Supplemental Information

Combining two distinctive intermolecular forces in designing ternary co-crystals and molecular salts of 1,3,5-trinitrobenzene, 9-anthracenecarboxylic acid and ten substituted pyridines.

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Experimental

All reagents used for synthesis and characterization were of analytical grade, purchased from Sigma-Aldrich, unless otherwise stated. Reagents were used as received, without further purification.

The general synthesis for the multi-component crystals is similar to the one given for compound **1**: 0.01 g TNB (0.046 mmol), 0.01 g 9-anthracene carboxylic acid (0.044 mmol) and 0.004 g pyridine (0.046 mmol) were dissolved in EtOH (60 °C) and stirred for 4 hrs. The solutions were filtered and allowed to crystallize via slow evaporation. Table S1 lists the respective masses for the substituted pyridines for **1**-**11**. Yields recorded were between 70 and 80%.

Table S1 Experimental masses of the substituted pyridine component

		mass (0.046 mmol)
1	$2NH_2py$	4 mg
2	$3NH_2py$	4 mg
3	$4NH_2py$	4 mg
4	$6Br\text{-}3NH_2py$	8 mg
5	$3Br\text{-}2NH_2py$	8 mg
6	$5Br\text{-}2NH_2py$	8 mg
7	$5Cl\text{-}2NH_2py$	6 mg
8	$3NO_2\text{-}2NH_2py$	6 mg
9	$5NO_2\text{-}2NH_2py$	6 mg
10	2,2'-bipy	7 mg

Figure S1 The ternary complexes arranged visually according to colour from yellow to red.

Elemental Analysis

Sample Reference **1**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	58.98	3.62	13.23		**59.08**	**3.653**	**13.15**	

Sample Reference **2**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	59.07	2.43	11.73		**58.84**	**3.314**	**11.79**	

Sample Reference **3**

Run no.	Expected values (%)				Results (%)			
	C	H	N	S	C	H	N	S
1	57.04	3.87	12.79		**57.27**	**3.828**	**12.38**	

Sample Reference **4**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	51.33	2.98	11.51		**51.16**	**2.838**	**12.58**	

Sample Reference **5**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	51.33	2.98	11.51		**51.16**	**2.474**	**11.06**	

Sample Reference **6**

Run no.	Expected values (%)	Results (%)

	C	H	N		C	H	N	
1	51.33	2.98	11.51		**51.48**	**2.439**	**10.65**	

Sample Reference **7**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	55.38	3.16	12.42		**55.10**	**3.263**	**12.65**	

Sample Reference **8**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	54.36	3.16	14.63		**54.38**	**3.055**	**14.21**	

Sample Reference **9**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	54.36	3.16	14.63		**54.62**	**2.744**	**14.65**	

Sample Reference **10**

Run no.	Expected values (%)				Results (%)			
	C	H	N		C	H	N	
1	62.95	3.58	11.84		**63.24**	**3.295**	**12.89**	

Crystallographic data for complexes 1 - 10

All data collections for **1-10** were obtained on a Bruker Venture D8 Photon CMOS diffractometer with graphite-monochromated MoKα_1 (λ = 0.71073 Å) radiation at 173 K using an Oxford Cryostream Plus cooler. The collection method involved ω-scans with a 0.5° width. *SAINT+* version 6.02.6[1] software was used for data reduction and *SADABS*[2] was used to make empirical absorption corrections. The crystal structures were solved using direct methods on *SHELXS-97*.[3] Non-hydrogen atoms were first refined isotropically, followed by anisotropic refinement by full matrix least-squares calculations based on F^2 using *SHELXL-2017*.[3] C-bound H atoms were located in the difference map, then positioned geometrically and were allowed to ride on their respective parent atoms, with thermal displacement parameters 1.2 times of the parent C atom. Where possible, the coordinates and isotropic displacement parameters of the N-bound and O-bound H atoms involved in hydrogen bonding interactions were allowed to refine freely. Diagrams and publication material were generated using *WinGX*,[4] *ORTEP-3*,[4] *PLATON*[5] and *MERCURY*.[6]

1. SAINT+, Version 6.02 (Includes XPREP and SADABS); Bruker AXS Inc: Madison, Wisconsin, USA, 2004.
2. Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst*. **48**, 3–10.
3. Sheldrick, G. M., Acta Crystallogr., Sect. C. 2015, 71 (Pt 1), 3-8.
4. Farrugia, L., J. Appl. Crystallogr. 2012, 45 (4), 849-854.
5. Spek, A., Acta Crystallogr., Sect. D. 2009, 65 (2), 148-155.
6. Macrae C.F., Edgington P.R., McCabe P., Pidcock E., Shields G.P., Taylor R., Towler M., van de Streek J., *J. Appl. Cryst.* 2006, **39-3**, 453.

Table S2. Crystal data and structure refinement for **1 (CSD Code: 1402877).**

Identification code	v14hth8_tp-1	
Empirical formula	C26 H19 N5 O8	
Formula weight	529.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 6.8850(11) Å	α= 90°.
	b = 13.936(2) Å	β= 102.600(5)°.
	c = 24.919(3) Å	γ = 90°.
Volume	2333.4(6) $Å^3$	
Z	4	
Density (calculated)	1.507 Mg/m^3	
Absorption coefficient	0.115 mm^{-1}	
F(000)	1096	
Crystal size	0.280 x 0.120 x 0.050 mm^3	
Theta range for data collection	2.907 to 25.499°.	
Index ranges	-8<=h<=8, -16<=k<=16, -30<=l<=30	
Reflections collected	29056	
Independent reflections	4373 [R(int) = 0.1282]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4373 / 0 / 361	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0856, wR2 = 0.2511	
R indices (all data)	R1 = 0.1083, wR2 = 0.2693	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.522 and -0.560 $e.Å^{-3}$	

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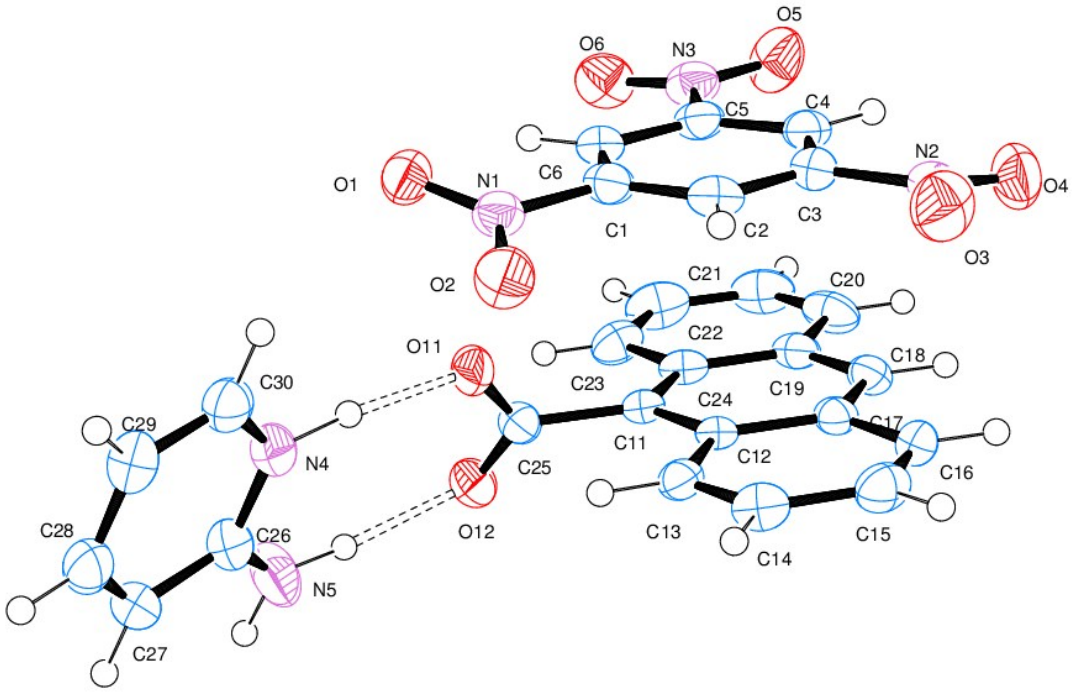


Figure S2 Asymmetric unit of TNB:9-anthroic acid:2-aminopyridine (**1**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond.

Table S3. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(21)-H(21)...O(11)	0.88	1.85	2.712(6)	167
N(22)-H(22A)...O(12)	0.95(8)	1.90(9)	2.841(6)	174(2)
N(22)-H(22B)...O(12)#1	0.92(6)	1.95(6)	2.859(7)	169(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

Table S4. Crystal data and structure refinement for **2 (CSD Code: 1402879).**

Identification code	mo_v14hth15_0m	
Empirical formula	C47 H32 N8 O16	
Formula weight	964.80	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 13.6779(11) Å	α= 90°.
	b = 18.3499(14) Å	β= 102.983(3)°.
	c = 17.2493(14) Å	γ = 90°.
Volume	4218.7(6) $Å^3$	
Z	4	
Density (calculated)	1.519 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	1992	
Crystal size	0.560 x 0.360 x 0.170 mm^3	
Theta range for data collection	2.811 to 25.498°.	
Index ranges	-16<=h<=16, -21<=k<=22, -20<=l<=20	
Reflections collected	44511	
Independent reflections	7826 [R(int) = 0.0352]	
Completeness to theta = 25.242°	99.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7826 / 0 / 649	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1378	
R indices (all data)	R1 = 0.0648, wR2 = 0.1550	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.390 and -0.252 $e.Å^{-3}$	

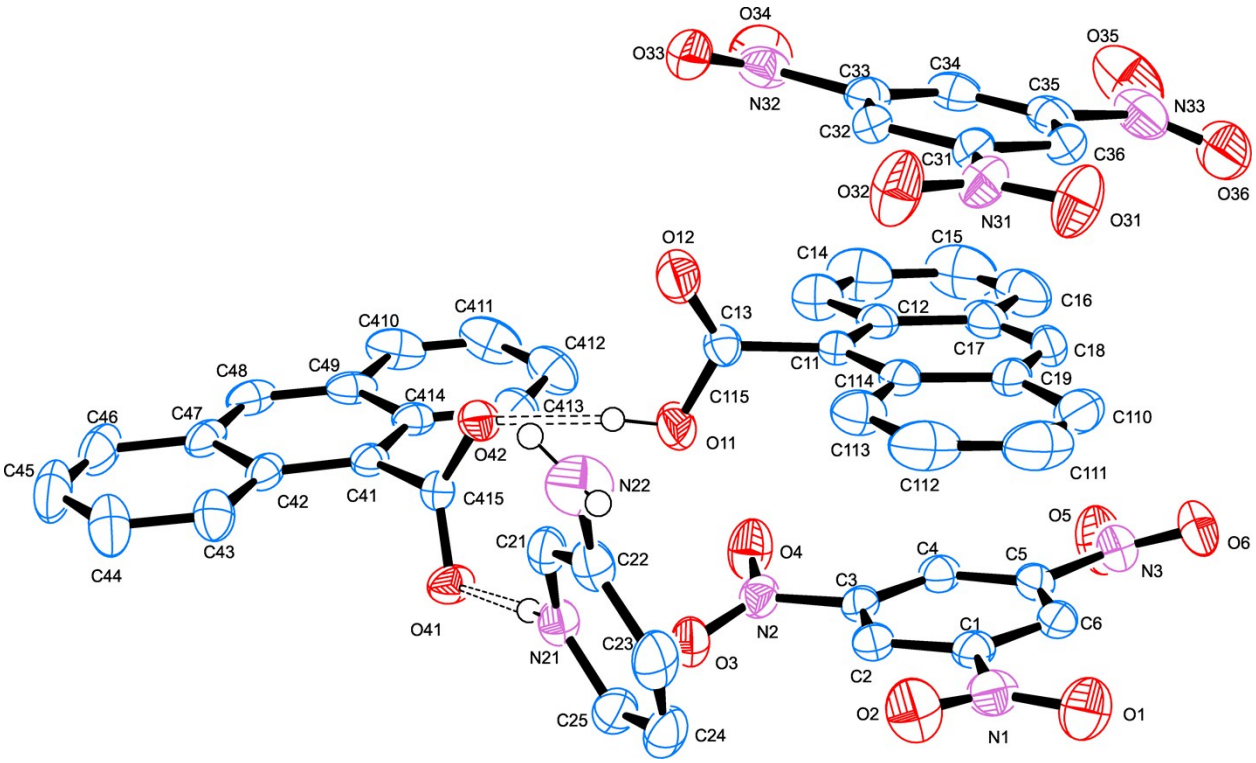


Figure S3 Asymmetric unit of TNB:9-anthroic acid:3-aminopyridine (**2**) (2:2:1), indicating the numbering scheme, ellipsoids at 50 % probability, only selected hydrogen atoms shown. Hydrogen bonding interactions shown with a dashed bond.

Table S7. Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(11)-H(11)...O(42)	0.84	1.74	2.5755(19)	172
N(21)-H(21A)...O(41)	0.88	1.71	2.581(2)	168
N(22)-H(22B)...O(12)#1	0.80(3)	2.52(3)	3.087(3)	129(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

Table S6. Crystal data and structure refinement for **3 (CSD Code: 1402880).**

Identification code	mo_v14hth13_0m	
Empirical formula	C26 H21 N5 O9	
Formula weight	547.48	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.234(2) Å	α= 89.798(6)°.
	b = 9.378(3) Å	β= 88.075(6)°.
	c = 35.927(11) Å	γ = 87.452(6)°.
Volume	2433.6(13) $Å^3$	
Z	4	
Density (calculated)	1.494 Mg/m^3	
Absorption coefficient	0.115 mm^{-1}	
F(000)	1136	
Crystal size	0.300 x 0.110 x 0.040 mm^3	
Theta range for data collection	2.836 to 25.499°.	
Index ranges	-8<=h<=8, -11<=k<=11, -43<=l<=43	
Reflections collected	24395	
Independent reflections	8989 [R(int) = 0.0506]	
Completeness to theta = 25.242°	99.1 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8989 / 0 / 761	
Goodness-of-fit on F^2	1.121	
Final R indices [I>2sigma(I)]	R1 = 0.0746, wR2 = 0.1680	
R indices (all data)	R1 = 0.1169, wR2 = 0.1837	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.500 and -0.254 $e.Å^{-3}$	

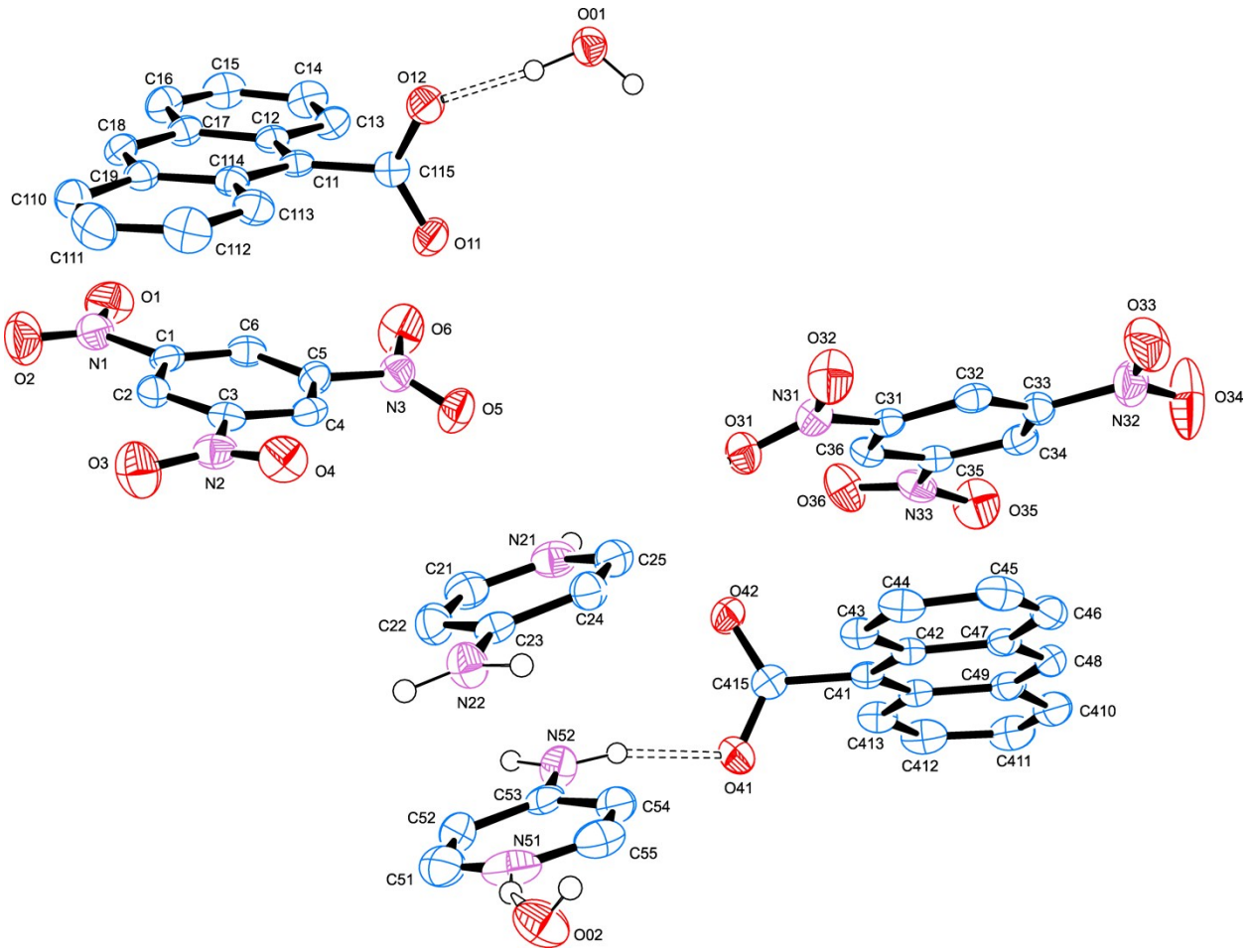


Figure S4 Asymmetric unit of TNB:9-anthroic acid:4-aminopyridine water solvate (**3**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability, only selected hydrogen atoms shown. Hydrogen bonding interactions shown with a dashed bond.

Table S7. Hydrogen bonds for **3** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(01)-H(01A)...O(12)	0.95(5)	1.73(5)	2.651(4)	163(4)
O(02)-H(02B)...O(41)#1	0.81(5)	2.05(5)	2.854(5)	176(5)
O(02)-H(02A)...O(01)#2	0.90(6)	2.01(6)	2.887(5)	167(5)
O(01)-H(01B)...O(42)#3	0.89(5)	1.94(6)	2.818(4)	167(5)
N(21)-H(21A)...O(01)#4	0.87(5)	1.91(5)	2.772(5)	168(4)
N(22)-H(22B)...O(11)#5	0.92(4)	2.14(4)	2.990(5)	153(4)
N(22)-H(22A)...O(42)#1	0.94(5)	1.98(5)	2.904(5)	168(4)
N(51)-H(51A)...O(02)	1.01(6)	1.78(6)	2.770(5)	165(5)
N(52)-H(52A)...O(41)	0.95(5)	1.93(5)	2.857(5)	166(4)

N(52)-H(52B)...O(11)#4	1.03(6)	1.94(6)	2.913(5)	157(5)

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 x+2,y-1,z #3 x-1,y,z #4 x+1,y,z #5 x+1,y-1,z

Table S8. Crystal data and structure refinement for **4 (CSD Code: 1402881).**

Identification code	mo_v14hth3_0m	
Empirical formula	C26 H18 Br N5 O8	
Formula weight	608.36	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.9809(6) Å	α= 90°.
	b = 7.3118(5) Å	β= 94.0950(10)°.
	c = 38.083(3) Å	γ = 90°.
Volume	2494.4(3) $Å^3$	
Z	4	
Density (calculated)	1.620 Mg/m^3	
Absorption coefficient	1.711 mm^{-1}	
F(000)	1232	
Crystal size	0.340 x 0.100 x 0.100 mm^3	
Theta range for data collection	2.985 to 25.496°.	
Index ranges	-10<=h<=10, -8<=k<=8, -46<=l<=46	
Reflections collected	23111	
Independent reflections	4616 [R(int) = 0.0288]	
Completeness to theta = 25.242°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4616 / 0 / 373	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0823	
R indices (all data)	R1 = 0.0451, wR2 = 0.0858	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.511 and -0.216 $e.Å^{-3}$	

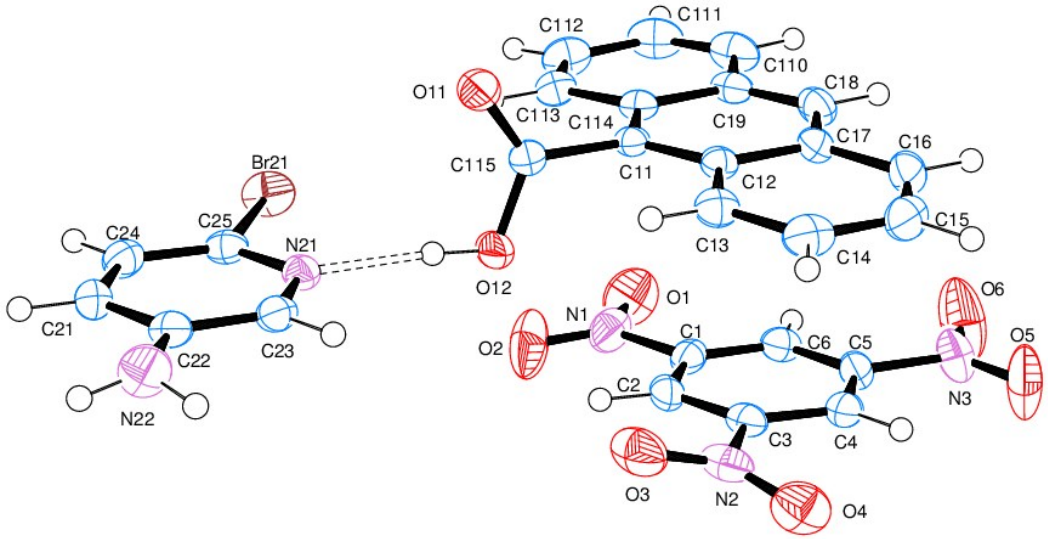


Figure S5 Asymmetric unit of TNB:9-anthroic acid:6-bromo-3-aminopyridine (**4**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond.

Table S9. Hydrogen bonds for **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(21)	0.84(4)	1.78(4)	2.613(3)	174(3)
N(22)-H(22A)...O(2)#1	0.85(3)	2.31(4)	3.157(4)	174(3)
N(22)-H(22B)...O(2)#2	0.85(3)	2.44(3)	3.267(3)	165(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x+1,y,z

Table S10. Crystal data and structure refinement for **5 (CSD Code: 1402882).**

Identification code	v14hth4	
Empirical formula	C26 H18 Br N5 O8	
Formula weight	608.36	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 21.301(5) Å	α= 90°.
	b = 7.2862(13) Å	β= 113.047(5)°.
	c = 17.188(3) Å	γ = 90°.
Volume	2454.7(8) $Å^3$	
Z	4	
Density (calculated)	1.646 Mg/m^3	
Absorption coefficient	1.738 mm^{-1}	
F(000)	1232	
Crystal size	0.280 x 0.130 x 0.040 mm^3	
Theta range for data collection	2.983 to 25.499°.	
Index ranges	-25<=h<=25, -8<=k<=8, -20<=l<=20	
Reflections collected	52199	
Independent reflections	4560 [R(int) = 0.1353]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4560 / 0 / 373	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1188	
R indices (all data)	R1 = 0.1062, wR2 = 0.1378	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.858 and -0.734 $e.Å^{-3}$	

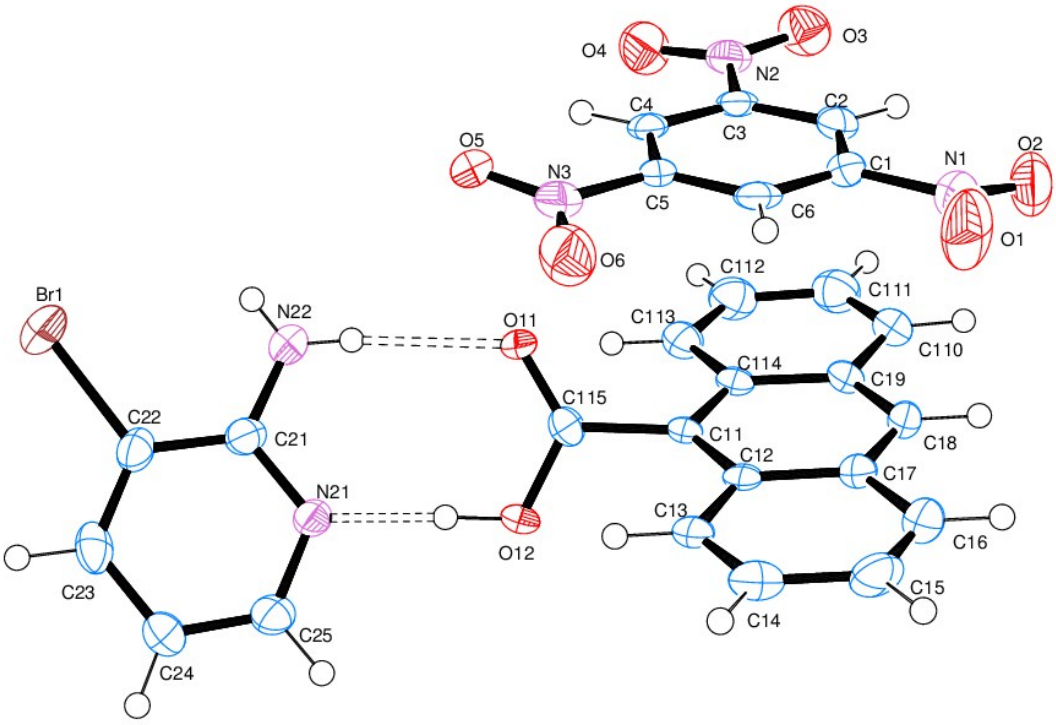


Figure S6 Asymmetric unit of TNB:9-anthroic acid:3-bromo-2-aminopyridine (**5**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond.

Table S11. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(21)	0.97(7)	1.67(7)	2.628(4)	171(6)
N(22)-H(22A)...O(11)	0.81(5)	2.16(5)	2.941(6)	164(4)
N(22)-H(22B)...Br(1)	0.75(5)	2.70(5)	3.109(5)	116(4)

Table S12. Crystal data and structure refinement for **6 (CSD Code: 1402883).**

Identification code	mo_v14hth12_0m	
Empirical formula	C26 H18 Br N5 O8	
Formula weight	608.36	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.9784(15) Å	α= 90°.
	b = 7.2372(12) Å	β= 94.321(4)°.
	c = 38.160(7) Å	γ = 90°.
Volume	2472.5(7) $Å^3$	
Z	4	
Density (calculated)	1.634 Mg/m^3	
Absorption coefficient	1.726 mm^{-1}	
F(000)	1232	
Crystal size	0.366 x 0.210 x 0.124 mm^3	
Theta range for data collection	2.865 to 25.499°.	
Index ranges	-10<=h<=10, -8<=k<=8, -46<=l<=46	
Reflections collected	28820	
Independent reflections	4588 [R(int) = 0.0486]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4588 / 0 / 373	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0426, wR2 = 0.1146	
R indices (all data)	R1 = 0.0476, wR2 = 0.1189	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.107 and -0.704 $e.Å^{-3}$	

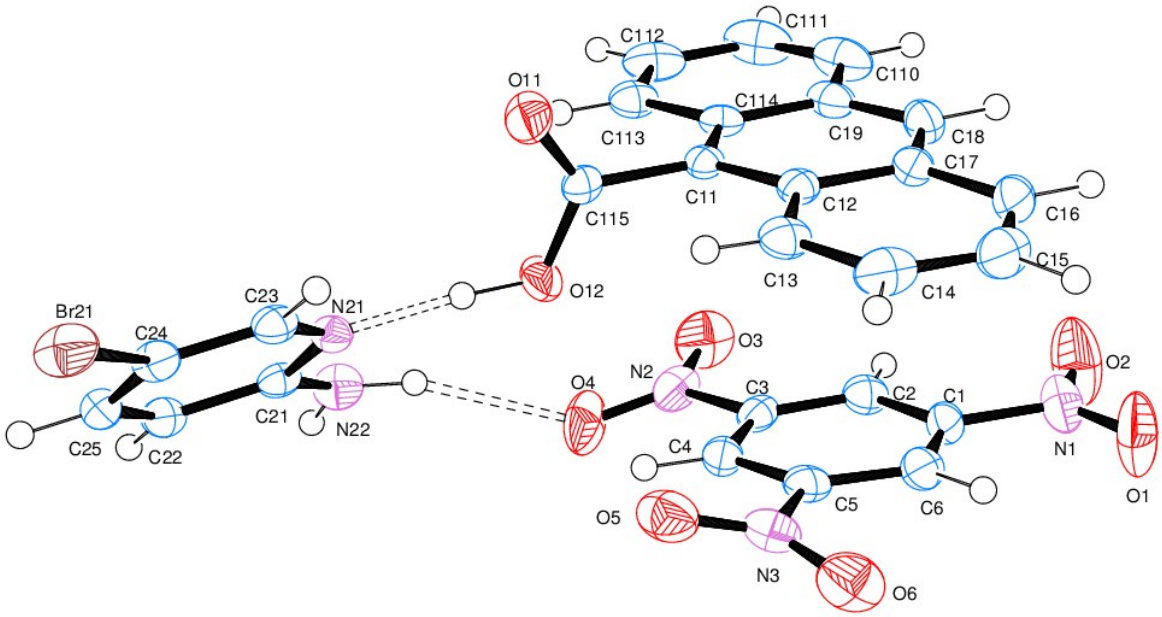


Figure S7 Asymmetric unit of TNB:9-anthroic acid:5-bromo-2-aminopyridine (**6**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond.

Table S13. Hydrogen bonds for **6** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(21)	0.98(3)	1.57(3)	2.542(3)	171(3)
N(22)-H(22A)...O(4)#1	0.88(4)	2.27(4)	3.109(3)	161(3)
N(22)-H(22B)...O(4)	0.92(4)	2.31(4)	3.173(3)	154(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z

Table S14. Crystal data and structure refinement for **7 (CSD Code: 1402884).**

Identification code	mo_v14hth5_0m	
Empirical formula	C26 H18 Cl N5 O8	
Formula weight	563.90	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.9310(10) Å	α= 90°.
	b = 7.2239(8) Å	β= 94.402(2)°.
	c = 38.218(5) Å	γ = 90°.
Volume	2458.4(5) $Å^3$	
Z	4	
Density (calculated)	1.524 Mg/m^3	
Absorption coefficient	0.219 mm^{-1}	
F(000)	1160	
Crystal size	0.09 x 0.09 x 0.34 mm^3	
Theta range for data collection	2.870 to 25.500°.	
Index ranges	-10<=h<=10, -8<=k<=8, -46<=l<=46	
Reflections collected	27353	
Independent reflections	4573 [R(int) = 0.0290]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4573 / 0 / 370	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.0902	
R indices (all data)	R1 = 0.0522, wR2 = 0.0981	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.288 and -0.235 $e.Å^{-3}$	

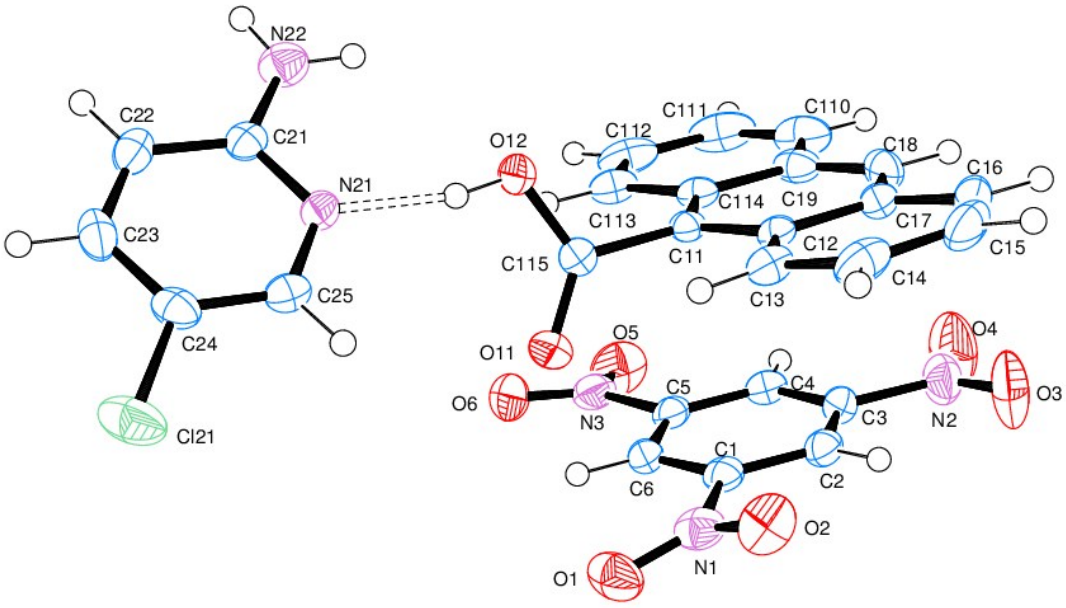


Figure S8 Asymmetric unit of TNB:9-anthroic acid:5-chloro-2-aminopyridine (**7**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond.

Table S15. Hydrogen bonds for **7** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(21)	0.84	1.71	2.5395(17)	167
N(22)-H(22A)...O(6)#1	0.88(2)	2.42(2)	3.192(2)	147(2)
N(22)-H(22B)...O(6)#2	0.83(2)	2.31(2)	3.116(2)	162(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 -x+1,-y+1,-z

Table S16. Crystal data and structure refinement for **8 (CSD Code: 1402885).**

Identification code	v14hth9_p.	
Empirical formula	C26 H18 N6 O10	
Formula weight	574.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 21.0640(17) Å	α= 90°.
	b = 7.3594(5) Å	β= 112.320(2)°.
	c = 17.0447(13) Å	γ = 90°.
Volume	2444.3(3) $Å^3$	
Z	4	
Density (calculated)	1.561 Mg/m^3	
Absorption coefficient	0.123 mm^{-1}	
F(000)	1184	
Crystal size	0.530 x 0.060 x 0.050 mm^3	
Theta range for data collection	3.384 to 25.498°.	
Index ranges	-25<=h<=25, -8<=k<=8, -20<=l<=20	
Reflections collected	49213	
Independent reflections	4543 [R(int) = 0.0635]	
Completeness to theta = 25.242°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4543 / 0 / 388	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0391, wR2 = 0.0861	
R indices (all data)	R1 = 0.0633, wR2 = 0.0984	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.203 and -0.191 $e.Å^{-3}$	

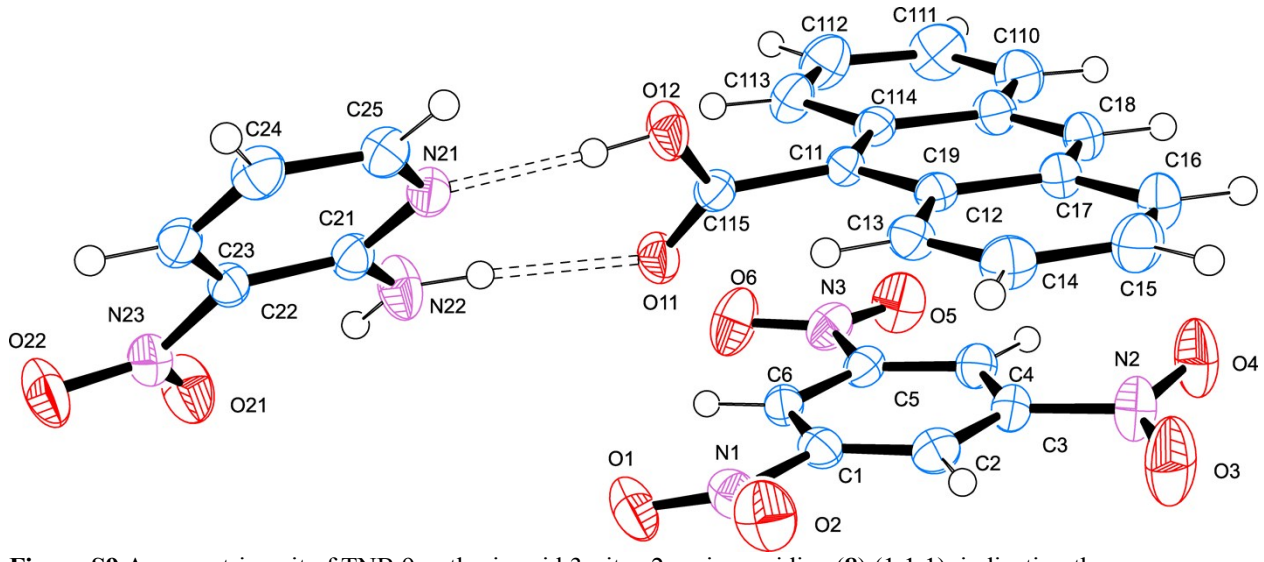


Figure S9 Asymmetric unit of TNB:9-anthroic acid:3-nitro-2-aminopyridine (**8**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond.

Table S17. Hydrogen bonds for **8** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(21)	0.84	1.86	2.6929(19)	171
N(22)-H(22A)...O(11)	0.91(2)	2.01(3)	2.918(2)	172(2)
N(22)-H(22B)...O(21)	0.87(2)	2.01(2)	2.636(2)	128(2)

Table S18. Crystal data and structure refinement for **9 (CSD Code: 1402886).**

Identification code	shelx	
Empirical formula	C26 H18 N6 O10	
Formula weight	574.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 8.8909(11) Å	α= 90°.
	b = 7.8185(10) Å	β= 96.018(4)°.
	c = 36.688(5) Å	γ = 90°.
Volume	2536.2(5) $Å^3$	
Z	4	
Density (calculated)	1.504 Mg/m^3	
Absorption coefficient	0.119 mm^{-1}	
F(000)	1184	
Crystal size	0.970 x 0.290 x 0.150 mm^3	
Theta range for data collection	2.834 to 25.497°.	
Index ranges	-10<=h<=10, -9<=k<=9, -44<=l<=44	
Reflections collected	44818	
Independent reflections	4716 [R(int) = 0.0297]	
Completeness to theta = 25.242°	99.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4716 / 0 / 388	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0748, wR2 = 0.1902	
R indices (all data)	R1 = 0.0810, wR2 = 0.1959	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.964 and -0.864 $e.Å^{-3}$	

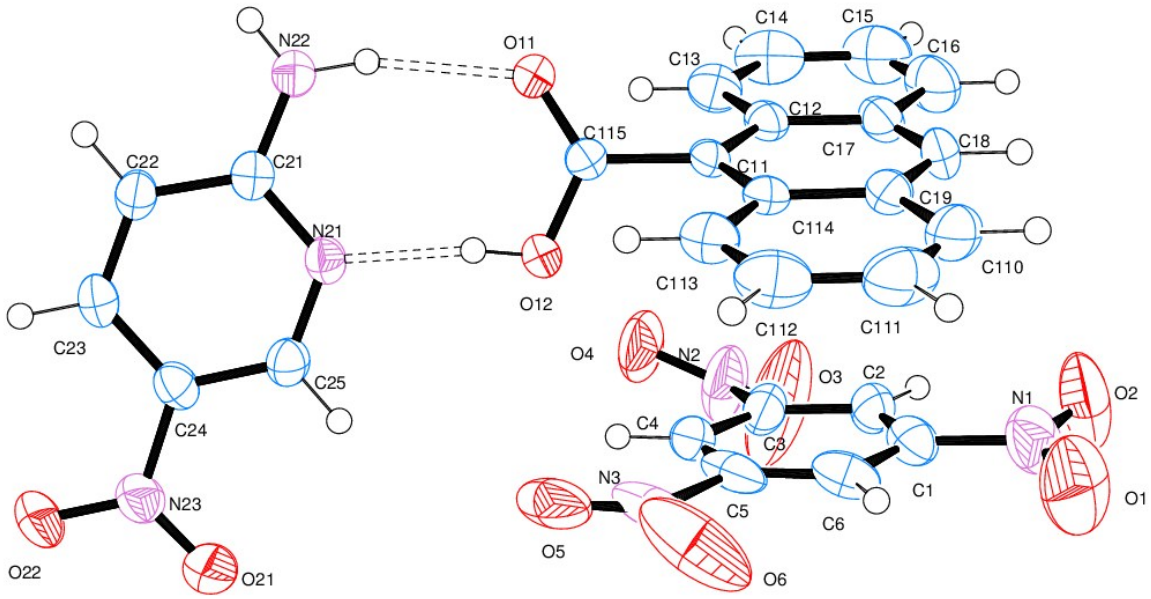


Figure S10 Asymmetric unit of TNB:9-anthroic acid:5-nitro-2-aminopyridine (**9**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond. Disorder shown for the oxygen atoms of the nitro group.

Table S19. Hydrogen bonds for **9** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(21)	0.84	1.80	2.633(3)	170.9
N(22)-H(22B)...O(11)	0.90(3)	2.04(3)	2.914(3)	165(3)
N(22)-H(22A)...O(21)#1	0.84(4)	2.40(4)	3.143(4)	149(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z

Table S20 Crystal data and structure refinement for **10 (CSD Code: 1402887).**

Identification code	mo_v14hth14_0m.	
Empirical formula	C31 H21 N5 O8	
Formula weight	591.53	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.037(3) Å	α= 87.593(11)°.
	b = 9.676(4) Å	β= 82.035(11)°.
	c = 19.738(8) Å	γ = 84.659(13)°.
Volume	1324.5(9) $Å^3$	
Z	2	
Density (calculated)	1.483 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	612	
Crystal size	1.230 x 0.130 x 0.060 mm^3	
Theta range for data collection	2.978 to 25.500°.	
Index ranges	-8<=h<=8, -10<=k<=11, -23<=l<=23	
Reflections collected	14591	
Independent reflections	4502 [R(int) = 0.0771]	
Completeness to theta = 25.242°	91.1 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4502 / 0 / 398	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.1019, wR2 = 0.2847	
R indices (all data)	R1 = 0.1522, wR2 = 0.3186	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.355 and -0.502 $e.Å^{-3}$	

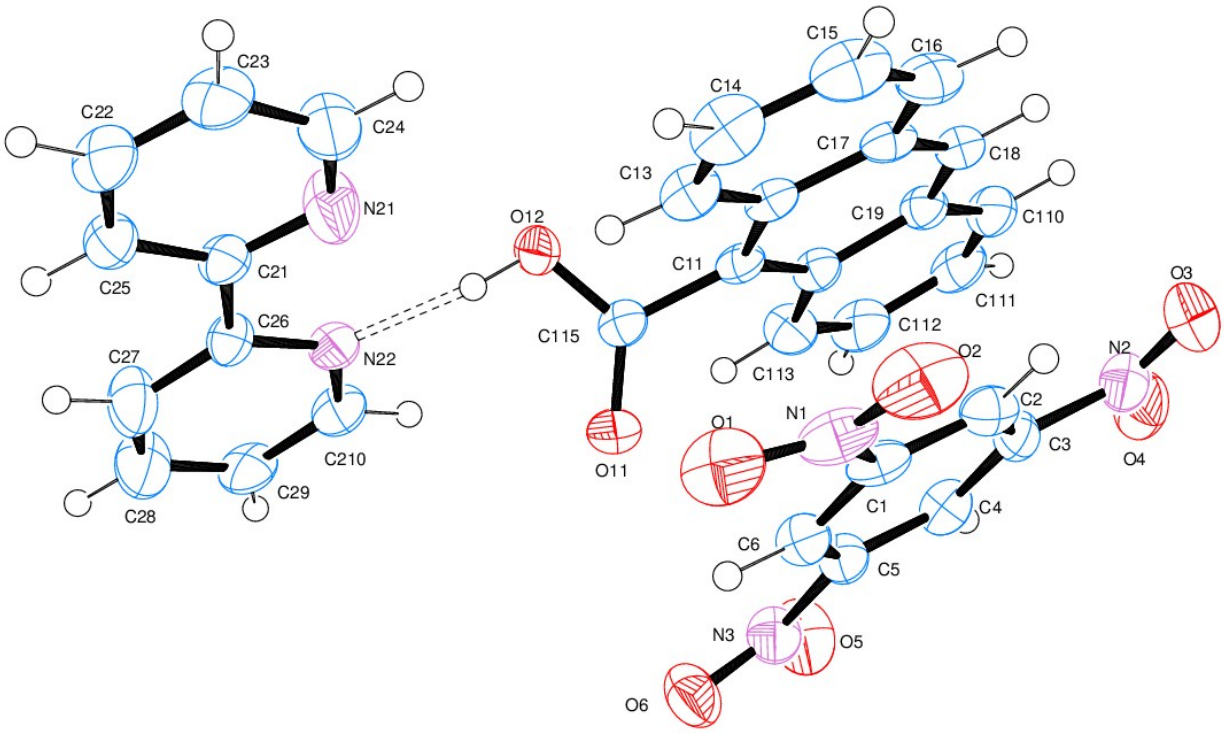


Figure S11 Asymmetric unit of TNB:9-anthroic acid:2,2'-bipyridine (**11**) (1:1:1), indicating the numbering scheme, ellipsoids at 50 % probability. Hydrogen bonding interactions shown with a dashed bond.

Table S21. Hydrogen bonds for **10** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(22)	0.84	1.74	2.568(5)	167

Symmetry transformations used to generate equivalent atoms:

Table S22 of carboxylic/carboxylate bond distances and their ratio's.

Compound	**C115-O11 / C415-O42**	**C115-O12 / C415-O41**	**Ratio (long over short)**
1 molecular salt	1.256(6)	1.244(6)	**1.010**
2 molecular salt	1.307(2) / 1.252(2)	1.200(3) / 1.255(2)	**1.089 / 1.002**
3 molecular salt hydrate	1.253(5) / 1.252(5)	1.250(5) / 1.253(5)	**1.002 / 1.001**
4 co-crystal	1.205(3)	1.301(3)	**1.080**
5 co-crystal	1.211(5)	1.312(5)	**1.083**
6 co-crystal	1.204(5)	1.298(3)	**1.078**
7 co-crystal	1.2106(19)	1.2980(19)	**1.072**
8 co-crystal	1.210(2)	1.308(3)	**1.081**
9 co-crystal	1.211(3)	1.298(3)	**1.072**
10 co-crystal	1.232(7)	1.283(7)	**1.041**

Powder X-ray diffraction patterns for complexes 1 - 10 (13)

Powder X-ray diffraction data patterns were collected at 293 K on a Bruker D2 Phaser diffractometer which employed a sealed tube Co X-ray source (λ = 1.78897 Å), operating at 30 kV and 10 mA, and LynxEye PSD detector in Bragg-Brentano geometry. The calculated powder diffraction patterns were computed from the single crystal data which was collected at 173 K using Mercury[11] version 3.5.1. The peak positions are shifted resulting from the different temperatures at which the samples were measured. The peak intensities vary due to preferred orientation.

1. Mercury: visualization and analysis of crystal structures C.F. Macrae, P.R. Edgington, P McCabe, E. Pidcock, G.P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Cryst.* (2006), 39-3, 453-457.

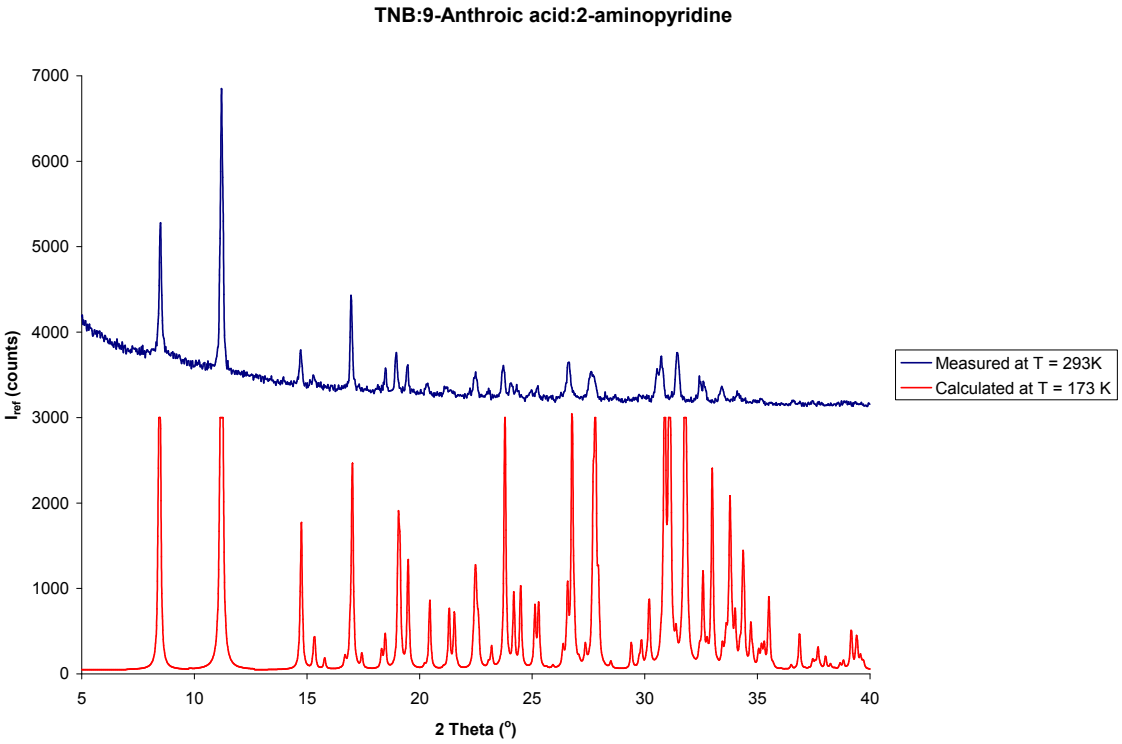


Figure S13 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:2-aminopyridine (1)

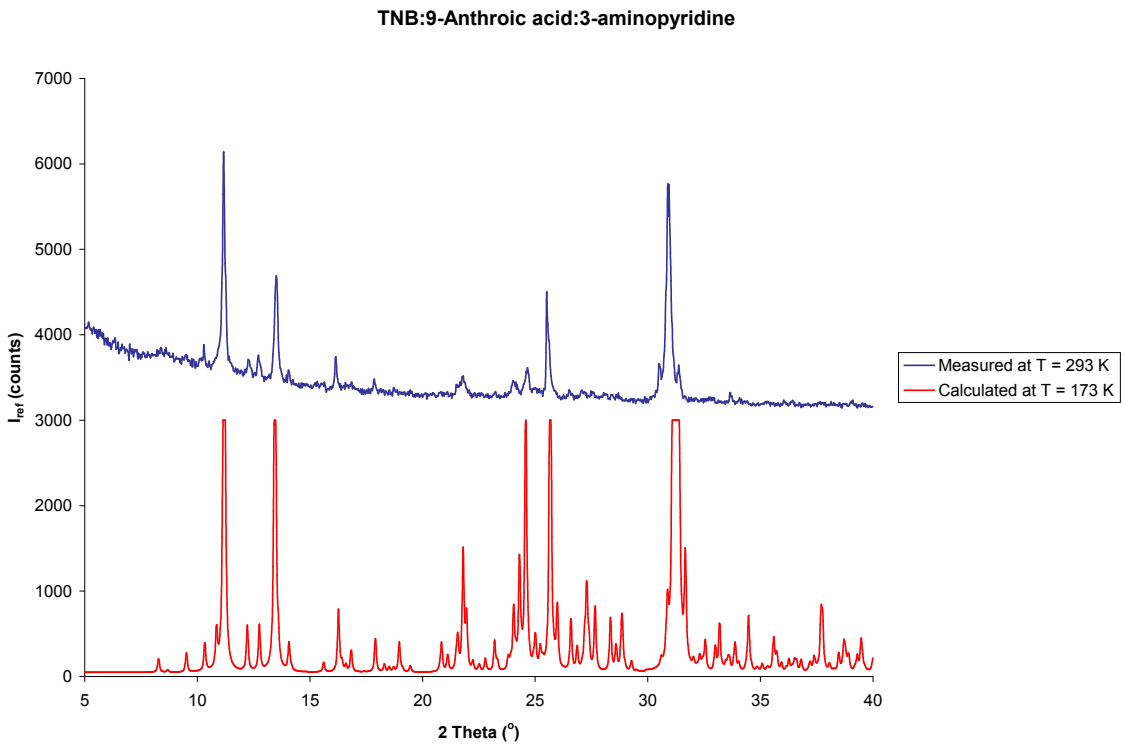


Figure S14 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:3-aminopyridine (2)

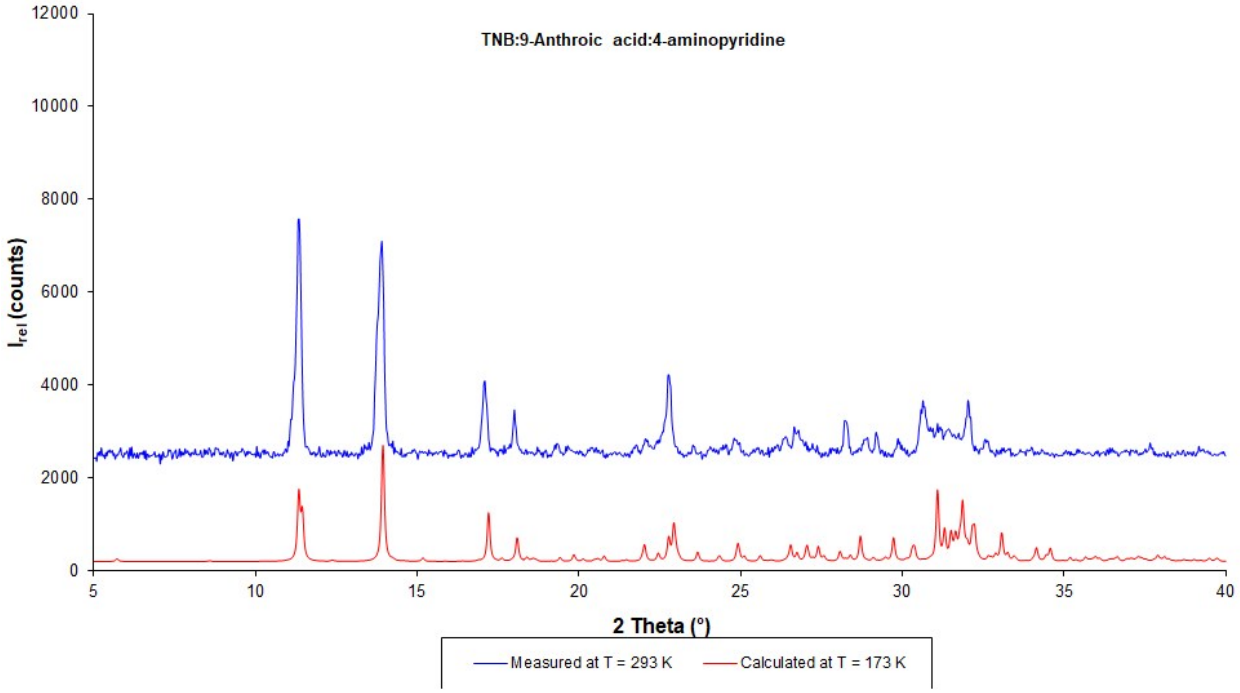


Figure S15 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:4-aminopyridine (3)

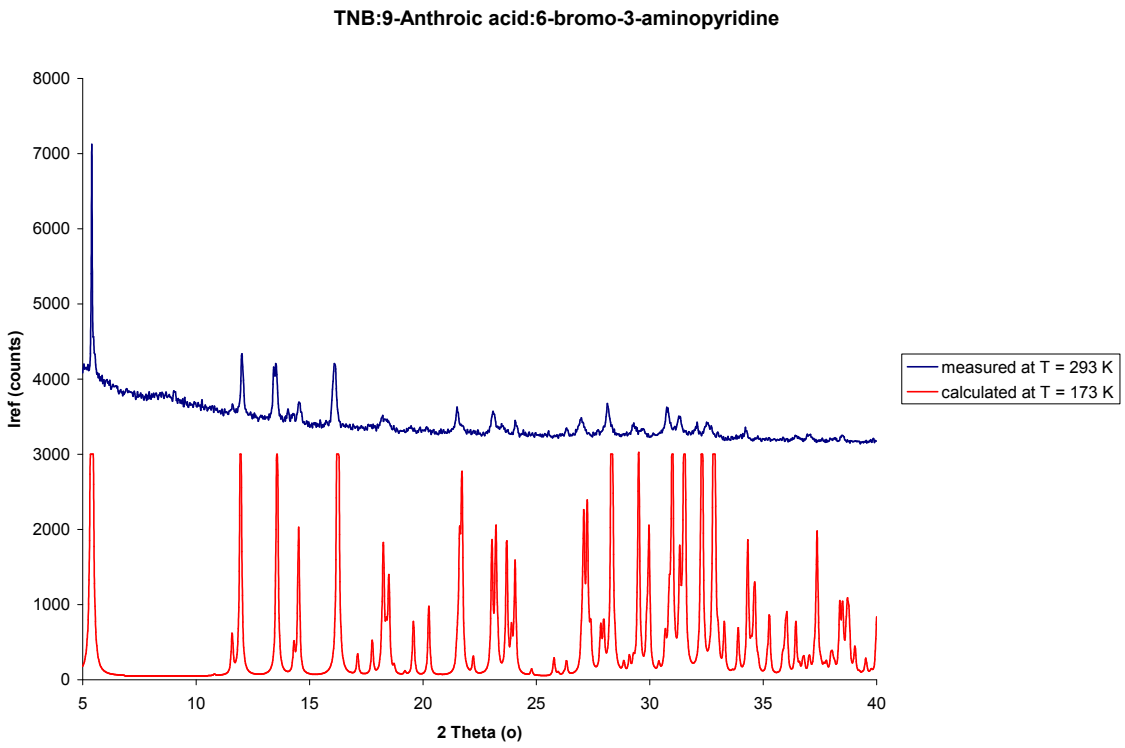


Figure S16 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:6-bromo-3-aminopyridine (4)

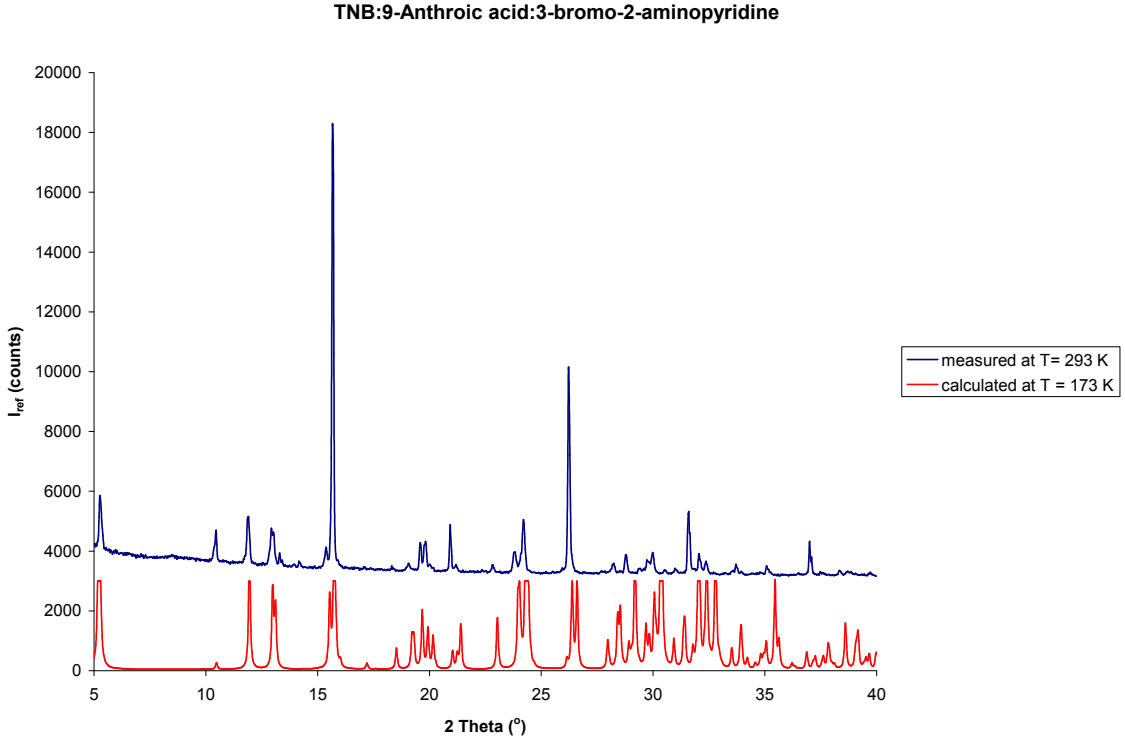


Figure S17 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:3-bromo-2-aminopyridine (5)

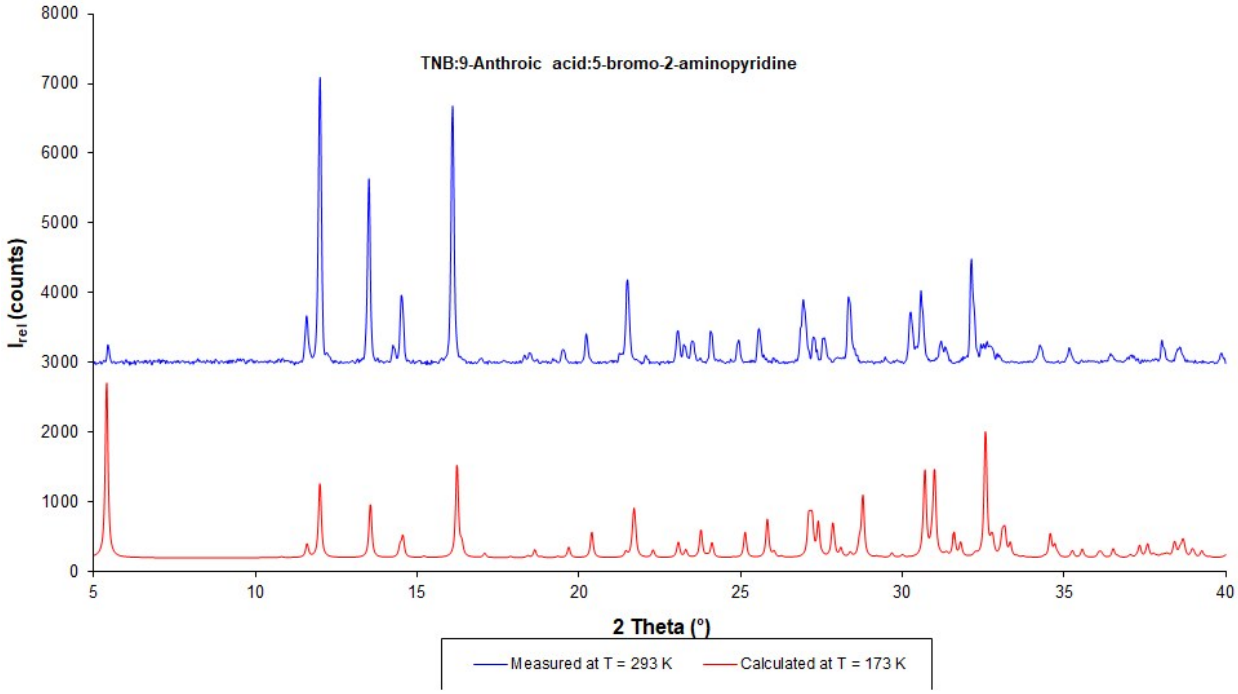


Figure S18 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:5-bromo-2-aminopyridine (6)

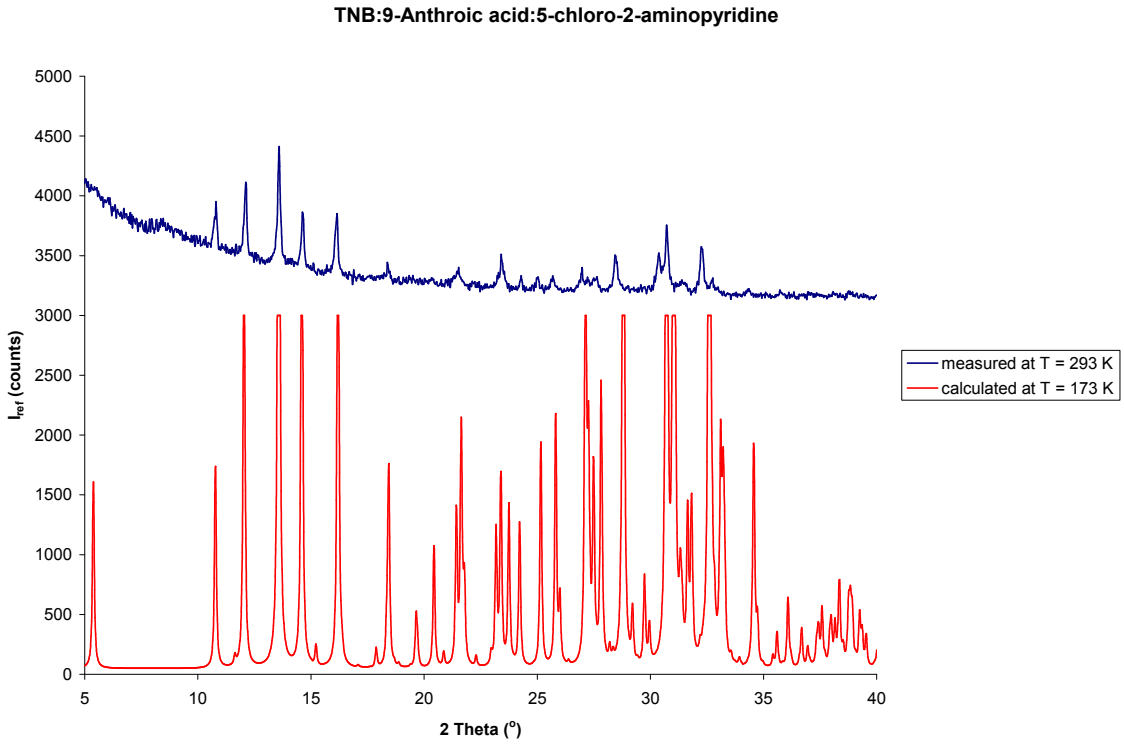


Figure S19 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:5-chloro-2-aminopyridine (7)

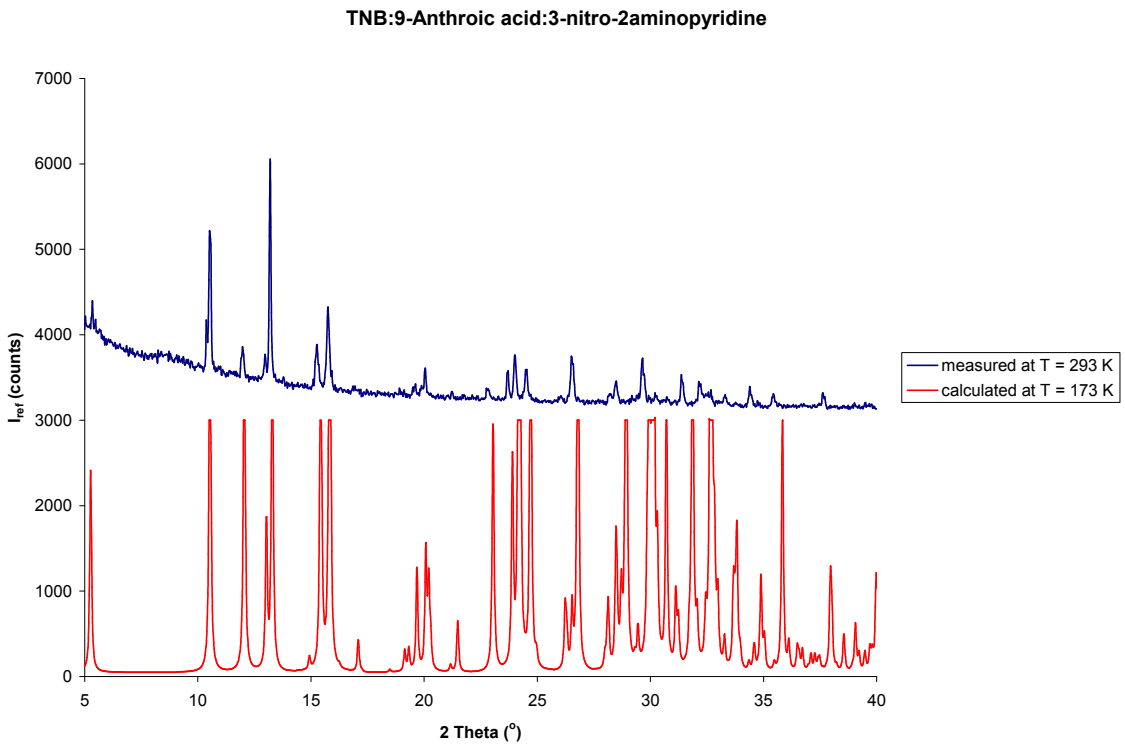


Figure S20 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:3-nitro-2-aminopyridine (8)

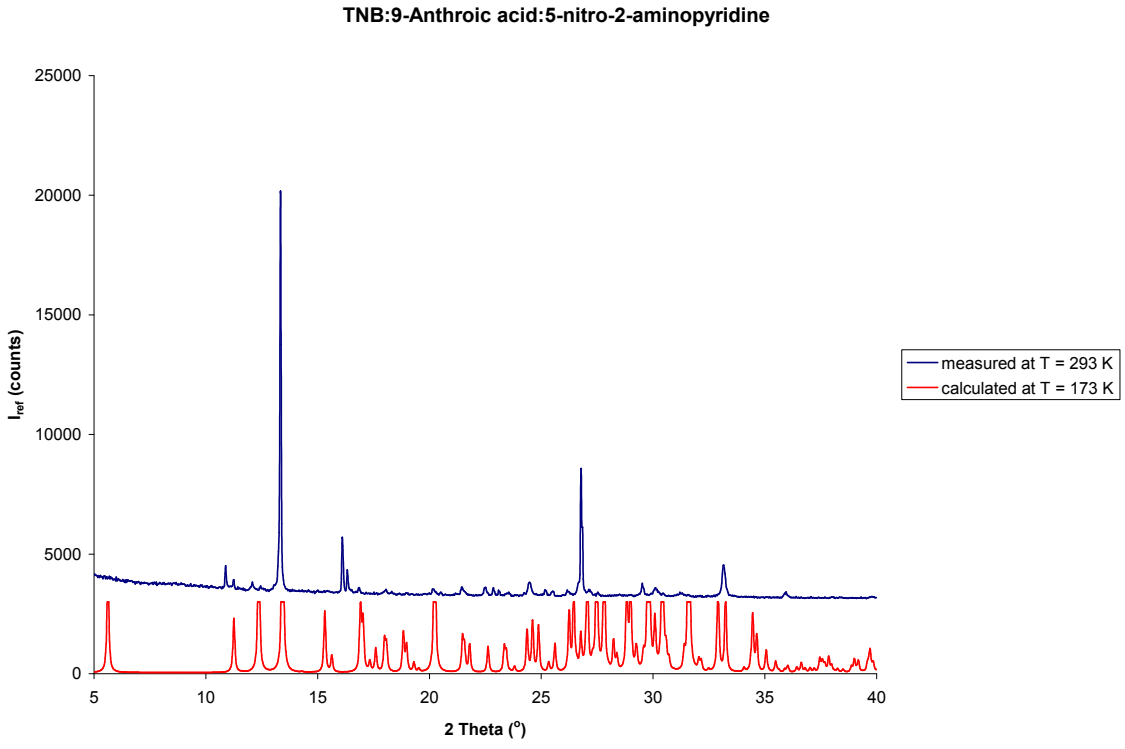


Figure S21 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:5-nitro-2-aminopyridine (9)

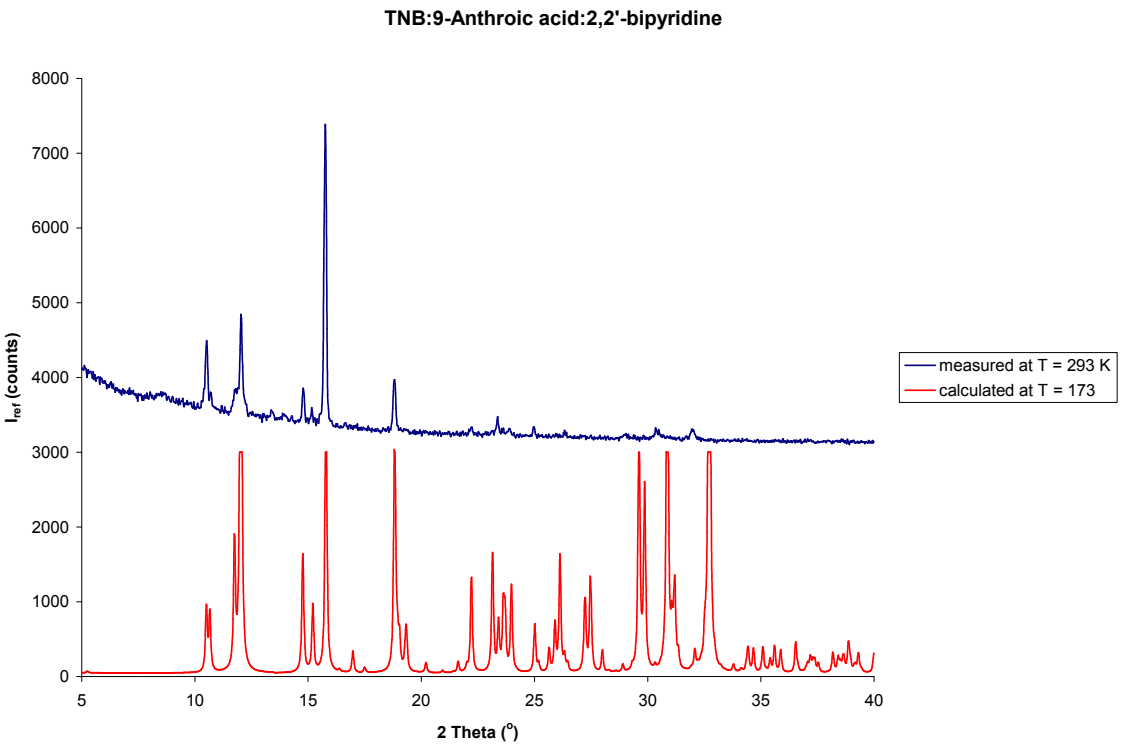
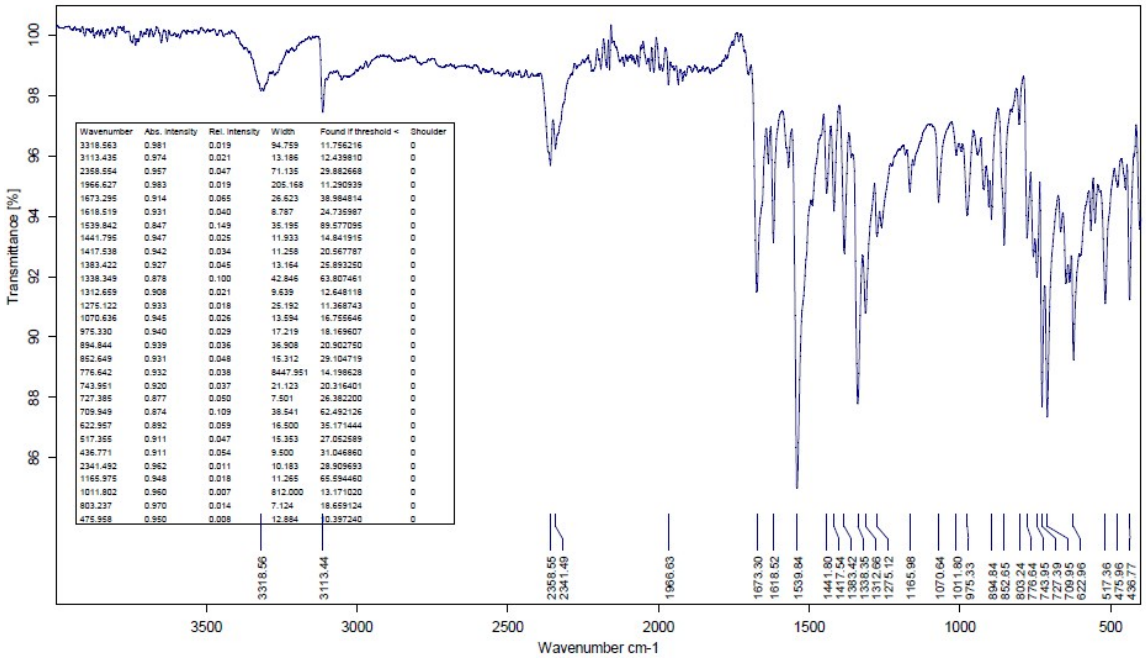


Figure S22 Measured *vs.* calculated PXRD of TNB:9-Anthroic acid:2,2'-bipyridine (10)

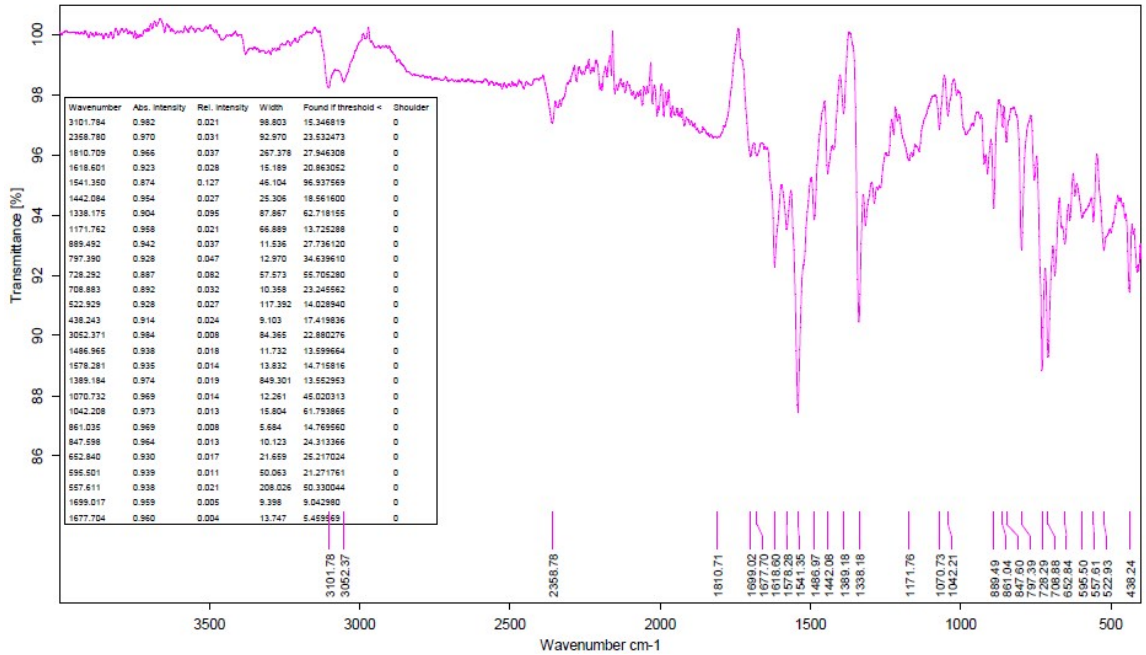
Infra-red spectroscopic data for complexes 1 - 10

All infra-red spectra were recorded on a Bruker Vertex 70 FT-IR spectrometer equipped with a Harrick MVP-Pro ATR. The spectral resolution was set to 4 cm^{-1} and the spectra were recorded between 400 - 4000 cm^{-1}.



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found If threshold <	Shoulder
3318.563	0.981	0.019	94.759	11.756216	0
3113.435	0.974	0.021	13.186	12.439810	0
2358.554	0.957	0.047	71.135	29.882668	0
1966.627	0.983	0.019	205.168	11.290939	0
1673.295	0.914	0.065	26.623	38.984814	0
1618.519	0.931	0.040	8.787	24.735987	0
1539.842	0.847	0.149	35.195	89.677095	0
1441.796	0.947	0.025	11.933	14.841915	0
1417.538	0.942	0.034	11.258	20.567787	0
1383.422	0.927	0.045	13.164	25.893260	0
1338.349	0.878	0.100	42.846	63.807461	0
1312.659	0.908	0.021	9.639	12.648118	0
1275.122	0.933	0.018	25.192	11.368743	0
1070.636	0.945	0.026	13.594	16.755646	0
975.330	0.940	0.029	17.219	18.169607	0
894.844	0.939	0.036	36.908	20.902750	0
852.649	0.931	0.048	15.312	29.104719	0
776.642	0.932	0.038	8447.951	14.198628	0
743.951	0.920	0.037	21.123	20.316401	0
727.385	0.877	0.050	7.501	26.382200	0
709.949	0.874	0.109	38.541	62.492126	0
622.957	0.892	0.059	16.500	35.171444	0
517.355	0.911	0.047	15.353	27.052589	0
436.771	0.911	0.054	9.500	31.046860	0
2341.492	0.962	0.011	10.183	28.909693	0
1165.975	0.948	0.018	11.265	65.594460	0
1011.802	0.960	0.007	812.000	13.171020	0
803.237	0.970	0.014	7.124	18.659124	0
475.958	0.950	0.008	12.884	10.397240	0

Figure S23 IR spectra of TNB:9-Anthroic acid:2-aminopyridine (**1**)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found If threshold <	Shoulder
3101.784	0.982	0.021	98.803	15.346819	0
2358.780	0.970	0.031	92.970	23.532473	0
1810.709	0.966	0.037	267.378	27.946308	0
1618.601	0.923	0.028	15.189	20.863052	0
1541.350	0.874	0.127	46.104	96.937569	0
1442.084	0.954	0.027	25.306	18.561600	0
1338.175	0.904	0.095	87.867	62.718155	0
1171.762	0.958	0.021	66.889	13.725288	0
889.492	0.942	0.037	11.536	27.736120	0
797.390	0.928	0.047	12.970	34.639610	0
728.292	0.887	0.082	57.573	55.705280	0
706.883	0.892	0.032	10.358	23.245562	0
522.929	0.928	0.027	117.392	14.028940	0
438.243	0.914	0.024	9.103	17.419836	0
3062.371	0.984	0.008	84.365	22.880276	0
1486.965	0.938	0.019	11.732	13.599664	0
1578.281	0.935	0.014	13.832	14.715816	0
1389.184	0.974	0.019	849.301	13.552953	0
1070.732	0.969	0.014	12.261	45.020313	0
1042.208	0.973	0.013	15.804	61.793865	0
861.035	0.969	0.008	5.684	14.769560	0
847.598	0.964	0.013	10.123	24.313366	0
652.840	0.930	0.017	21.659	25.217024	0
595.501	0.939	0.011	50.063	21.271761	0
557.611	0.938	0.021	208.026	50.330044	0
1699.017	0.959	0.005	9.398	9.042980	0
1677.704	0.960	0.004	13.747	5.459669	0

Figure S24 IR spectra of TNB:9-Anthroic acid:3-aminopyridine (**2**)

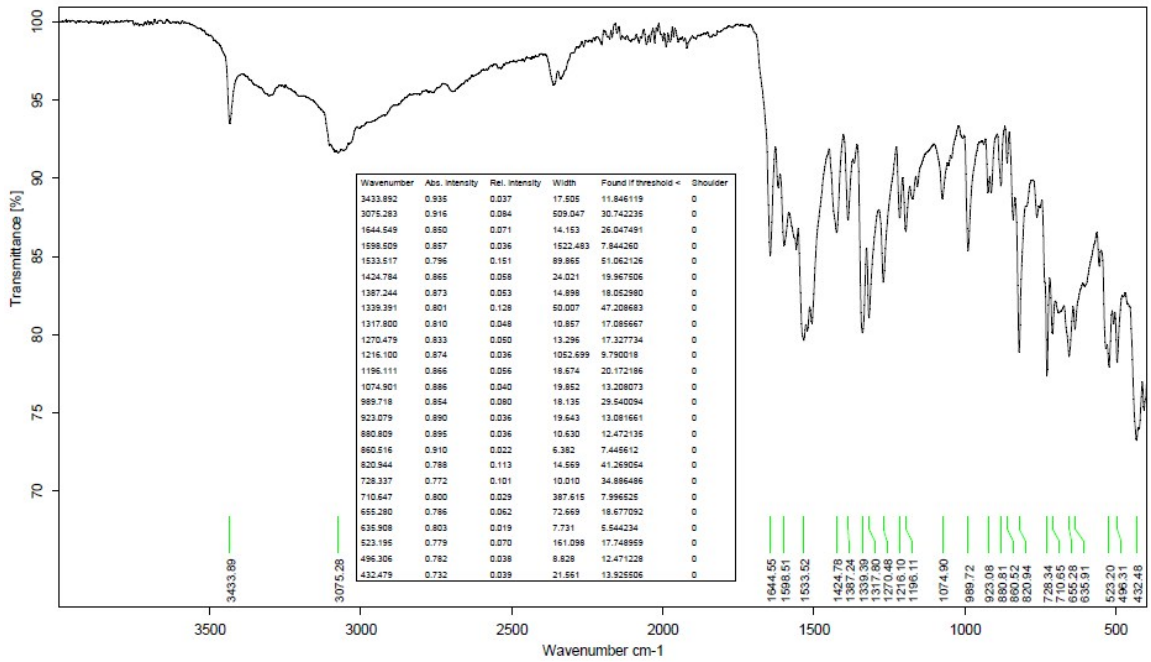


Figure S25 IR spectra of TNB:9-Anthroic acid:4-aminopyridine (**3**)

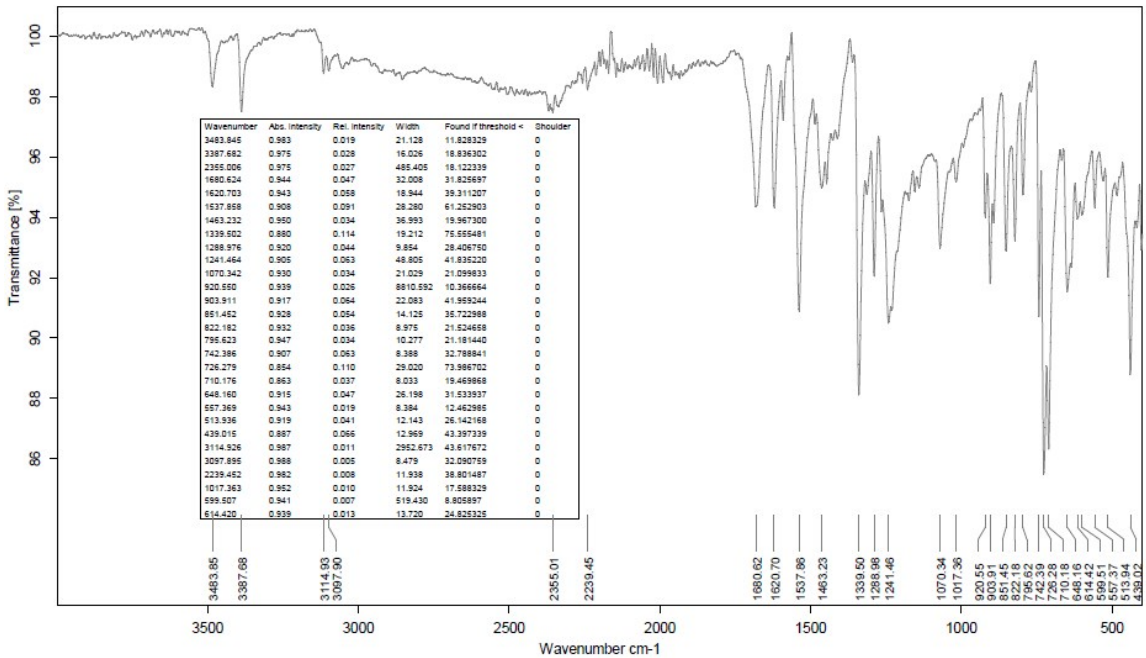
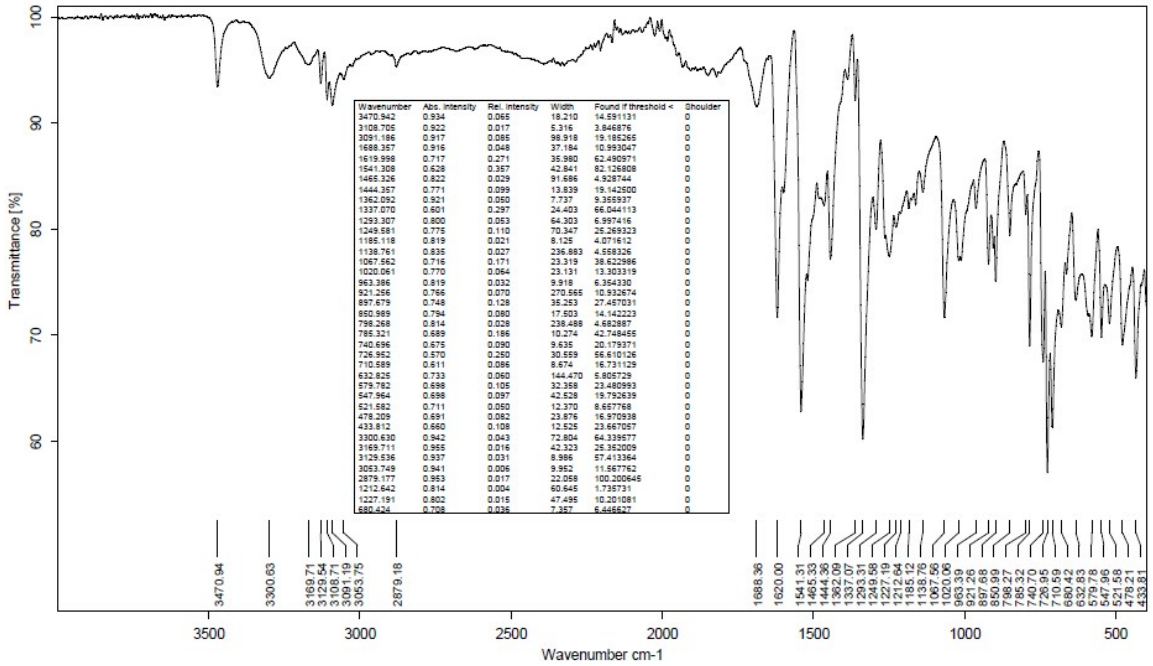
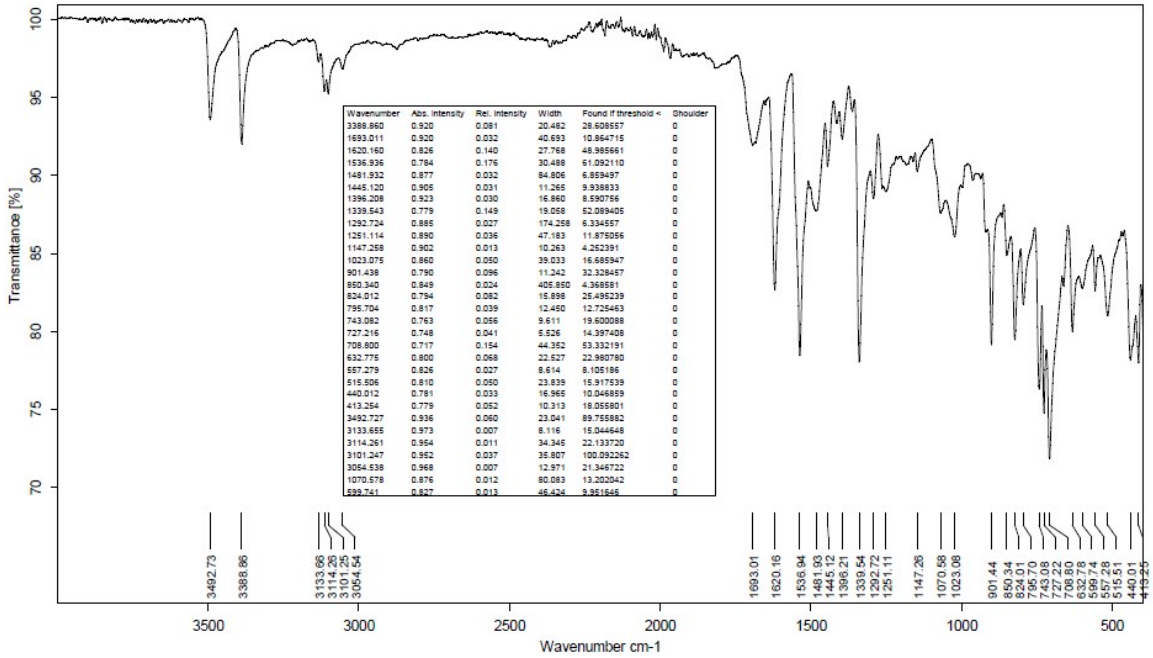


Figure S26 IR spectra of TNB:9-Anthroic acid:6-bromo-3-aminopyridine (**4**)



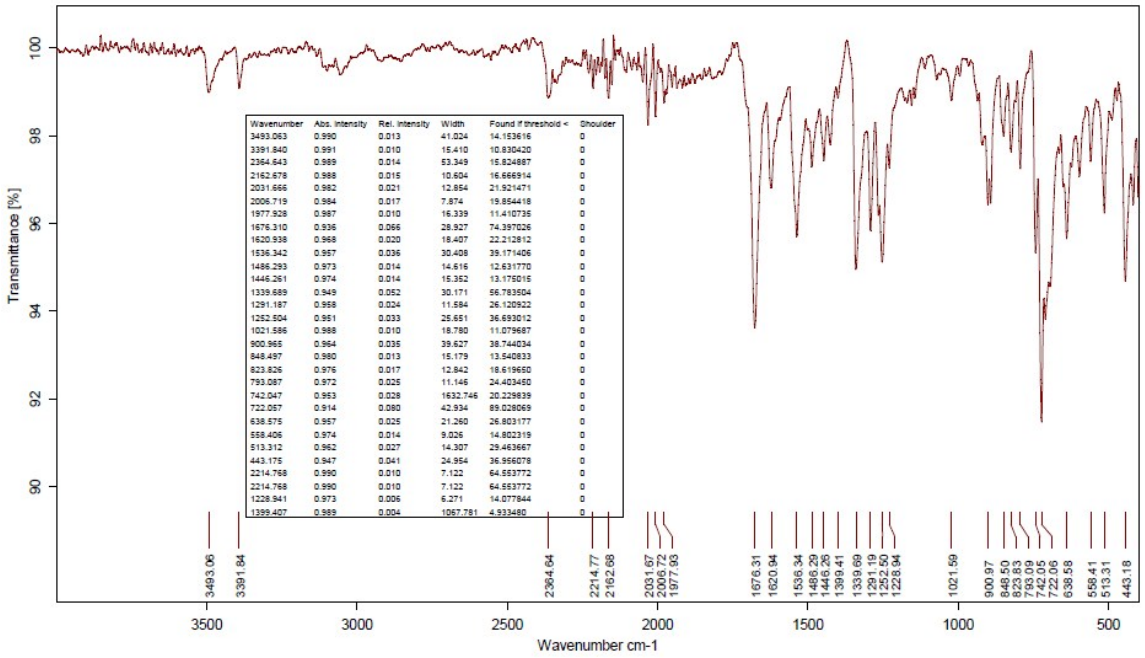
Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found If threshold <	Shoulder
3470.942	0.934	0.065	18.210	14.591131	0
3108.705	0.922	0.017	5.316	3.846876	0
3091.186	0.917	0.085	98.918	19.185265	0
1688.357	0.916	0.048	37.184	10.993047	0
1619.998	0.717	0.271	35.980	62.480971	0
1541.308	0.628	0.357	42.841	82.126808	0
1465.326	0.822	0.029	91.686	4.928744	0
1444.357	0.771	0.099	13.839	19.142500	0
1362.092	0.921	0.050	7.737	9.355937	0
1337.070	0.601	0.297	24.403	66.044113	0
1293.307	0.800	0.053	64.303	6.997416	0
1249.581	0.775	0.110	70.347	25.269323	0
1195.118	0.819	0.021	8.125	4.071612	0
1138.761	0.835	0.027	236.883	4.568326	0
1067.562	0.716	0.171	23.319	38.622986	0
1020.061	0.770	0.064	23.131	13.303319	0
963.386	0.819	0.032	9.918	6.354330	0
921.256	0.766	0.070	270.565	10.932674	0
897.679	0.748	0.128	35.253	27.457031	0
850.989	0.794	0.080	17.503	14.142223	0
798.268	0.814	0.028	238.486	4.682887	0
785.321	0.689	0.186	10.274	42.748465	0
740.696	0.675	0.090	9.635	20.179371	0
726.952	0.570	0.260	30.569	56.610126	0
710.589	0.611	0.086	8.674	16.731129	0
632.825	0.733	0.060	144.470	5.805729	0
579.782	0.698	0.105	32.358	23.480993	0
547.964	0.698	0.097	42.528	19.792639	0
521.582	0.711	0.050	12.370	8.667768	0
478.209	0.691	0.082	23.876	16.970938	0
433.812	0.660	0.108	12.525	23.667057	0
3300.630	0.942	0.043	72.804	64.339577	0
3169.711	0.955	0.016	42.323	25.362009	0
3129.536	0.937	0.031	8.986	57.413364	0
3053.749	0.941	0.006	9.952	11.567762	0
2879.177	0.953	0.017	22.059	100.200645	0
1212.642	0.814	0.004	60.645	1.735731	0
1227.191	0.802	0.015	47.495	10.201081	0
680.424	0.708	0.036	7.357	6.446527	0

Figure S27 IR spectra of TNB:9-Anthroic acid:3-bromo-2-aminopyridine (**5**)



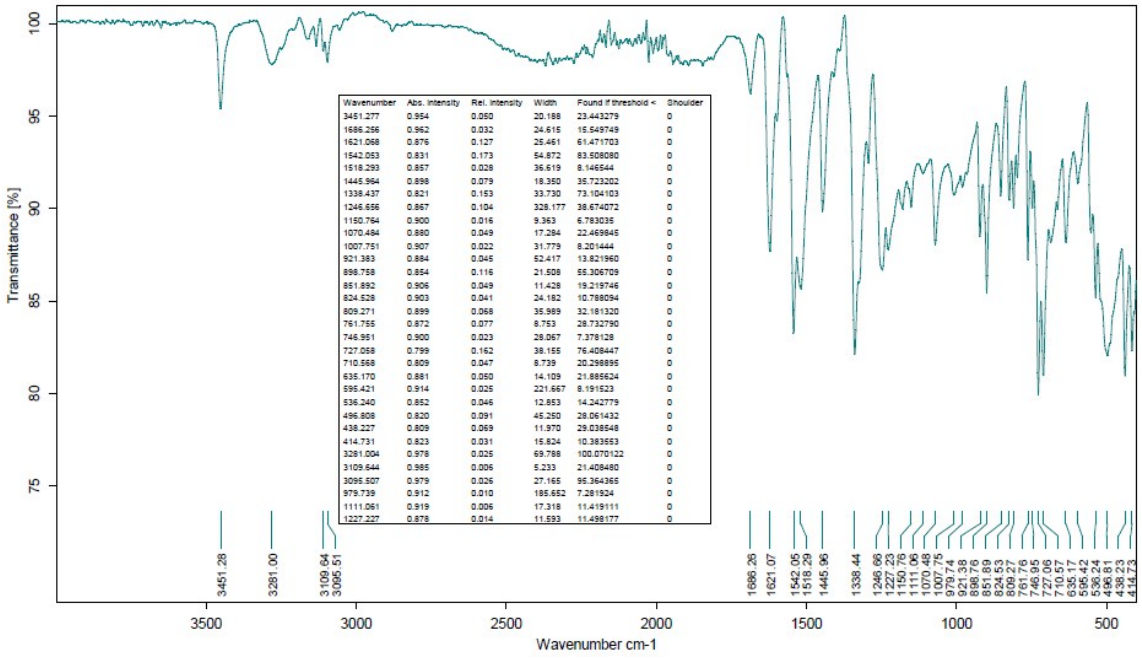
Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found If threshold <	Shoulder
3388.860	0.920	0.081	20.482	28.608557	0
1693.011	0.920	0.032	40.693	10.864715	0
1620.160	0.826	0.140	27.768	48.985661	0
1536.936	0.784	0.176	30.488	61.092110	0
1481.932	0.877	0.032	84.606	6.859497	0
1445.120	0.905	0.031	11.265	9.938833	0
1396.208	0.923	0.030	16.860	8.590756	0
1339.543	0.779	0.149	19.058	52.089405	0
1292.724	0.885	0.027	174.258	6.334557	0
1251.114	0.890	0.036	47.183	11.875056	0
1147.268	0.902	0.013	10.263	4.252391	0
1023.075	0.860	0.050	39.033	16.685947	0
901.438	0.790	0.096	11.242	32.328457	0
850.340	0.849	0.024	405.850	4.368581	0
824.012	0.794	0.082	15.899	25.495239	0
795.704	0.817	0.039	12.450	12.725463	0
743.082	0.763	0.056	9.611	19.600088	0
727.216	0.748	0.041	5.526	14.397408	0
708.800	0.717	0.154	44.352	53.332191	0
632.776	0.800	0.068	22.527	22.980780	0
557.279	0.826	0.027	8.614	8.105186	0
515.506	0.810	0.050	23.839	15.917539	0
440.012	0.781	0.033	16.965	10.046859	0
413.254	0.779	0.052	10.313	18.055801	0
3492.727	0.936	0.060	23.041	89.755882	0
3133.655	0.973	0.007	8.116	15.044648	0
3114.261	0.954	0.011	34.345	22.133720	0
3101.247	0.952	0.037	35.607	100.092262	0
3054.538	0.968	0.007	12.971	21.346722	0
1070.578	0.876	0.012	80.083	13.202042	0
599.741	0.827	0.013	46.424	9.951646	0

Figure S28 IR spectra of TNB:9-Anthroic acid:5-bromo-2-aminopyridine (**6**)



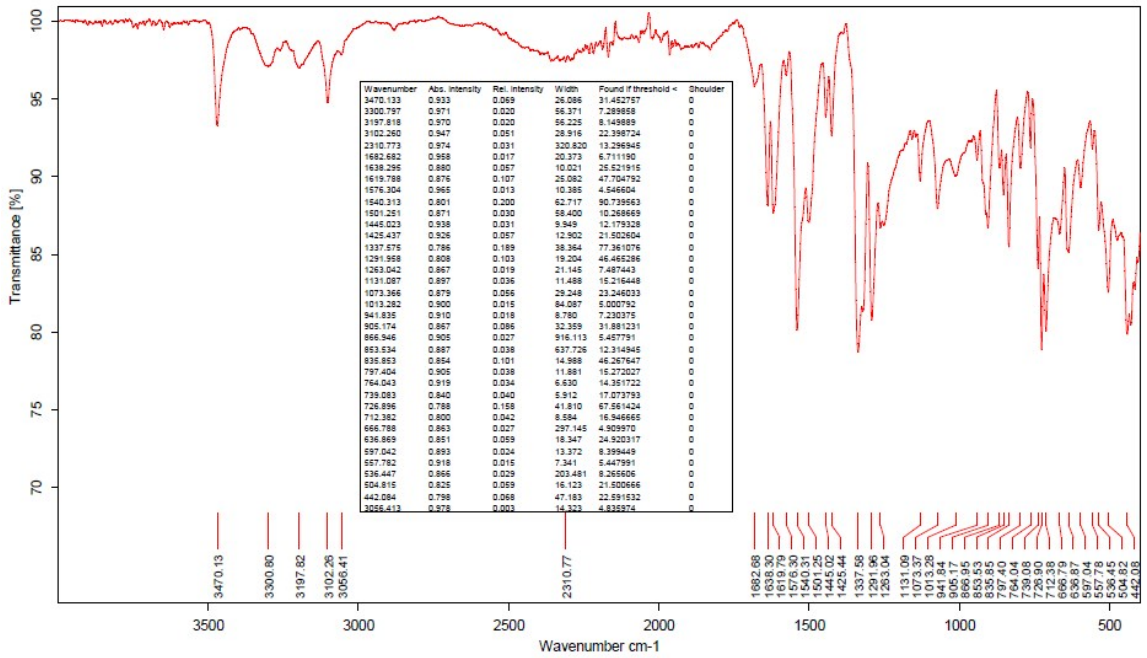
Wavenumber	Abs. intensity	Rel. intensity	Width	Found if threshold <	Shoulder
3493.063	0.990	0.013	41.024	14.153616	0
3391.840	0.991	0.010	15.410	10.830420	0
2364.643	0.989	0.014	53.349	15.824887	0
2162.678	0.988	0.015	10.604	16.666914	0
2031.666	0.982	0.021	12.854	21.921471	0
2006.719	0.984	0.017	7.874	19.854418	0
1977.928	0.987	0.010	16.339	11.410735	0
1676.310	0.936	0.066	28.927	74.397026	0
1620.938	0.968	0.020	18.407	22.212812	0
1536.342	0.957	0.036	30.408	39.171406	0
1486.293	0.973	0.014	14.616	12.631770	0
1446.261	0.974	0.014	15.352	13.175015	0
1339.689	0.949	0.052	30.171	56.783504	0
1291.187	0.958	0.024	11.584	26.120922	0
1252.504	0.951	0.033	25.651	36.693012	0
1021.586	0.988	0.010	18.780	11.079687	0
900.965	0.964	0.035	39.627	38.744034	0
848.497	0.980	0.013	15.179	13.540833	0
823.826	0.976	0.017	12.842	18.619650	0
793.087	0.972	0.025	11.146	24.403450	0
742.047	0.953	0.028	1632.746	20.229839	0
722.057	0.914	0.080	42.934	89.028069	0
638.575	0.957	0.025	21.260	26.803177	0
558.406	0.974	0.014	9.026	14.802319	0
513.312	0.962	0.027	14.307	29.463667	0
443.175	0.947	0.041	24.954	36.956078	0
2214.768	0.990	0.010	7.122	64.553772	0
2214.768	0.990	0.010	7.122	64.553772	0
1228.941	0.973	0.006	6.271	14.077844	0
1399.407	0.989	0.004	1067.781	4.933480	0

Figure S29 IR spectra of TNB:9-Anthroic acid:5-chloro-2-aminopyridine (**7**)



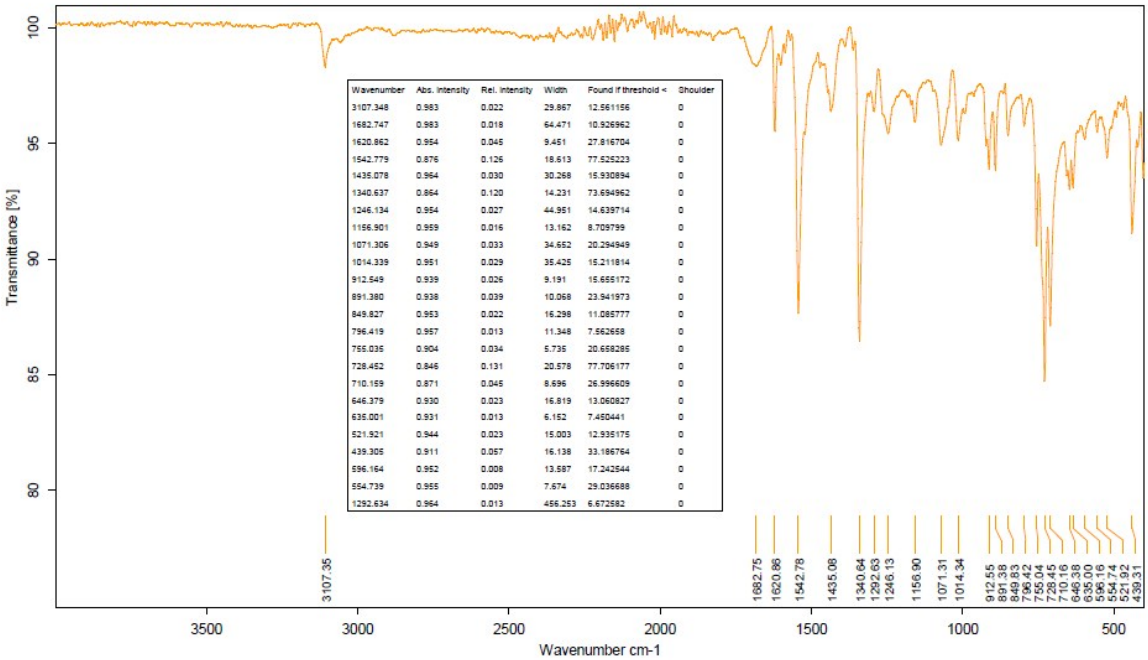
Wavenumber	Abs. intensity	Rel. intensity	Width	Found if threshold <	Shoulder
3451.277	0.954	0.050	20.188	23.443279	0
1686.256	0.962	0.032	24.615	15.549749	0
1621.068	0.876	0.127	25.461	61.471703	0
1542.053	0.831	0.173	54.872	83.508080	0
1518.293	0.857	0.028	36.619	8.146544	0
1445.964	0.898	0.079	18.350	35.723202	0
1338.437	0.821	0.153	33.730	73.104103	0
1246.656	0.867	0.104	328.177	38.674072	0
1150.764	0.900	0.016	9.363	6.783035	0
1070.484	0.880	0.049	17.284	22.469845	0
1007.751	0.907	0.022	31.779	8.201444	0
921.383	0.884	0.045	52.417	13.821960	0
898.758	0.854	0.116	21.508	55.306709	0
851.892	0.906	0.049	11.428	19.219746	0
824.528	0.903	0.041	24.182	10.788094	0
809.271	0.899	0.068	35.989	32.181320	0
761.755	0.872	0.077	8.753	28.732790	0
746.951	0.900	0.023	28.067	7.378128	0
727.058	0.799	0.162	38.155	76.408447	0
710.568	0.809	0.047	8.739	20.298895	0
635.170	0.881	0.050	14.109	21.666624	0
595.421	0.914	0.025	221.667	8.191523	0
536.240	0.852	0.046	12.853	14.242779	0
496.808	0.820	0.091	45.250	28.061432	0
438.227	0.809	0.069	11.970	29.036548	0
414.731	0.823	0.031	15.824	10.383553	0
3281.004	0.978	0.025	69.788	100.070122	0
3109.644	0.985	0.006	5.233	21.408480	0
3095.507	0.979	0.026	27.165	95.364366	0
979.739	0.912	0.010	185.652	7.281924	0
1111.061	0.919	0.006	17.318	11.419111	0
1227.227	0.878	0.014	11.593	11.499177	0

Figure S30 IR spectra of TNB:9-Anthroic acid:3-nitro-2-aminopyridine (**8**)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if threshold <	Shoulder
3470.133	0.933	0.069	26.086	31.452757	0
3300.797	0.971	0.020	56.371	7.289858	0
3197.818	0.970	0.020	56.225	8.149889	0
3102.260	0.947	0.051	28.916	22.398724	0
2310.773	0.974	0.031	320.820	13.296945	0
1682.682	0.958	0.017	20.373	6.711190	0
1638.296	0.880	0.057	10.021	25.521915	0
1619.788	0.876	0.107	25.082	47.704792	0
1576.304	0.965	0.013	10.385	4.546604	0
1540.313	0.801	0.200	62.717	90.739563	0
1501.251	0.871	0.030	58.400	10.268669	0
1445.023	0.938	0.031	9.949	12.179328	0
1425.437	0.926	0.057	12.902	21.502604	0
1337.575	0.786	0.189	38.364	77.361076	0
1291.958	0.808	0.103	19.204	46.466286	0
1263.042	0.867	0.019	21.145	7.487443	0
1131.087	0.897	0.036	11.488	15.216448	0
1073.366	0.879	0.056	29.248	23.246033	0
1013.282	0.900	0.015	84.087	5.000792	0
941.835	0.910	0.018	8.780	7.230375	0
905.174	0.867	0.086	32.359	31.881231	0
866.946	0.905	0.027	916.113	5.457791	0
853.534	0.887	0.038	637.726	12.314945	0
835.853	0.854	0.101	14.988	46.267647	0
797.404	0.905	0.038	11.881	15.272027	0
764.043	0.919	0.034	6.630	14.351722	0
739.083	0.840	0.040	5.912	17.073793	0
726.896	0.788	0.158	41.810	67.561424	0
712.382	0.800	0.042	8.584	16.946665	0
666.788	0.863	0.027	297.145	4.909970	0
636.869	0.851	0.059	18.347	24.520317	0
597.042	0.893	0.024	13.372	8.399449	0
557.782	0.918	0.015	7.341	5.447991	0
536.447	0.866	0.029	203.481	8.265606	0
504.815	0.825	0.059	16.123	21.600666	0
442.084	0.798	0.068	47.183	22.691832	0
3056.413	0.978	0.003	14.323	4.835974	0

Figure S31 IR spectra of TNB:9-Anthroic acid:5-nitro-2-aminopyridine (**9**)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if threshold <	Shoulder
3107.348	0.983	0.022	29.867	12.561156	0
1682.747	0.983	0.018	64.471	10.926962	0
1620.862	0.954	0.045	9.451	27.816704	0
1542.779	0.876	0.126	18.613	77.525223	0
1435.078	0.964	0.030	30.268	15.930894	0
1340.637	0.864	0.120	14.231	73.694962	0
1246.134	0.954	0.027	44.951	14.639714	0
1156.901	0.959	0.016	13.162	8.709799	0
1071.306	0.949	0.033	34.652	20.294949	0
1014.339	0.951	0.029	35.425	15.211814	0
912.549	0.939	0.026	9.191	15.655172	0
891.380	0.938	0.039	10.068	23.941973	0
849.827	0.953	0.022	16.298	11.085777	0
796.419	0.957	0.013	11.348	7.562658	0
755.035	0.904	0.034	5.735	20.659285	0
728.452	0.846	0.131	20.578	77.706177	0
710.159	0.871	0.045	8.696	26.996609	0
646.379	0.930	0.023	16.819	13.060827	0
635.001	0.931	0.013	6.152	7.460441	0
521.921	0.944	0.023	15.003	12.935175	0
439.305	0.911	0.057	16.138	33.186764	0
596.164	0.952	0.008	13.587	17.242544	0
554.739	0.955	0.009	7.674	29.036688	0
1292.634	0.964	0.013	456.253	6.672582	0

Figure S32 IR spectra of TNB:9-Anthroic acid:2,2'-dipyridyl (**10**)

Diffuse Reflectance data for complexes 1 - 10

Diffuse reflectance spectra were collected at room temperature using a Praying Mantis DRS attachment with a Varian Cary 500 UV-Vis-NIR spectrophotometer. Each spectrum was scanned from 800 nm to 200 nm at 600 nm/min. The small step at 350 nm in some spectra is an instrumental artefact associated with a change in lamp source.

Raman spectroscopic data for complexes 1 - 10

Raman spectra were acquired using the 785 nm line of a diode laser and a Horiba LabRAM HR Raman spectrometer equipped with an Olympus BX41 microscope attachment. The incident beam was focused onto the sample using a 100x objective (N.A. = 0.90) and the backscattered light was dispersed via a 600 lines/mm grating onto a liquid nitrogen cooled CCD detector. Spectral resolution was better than 1 cm^{-1}. LabSpec v5 software was used to acquire and analyse the spectra. It was necessary to use 785 nm excitation, as 514.5 nm excitation gave intense background fluorescence for several samples. Due to detector range limitations, it was not possible to acquire Raman peaks above about 2000 cm^{-1} with our instrument, so the Raman spectra do not show the C-H vibrations between 2800 cm^{-1} and 3200 cm^{-1}.

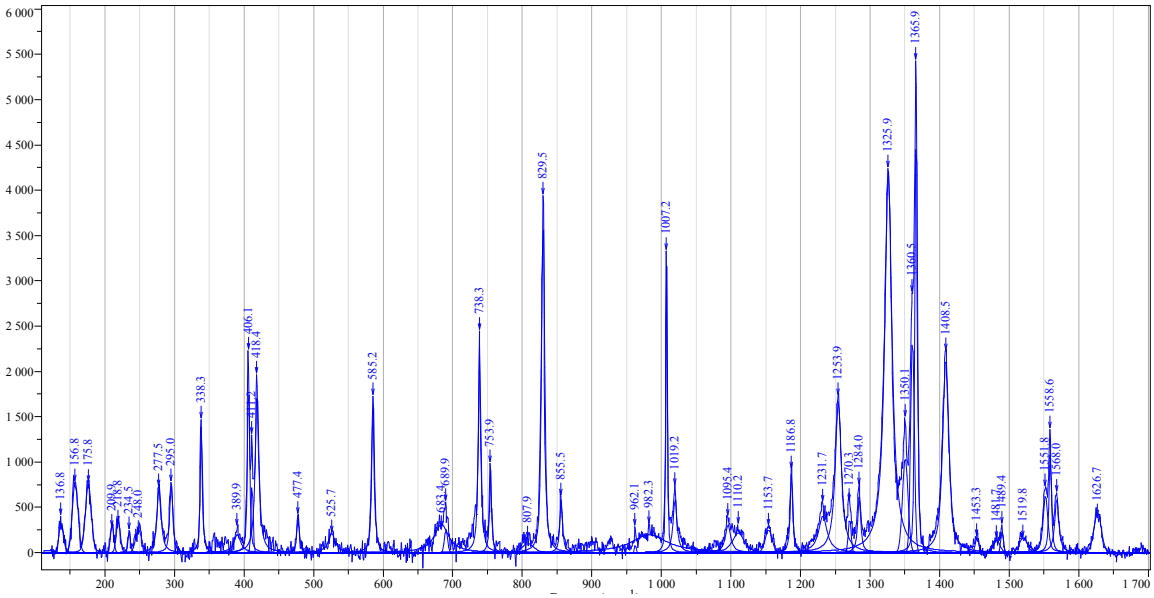


Figure S34 Raman spectrum of TNB:9-Anthroic acid:2-aminopyridine (**1**)

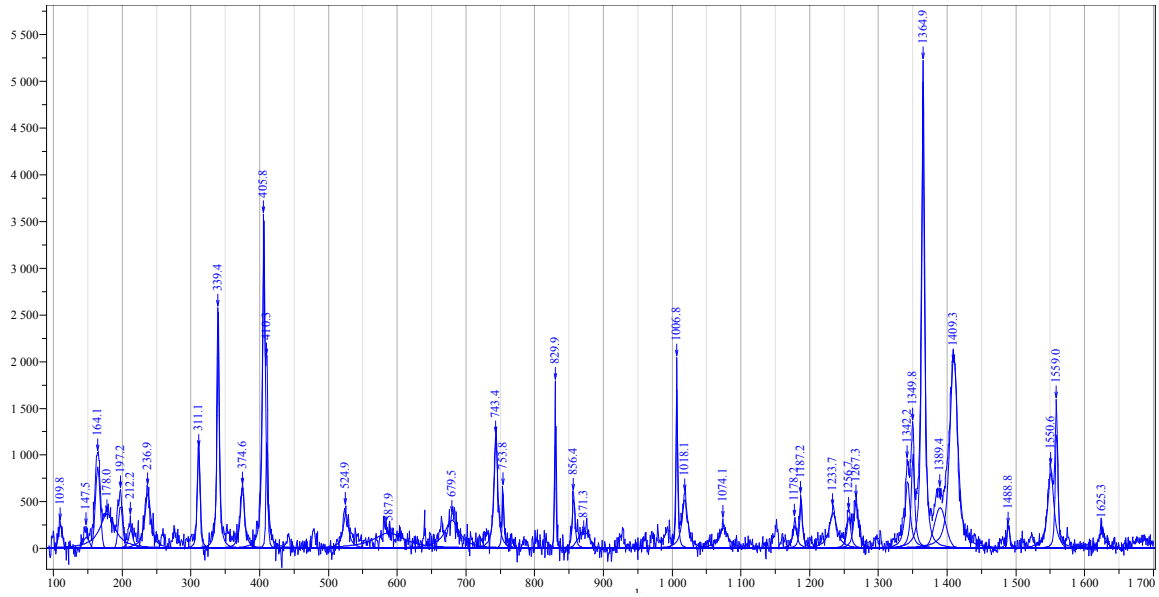


Figure S35 Raman spectrum of TNB:9-Anthroic acid:3-aminopyridine (**2**)

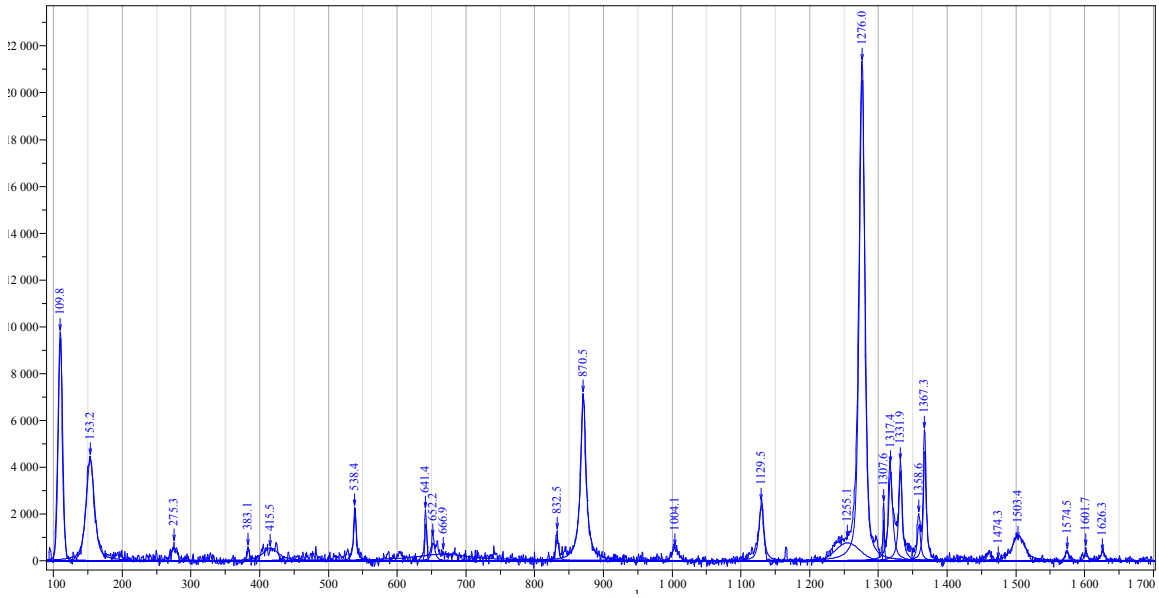


Figure S36 Raman spectrum of TNB:9-Anthroic acid:4-aminopyridine (**3**)

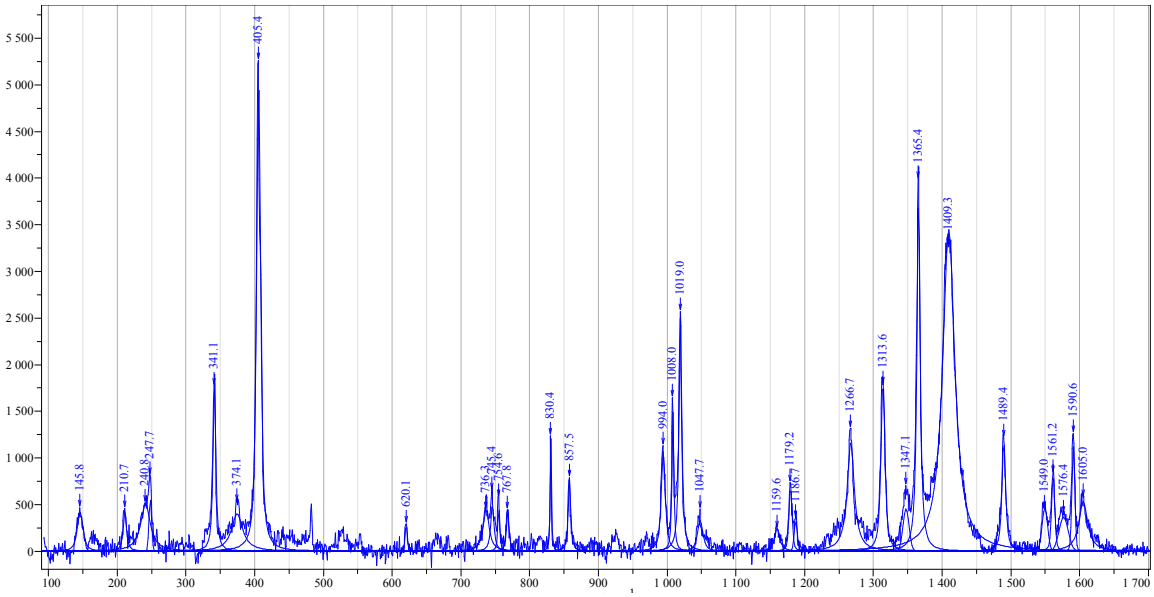


Figure S37 Raman spectrum of TNB:9-Anthroic acid:6-bromo-3-aminopyridine (**4**)

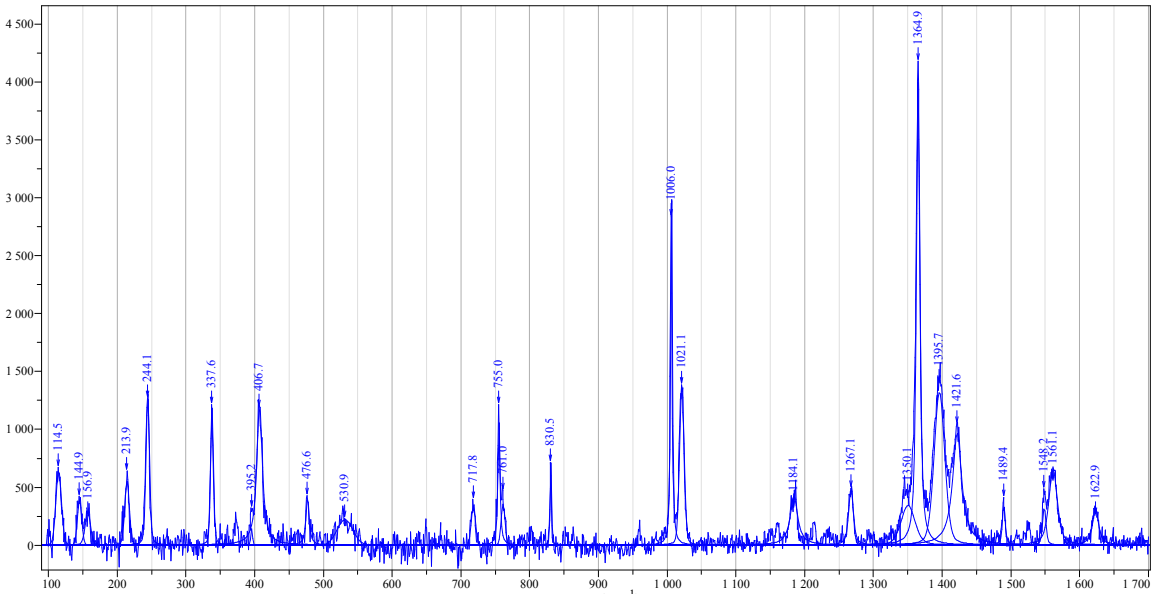


Figure S38 Raman spectrum of TNB:9-Anthroic acid:3-bromo-2-aminopyridine (**5**)

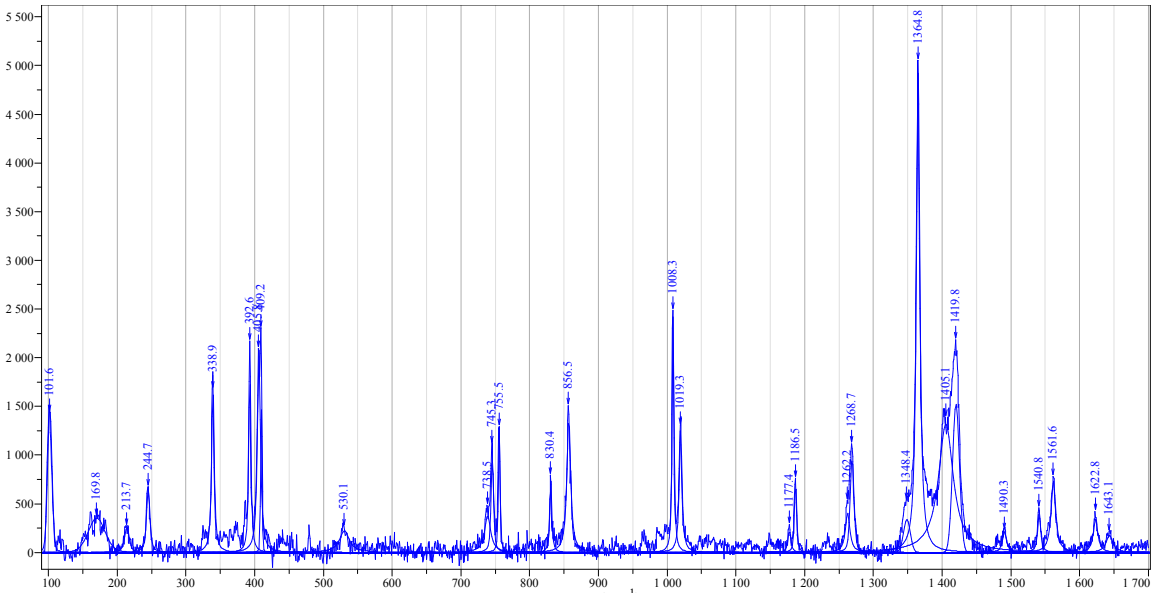


Figure S39 Raman spectrum of TNB:9-Anthroic acid:5-bromo-2-aminopyridine (**6**)

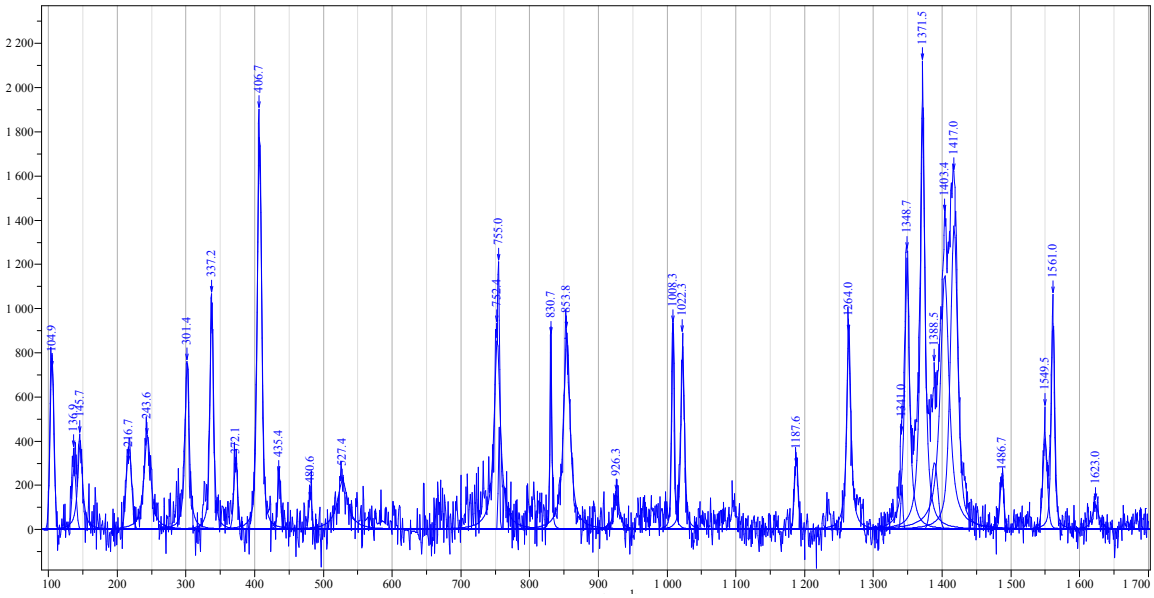


Figure S40 Raman spectrum of TNB:9-Anthroic acid:5-chloro-2-aminopyridine (**7**)

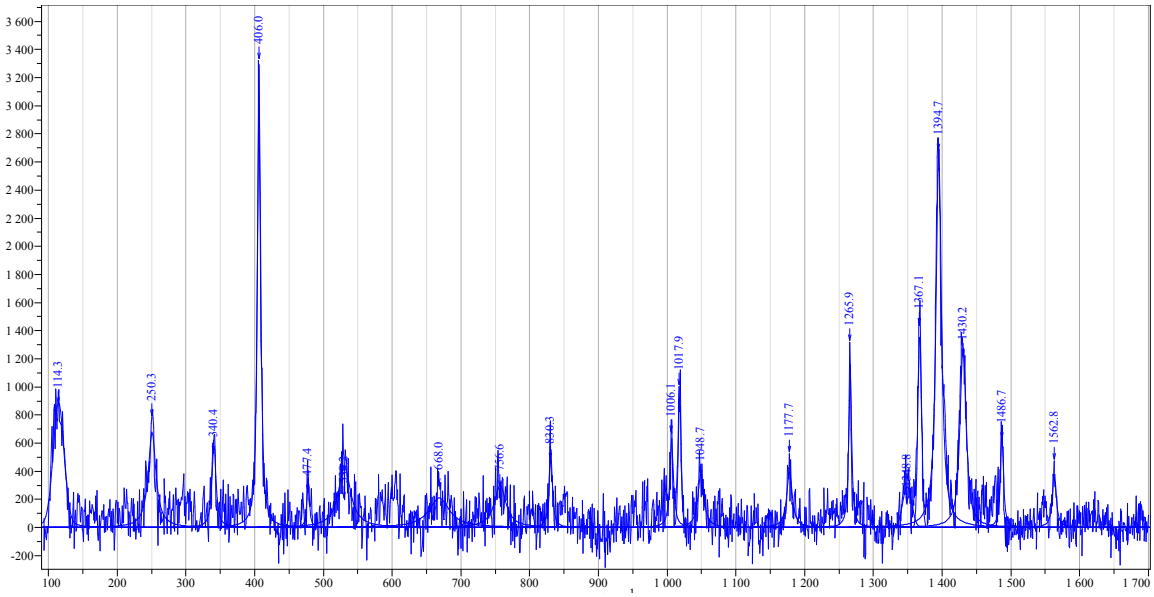


Figure S41 Raman spectrum of TNB:9-Anthroic acid:3-nitro-2-aminopyridine (**8**)

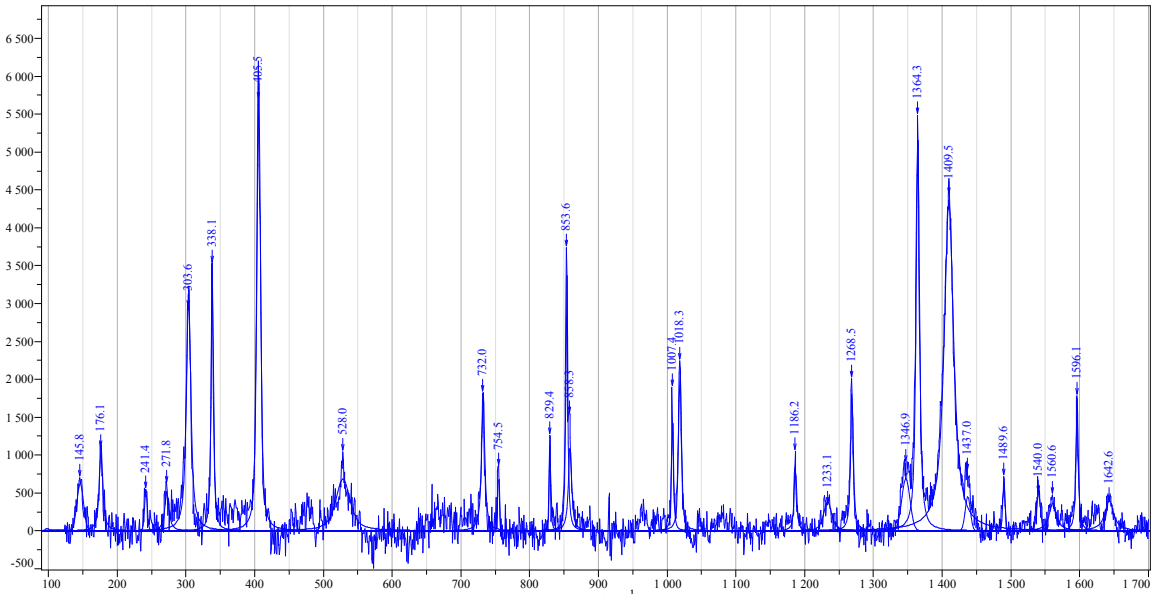


Figure S42 Raman spectrum of TNB:9-Anthroic acid:5-nitro-2-aminopyridine (**9**)

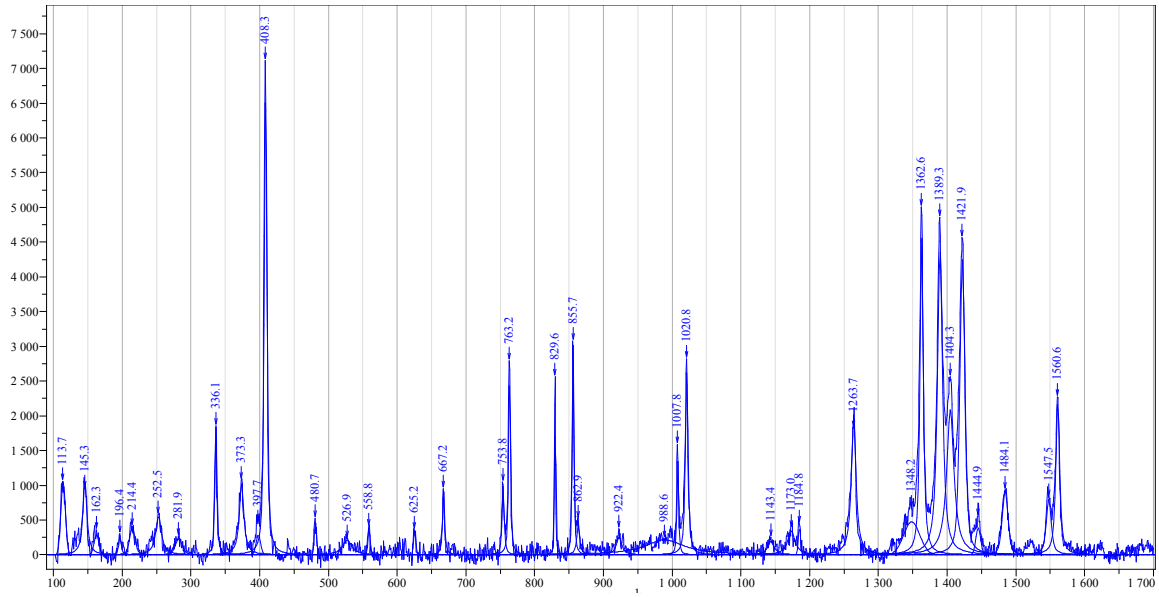


Figure S43 Raman spectrum of TNB:9-Anthroic acid:2,2'-dipyridyl (**10**)