

S1 Figure S4 The plot of orientation Polarizability Vs Stokes shift for **4b** and **5b**

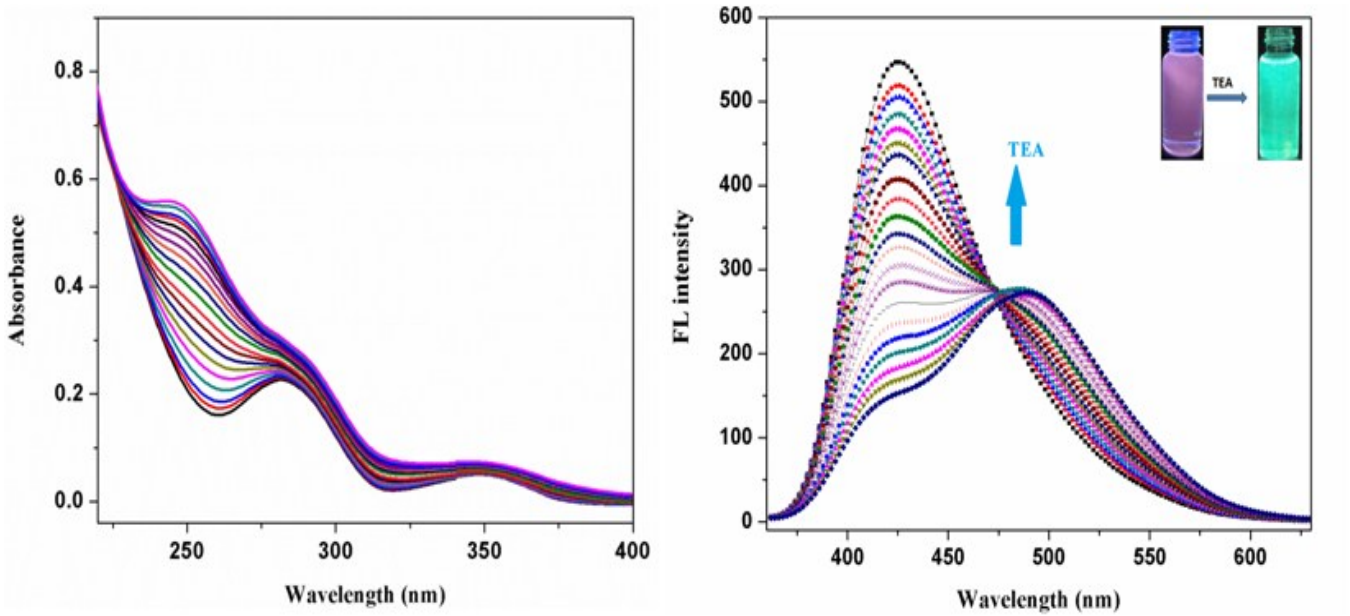


S1 Figure S5 Reversible absorption and Emission spectra of dye **4b** and **5b** (containing **TFA**) recorded with different concentrations of **TEA**

4b

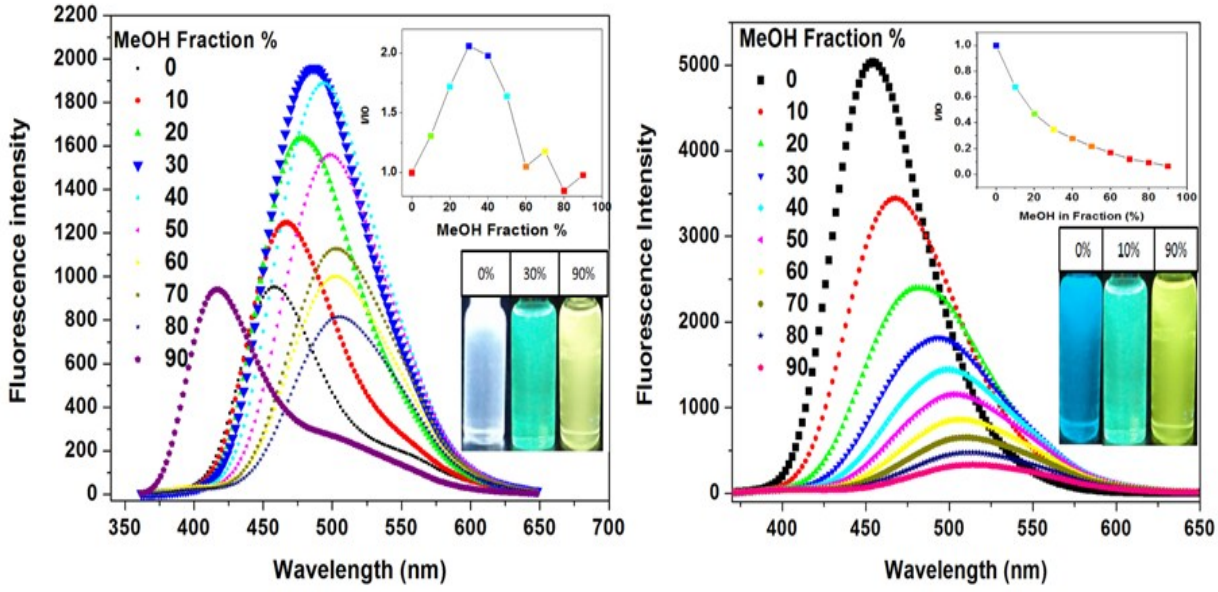


5b

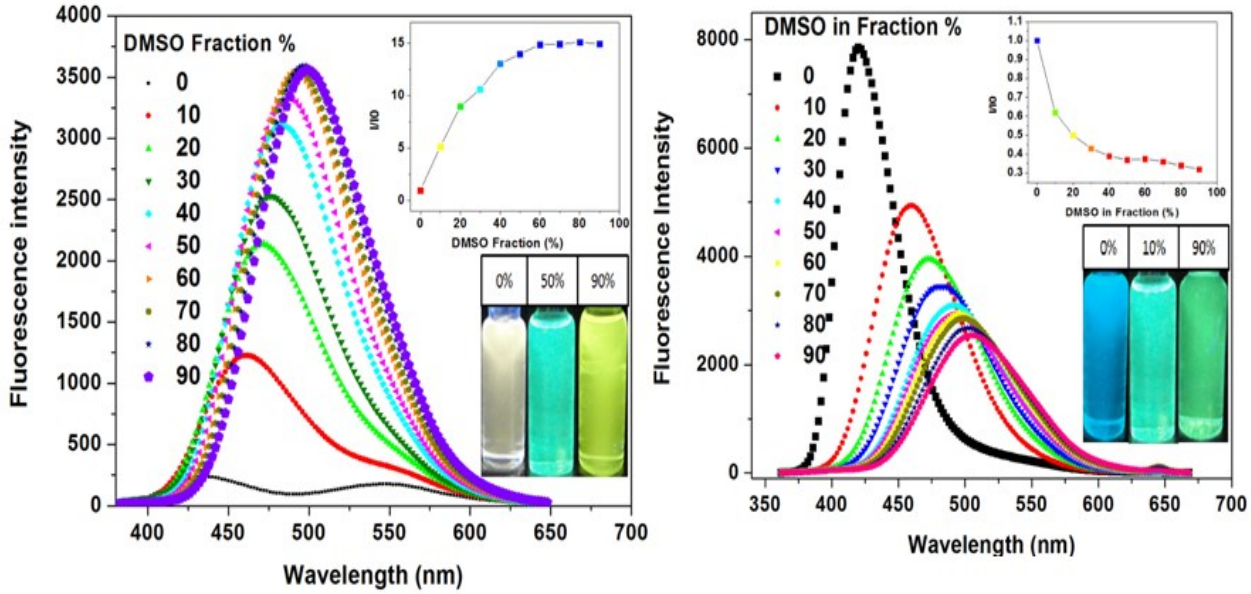


S1 Figure S6 Emission spectra of compound **4b (left)** and **5b (right)** in THF and Methanol solvent mixture

4b and 5b



S1 Figure S7 Emission spectra of compound **4b (left)** and **5b (right)** in Toluene and DMSO solvent mixture



SI Table 1 Absorption, Fluorescence, Quantum yield and Lifetime Data for **4a-j** and **5a-j**[a]

Compounds	$\lambda_{max, abs}$ (nm) ε (10^4 $M^{-1}cm^{-1}$)	$\lambda_{max, fl}$ (nm)[b]		Stokes shift Δss (cm^{-1})[c]	Quantum yield (ϕ_{fl})[d]	[e]τ_f (ns)	[f]k_r (10^8 s^{-1})	[g]k_{nr} (10^8 s^{-1})
		solution	solid					
4a	284 (3.4), 341 (0.5)	437	450	6442	0.22	5.54	0.39	1.38
4b	241 (1.65), 283 (2.95) , 340 (0.7)	443	480	6939	0.12	6.34	0.18	1.32
4c	276 (2.15), 347 (0.49)	436	438	5882	0.26	5.67	0.45	1.28
4d	236 (1.6), 281 (3.25), 362 (0.36)	445	453	5101	0.27	5.88	0.46	1.24
4e	242 (1.65), 283 (3.05), 340 (0.44)	411, 437	-	5080, 6528	0.33	1.52	2.17	4.40
4f	242 (1.35), 282 (2.4), 341 (0.6)	436	-	6389	0.12	5.67	0.21	1.54
4g	241 (1.30), 283 (2.9), 342 (0.6)	436	445	6303	0.08	1.74	0.45	5.17
4h	244 (1.44), 286 (2.67), 340 (0.63)	413	-	5198	0.18	1.71	1.05	4.78
4i	244 (1.35), 284 (2.79), 340 (0.54)	405		4720	0.29	6.16	0.47	1.15
4j	243 (1.32), 283 (2.78), 340 (0.66)	410		5021	0.23	7.36	0.31	1.03
5a	253 (1.41), 281 (2.54), 350 (0.59)	406	425	3940	0.25	4.21	0.59	1.77
5b	255 (1.58), 281 (2.22), 353 (0.48)	437	536	5445	0.40	3.64	1.09	1.63
5c	242 (1.39), 282 (3.51), 350 (0.72)	401	409	3633	0.26	2.26	1.15	3.27
5d	245 (2.2), 280 (3.07), 355 (0.81)	440	433	5441	0.41	5.15	0.79	1.13
5e	234 (1.42), 278 (3.53), 358 (0.34)	411, 434	-	3602, 4891	0.14	1.74	0.80	4.91
5f	234 (1.00), 281 (2.37), 350 (0.40)	404	407, 513	2875	0.28	4.20	0.66	1.69
5g	279 (2.35), 349 (0.60)	403	-	3839	0.28	3.76	0.74	1.90
5h	241 (1.37), 281 (2.95), 350 (0.75)	402	-	3695	0.47	3.35	1.40	1.57
5i	246 (1.35), 286 (2.82), 351 (0.78)	407	-	3920	0.16	4.21	0.38	1.99
5j	242 (1.37), 284 (2.98), 351 (0.67)	403	-	3676	0.53	3.59	1.47	1.30

[a]The UV and FL Experiments were performed in Chloroform solvents. [b]Excitation at either 320 or 330 nm. [c]Δss = UV-FL. [d]Quantum yields were reported relative to Anthracene (ϕ_{fl} = 0.27 in ethanol). [e]Fluorescence lifetime was measured by exciting the samples at 320 nm using time-correlated single-photon-counting technique using 150 ps nanoleds; [f]k_r measured by using $k_r = [\Phi_{fl}/\tau_F]$; [g]k_{nr} measured by using $k_{nr} = k_r[(1/\Phi_{fl})-1]$.

SI Table 2 UV-Visible Absorption and Fluorescence Properties of **4a-e** in various solvents[a]

Entry		Toluene	$CHCl_3$	Hexane	Acetone	THF	DMF	DMSO	ACN	EA	MeOH
4a	λ_{abs}	287, 341	287, 342	286, 340	329	284, 340	286, 340	286, 339	241, 283, 339	285, 339	281, 339
	λ_{fl} (ϕ_{fl})[b]	435 (0.036)	416 (0.053)	428 (0.088)	441 (0.013)	433 (0.036)	443 (0.051)	440 (0.073)	443 (0.039)	432 (0.046)	441 (0.059)
	Δss (cm^{-1})	6337	5201	6047	7720	6317	6838	6771	6925	6350	5823
4b	λ_{abs}	287, 354	282, 354	285, 350	355	282, 356	284, 357	283, 357	279, 355	284, 354	274, 356
	λ_{fl} (ϕ_{fl})	433, 546 (0.021)	442 (0.051)	402, 544 (0.042)	475 (0.061)	454 (0.088)	491 (0.209)	499 (0.241)	489 (0.244)	452 (0.090)	508 (0.053)
	Δss (cm^{-1})	5154, 9933	5624	3695, 10188	7117	6063, 9908	7645	7971	7720	6125, 9933	8404
4c	λ_{abs}	341	280, 342	280, 340	334	280, 342	283, 341	283, 342	236, 280, 340	281, 340	278, 339
	λ_{fl} (ϕ_{fl})	435 (0.02)	417 (0.041)	405 (0.048)	433 (0.006)	438 (0.25)	447 (0.42)	443 (0.06)	448 (0.23)	436 (0.30)	441 (0.26)
	Δss (cm^{-1})	6337	6328	4720	6846	6408, 10789	6954	6666	7090	6476	6823
4d	λ_{abs}	288, 346	276, 346	276, 347	341	279, 346	282, 344	276, 349	236, 275, 343	278, 346	272, 344
	λ_{fl} (ϕ_{fl})	439 (0.126)	443 (0.28)	429 (0.33)	445 (0.072)	441 (0.238)	448 (0.47)	451 (0.39)	448 (0.25)	440 (0.24)	447 (0.43)
	Δss (cm^{-1})	6122	6328	5508	6854	6226	6748	6332	6833	6174	6698
4e	λ_{abs}	288, 359	281, 360	280, 360	343	281, 357	283, 356	284, 356	235, 279, 355	281, 354	277, 353
	λ_{fl} (ϕ_{fl})	408 (0.079)	416 (0.017)	405 (0.066)	407 (0.055)	408 (0.11)	472 (0.04)	411, 479 (0.16)	408, 468 (0.10)	410, 436 (0.15)	391 (0.063)
	Δss (cm^{-1})	3346	3739	3086	4584	3502	6903	3759, 7213	3660, 6802	3858, 5313	2753

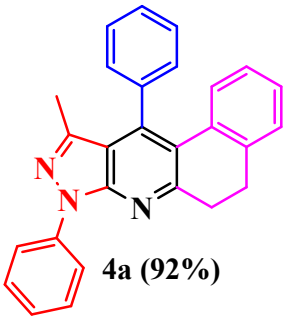
[a]The excitation wavelength (λ_{abs}) of **4a-e** is 320 nm. [b]Quantum yields (ϕ_{fl}) were determined in various solvents using Anthracene 320 as standard (ϕ_{fl} = 0.27 in ethanol).

SI Table 3 UV-Visible Absorption and Fluorescence Properties of **5a-b** and **5e** in various solvents[a]

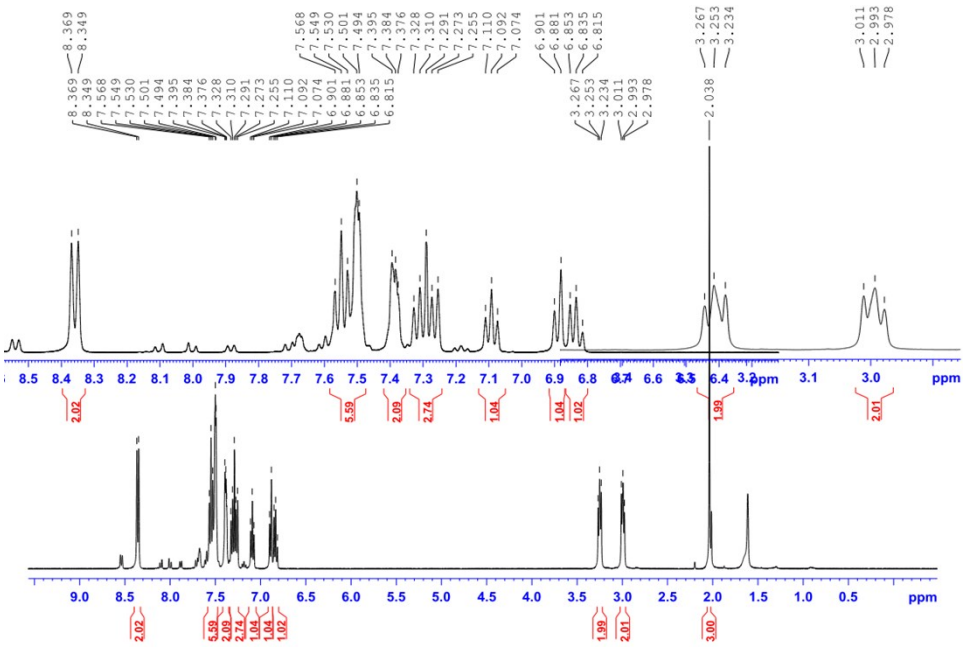
		Toluene	$CHCl_3$	Hexane	Acetone	THF	DMF	DMSO	ACN	EA	MeOH
5a	λ_{abs}	281, 350	282, 350	283, 350	346	241, 281, 350	282, 354	283, 350	247, 281, 346	282, 348	279, 348
	λ_{fl} (ϕ_{fl})[b]	402 (0.13)	406 (0.20)	397 (0.19)	404 (0.12)	403 (0.15)	408 (0.17)	410 (0.11)	406 (0.22)	402 (0.11)	376 (0.11)
	Δss (cm^{-1})	3696	3941	3383	4149	3938	3739	4181	4271	3860	2140
5b	λ_{abs}	289, 356	281, 355	257, 285, 355	353	282, 354	283, 355	283, 354	280, 352	282, 354	270, 352
	λ_{fl} (ϕ_{fl})	419 (0.20)	435 (0.35)	403 (0.41)	478 (0.09)	451 (0.56)	494 (0.30)	503 (0.26)	494 (0.13)	448 (0.34)	515 (0.30)
	Δss (cm^{-1})	4223	5181	3355	7408	6076	7927	8368	8167	5927	8992
5e	λ_{abs}	357	280, 356	275, 359	351	280, 354	282, 354	282, 353	239, 279, 350	280, 352	275, 353
	λ_{fl} (ϕ_{fl})	410 (0.89)	416, 439 (0.023)	407, 428 (0.027)	425 (0.081)	431, 505 (0.17)	410, 489 (0.079)	410, 489 (0.12)	448 (0.12)	432 (0.22)	397, 468 (0.13)
	Δss (cm^{-1})	3621	4051, 5310	3285, 4491	4961	5047, 8447	3858, 7799	3938, 7879	6250	5261	3140, 6961

[a] The excitation wavelength (λ_{abs}) of **5a-b** and **5e** is 320 nm. [b] Quantum yields (ϕ_{fl}) were determined in various solvents using Anthracene 320 as standard (ϕ_{fl} = 0.27 in ethanol).

^{1}H NMR Data of Compound 4a:



4a (92%)



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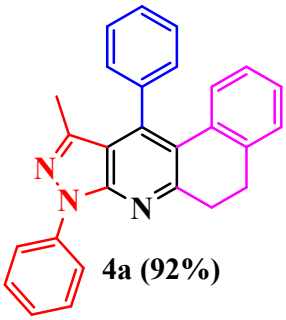
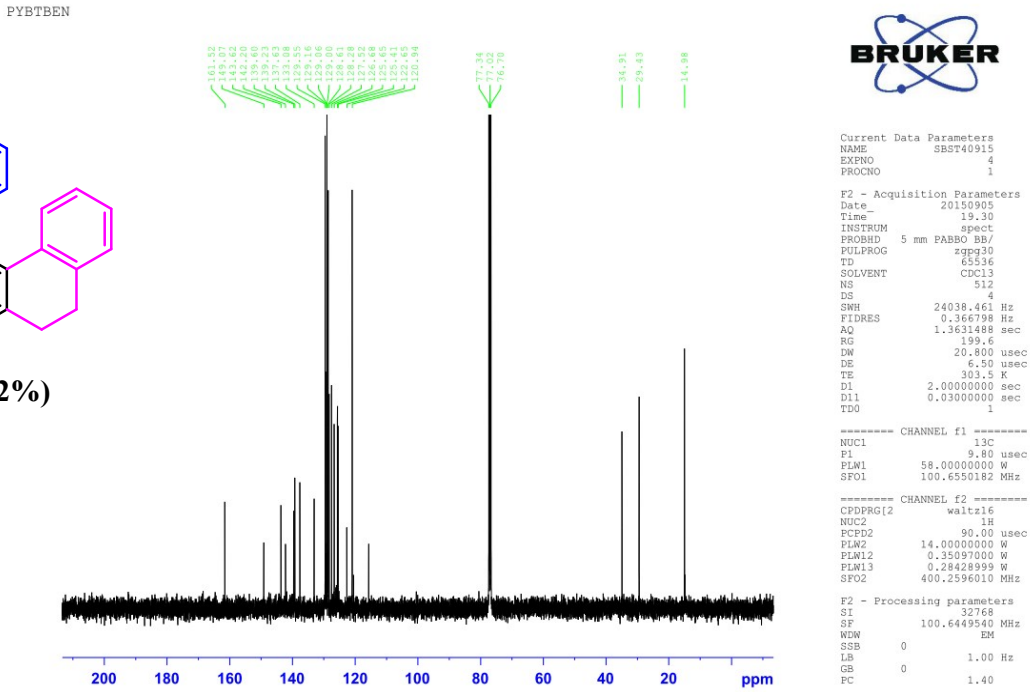


4a (92%)



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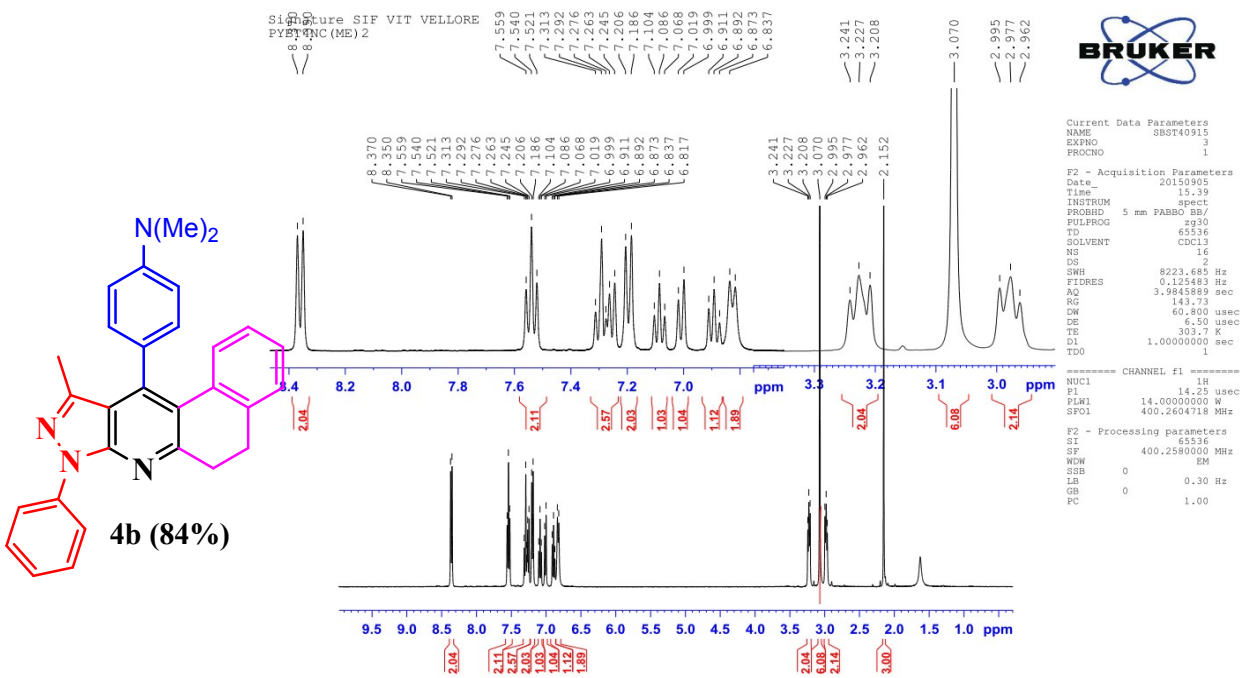

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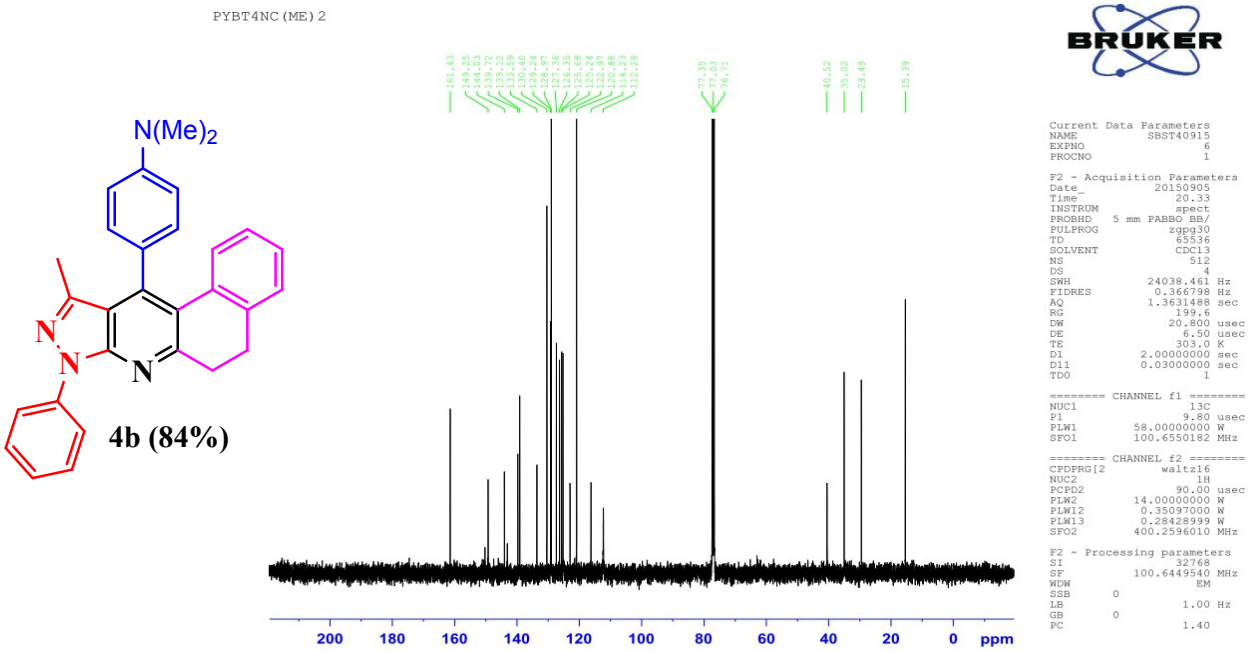

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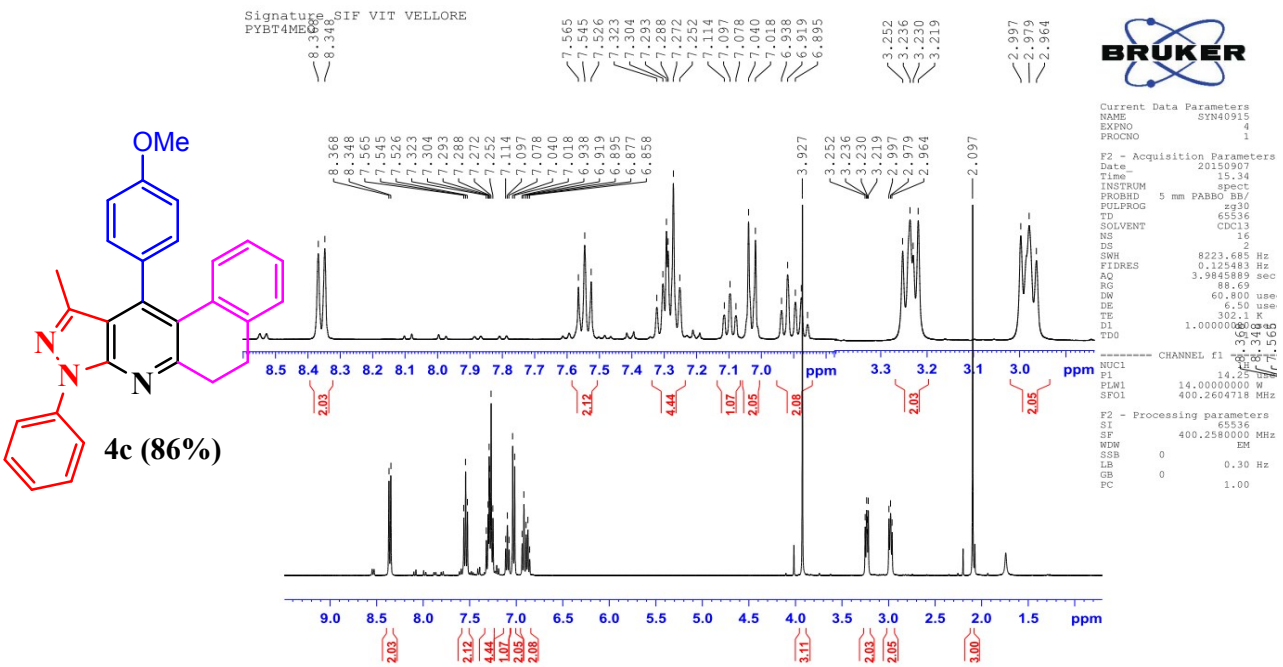
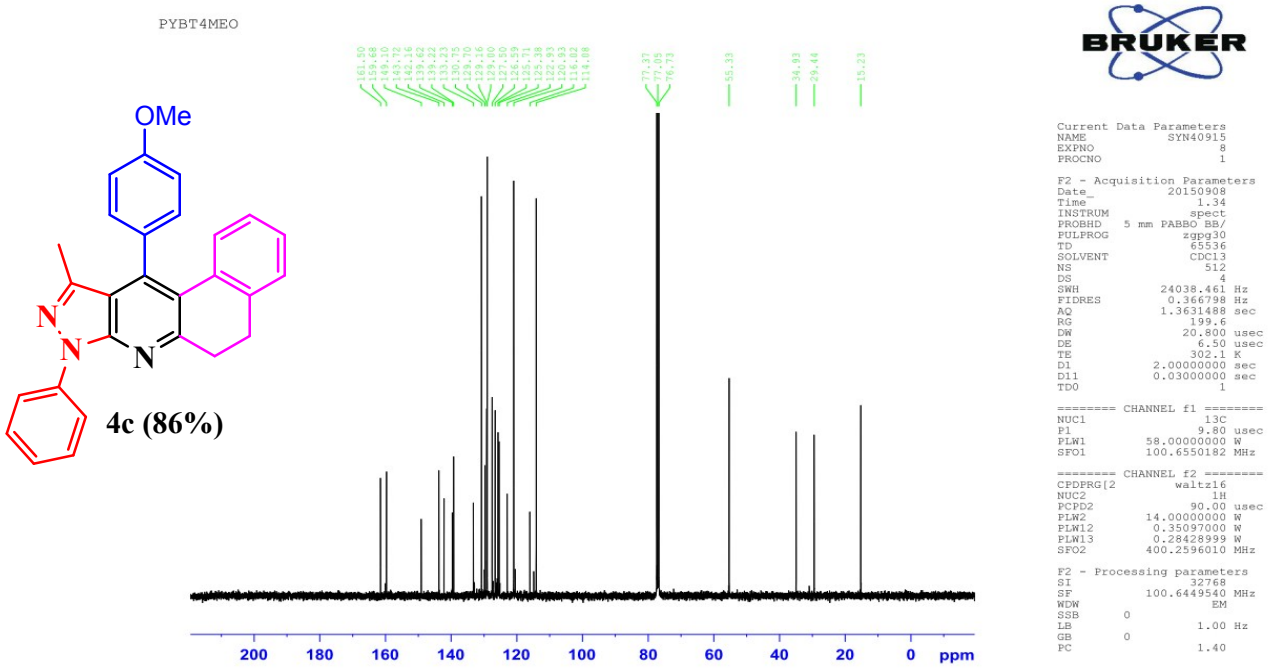
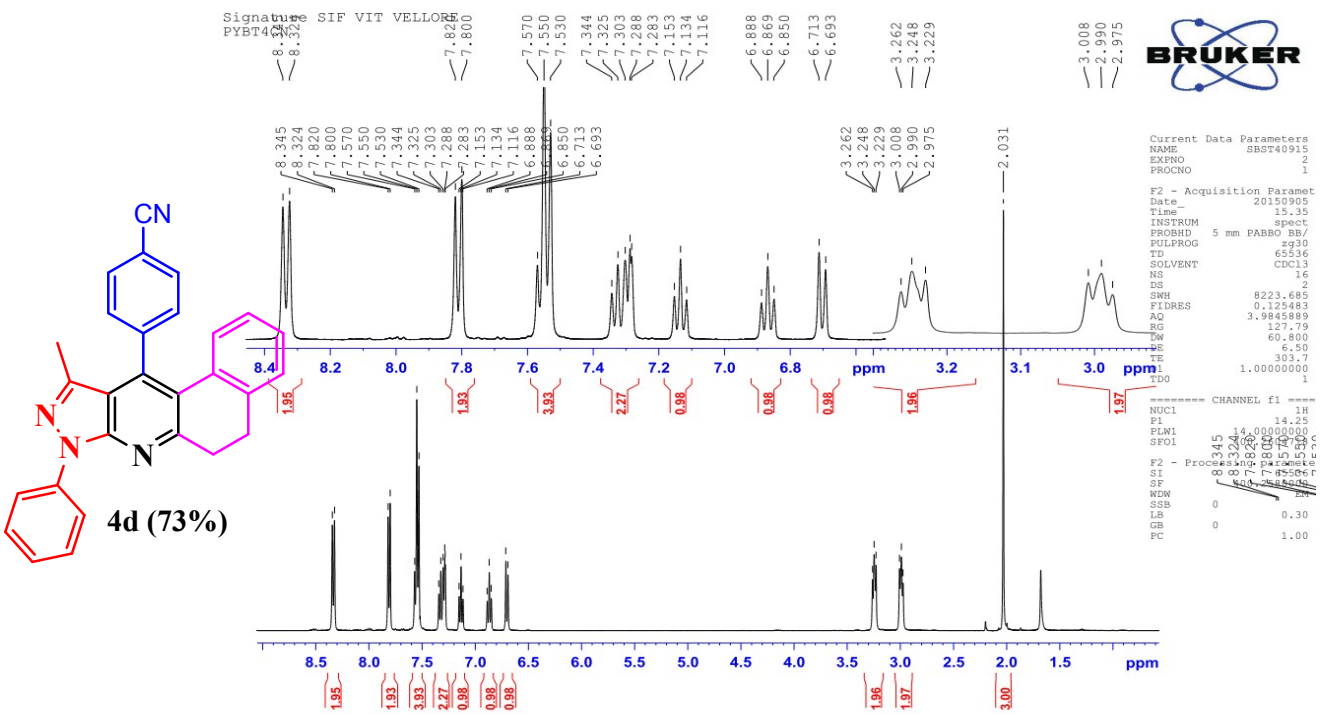


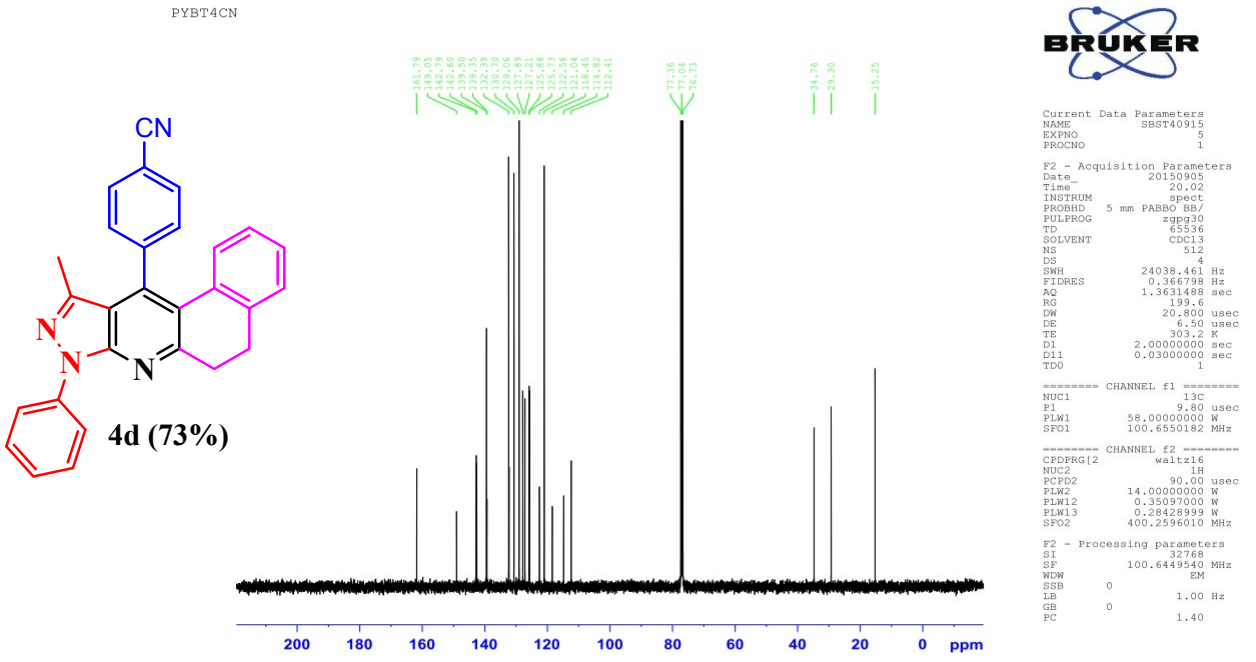
^{13}C NMR Data of Compound 4c:



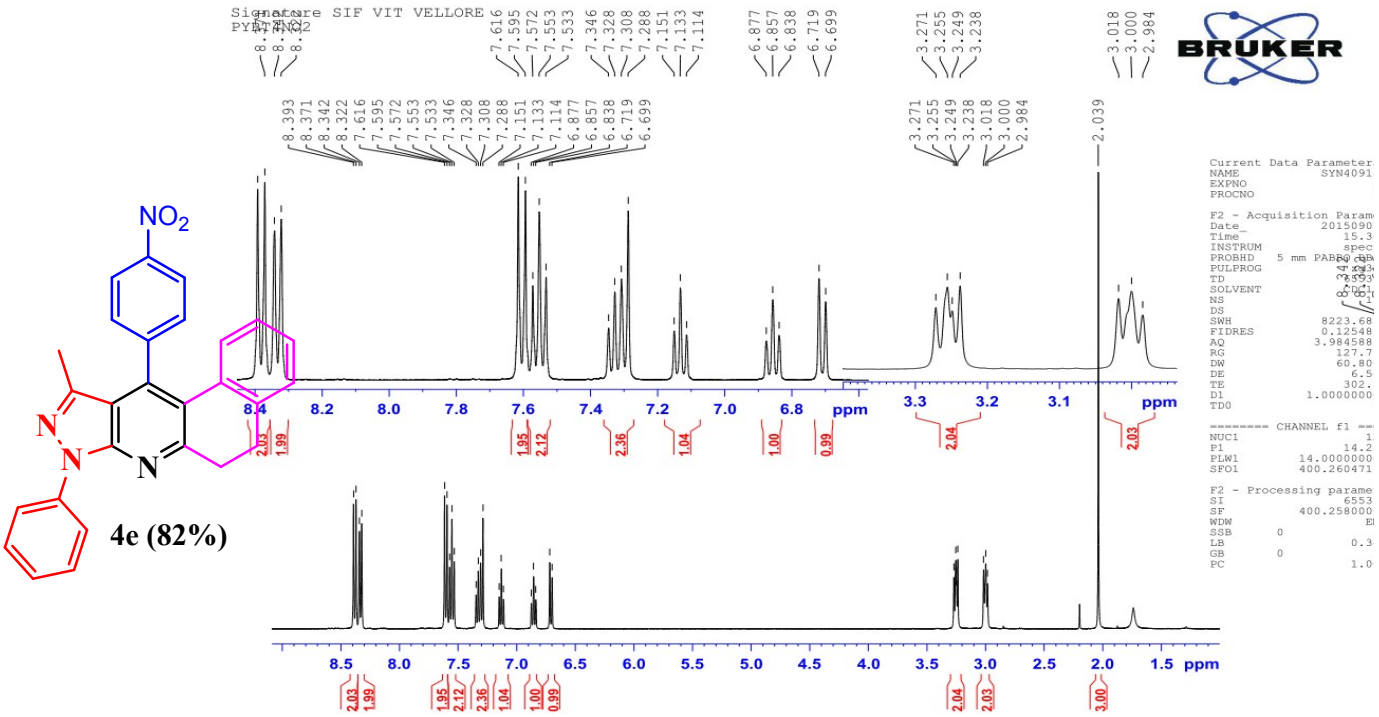
[1]H NMR Data of Compound 4d:



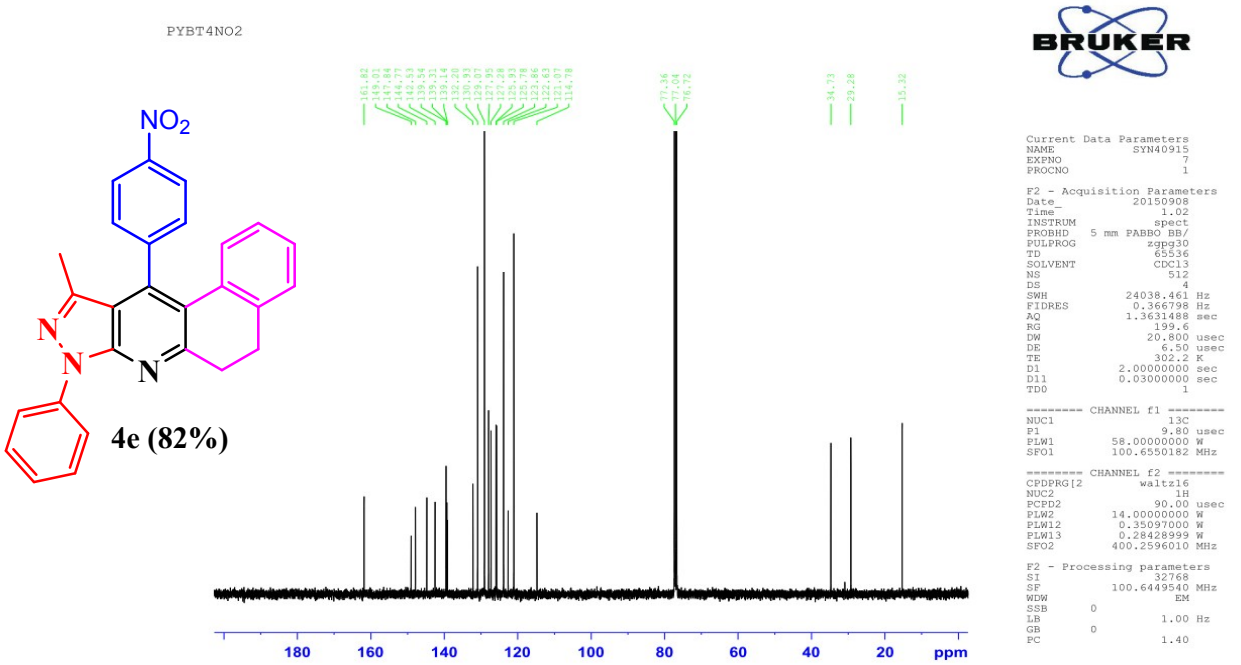
[13]C NMR Data of Compound 4d:



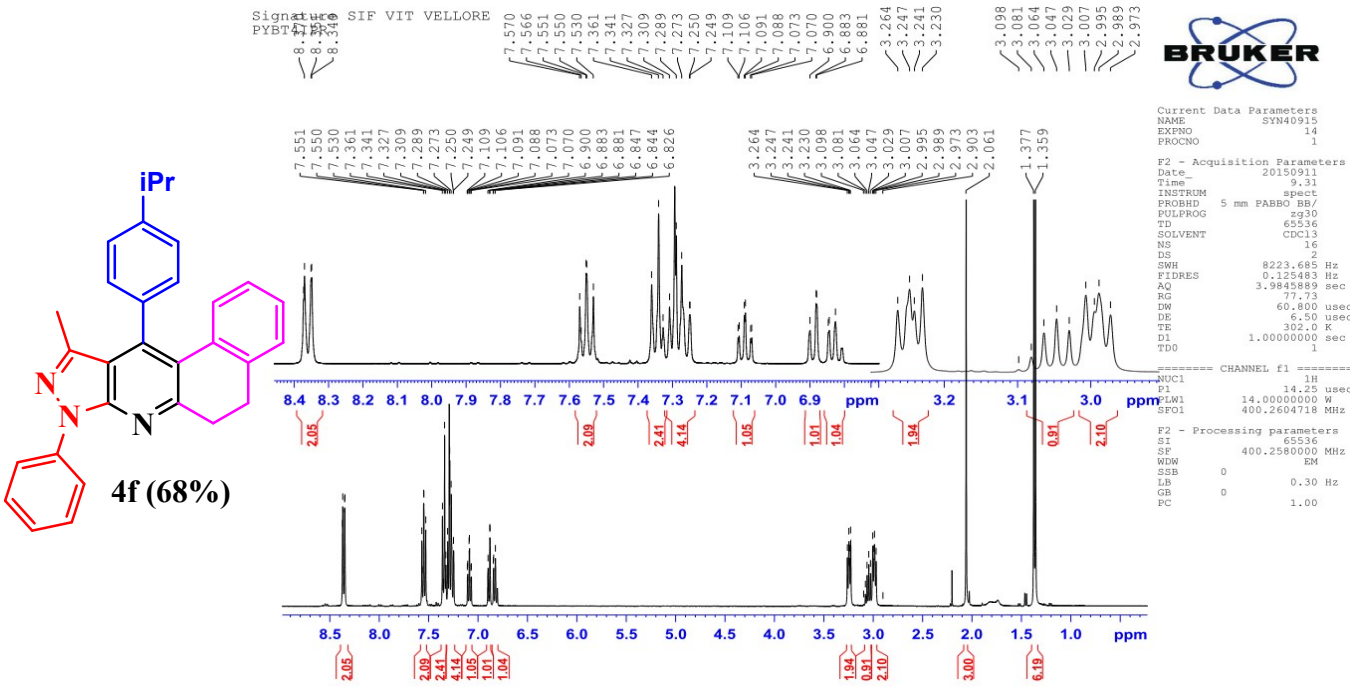
^{1}H NMR Data of Compound 4e:



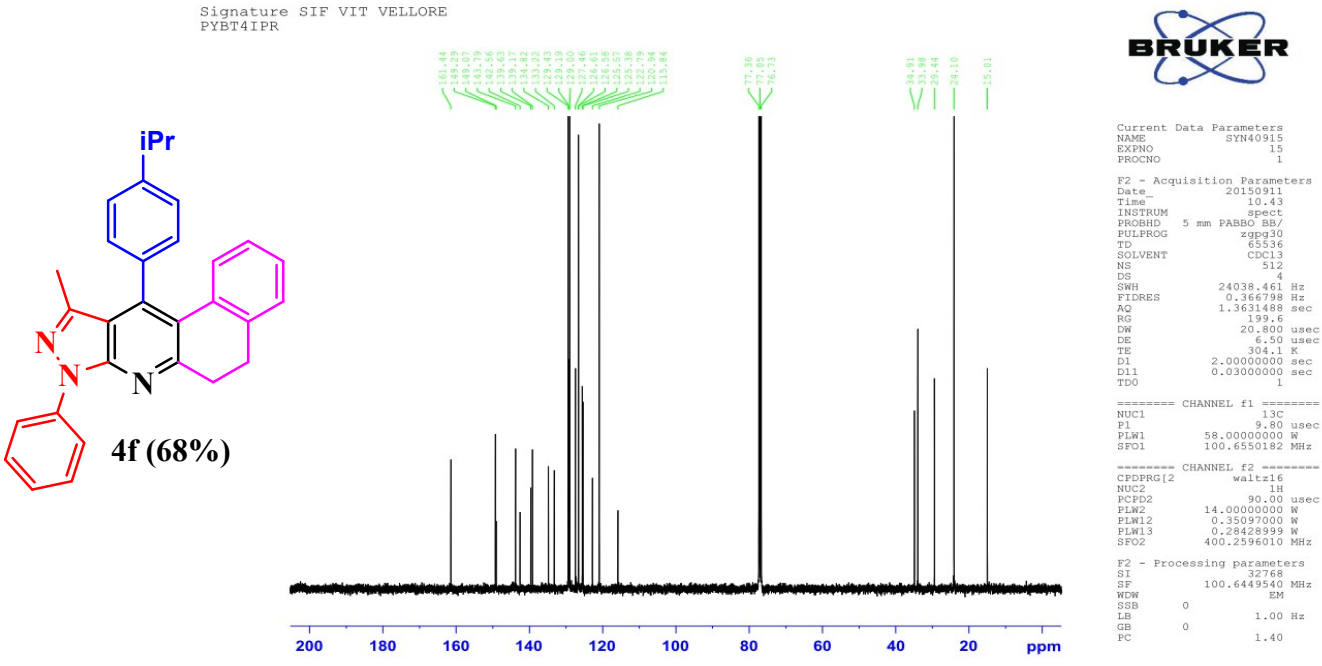
^{13}C NMR Data of Compound 4e:



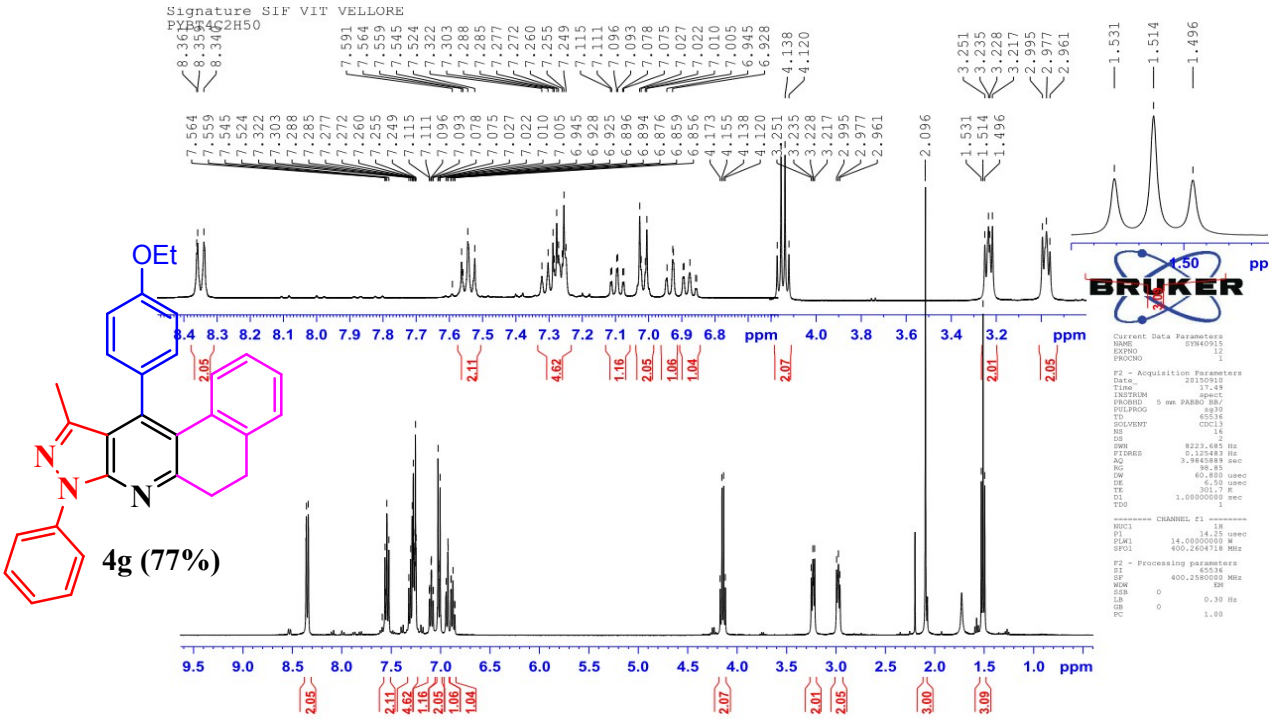
^{1}H NMR Data of Compound 4f:



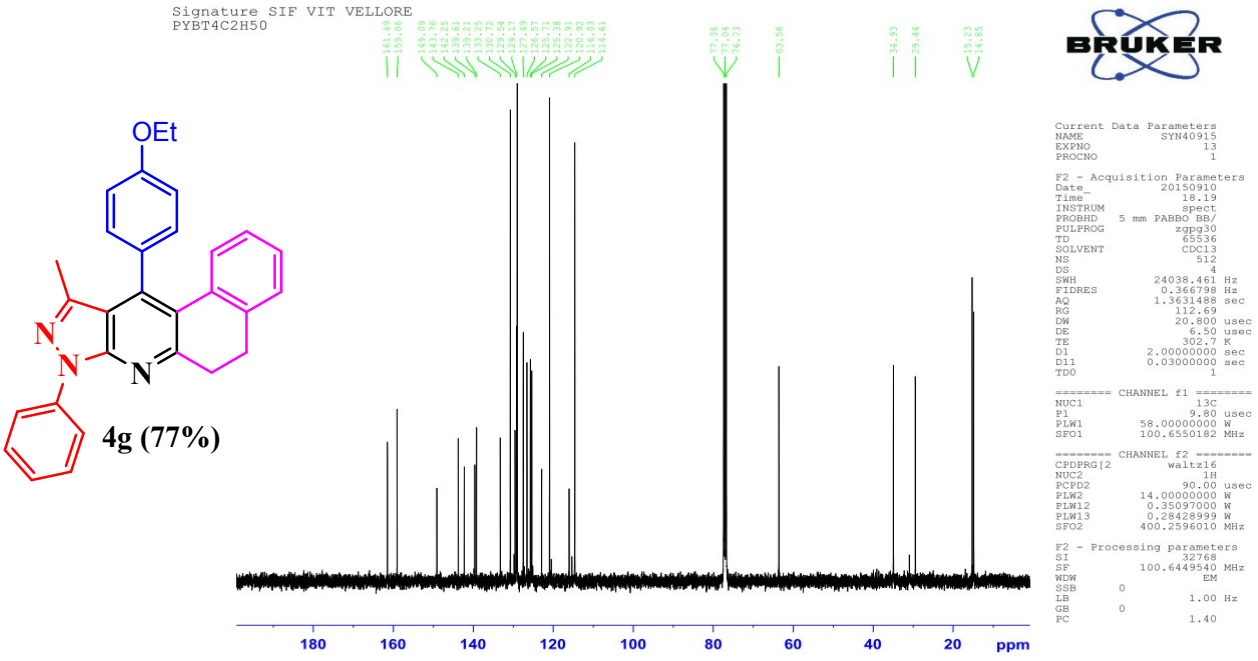
^{13}C NMR Data of Compound 4f:



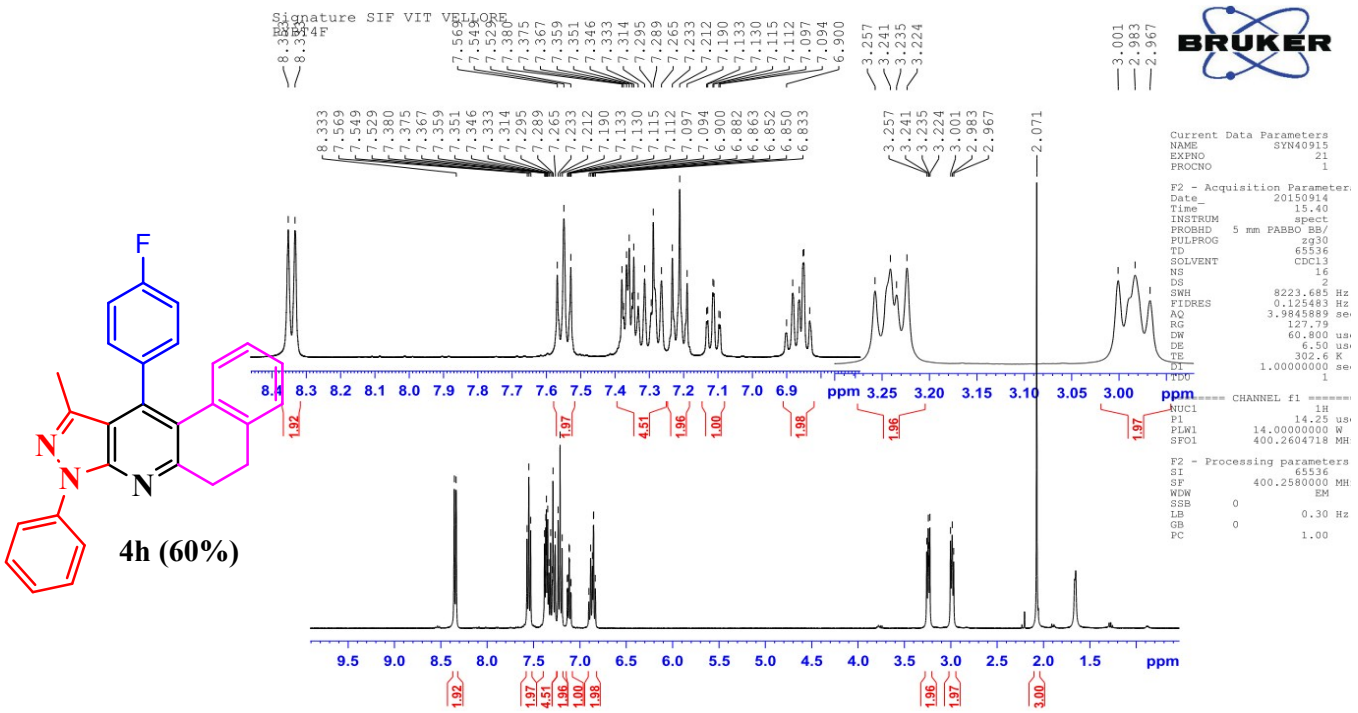
^{1}H NMR Data of Compound 4g:



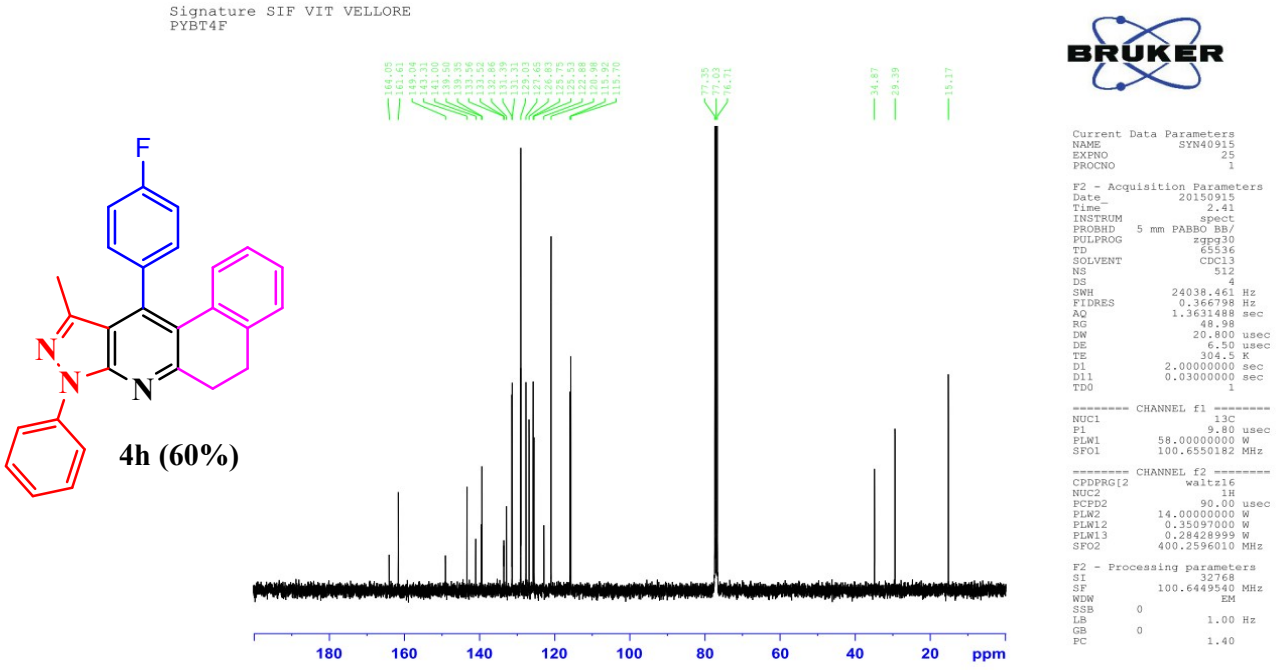
^{13}C NMR Data of Compound 4g:



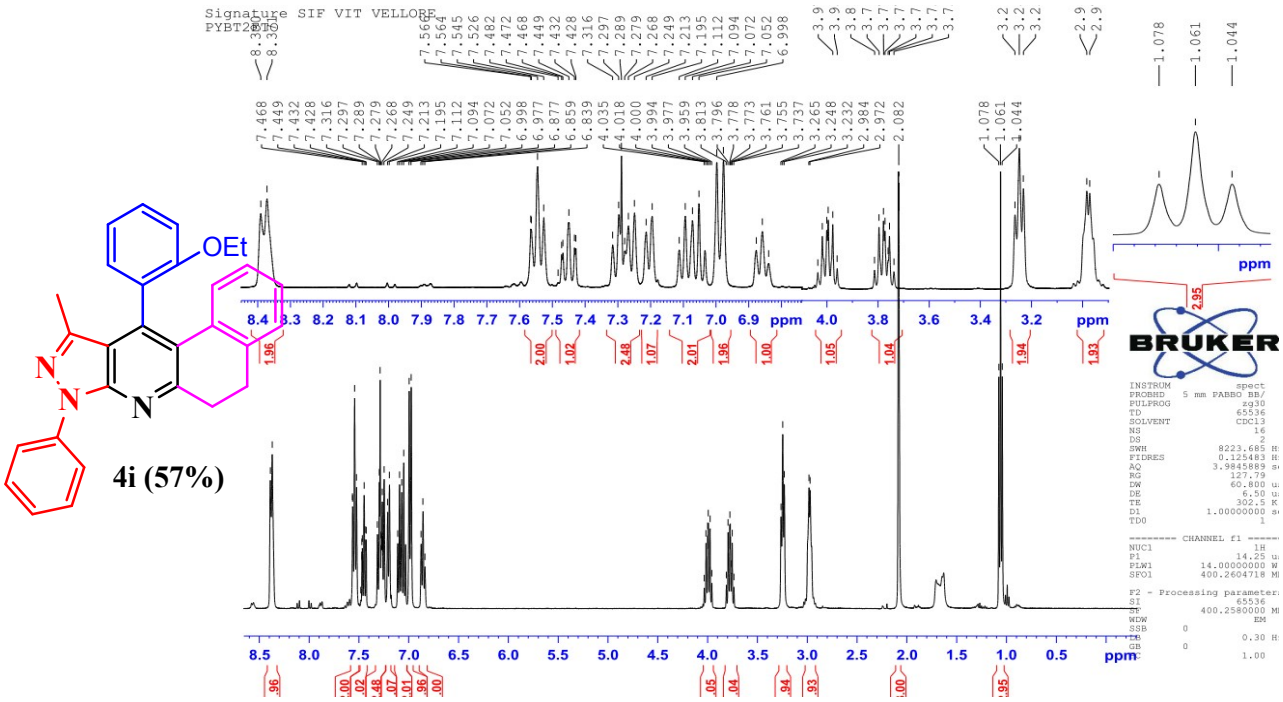
[1]H NMR Data of Compound 4h:



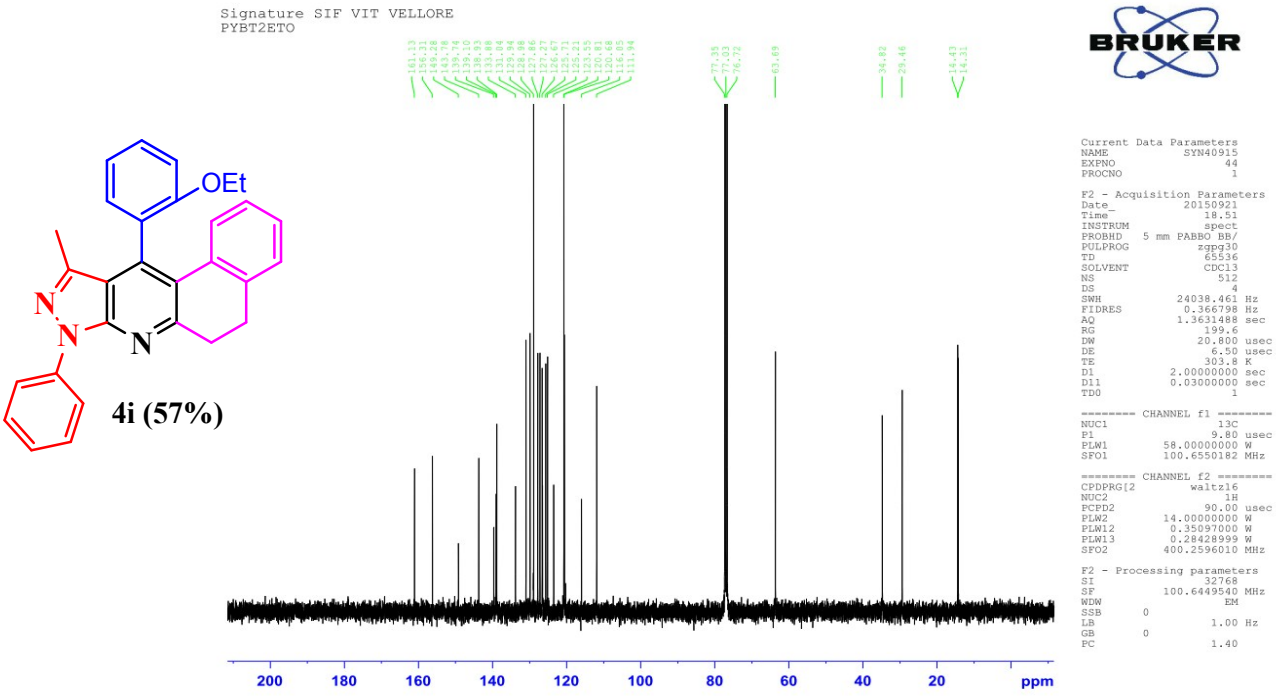
[13]C NMR Data of Compound 4h:



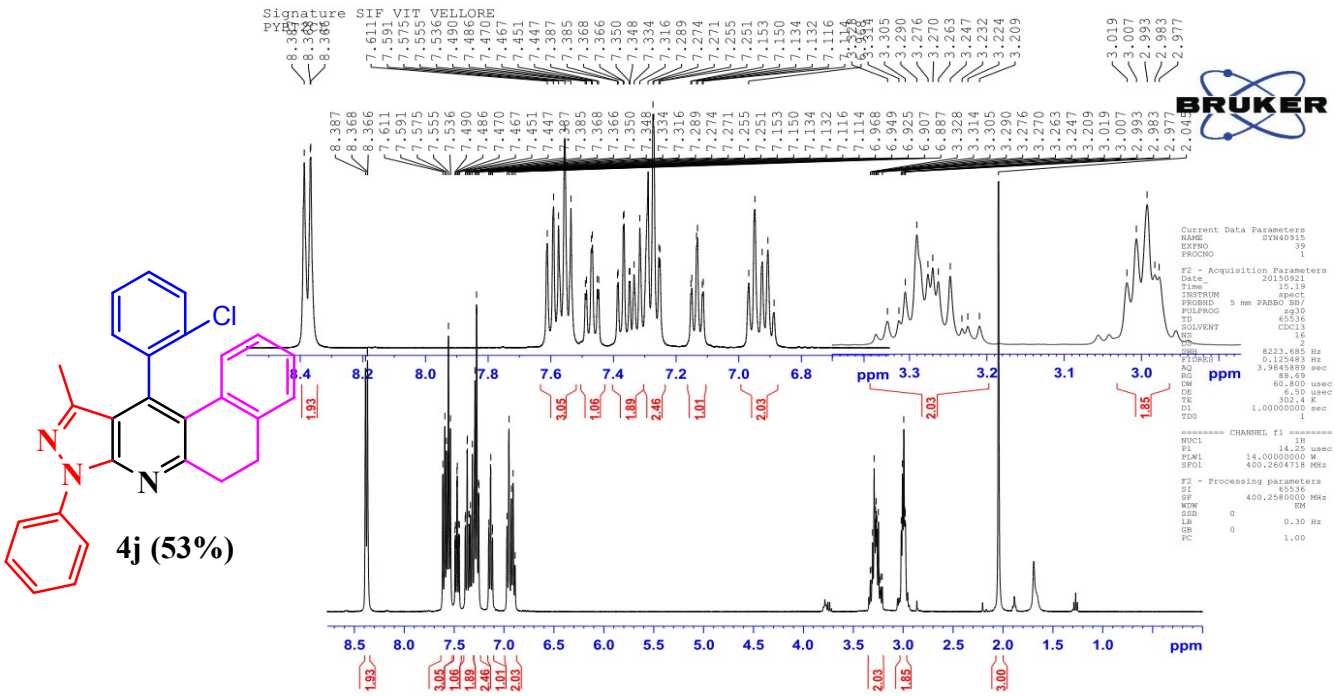
^{1}H NMR Data of Compound 4i:



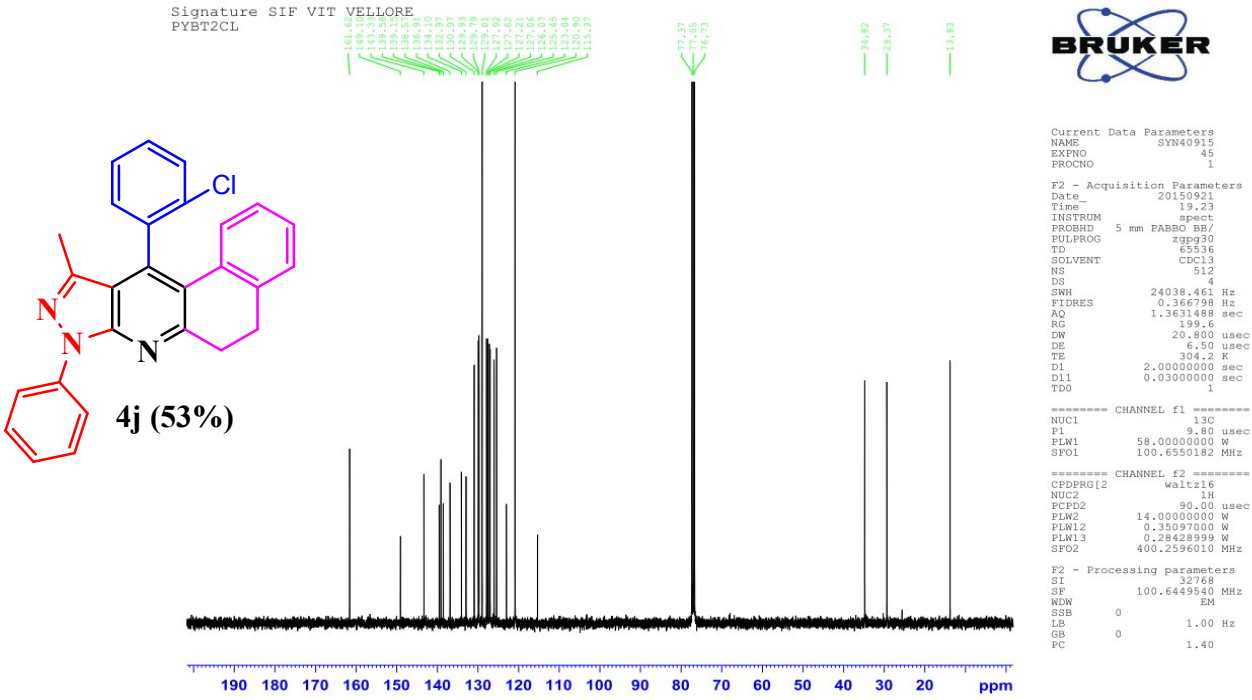
^{13}C NMR Data of Compound 4i:



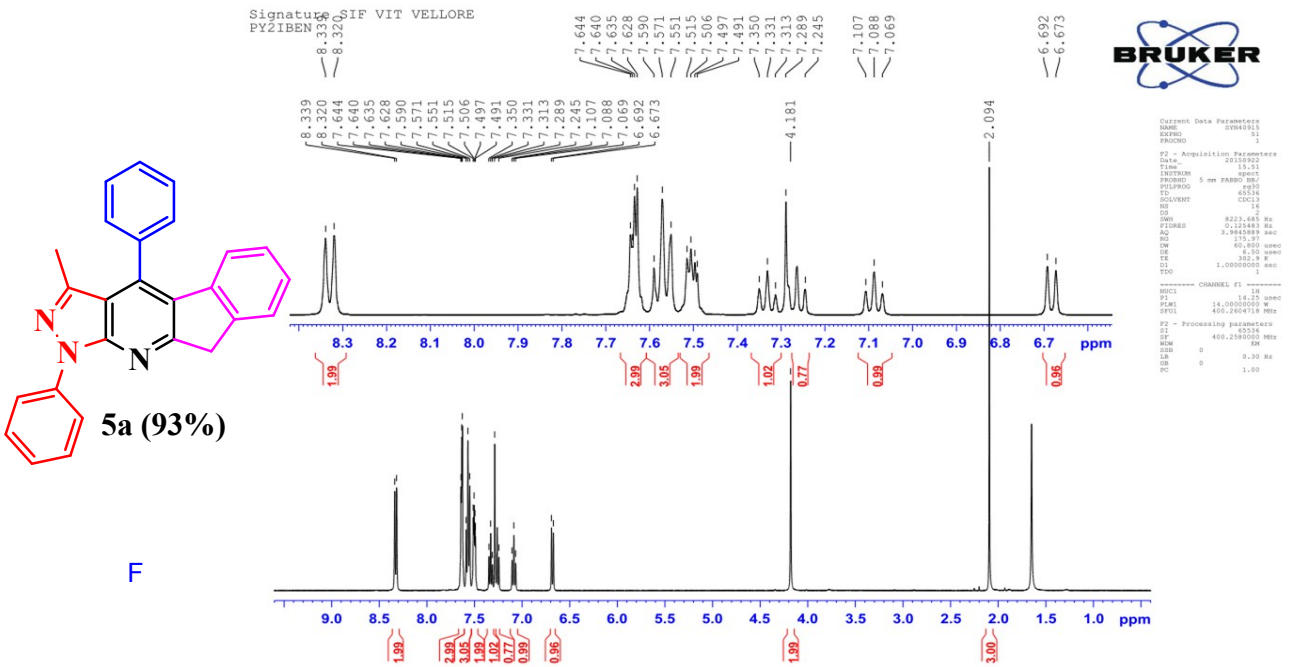
^{1}H NMR Data of Compound 4j:



^{13}C NMR Data of Compound 4j:



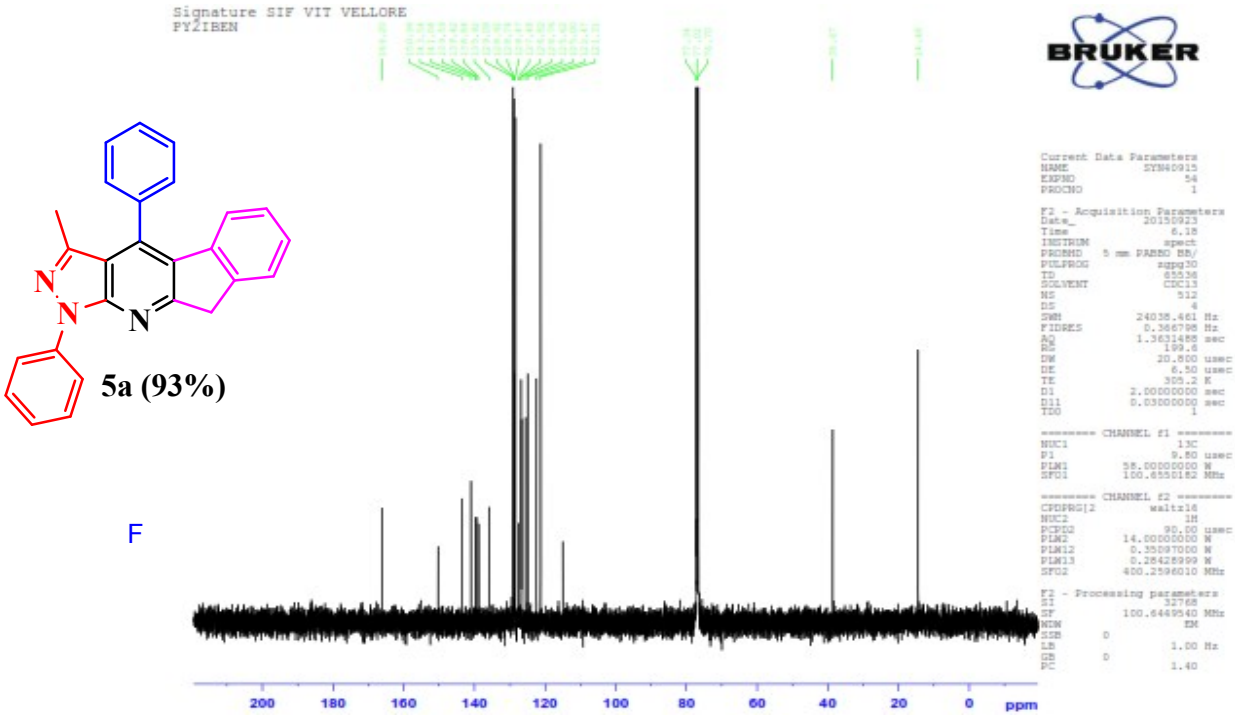
[1]H NMR Data of Compound 5a:



5a (93%)

F

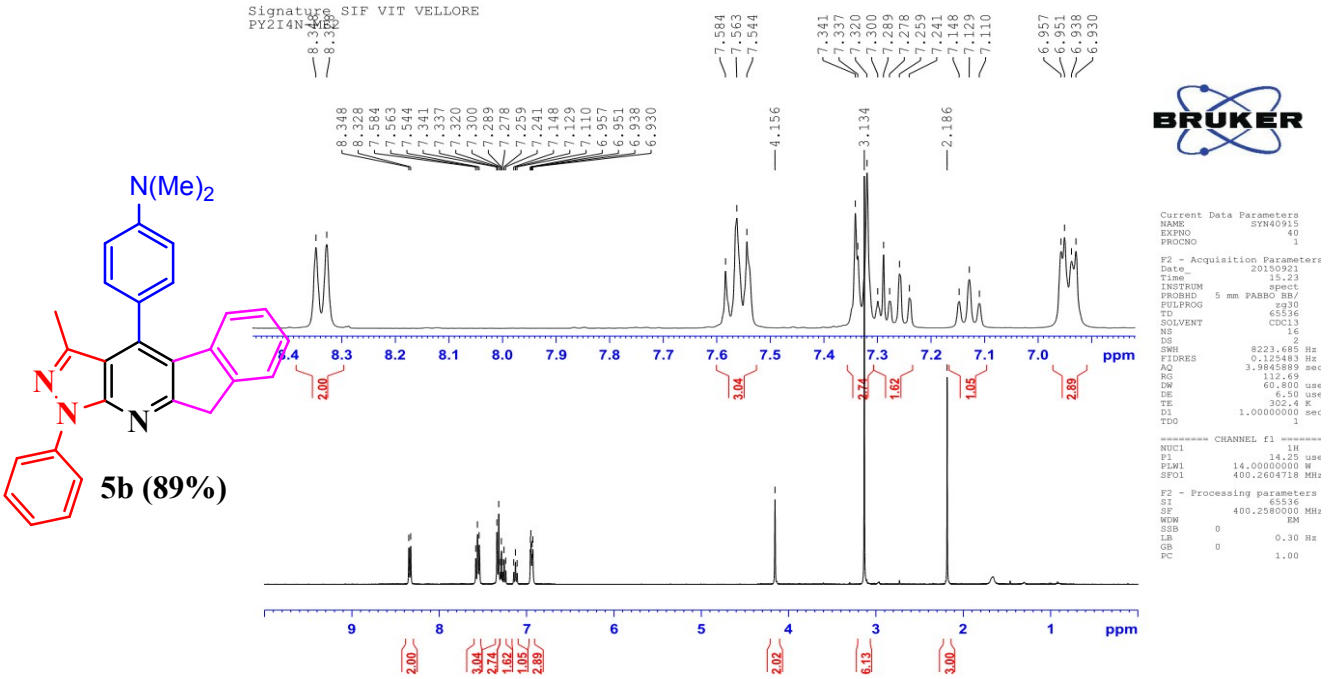
[13] C NMR Data of Compound 5a:



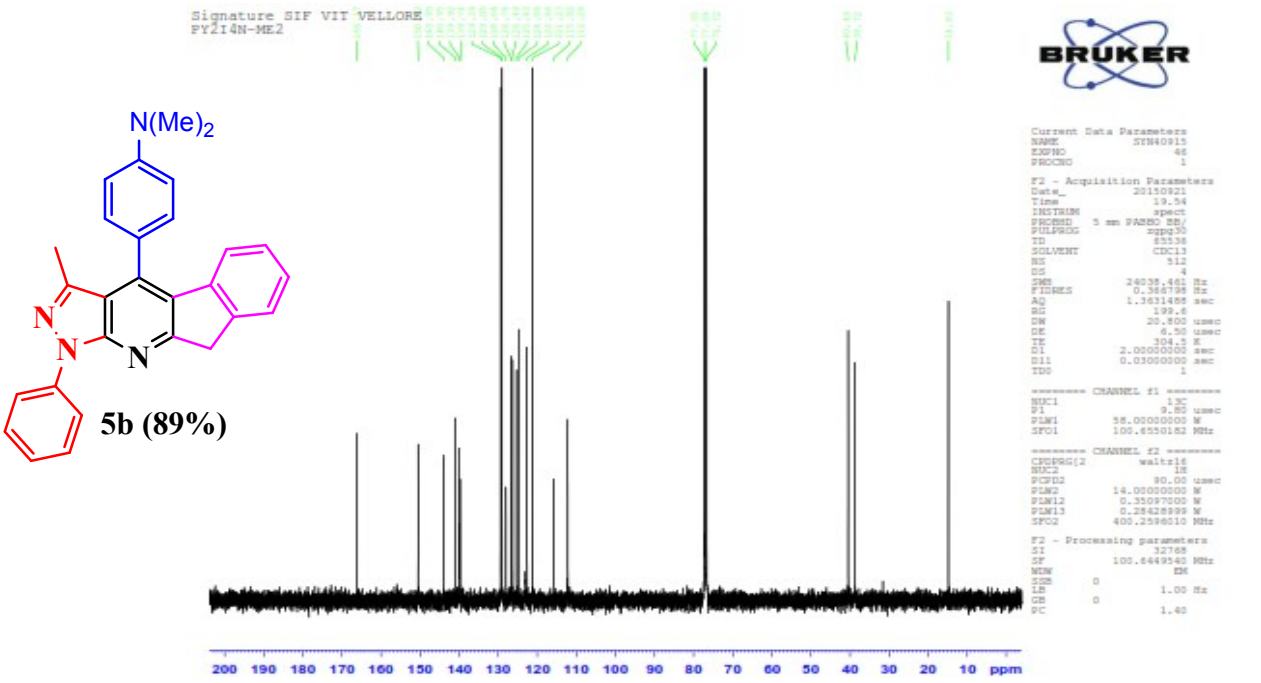
5a (93%)

F

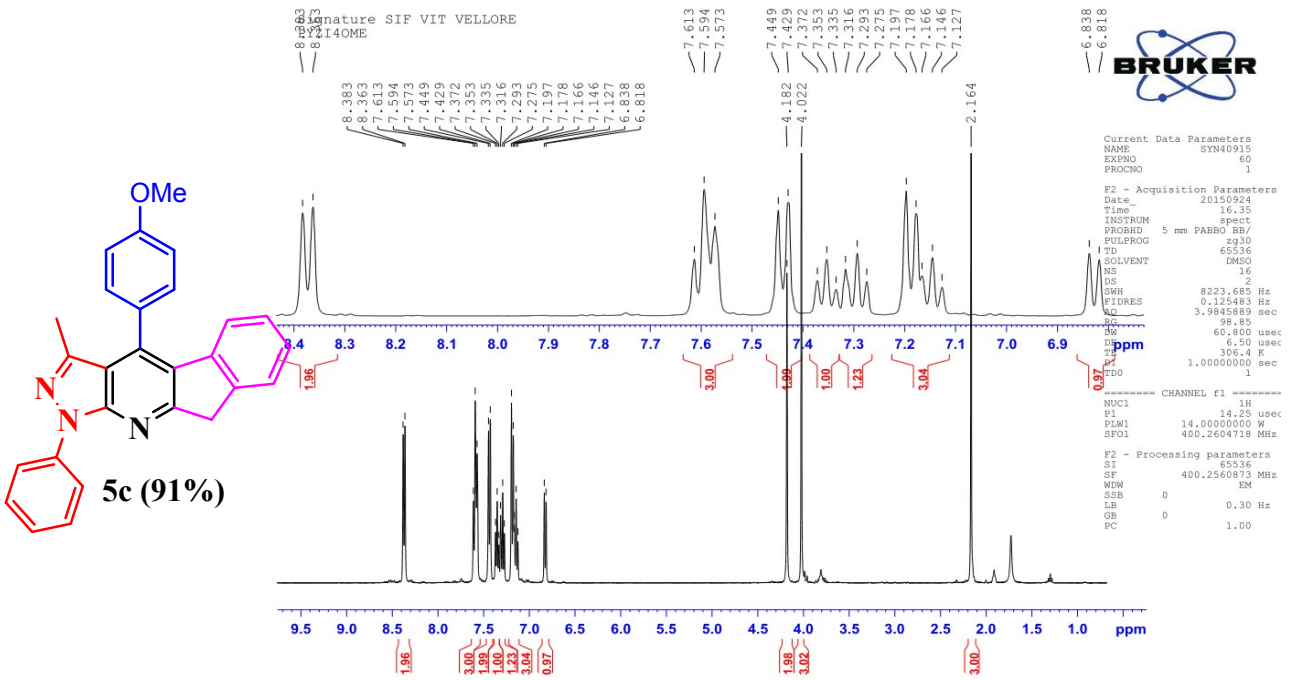
^{1}H NMR Data of Compound 5b:



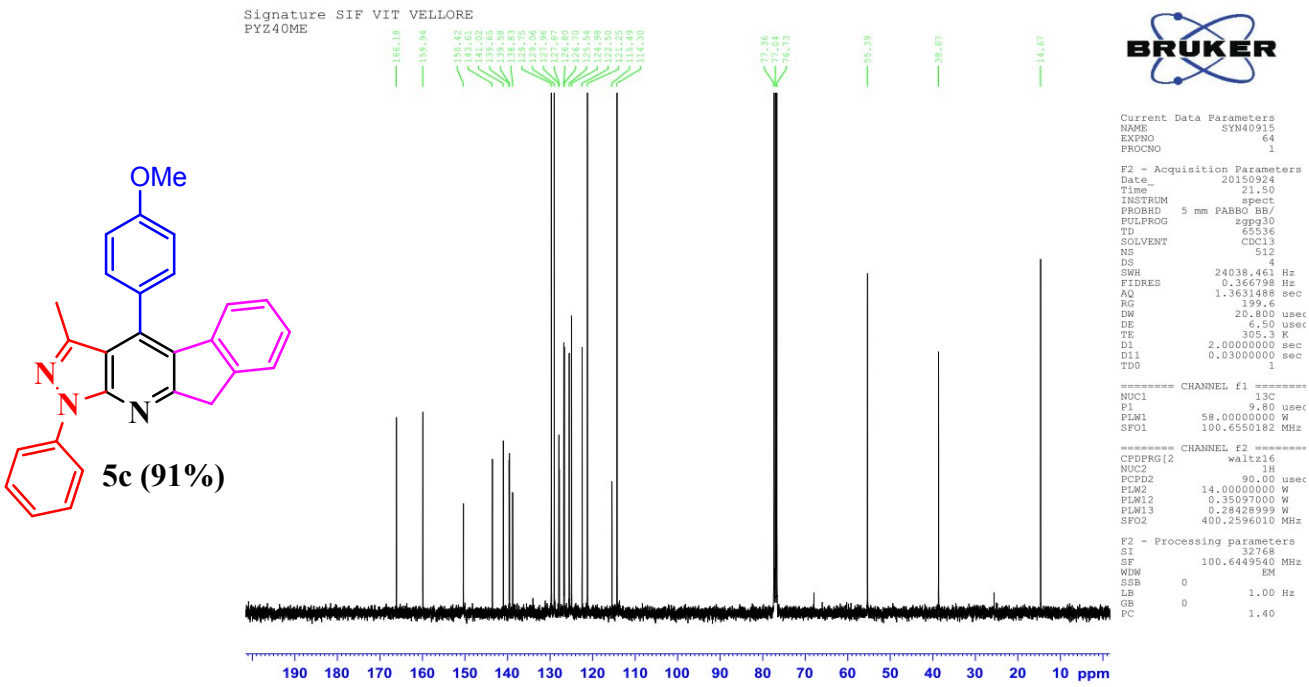
^{13}C NMR Data of Compound 5b:



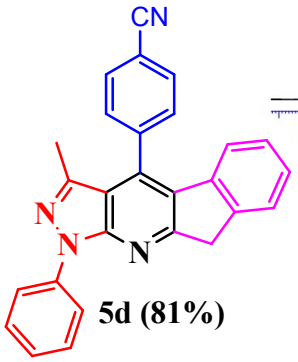
[1]H NMR Data of Compound 5c:



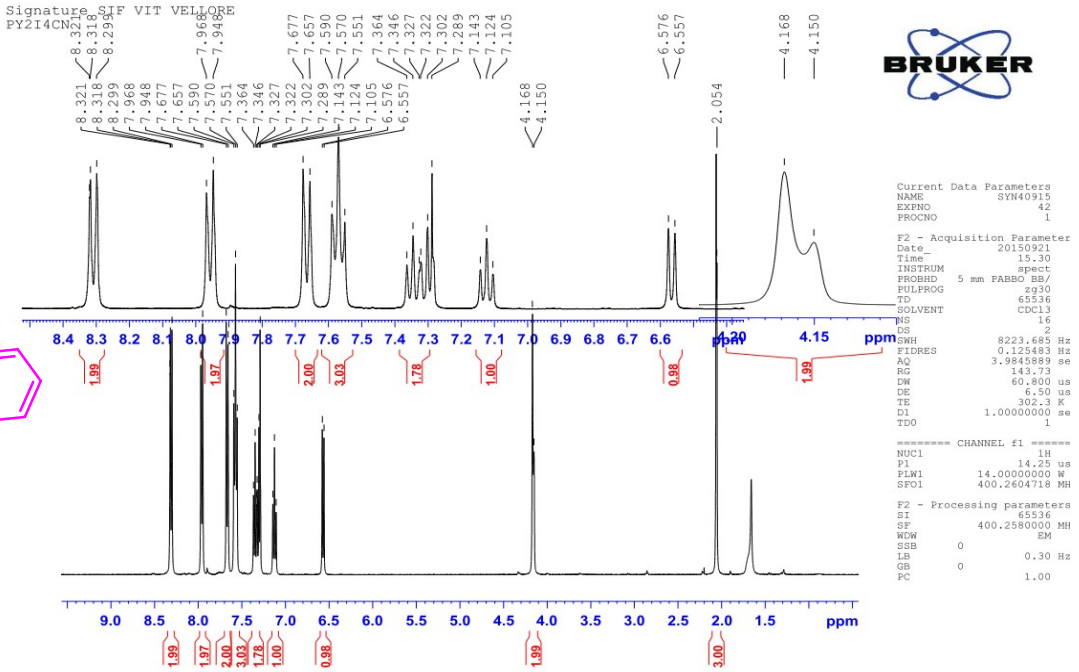
[13] C NMR Data of Compound 5c:



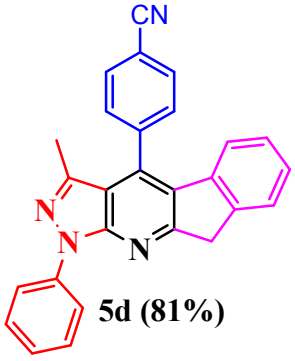
[1]H NMR Data of Compound 5d:



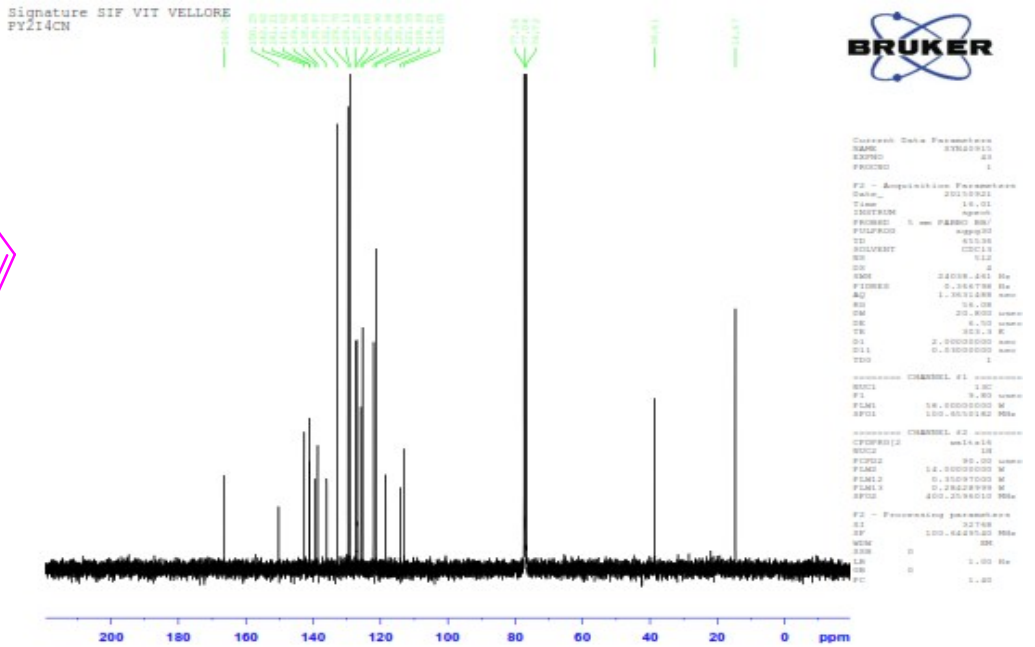
5d (81%)



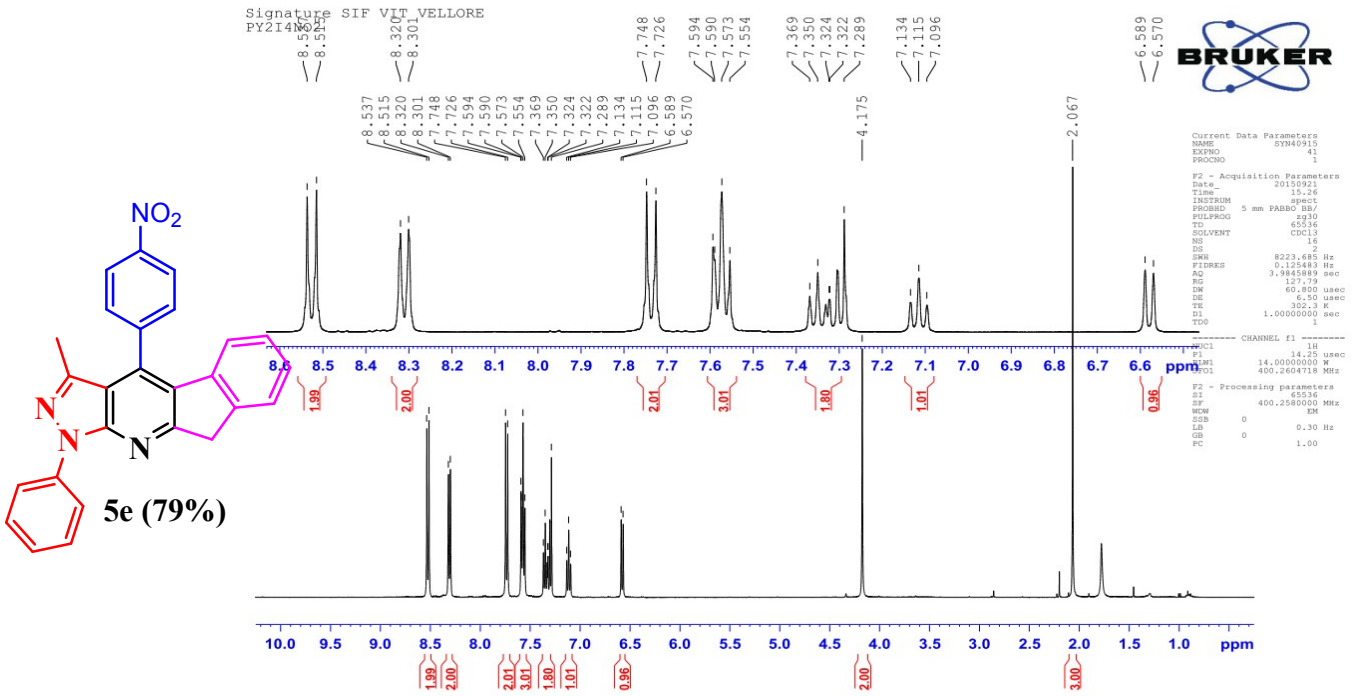
[13] C NMR Data of Compound 5d:



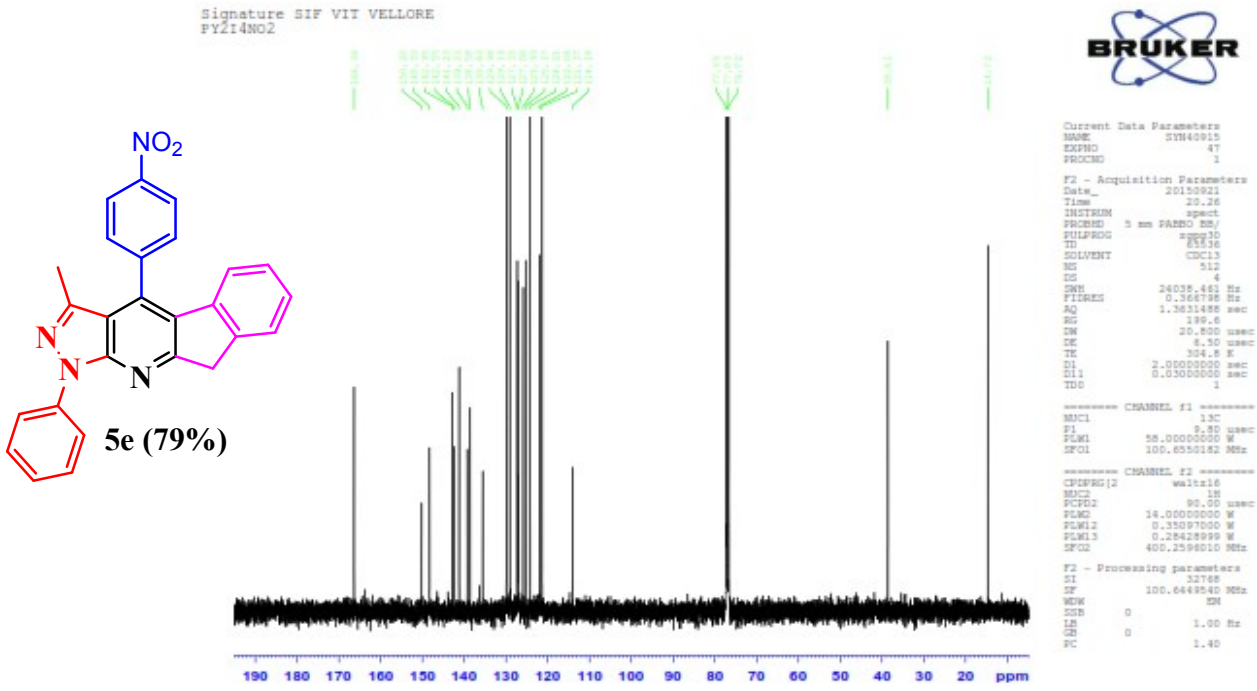
5d (81%)



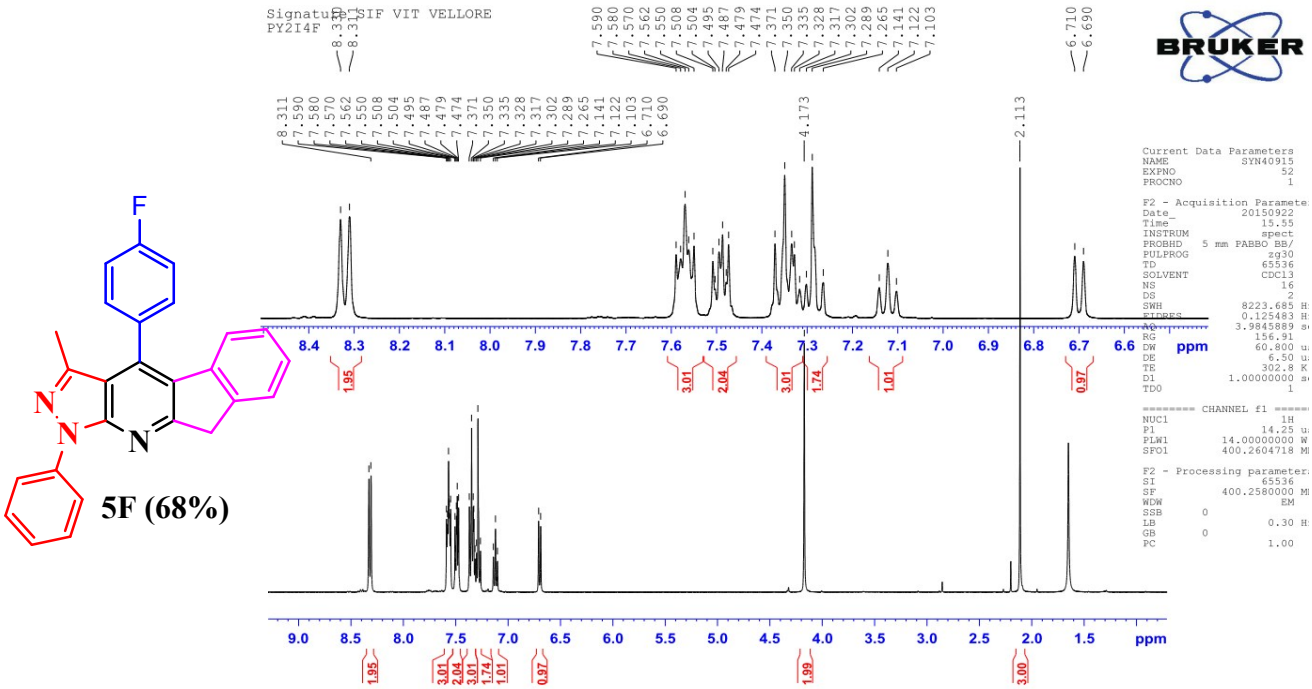
[1]H NMR Data of Compound 5e:



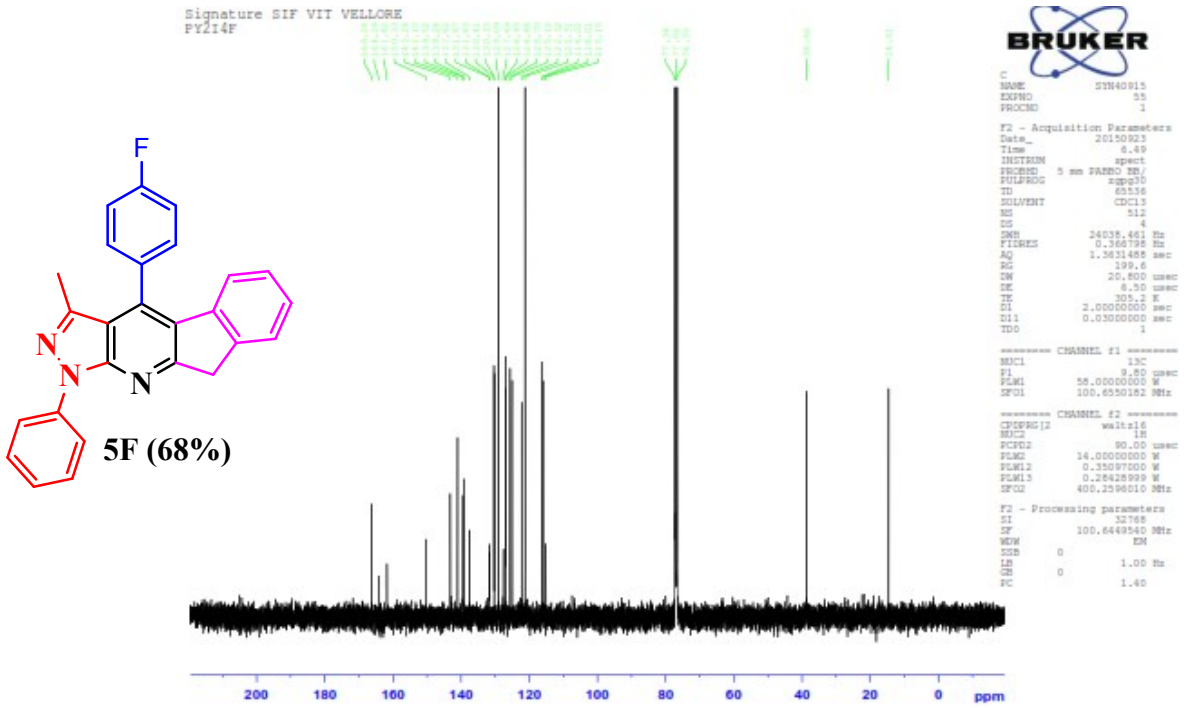
[13] C NMR Data of Compound 5e:



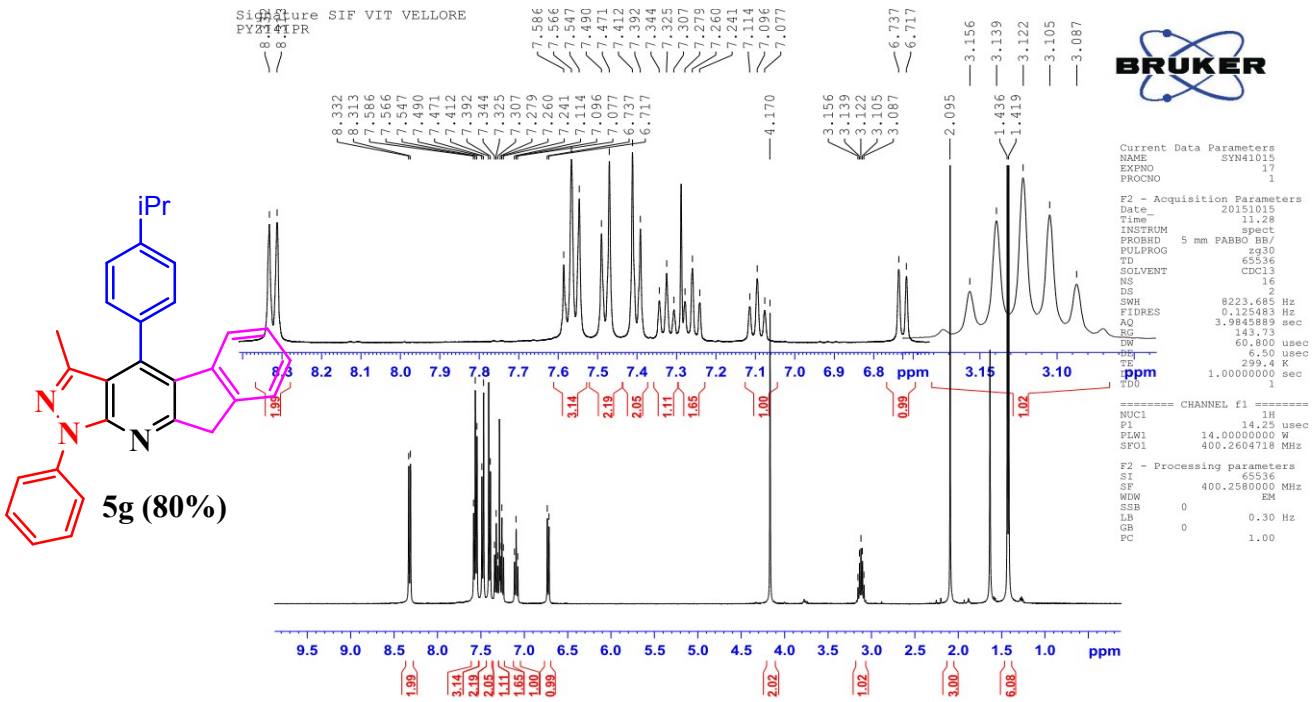
[1]H NMR Data of Compound 5f:



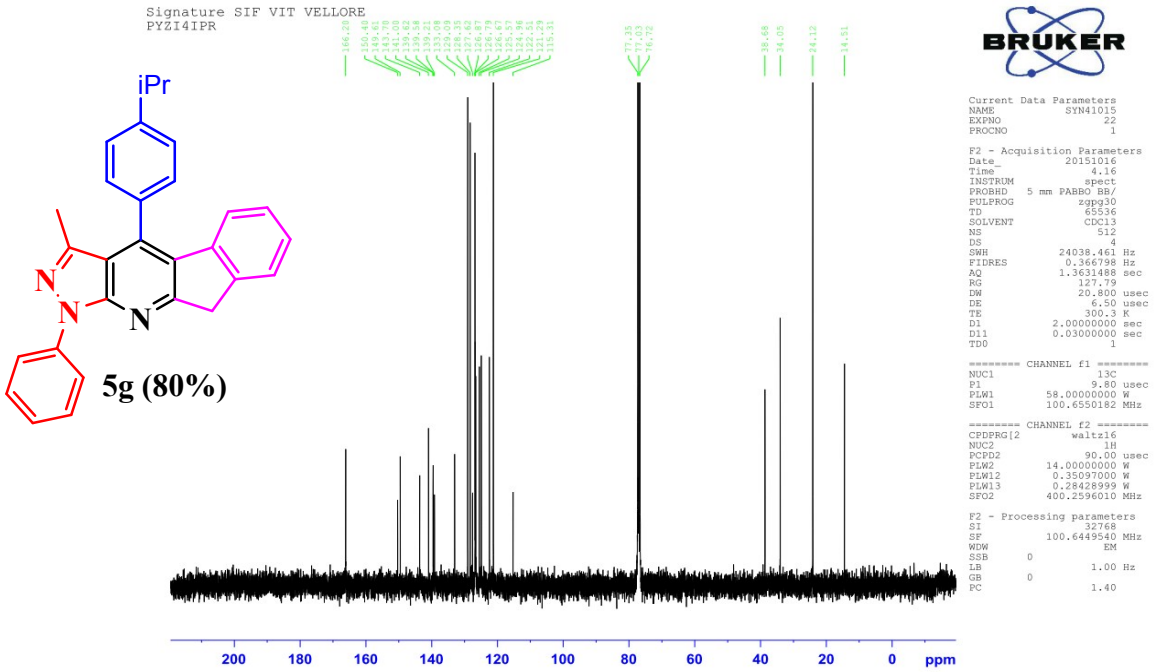
[13] C NMR Data of Compound 5f:



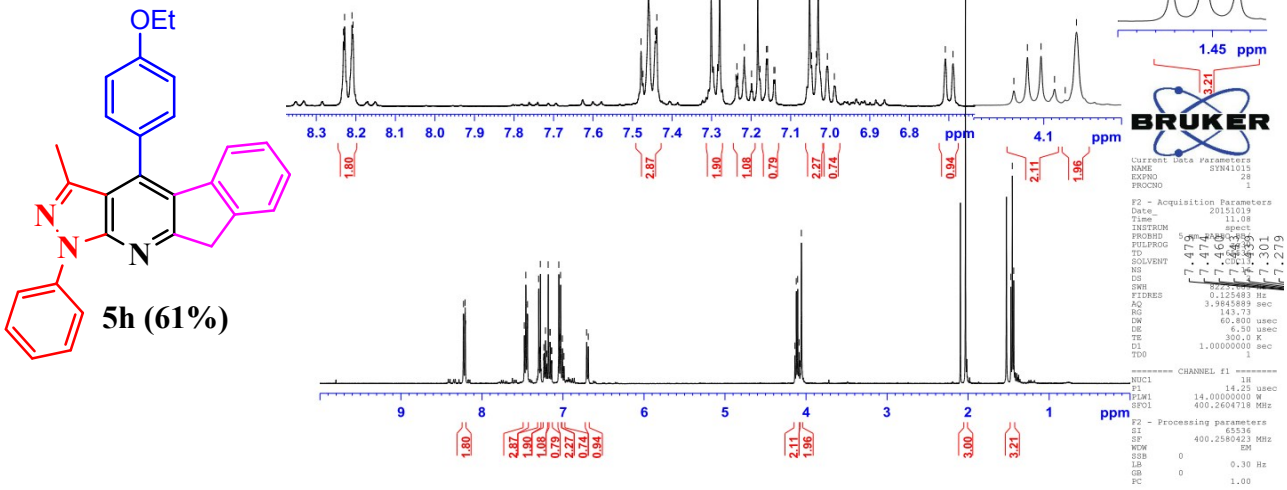
^{1}H NMR Data of Compound 5g:



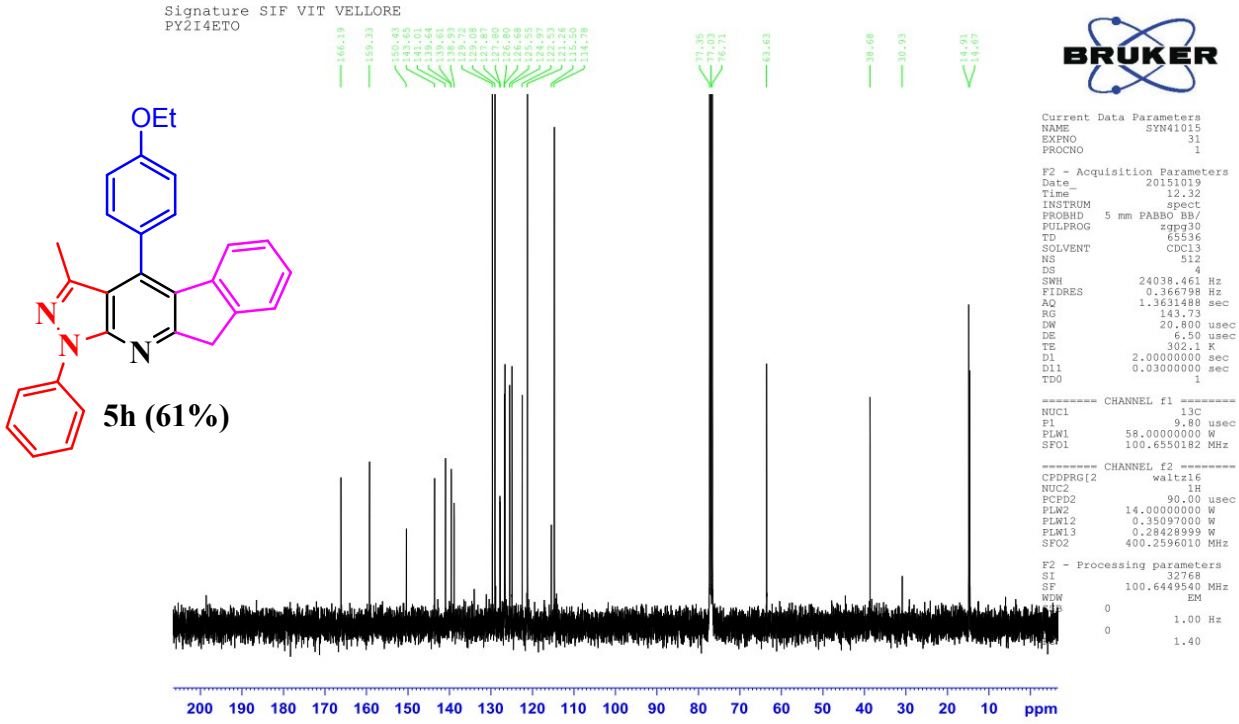
^{13}C NMR Data of Compound 5g:



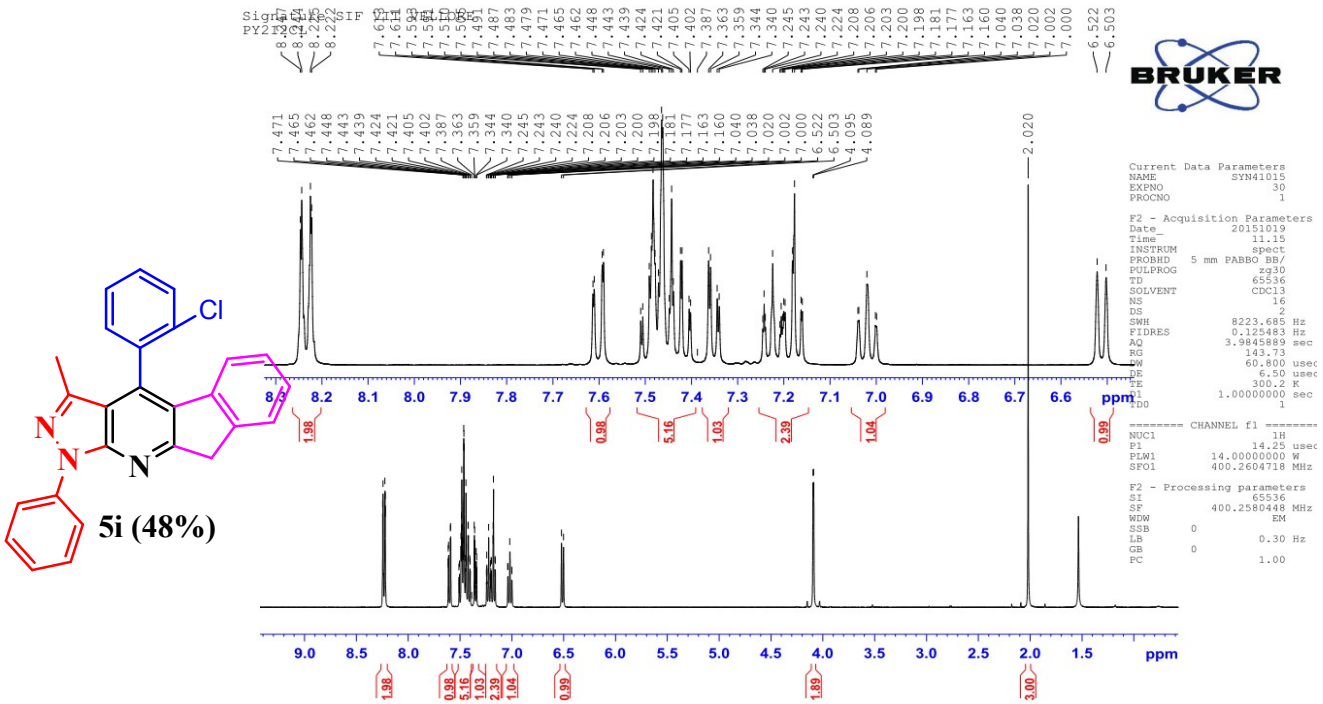
[1]H NMR Data of Compound 5h:



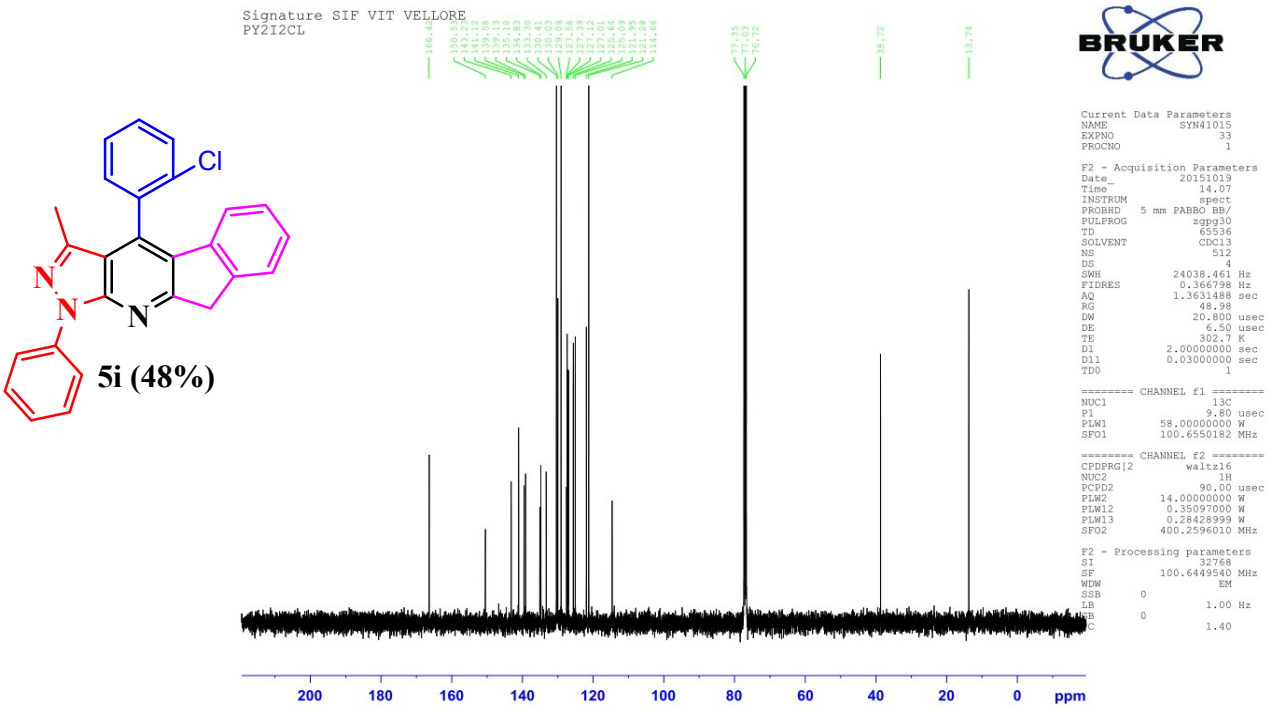
[13] C NMR Data of Compound 5h:



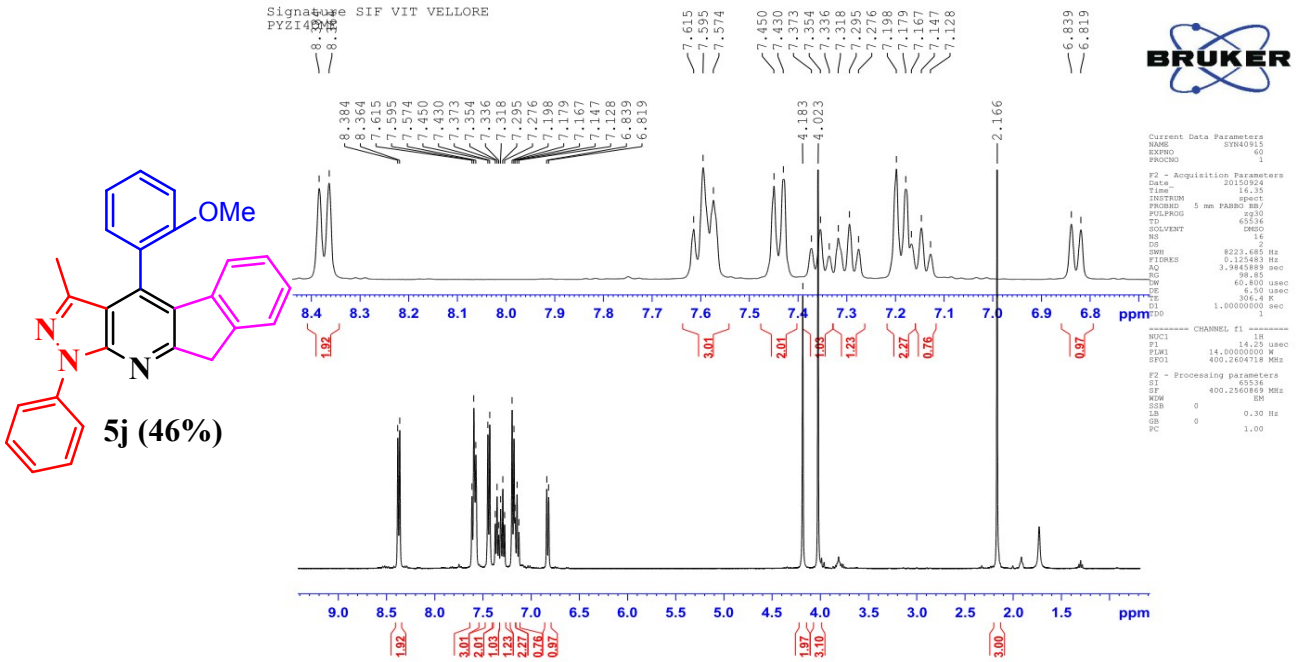
[1]H NMR Data of Compound 5i:



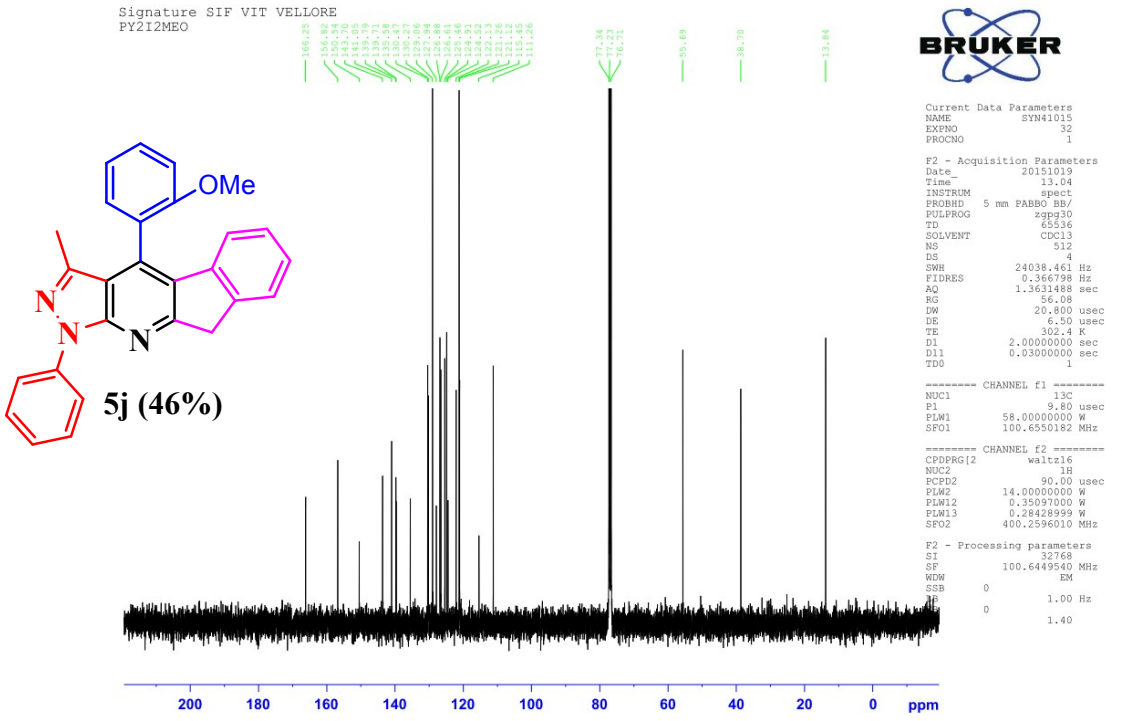
[13] C NMR Data of Compound 5i:



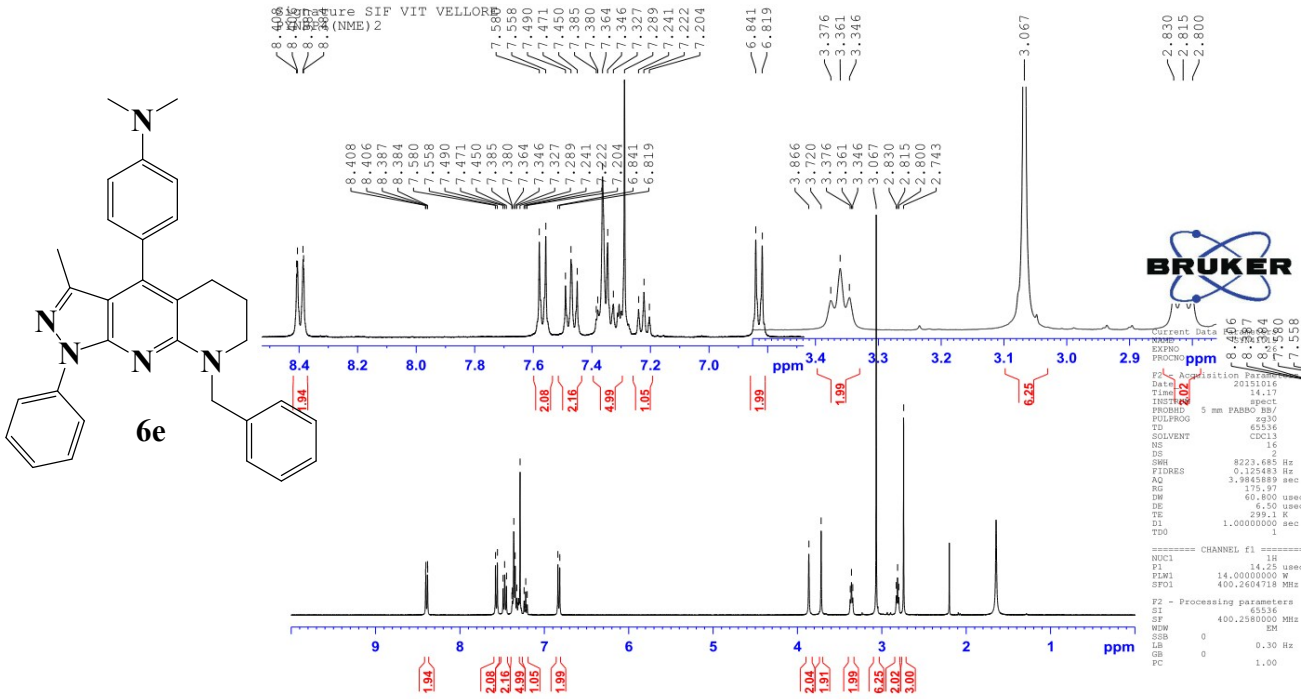
^{1}H NMR Data of Compound 5j:



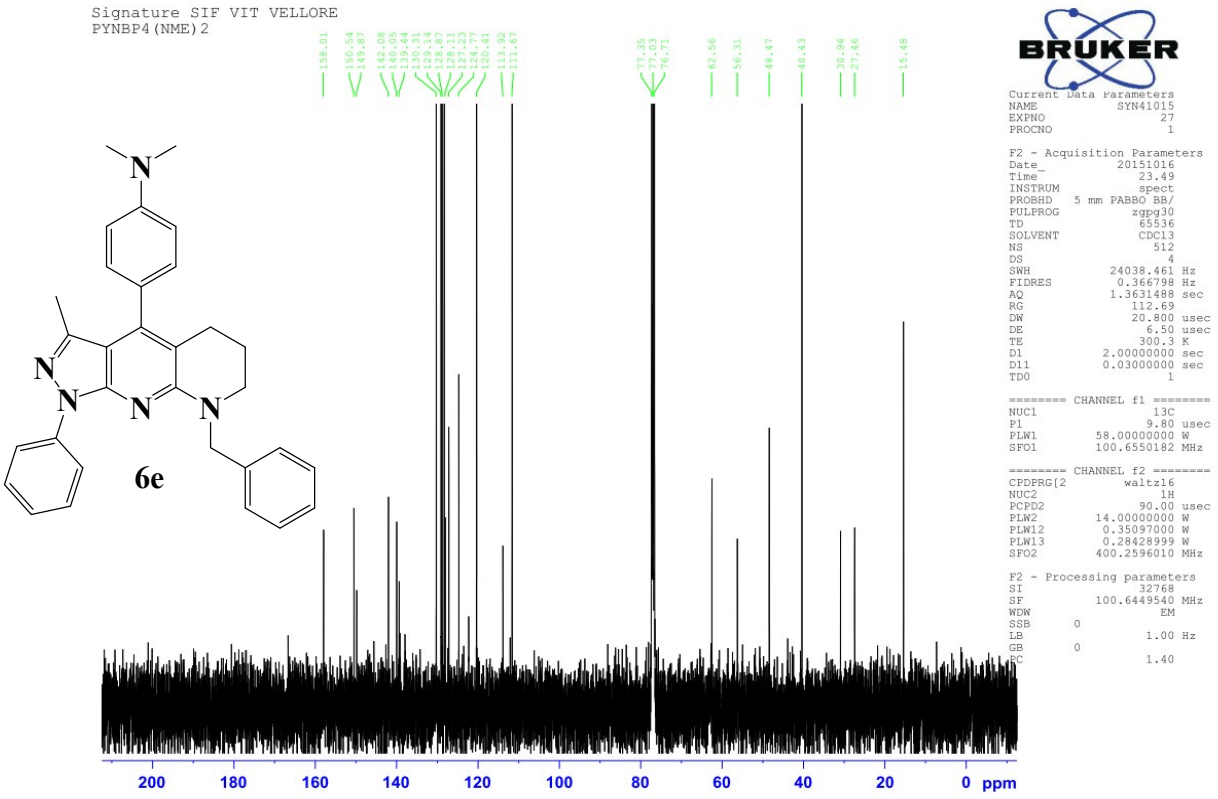
^{13}C NMR Data of Compound 5j:



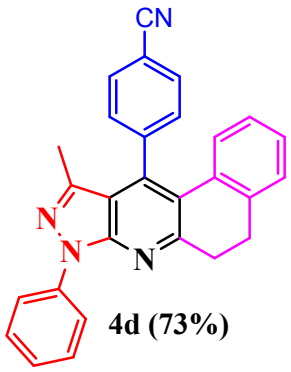
[1]H NMR Data of Compound 6e:



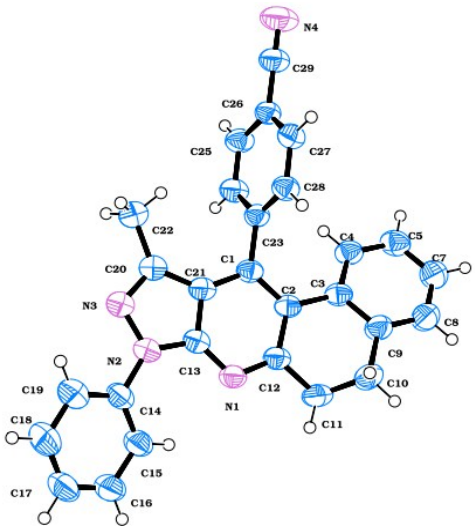
[13] C NMR Data of Compound 6e:



Single Crystal XRD Data for Compound 4d



4d (73%)



SI Table S4. Crystal data and structure refinement for **4d**

Identification code	**4d**	
Empirical formula	C28 H0 N4	
Formula weight	392.32	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.3474(3) Å	a= 95.021(3)°.
	b = 8.9699(4) Å	b= 95.805(2)°.
	c = 16.5075(7) Å	g = 91.637(2)°.
Volume	1077.43(8) $Å^3$	
Z	2	
Density (calculated)	1.209 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	392	
Theta range for data collection	1.245 to 27.110°.	
Index ranges	-9<=h<=9, -11<=k<=11, -21<=l<=21	
Reflections collected	23605	

Independent reflections	4661 [R(int) = 0.0405]
Completeness to theta = 25.242°	99.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4661 / 0 / 289
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0545, wR2 = 0.1492
R indices (all data)	R1 = 0.1060, wR2 = 0.1918
Extinction coefficient	n/a
Largest diff. peak and hole	0.334 and -0.226 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)
for BTCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3198(3)	56(2)	7530(1)	43(1)
C(2)	2193(3)	-1289(2)	7539(1)	44(1)
C(3)	2722(3)	-2519(2)	8053(1)	47(1)
C(4)	4522(3)	-2771(3)	8350(1)	52(1)
C(5)	4947(3)	-3900(3)	8839(2)	60(1)
C(7)	3580(4)	-4826(3)	9046(2)	65(1)
C(8)	1799(3)	-4633(3)	8744(2)	66(1)
C(9)	1351(3)	-3505(3)	8252(2)	56(1)
C(10)	-587(3)	-3343(3)	7896(2)	69(1)
C(11)	-598(3)	-2921(3)	7036(2)	68(1)
C(12)	510(3)	-1513(3)	7016(1)	48(1)
C(13)	844(3)	717(3)	6522(1)	46(1)
C(14)	-1113(3)	2164(3)	5527(1)	53(1)
C(15)	-2255(3)	1006(3)	5162(1)	59(1)
C(16)	-3715(3)	1319(4)	4612(2)	71(1)
C(17)	-4034(4)	2747(4)	4436(2)	83(1)
C(18)	-2892(4)	3891(4)	4800(2)	88(1)
C(19)	-1433(4)	3611(3)	5347(2)	71(1)

C(20)	3037(3)	2531(3)	6780(1)	55(1)
C(21)	2513(3)	1083(3)	6994(1)	47(1)
C(22)	4717(4)	3498(3)	7041(2)	73(1)
C(23)	4905(3)	499(2)	8083(1)	43(1)
C(24)	6590(3)	550(3)	7778(1)	52(1)
C(25)	8147(3)	989(3)	8281(1)	53(1)
C(26)	8048(3)	1396(2)	9100(1)	46(1)
C(27)	6365(3)	1372(3)	9409(1)	50(1)
C(28)	4810(3)	924(2)	8903(1)	47(1)
C(29)	9694(3)	1819(3)	9623(2)	58(1)
N(1)	-184(2)	-533(2)	6524(1)	48(1)
N(2)	430(2)	1899(2)	6079(1)	54(1)
N(3)	1788(3)	3003(2)	6241(1)	62(1)
N(4)	11026(3)	2130(3)	10025(2)	84(1)

Table 3. Bond lengths [Å] and angles [°] for 4d

C(1)-C(21)	1.402(3)
C(1)-C(2)	1.398(3)
C(1)-C(23)	1.496(3)
C(2)-C(12)	1.433(3)
C(2)-C(3)	1.486(3)
C(3)-C(4)	1.396(3)
C(3)-C(9)	1.405(3)
C(4)-C(5)	1.373(3)
C(4)-H(4)	0.9300
C(5)-C(7)	1.373(4)
C(5)-H(5)	0.9300
C(7)-C(8)	1.374(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.378(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.501(3)
C(10)-C(11)	1.500(4)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700

C(11)-C(12)	1.489(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-N(1)	1.327(3)
C(13)-N(1)	1.334(3)
C(13)-N(2)	1.363(3)
C(13)-C(21)	1.399(3)
C(14)-C(15)	1.373(3)
C(14)-C(19)	1.378(4)
C(14)-N(2)	1.420(3)
C(15)-C(16)	1.385(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.360(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.364(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.374(4)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-N(3)	1.317(3)
C(20)-C(21)	1.428(3)
C(20)-C(22)	1.493(3)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-C(28)	1.383(3)
C(23)-C(24)	1.385(3)
C(24)-C(25)	1.370(3)
C(24)-H(24)	0.9300
C(25)-C(26)	1.378(3)
C(25)-H(25)	0.9300
C(26)-C(27)	1.385(3)
C(26)-C(29)	1.435(3)
C(27)-C(28)	1.374(3)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300

C(29)-N(4)	1.139(3)
N(2)-N(3)	1.375(3)

C(21)-C(1)-C(2)	117.68(18)
C(21)-C(1)-C(23)	117.96(19)
C(2)-C(1)-C(23)	124.30(19)
C(1)-C(2)-C(12)	118.1(2)
C(1)-C(2)-C(3)	125.25(18)
C(12)-C(2)-C(3)	116.69(19)
C(4)-C(3)-C(9)	117.1(2)
C(4)-C(3)-C(2)	123.9(2)
C(9)-C(3)-C(2)	119.03(19)
C(5)-C(4)-C(3)	122.0(2)
C(5)-C(4)-H(4)	119.0
C(3)-C(4)-H(4)	119.0
C(4)-C(5)-C(7)	119.9(2)
C(4)-C(5)-H(5)	120.0
C(7)-C(5)-H(5)	120.0
C(8)-C(7)-C(5)	119.5(2)
C(8)-C(7)-H(7)	120.3
C(5)-C(7)-H(7)	120.3
C(7)-C(8)-C(9)	121.2(2)
C(7)-C(8)-H(8)	119.4
C(9)-C(8)-H(8)	119.4
C(8)-C(9)-C(3)	120.2(2)
C(8)-C(9)-C(10)	120.9(2)
C(3)-C(9)-C(10)	118.9(2)
C(11)-C(10)-C(9)	109.5(2)
C(11)-C(10)-H(10A)	109.8
C(9)-C(10)-H(10A)	109.8
C(11)-C(10)-H(10B)	109.8
C(9)-C(10)-H(10B)	109.8
H(10A)-C(10)-H(10B)	108.2
C(12)-C(11)-C(10)	110.6(2)
C(12)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11A)	109.5

C(12)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
N(1)-C(12)-C(2)	125.0(2)
N(1)-C(12)-C(11)	116.38(19)
C(2)-C(12)-C(11)	118.6(2)
N(1)-C(13)-N(2)	126.25(19)
N(1)-C(13)-C(21)	126.5(2)
N(2)-C(13)-C(21)	107.25(19)
C(15)-C(14)-C(19)	120.0(2)
C(15)-C(14)-N(2)	121.2(2)
C(19)-C(14)-N(2)	118.8(2)
C(14)-C(15)-C(16)	119.0(3)
C(14)-C(15)-H(15)	120.5
C(16)-C(15)-H(15)	120.5
C(17)-C(16)-C(15)	121.1(3)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(16)-C(17)-C(18)	119.6(3)
C(16)-C(17)-H(17)	120.2
C(18)-C(17)-H(17)	120.2
C(17)-C(18)-C(19)	120.4(3)
C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(18)-C(19)-C(14)	119.9(3)
C(18)-C(19)-H(19)	120.0
C(14)-C(19)-H(19)	120.0
N(3)-C(20)-C(21)	110.4(2)
N(3)-C(20)-C(22)	118.5(2)
C(21)-C(20)-C(22)	131.0(2)
C(13)-C(21)-C(1)	118.0(2)
C(13)-C(21)-C(20)	104.73(19)
C(1)-C(21)-C(20)	137.27(19)
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5

C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(28)-C(23)-C(24)	118.89(19)
C(28)-C(23)-C(1)	120.28(18)
C(24)-C(23)-C(1)	120.79(19)
C(25)-C(24)-C(23)	120.7(2)
C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(24)-C(25)-C(26)	120.2(2)
C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(25)-C(26)-C(27)	119.65(19)
C(25)-C(26)-C(29)	119.5(2)
C(27)-C(26)-C(29)	120.8(2)
C(28)-C(27)-C(26)	119.9(2)
C(28)-C(27)-H(27)	120.0
C(26)-C(27)-H(27)	120.0
C(27)-C(28)-C(23)	120.6(2)
C(27)-C(28)-H(28)	119.7
C(23)-C(28)-H(28)	119.7
N(4)-C(29)-C(26)	178.2(3)
C(12)-N(1)-C(13)	114.78(18)
C(13)-N(2)-N(3)	110.26(17)
C(13)-N(2)-C(14)	131.7(2)
N(3)-N(2)-C(14)	118.05(19)
C(20)-N(3)-N(2)	107.3(2)

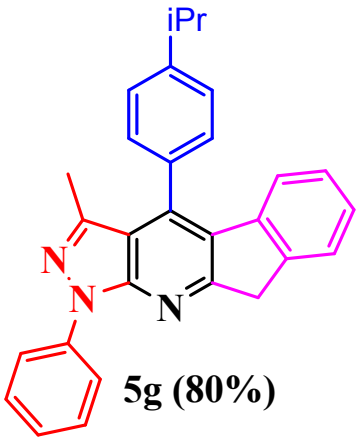
Symmetry transformations used to generate equivalent atoms:

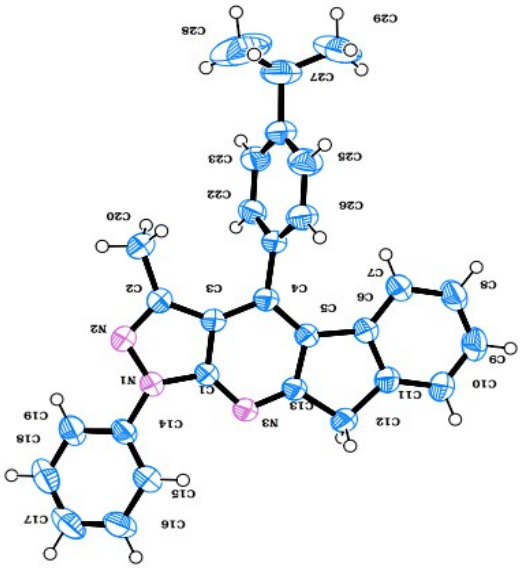
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 4d. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(1)	51(1)	42(1)	-1(1)	4(1)	2(1)

C(2)	36(1)	48(1)	47(1)	1(1)	2(1)	2(1)
C(3)	38(1)	50(1)	53(1)	1(1)	2(1)	3(1)
C(4)	40(1)	51(1)	63(2)	5(1)	1(1)	4(1)
C(5)	49(1)	59(2)	69(2)	5(1)	-4(1)	11(1)
C(7)	64(2)	59(2)	74(2)	17(1)	-3(1)	6(1)
C(8)	57(2)	61(2)	80(2)	19(1)	2(1)	-4(1)
C(9)	43(1)	54(1)	70(2)	11(1)	0(1)	-1(1)
C(10)	41(1)	74(2)	94(2)	31(2)	-4(1)	-9(1)
C(11)	53(1)	64(2)	82(2)	10(1)	-17(1)	-15(1)
C(12)	40(1)	54(1)	49(1)	3(1)	-1(1)	0(1)
C(13)	43(1)	52(1)	43(1)	2(1)	0(1)	3(1)
C(14)	46(1)	71(2)	41(1)	11(1)	1(1)	5(1)
C(15)	54(1)	78(2)	45(1)	10(1)	-2(1)	-2(1)
C(16)	57(2)	102(2)	53(2)	17(2)	-5(1)	-11(2)
C(17)	57(2)	118(3)	76(2)	42(2)	-12(1)	1(2)
C(18)	73(2)	95(2)	97(2)	38(2)	-14(2)	11(2)
C(19)	65(2)	73(2)	73(2)	16(1)	-8(1)	5(1)
C(20)	52(1)	57(2)	53(1)	6(1)	-2(1)	-6(1)
C(21)	41(1)	53(1)	45(1)	1(1)	1(1)	-2(1)
C(22)	71(2)	66(2)	78(2)	16(1)	-15(1)	-19(1)
C(23)	38(1)	44(1)	46(1)	4(1)	1(1)	1(1)
C(24)	43(1)	67(2)	44(1)	-3(1)	4(1)	-1(1)
C(25)	40(1)	67(2)	51(1)	0(1)	6(1)	-4(1)
C(26)	40(1)	47(1)	49(1)	5(1)	-4(1)	-1(1)
C(27)	50(1)	56(1)	43(1)	0(1)	1(1)	2(1)
C(28)	40(1)	54(1)	49(1)	4(1)	5(1)	3(1)
C(29)	48(1)	67(2)	57(1)	0(1)	-4(1)	-3(1)
N(1)	40(1)	57(1)	47(1)	3(1)	-1(1)	-2(1)
N(2)	47(1)	60(1)	52(1)	10(1)	-7(1)	-3(1)
N(3)	58(1)	62(1)	64(1)	14(1)	-10(1)	-8(1)
N(4)	59(1)	111(2)	75(2)	-6(1)	-14(1)	-12(1)

Single Crystal XRD Data for Compound 5g





SI Table S5. Crystal data and structure refinement for **5g**.

Identification code	**5g**	
Empirical formula	C58 H48 N6	
Formula weight	829.02	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 18.1618(6) Å	□= 90°.
	b = 12.4595(4) Å	□= 101.4420(10)°.
	c = 20.2872(8) Å	□ = 90°.
Volume	4499.5(3) $Å^3$	
Z	4	
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	1752	
Theta range for data collection	1.995 to 29.772°.	
Index ranges	-24<=h<=24, -17<=k<=17, -26<=l<=28	
Reflections collected	26026	
Independent reflections	5742 [R(int) = 0.0325]	

Completeness to theta = 25.242°	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5742 / 0 / 292
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0568, wR2 = 0.1507
R indices (all data)	R1 = 0.1008, wR2 = 0.1831
Extinction coefficient	n/a
Largest diff. peak and hole	0.383 and -0.220 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)
for pq. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4111(1)	926(1)	6900(1)	42(1)
C(2)	3688(1)	1967(1)	7649(1)	45(1)
C(3)	3812(1)	872(1)	7485(1)	41(1)
C(4)	3697(1)	-141(1)	7755(1)	41(1)
C(5)	3870(1)	-1010(1)	7386(1)	41(1)
C(6)	3845(1)	-2186(1)	7489(1)	45(1)
C(7)	3646(1)	-2800(2)	7996(1)	57(1)
C(8)	3685(1)	-3913(2)	7956(1)	67(1)
C(9)	3916(1)	-4409(2)	7426(1)	68(1)
C(10)	4115(1)	-3804(2)	6919(1)	61(1)
C(11)	4086(1)	-2697(1)	6955(1)	49(1)
C(12)	4300(1)	-1888(1)	6477(1)	52(1)
C(13)	4160(1)	-842(1)	6794(1)	43(1)
C(14)	4460(1)	2483(1)	6225(1)	47(1)
C(15)	4417(1)	1966(2)	5618(1)	58(1)
C(16)	4702(1)	2451(2)	5112(1)	69(1)
C(17)	5028(1)	3451(2)	5209(1)	77(1)
C(18)	5061(1)	3966(2)	5809(1)	72(1)
C(19)	4785(1)	3491(2)	6325(1)	60(1)
C(20)	3332(1)	2422(2)	8190(1)	59(1)

C(21)	3422(1)	-222(1)	8397(1)	42(1)
C(22)	3857(1)	176(2)	8987(1)	50(1)
C(23)	3586(1)	192(2)	9573(1)	55(1)
C(24)	2877(1)	-189(2)	9597(1)	58(1)
C(25)	2456(1)	-620(2)	9012(1)	63(1)
C(26)	2721(1)	-641(2)	8419(1)	54(1)
C(27)	2592(2)	-110(2)	10253(1)	84(1)
C(28)	2034(3)	779(4)	10214(2)	167(2)
C(29)	2321(2)	-1161(3)	10471(2)	136(1)
N(1)	4173(1)	1994(1)	6753(1)	48(1)
N(2)	3908(1)	2623(1)	7215(1)	51(1)
N(3)	4298(1)	101(1)	6540(1)	45(1)

_Table 3. Bond lengths [Å] and angles [°] for pq.

C(1)-N(3)	1.342(2)
C(1)-N(1)	1.373(2)
C(1)-C(3)	1.402(2)
C(2)-N(2)	1.320(2)
C(2)-C(3)	1.433(2)
C(2)-C(20)	1.493(2)
C(3)-C(4)	1.408(2)
C(4)-C(5)	1.388(2)
C(4)-C(21)	1.488(2)
C(5)-C(13)	1.419(2)
C(5)-C(6)	1.481(2)
C(6)-C(7)	1.387(2)
C(6)-C(11)	1.399(2)
C(7)-C(8)	1.392(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.377(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.380(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.383(3)
C(10)-H(10)	0.9300

C(11)-C(12)	1.504(3)
C(12)-C(13)	1.499(2)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-N(3)	1.326(2)
C(14)-C(15)	1.379(3)
C(14)-C(19)	1.385(3)
C(14)-N(1)	1.419(2)
C(15)-C(16)	1.378(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.376(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.367(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.379(3)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-C(26)	1.384(3)
C(21)-C(22)	1.388(2)
C(22)-C(23)	1.375(3)
C(22)-H(22)	0.9300
C(23)-C(24)	1.382(3)
C(23)-H(23)	0.9300
C(24)-C(25)	1.385(3)
C(24)-C(27)	1.523(3)
C(25)-C(26)	1.382(3)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-C(28)	1.491(4)
C(27)-C(29)	1.497(4)
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600

C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
N(1)-N(2)	1.379(2)

N(3)-C(1)-N(1)	125.77(15)
N(3)-C(1)-C(3)	127.28(15)
N(1)-C(1)-C(3)	106.94(14)
N(2)-C(2)-C(3)	110.63(15)
N(2)-C(2)-C(20)	119.24(16)
C(3)-C(2)-C(20)	130.06(16)
C(1)-C(3)-C(4)	119.03(14)
C(1)-C(3)-C(2)	104.84(14)
C(4)-C(3)-C(2)	136.12(16)
C(5)-C(4)-C(3)	114.97(15)
C(5)-C(4)-C(21)	124.81(14)
C(3)-C(4)-C(21)	120.21(14)
C(4)-C(5)-C(13)	120.18(15)
C(4)-C(5)-C(6)	132.75(16)
C(13)-C(5)-C(6)	107.02(14)
C(7)-C(6)-C(11)	119.34(17)
C(7)-C(6)-C(5)	132.11(17)
C(11)-C(6)-C(5)	108.54(15)
C(6)-C(7)-C(8)	118.89(19)
C(6)-C(7)-H(7)	120.6
C(8)-C(7)-H(7)	120.6
C(9)-C(8)-C(7)	121.3(2)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(8)-C(9)-C(10)	120.21(19)
C(8)-C(9)-H(9)	119.9
C(10)-C(9)-H(9)	119.9
C(9)-C(10)-C(11)	119.12(19)
C(9)-C(10)-H(10)	120.4
C(11)-C(10)-H(10)	120.4
C(10)-C(11)-C(6)	121.12(17)

C(10)-C(11)-C(12)	128.05(17)
C(6)-C(11)-C(12)	110.83(15)
C(13)-C(12)-C(11)	102.54(14)
C(13)-C(12)-H(12A)	111.3
C(11)-C(12)-H(12A)	111.3
C(13)-C(12)-H(12B)	111.3
C(11)-C(12)-H(12B)	111.3
H(12A)-C(12)-H(12B)	109.2
N(3)-C(13)-C(5)	126.22(15)
N(3)-C(13)-C(12)	122.77(15)
C(5)-C(13)-C(12)	111.02(14)
C(15)-C(14)-C(19)	120.11(18)
C(15)-C(14)-N(1)	120.62(17)
C(19)-C(14)-N(1)	119.27(17)
C(16)-C(15)-C(14)	119.8(2)
C(16)-C(15)-H(15)	120.1
C(14)-C(15)-H(15)	120.1
C(17)-C(16)-C(15)	120.4(2)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	119.6(2)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(17)-C(18)-C(19)	121.1(2)
C(17)-C(18)-H(18)	119.5
C(19)-C(18)-H(18)	119.5
C(18)-C(19)-C(14)	119.1(2)
C(18)-C(19)-H(19)	120.5
C(14)-C(19)-H(19)	120.5
C(2)-C(20)-H(20A)	109.5
C(2)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(26)-C(21)-C(22)	118.47(16)

C(26)-C(21)-C(4)	121.67(16)
C(22)-C(21)-C(4)	119.80(15)
C(23)-C(22)-C(21)	120.68(17)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	121.44(18)
C(22)-C(23)-H(23)	119.3
C(24)-C(23)-H(23)	119.3
C(23)-C(24)-C(25)	117.54(17)
C(23)-C(24)-C(27)	119.29(19)
C(25)-C(24)-C(27)	123.2(2)
C(26)-C(25)-C(24)	121.63(18)
C(26)-C(25)-H(25)	119.2
C(24)-C(25)-H(25)	119.2
C(25)-C(26)-C(21)	120.16(18)
C(25)-C(26)-H(26)	119.9
C(21)-C(26)-H(26)	119.9
C(28)-C(27)-C(29)	113.9(3)
C(28)-C(27)-C(24)	110.3(2)
C(29)-C(27)-C(24)	113.0(2)
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(1)-N(1)-N(2)	110.46(13)
C(1)-N(1)-C(14)	129.59(15)
N(2)-N(1)-C(14)	119.95(14)
C(2)-N(2)-N(1)	107.10(14)

C(13)-N(3)-C(1) 112.25(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 5g. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	51(1)	37(1)	38(1)	3(1)	13(1)	1(1)
C(2)	55(1)	40(1)	42(1)	-2(1)	13(1)	1(1)
C(3)	48(1)	39(1)	36(1)	0(1)	11(1)	0(1)
C(4)	45(1)	41(1)	37(1)	1(1)	10(1)	1(1)
C(5)	48(1)	38(1)	38(1)	3(1)	11(1)	2(1)
C(6)	52(1)	40(1)	44(1)	3(1)	12(1)	2(1)
C(7)	74(1)	45(1)	57(1)	7(1)	26(1)	2(1)
C(8)	85(2)	45(1)	78(2)	14(1)	33(1)	2(1)
C(9)	85(2)	37(1)	84(2)	5(1)	24(1)	5(1)
C(10)	83(1)	39(1)	64(1)	-1(1)	22(1)	7(1)
C(11)	61(1)	40(1)	46(1)	2(1)	13(1)	5(1)
C(12)	71(1)	42(1)	44(1)	0(1)	19(1)	10(1)
C(13)	53(1)	40(1)	37(1)	3(1)	12(1)	5(1)
C(14)	55(1)	42(1)	45(1)	11(1)	15(1)	5(1)
C(15)	76(1)	52(1)	51(1)	8(1)	21(1)	-3(1)
C(16)	89(2)	72(2)	53(1)	15(1)	30(1)	7(1)
C(17)	82(2)	77(2)	78(2)	37(1)	34(1)	5(1)
C(18)	81(2)	52(1)	87(2)	22(1)	23(1)	-5(1)
C(19)	69(1)	48(1)	64(1)	11(1)	17(1)	0(1)
C(20)	82(1)	47(1)	55(1)	-6(1)	28(1)	7(1)
C(21)	51(1)	39(1)	37(1)	1(1)	14(1)	1(1)
C(22)	56(1)	54(1)	42(1)	1(1)	11(1)	-9(1)
C(23)	69(1)	59(1)	38(1)	-2(1)	11(1)	-6(1)
C(24)	73(1)	60(1)	45(1)	-1(1)	24(1)	5(1)
C(25)	54(1)	77(1)	64(1)	-5(1)	26(1)	-9(1)
C(26)	54(1)	63(1)	45(1)	-8(1)	15(1)	-7(1)
C(27)	96(2)	106(2)	64(2)	-4(1)	46(1)	4(2)

C(28)	188(4)	211(5)	127(3)	-14(3)	91(3)	91(4)
C(29)	176(3)	159(3)	103(2)	-3(2)	97(3)	-45(3)
N(1)	65(1)	37(1)	45(1)	3(1)	20(1)	2(1)
N(2)	68(1)	38(1)	48(1)	-3(1)	20(1)	3(1)
N(3)	59(1)	40(1)	39(1)	4(1)	17(1)	4(1)