Supplementary Materials: Nuclear Magnetic Resonance Spectroscopy Investigations of Naphthalene Based 1,2,3-Triazole Systems for Anion Sensing.

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General Considerations:

All chemicals and reactants were obtained from commercial sources and used without further purification.

NMR spectra were recorded on an Agilent MR400DD2 spectrometer, with a multinuclear probe with two RF channels and variable temperature capability (^{1}H-NMR: 400 MHz, ^{13}C-NMR: 100 MHz, ^{19}F-NMR: 376 MHz). The solvent used was deuterated acetonitrile (CD_3CN), dimethylsulfoxide ($[(CD_3)_2S=O]$, DMSO), acetone ($[(CD_3)_2C=O]$) with tetramethylsilane (TMS) as an internal standard set at 0 *ppm* in both ^{1}H-NMR and ^{13}C NMR spectra. The NMR signals are reported in parts per million (*ppm*) relative to the residual in the solvent. Signals are described with multiplicity, singlet (*s*), doublet (*d*), triplet (*t*), doublet of doublet (*dd*), triplet of doublet (*td*), quartet (*q*) and multiplet (*m*); coupling constants (*J*; *Hz*) and integration.

All reactions were monitored by thin–layer chromatography (TLC) using Merck silica gel plates 60 F_{254}; visualization was accomplished with UV light and/or staining with appropriate stains (Iodine, Vanillin).

Column Chromatography was performed with Selecto Scientific Silica-gel (particle size 100–200 microns).

Melting point were measured with Vernier Melt Station using Vernier LabQuest 2 and are uncorrected.

Room temperature (RT) absorption and steady state fluorescence measurements were performed using a Shimadzu UV-2450 spectrophotometer and PerkinElmer LS55 with well plate reader fluorimeter respectively. Concentration of **NpTP** was kept at ~1.0×10^{-6} mol dm^{-3} in acetonitrile to avoid any possible intermolecular effect. Stock concentrations of ~1.0×10^{-2} mol dm^{-3} for the tetrabutylammonium salts of anions were also prepared in acetonitrile. The solvents used are of HPLC grade and all the experiments are performed at ambient temperature (27 °C) with air-equilibrated solutions.

The Electrospray Ionization mass spectrometry (ESI-MS) was conducted using Shimadzu LCMS-2020 Single Quad respectively. All the experiments were performed at ambient temperature (27 ^{0}C) with air-equilibrated solutions.

High Resolution MS (HRMS) analyses were performed using MALDI, Q-TOF micro, 3200API, LCMS, GCMS EI (DI).

The single x-ray crystal structure measurements were made on a Bruker D8 Venture Photon 100 diffractometer using Mo-Kα radiation.

Nuclear Magnetic Resonance Spectroscopy Characterization of NpTP:

^{1}H NMR Spectrum in DMSO-d_6

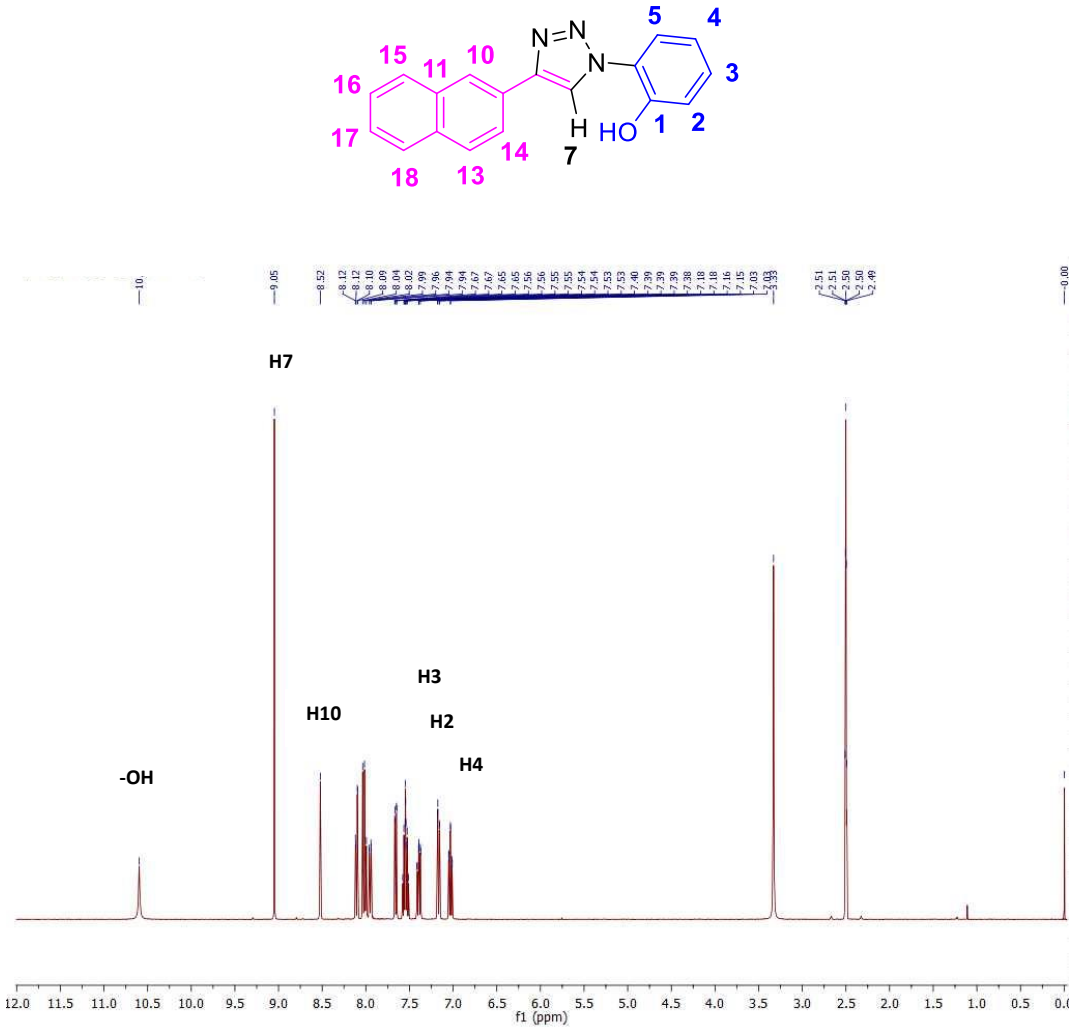

Figure S1. Full ^{1}H NMR spectrum in $(CD_3)_2S{=}O$ (400 MHz, RT) of **NpTP**; selected few peak are assigned (for the expanded version of the aromatic region and assignments, refer to the article).

^{13}C NMR Spectrum in DMSO-d_6

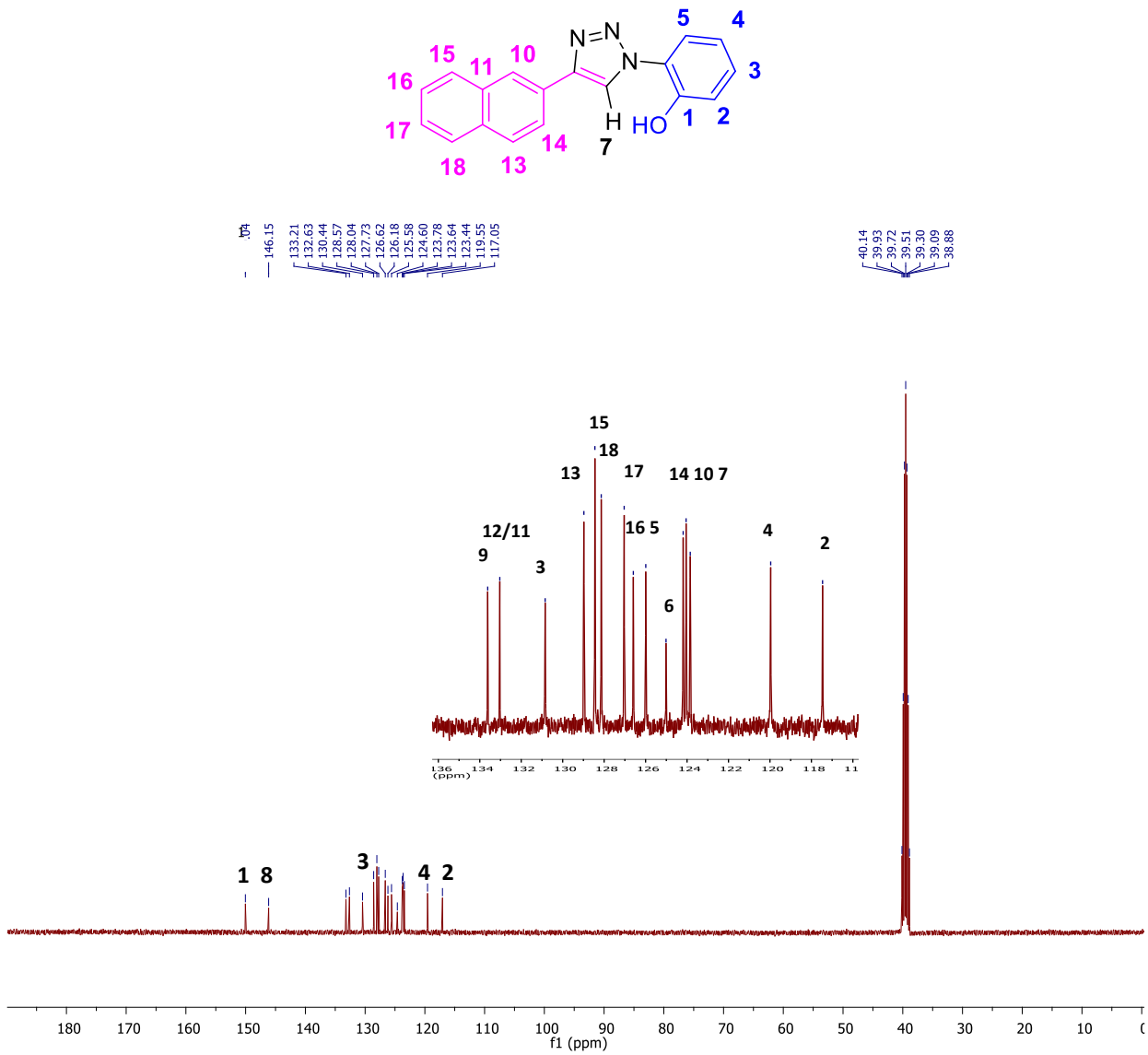

Figure S2. ^{13}C-NMR spectrum in $(CD_3)_2S{=}O$ (100 MHz, RT) of **NpTP**; expanded aromatic region in the inset.

^{13}C NMR Spectrum in Acetone-*d*$_6$

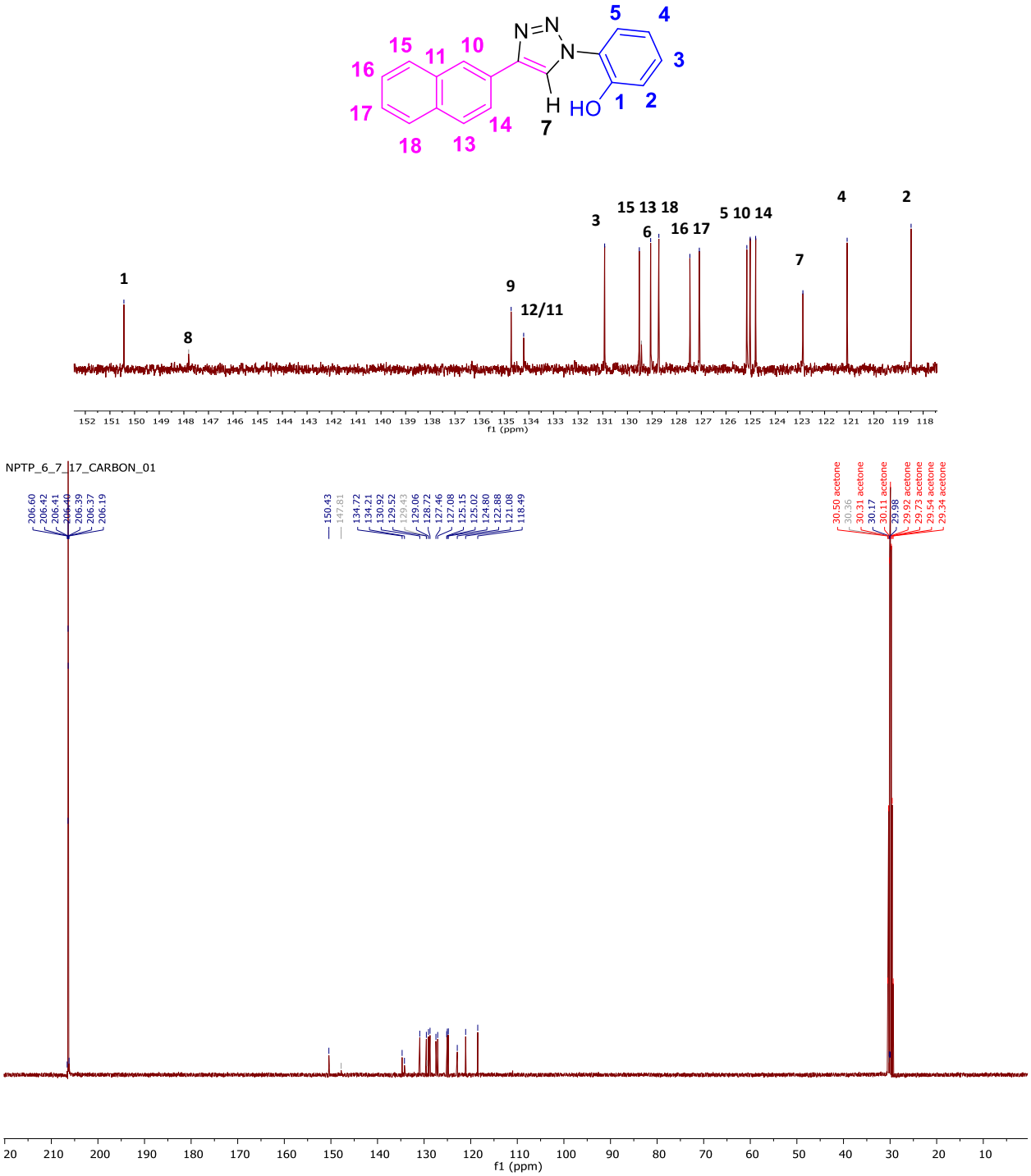

Figure S3. ^{13}C-NMR spectrum in $(CD_3)_2C{=}O$ (100 MHz, RT) of **NpTP**; expanded aromatic region in the inset.

1D DEPT90 spectrum of NpTP.

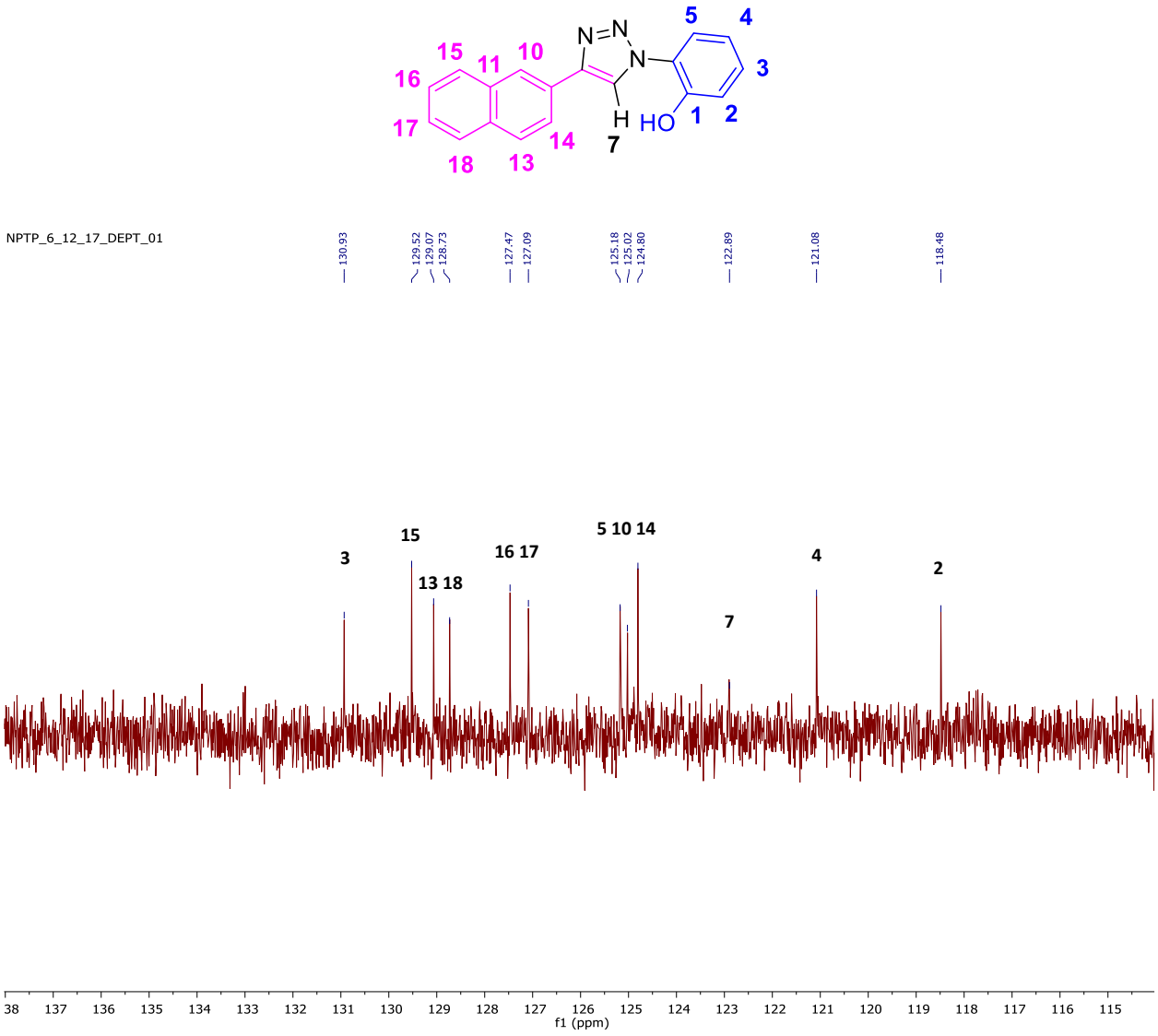

Figure S4. The 1D DEPT 90 spectrum in $(CD_3)_2C=O$ (100 MHz, RT) of **NpTP**, Only C-H signals are visible. The quaternary carbons (1, 6, 8, 9, 11, 12) are missing.

2D HMBC spectrum of NpTP.

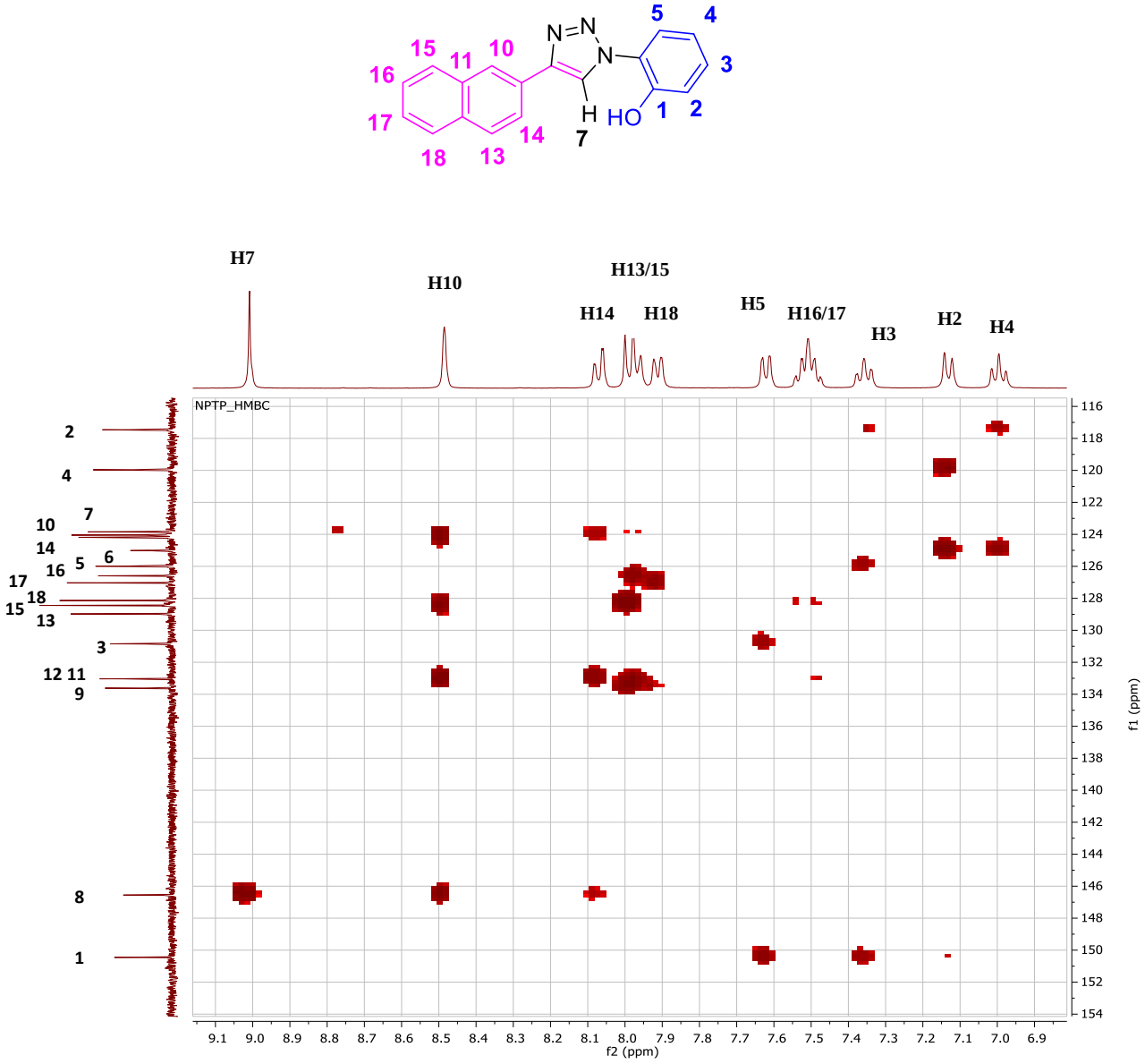

Figure S5. The 2D HMBC spectrum of **NpTP** in $(CD_3)_2S{=}O$, showing multiple bond carbon hydrogen correlation. The strong peaks are three-bond correlations and the weak peaks are two-bond correlations.

2D NOESY spectrum of NpTP.

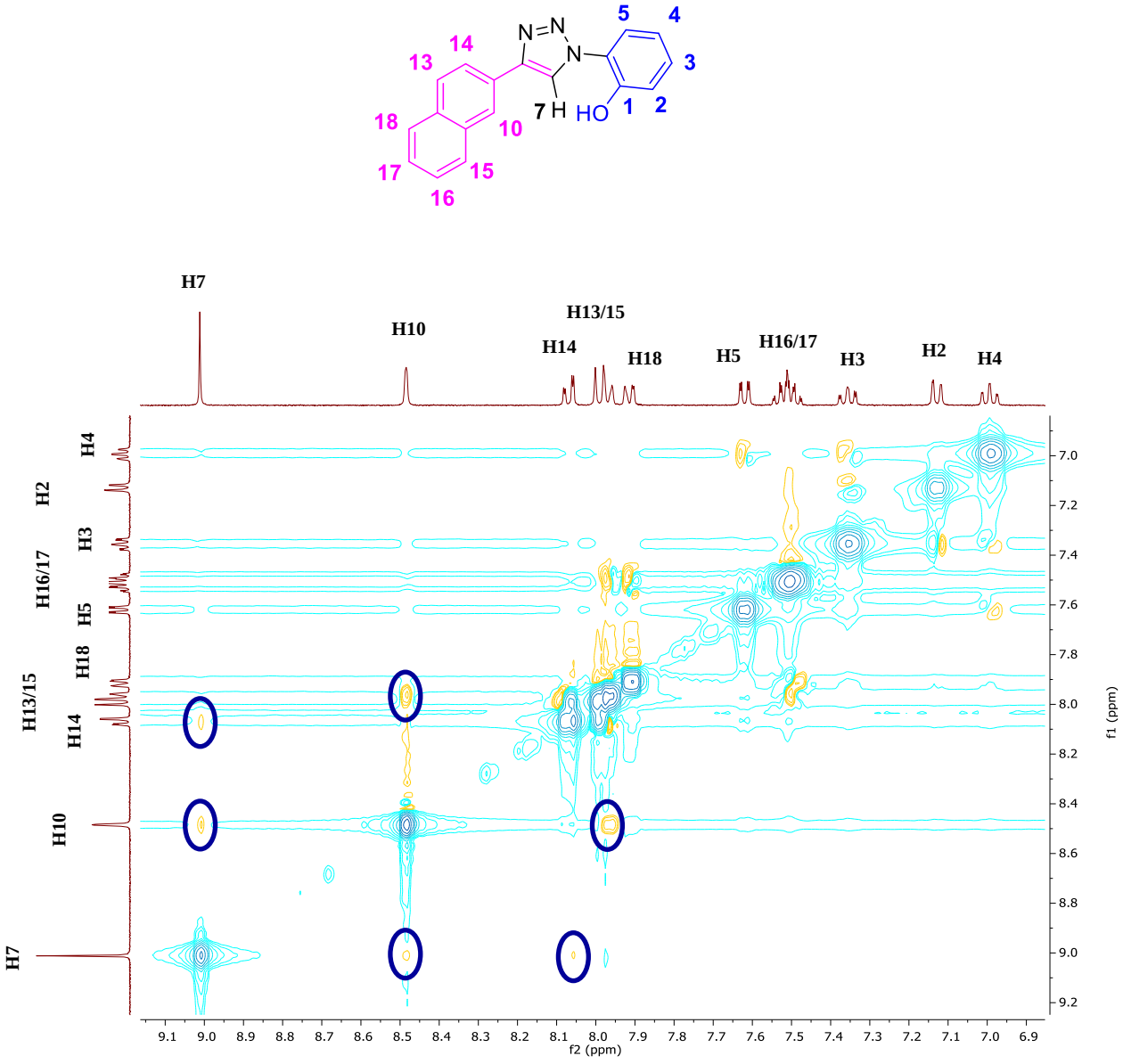

Figure S6. The 2D NOESY spectrum of **NpTP** in ($(CD_3)_2S=O$, RT) showing the correlation between the H7 proton and H10 and H14 protons and in between H10 and H15 proton.

2D NOESY spectrum of NpTP – OH correlation.

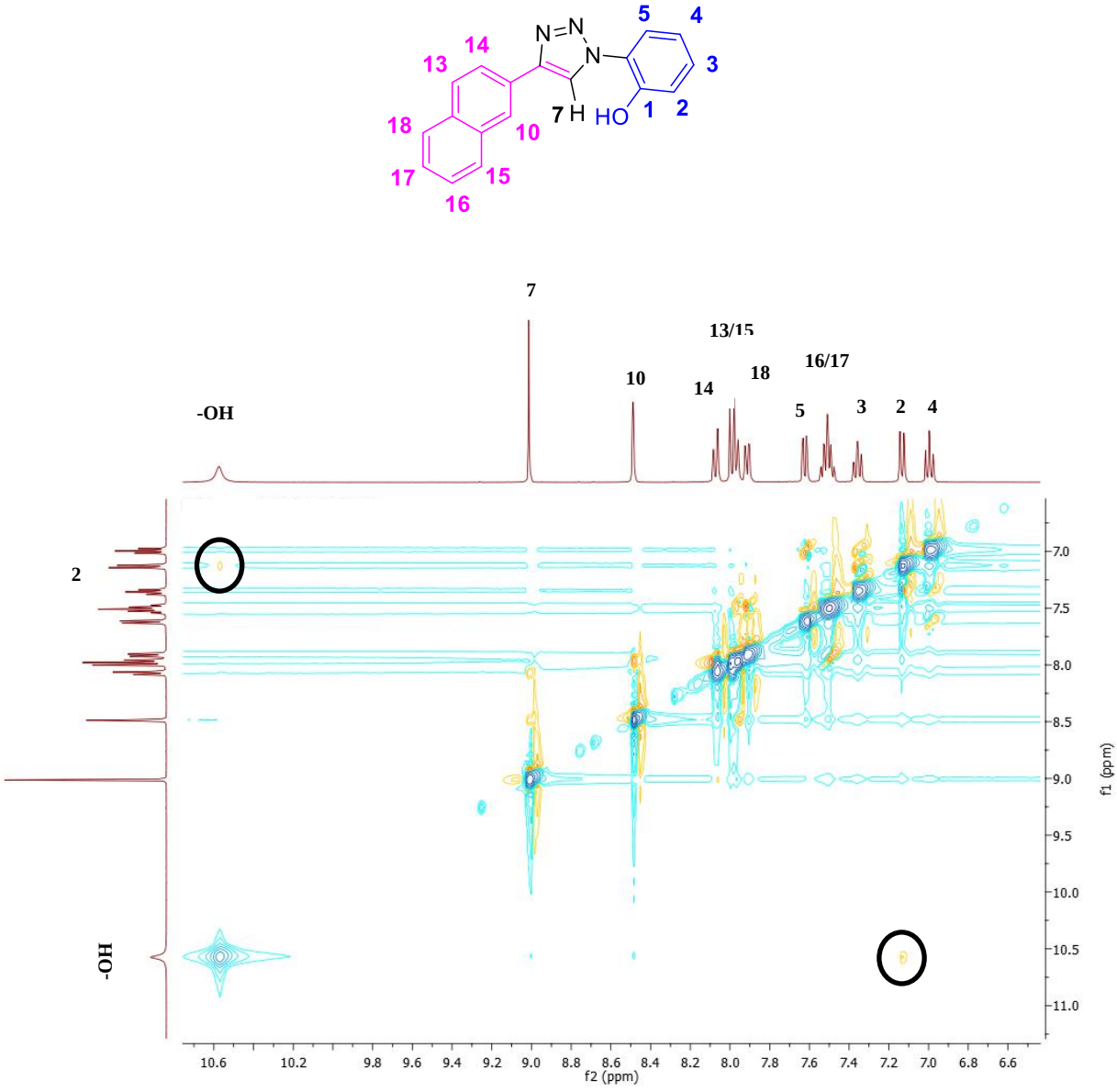

Figure S7. The 2D NOESY spectrum of **NpTP** in ($(CD_3)_2S{=}O$, RT) showing the correlation between the -OH proton and H2 proton.

2D NOESY spectrum of NpTP + 4 equivalence of TBAF.

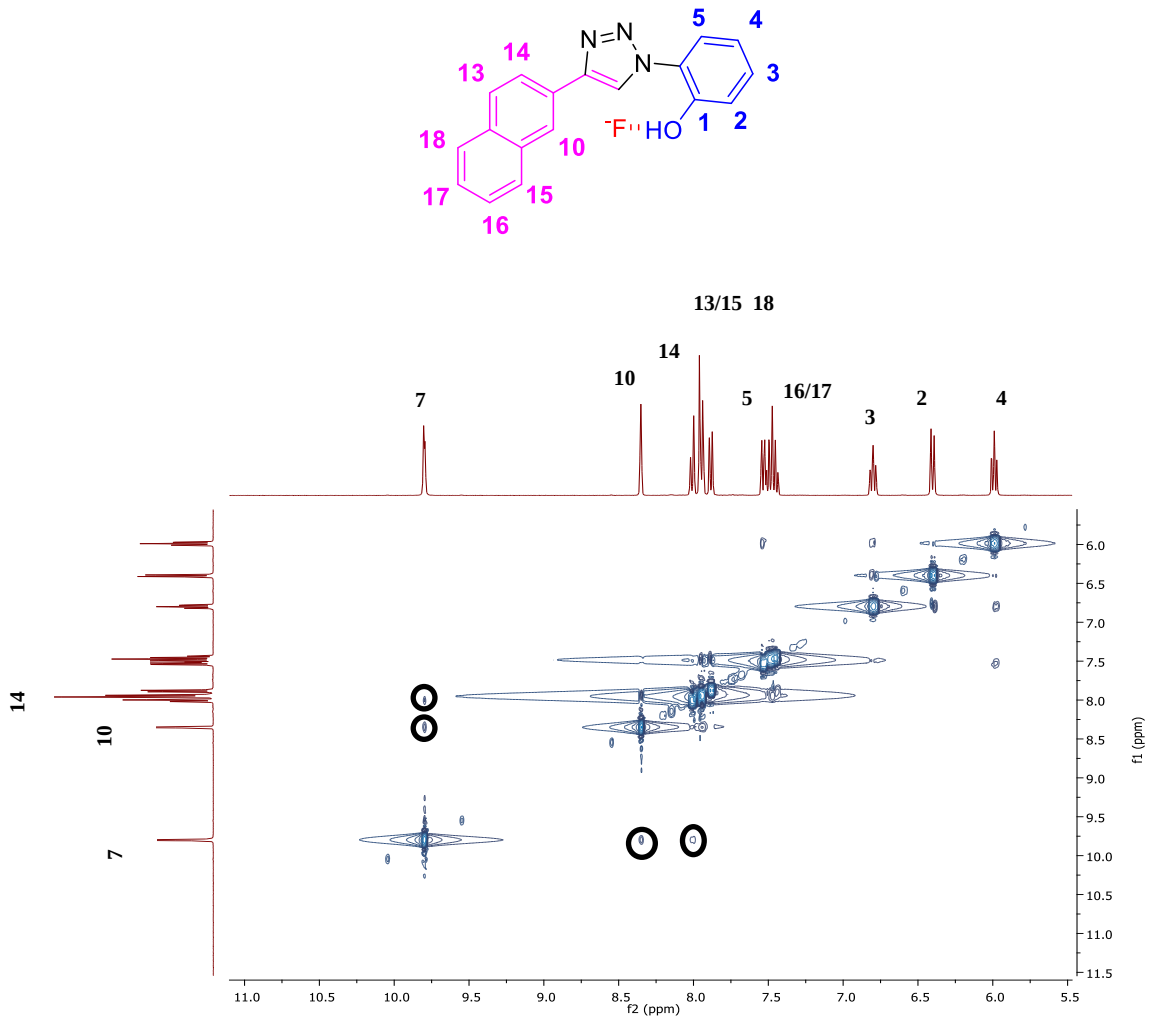

Figure S8. The 2D NOESY spectrum of **NpTP** with 4 equivalence of TBAF in ($(CD_3)_2S=O$, RT).

Titration experiments of NpTP with TBAF in DMSO-d_6

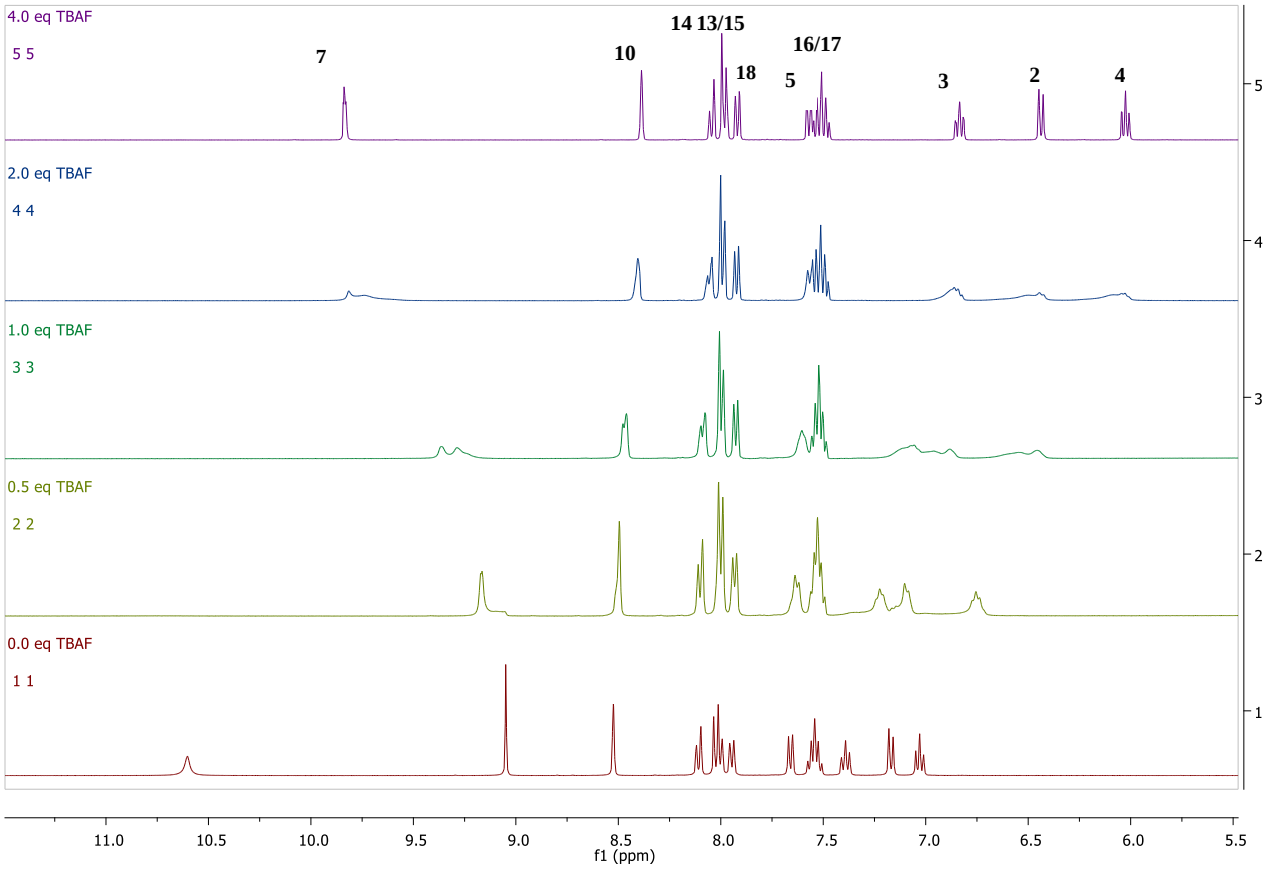

Figure S9. Changes in partial ^{1}H NMR (400 MHz) spectra of **NpTP** (6.2 x 10^{-2} M) in ($(CD_3)_2S=O$, RT) upon increasing equivalents of TBAF (0 to 4.0 eq.).

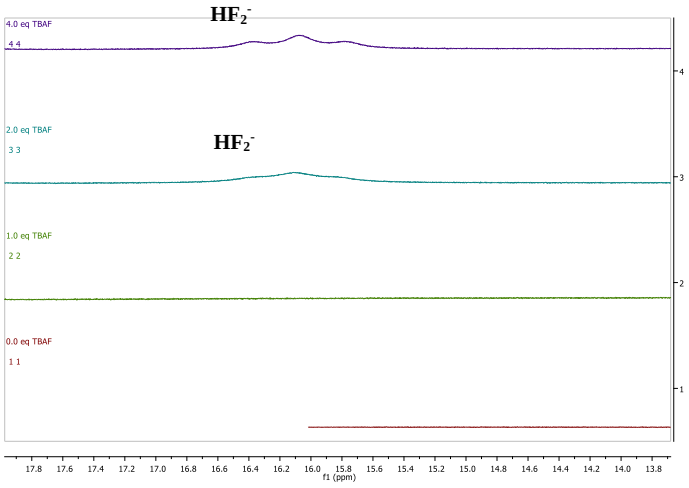

Figure S10. Changes in partial ^{1}H NMR (400 MHz) spectra of **NpTP** (6.2 x 10^{-2} M) in ($(CD_3)_2S=O$, RT) upon increasing equivalents of TBAF (0 to 4.0 eq.), region expanded from 13.5 to 18.0 ppm.

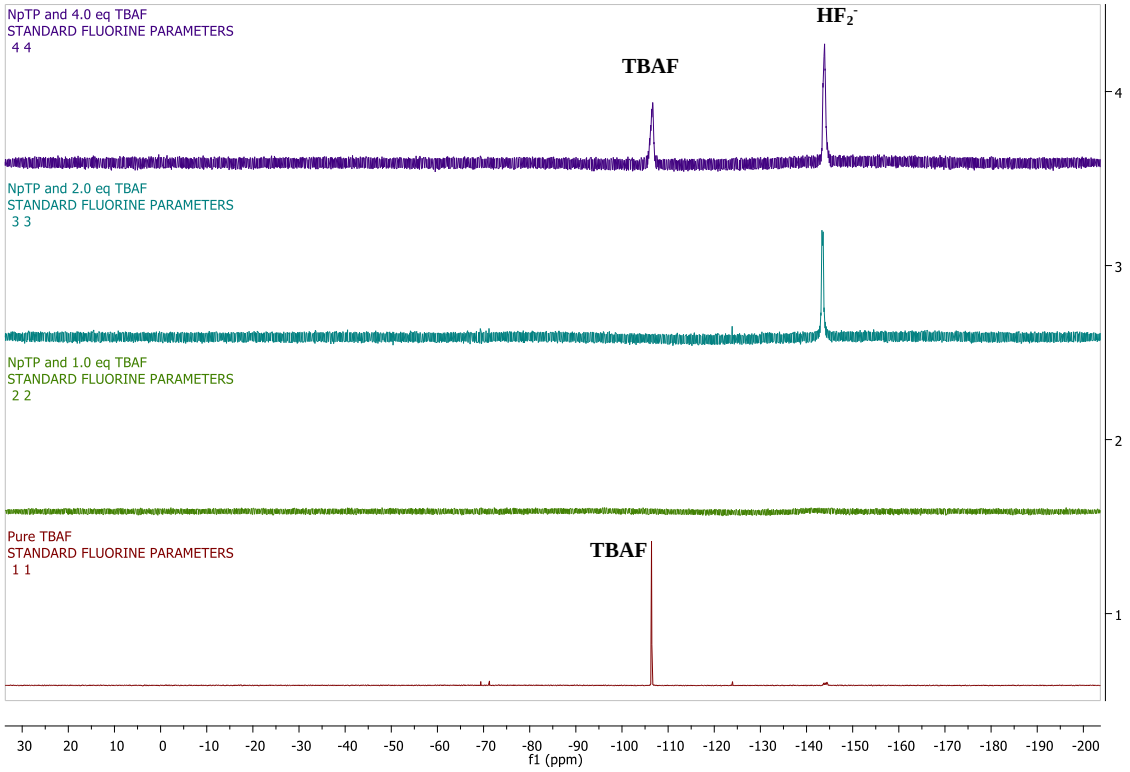

Figure S11. Changes in partial ^{19}F NMR (376 MHz) spectra of **NpTP** (6.2 x 10^{-2} M) in ($(CD_3)_2S=O$, RT) upon increasing equivalents of TBAF (0 to 4.0 eq.).

Benesi-Hildebrand plot for binding study.

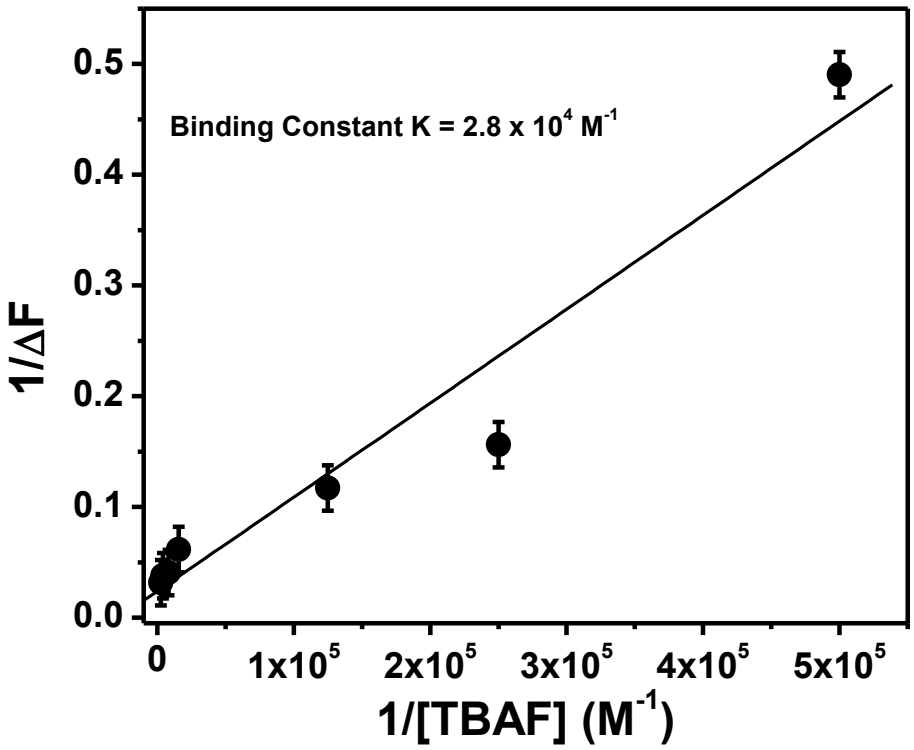

Figure S12. Benesi-Hildebrand plot of **NpTP** with addition of TBAF in acetonitrile. The fluorescence was monitored at 530 nm for the plot.

HRMS spectrum of NpTP.

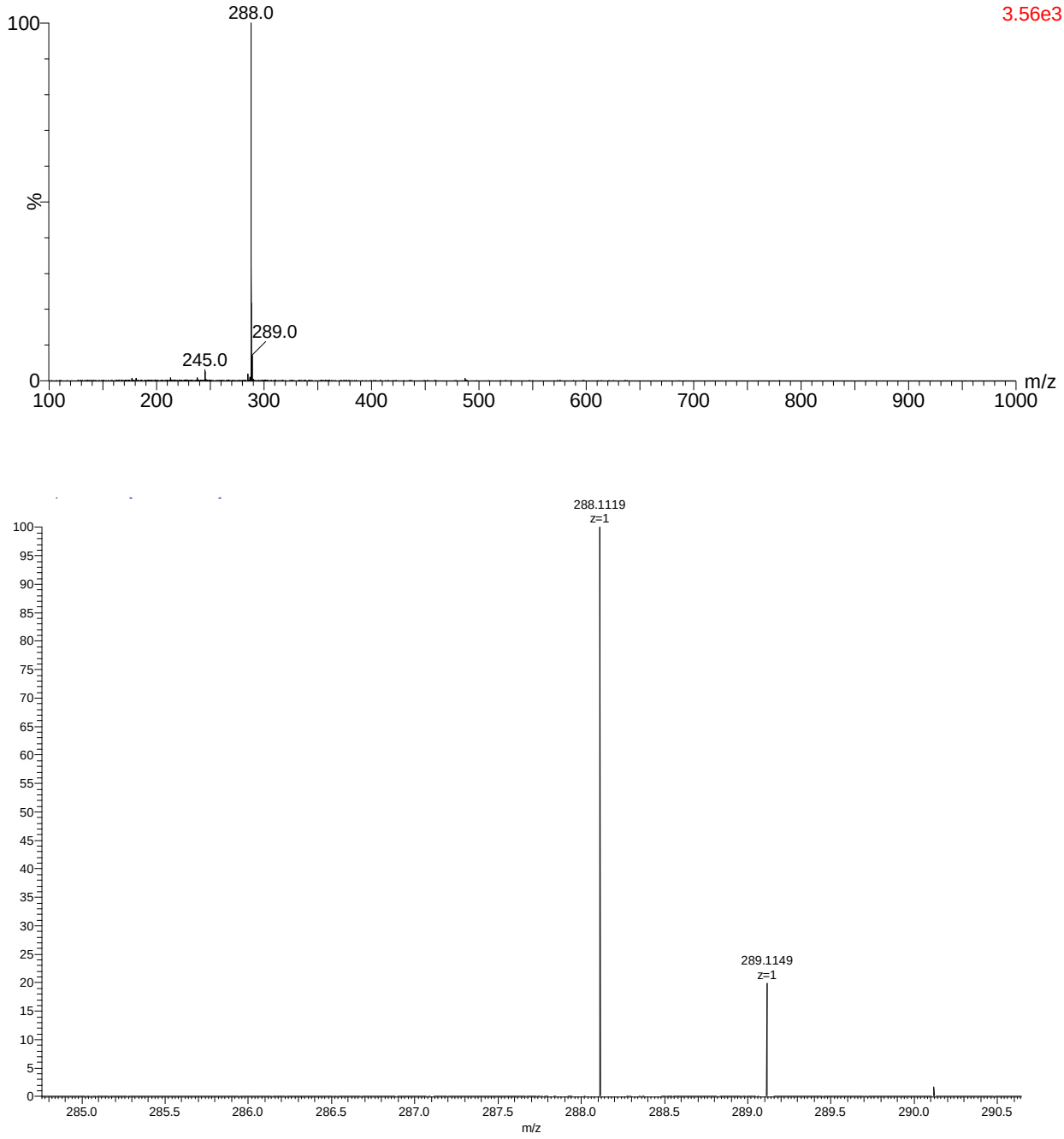

Figure S13. The HRMS spectrums of **NpTP** showing the *m*/*z* of 288.1119 [**NpTP** +H]$^+$.

ESI spectrum of NpTP.

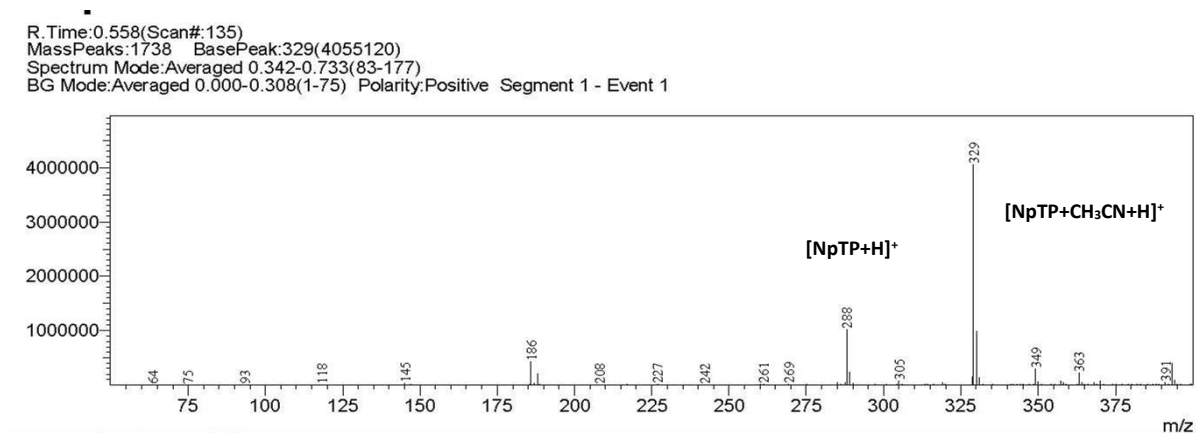

Figure S14. The ESI-MS spectrum of **NpTP** showing the *m*/*z* of 288 [**NpTP** +H]$^+$

Single Crystal X-ray spectroscopic study.

Crystal Structure Report for NpTP

A specimen of $C_{18}H_{13}N_3O$, approximate dimensions 0.067 mm x 0.068 mm x 0.071 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

The integration of the data using a tetragonal unit cell yielded a total of 17713 reflections to a maximum θ angle of 26.00° (0.81 Å resolution), of which 5409 were independent (average redundancy 3.275, completeness = 99.9%, R_{int} = 4.48%, R_{sig} = 6.43%) and 4263 (78.81%) were greater than $2\sigma(F^2)$. The final cell constants of a = 7.3806(16) Å, b = 7.3806(16) Å, c = 50.665(11) Å, volume = 2759.9(13) Å^3, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8829 and 1.0000.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 43, with Z = 8 for the formula unit, $C_{18}H_{13}N_3O$. The final anisotropic full-matrix least-squares refinement on F^2 with 398 variables converged at R1 = 4.88%, for the observed data and wR2 = 9.55% for all data. The goodness-of-fit was 1.024. The largest peak in the final difference electron density synthesis was 0.158 e$^-$/Å^3 and the largest hole was -0.203 e$^-$/Å^3 with an RMS deviation of 0.045 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.383 g/cm^3 and F(000), 1200 e$^-$. For the detail reports see below (Tables S1–S7). For Single X-ray crystal structure: Computer programs: Data collection: Bruker APEX3; cell refinement: Bruker SAINT; data reduction: Bruker SAINT; program(s) used to solve structure: SHELXT-2014 (Sheldrick 2014); program(s) used to refine structure: SHELXL2014 (Sheldrick 2014).

The structure has two independent **NpTP** molecules in the asymmetric unit that only differ in the orientation of the naphthyl ring to the triazole. The structure is held together to two independent hydrogen bonding chains with H-bonds between the phenolic O-H and triazole nitrogen of neighboring molecules. The first chain runs parallel to the a-axis, the second runs parallel to the b-axis (Figures S15–16). Combined, these form a network of hydrogen bonds that hold the structure together.

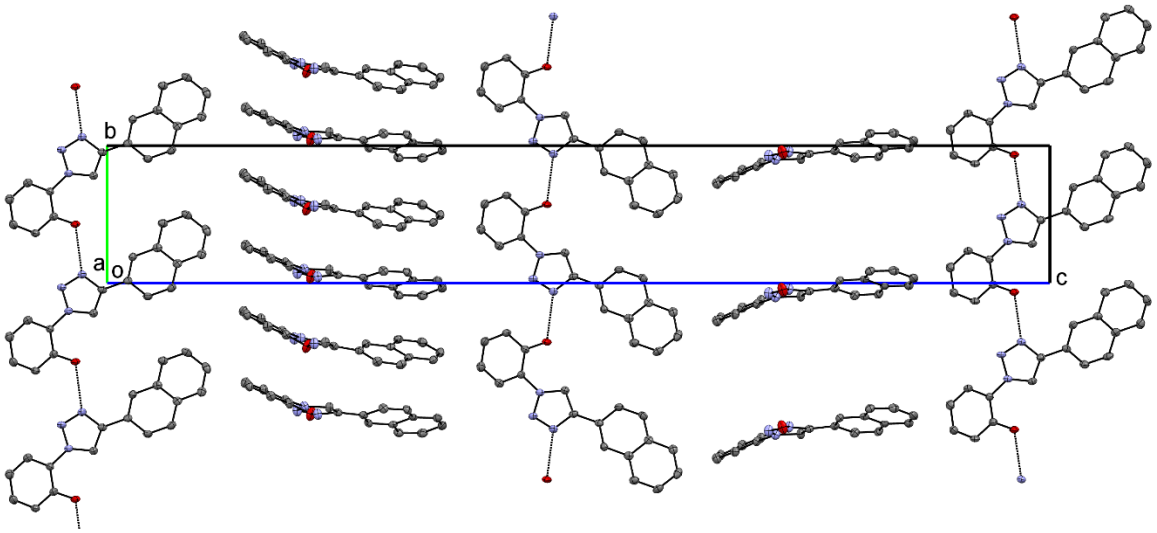

Figure S15. Crystal packing diagram of **NpTP** viewed along the a axis, H atoms have been omitted for clarity.

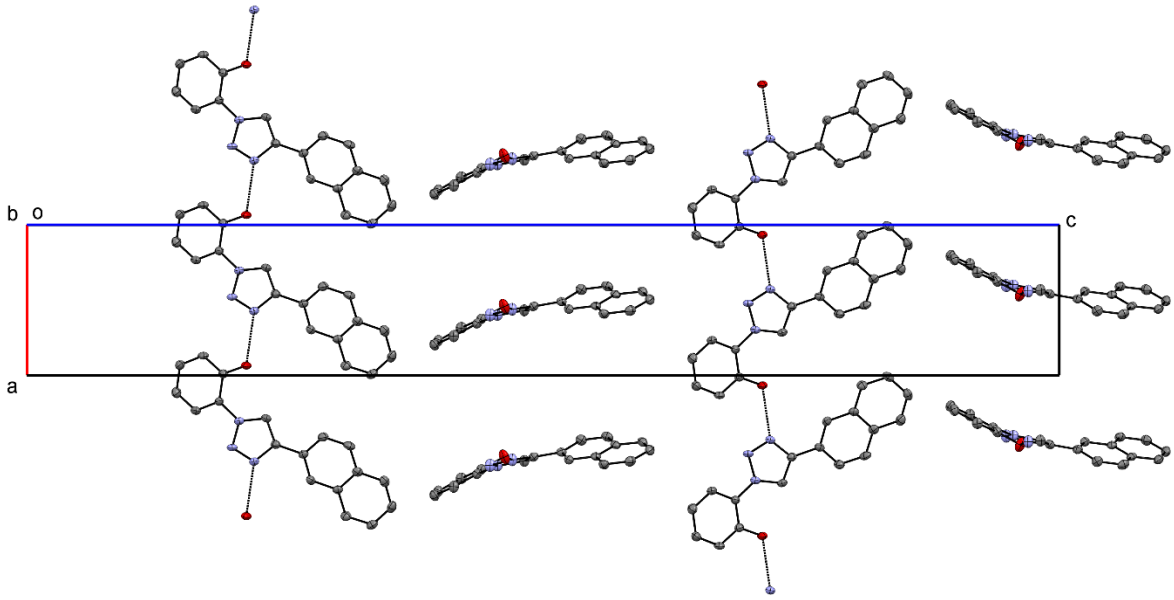

Figure S16. Crystal packing diagram of **NpTP** viewed along the b axis, H atoms have been omitted for clarity.

Table S1. Sample and crystal data for NpTP.

Chemical formula	$C_{18}H_{13}N_3O$	
Formula weight	287.31 g/mol	
Temperature	140(2) K	
Wavelength	0.71073 Å	
Crystal size	0.067 x 0.068 x 0.071 mm	
Crystal system	tetragonal	
Space group	P 43	
Unit cell dimensions	a = 7.3806(16) Å	α = 90°
	b = 7.3806(16) Å	β = 90°
	c = 50.665(11) Å	γ = 90°
Volume	2759.9(13) $Å^3$	
Z	8	
Density (calculated)	1.383 g/cm^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	1200	

Table S2. Data collection and structure refinement for NpTP.

Theta range for data collection	2.76 to 26.00°	
Index ranges	-9<=h<=8, -9<=k<=8, -62<=l<=62	
Reflections collected	17713	
Independent reflections	5409 [R(int) = 0.0448]	
Max. and min. transmission	1.0000 and 0.8829	
Structure solution technique	direct methods	
Structure solution program	SHELXT-2014 (Sheldrick 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014 (Sheldrick 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5409 / 1 / 398	
Goodness-of-fit on F^2	1.024	
Δ/σ_{max}	0.001	
Final R indices	4263 data; I>2σ(I)	R1 = 0.0488, wR2 = 0.0883
	all data	R1 = 0.0734, wR2 = 0.0955
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0469P)^2+0.0103P]$ where $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	-0.1(19)	
Largest diff. peak and hole	0.158 and -0.203 $eÅ^{-3}$	
R.M.S. deviation from mean	0.045 $eÅ^{-3}$	

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²) for NpTP.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.5405(3)	0.0658(3)	0.46222(4)	0.0315(7)
O2	0.0482(3)	0.5717(3)	0.46643(4)	0.0327(7)
N1	0.6013(4)	0.6968(4)	0.45549(5)	0.0216(7)
N2	0.5974(4)	0.5211(4)	0.44850(5)	0.0261(7)
N3	0.5604(4)	0.4279(4)	0.46988(5)	0.0253(7)
N4	0.1035(4)	0.2036(4)	0.45926(5)	0.0223(7)
N5	0.0739(4)	0.0315(4)	0.45178(5)	0.0264(7)
N6	0.0463(4)	0.9382(4)	0.47341(5)	0.0253(7)
C1	0.6244(5)	0.0109(4)	0.43986(6)	0.0228(8)
C2	0.6828(5)	0.1317(5)	0.42058(6)	0.0239(8)
C3	0.7700(5)	0.0700(5)	0.39808(7)	0.0266(8)
C4	0.7973(5)	0.8858(5)	0.39451(7)	0.0278(9)
C5	0.7386(5)	0.7663(5)	0.41333(6)	0.0251(8)
C6	0.6542(4)	0.8272(4)	0.43596(6)	0.0212(8)
C7	0.5674(5)	0.7150(4)	0.48158(6)	0.0241(8)
C8	0.5416(5)	0.5419(4)	0.49063(6)	0.0219(8)
C9	0.5089(4)	0.4769(4)	0.51767(6)	0.0214(8)
C10	0.5594(4)	0.3042(5)	0.52473(6)	0.0215(8)
C11	0.5373(4)	0.2410(4)	0.55091(6)	0.0211(8)
C12	0.4608(5)	0.3591(5)	0.57001(6)	0.0226(8)
C13	0.4074(5)	0.5333(5)	0.56203(7)	0.0269(9)
C14	0.4291(5)	0.5914(5)	0.53671(7)	0.0257(8)
C15	0.5910(5)	0.0656(5)	0.55880(7)	0.0248(8)
C16	0.5695(5)	0.0093(5)	0.58426(6)	0.0282(9)
C17	0.4952(5)	0.1260(5)	0.60318(7)	0.0292(9)
C18	0.4422(5)	0.2964(5)	0.59624(7)	0.0267(9)
C19	0.1248(5)	0.5177(4)	0.44349(6)	0.0234(8)
C20	0.1784(5)	0.6376(5)	0.42382(6)	0.0240(8)
C21	0.2529(5)	0.5745(5)	0.40059(7)	0.0288(9)
C22	0.2765(5)	0.3910(5)	0.39661(7)	0.0290(9)
C23	0.2264(5)	0.2713(5)	0.41597(6)	0.0252(8)
C24	0.1515(4)	0.3337(4)	0.43932(6)	0.0211(8)
C25	0.0964(5)	0.2198(5)	0.48573(6)	0.0235(8)
C26	0.0595(4)	0.0487(4)	0.49487(6)	0.0213(8)
C27	0.0396(4)	0.9825(4)	0.52197(7)	0.0208(8)

C28	0.9812(4)	0.8098(4)	0.52717(6)	0.0205(8)
C29	0.9714(4)	0.7438(4)	0.55338(6)	0.0209(8)
C30	0.0236(4)	0.8576(5)	0.57457(6)	0.0209(8)
C31	0.0790(5)	0.0355(5)	0.56848(6)	0.0242(9)
C32	0.0881(4)	0.0972(5)	0.54311(6)	0.0239(8)
C33	0.9123(5)	0.5655(4)	0.55917(7)	0.0257(8)
C34	0.9098(5)	0.5039(5)	0.58452(7)	0.0282(9)
C35	0.9637(5)	0.6166(5)	0.60544(7)	0.0295(9)
C36	0.0187(5)	0.7898(5)	0.60045(7)	0.0259(9)

Table S4. Bond lengths (Å) for NpTP.

O1-C1	1.353(4)	O1-H1	0.84
O2-C19	1.353(4)	O2-H2A	0.84
N1-N2	1.345(4)	N1-C7	1.352(4)
N1-C6	1.434(4)	N2-N3	1.312(4)
N3-C8	1.354(4)	N4-N5	1.343(4)
N4-C25	1.347(4)	N4-C24	1.438(4)
N5-N6	1.311(4)	N6-C26	1.363(4)
C1-C6	1.388(5)	C1-C2	1.391(4)
C2-C3	1.386(5)	C2-H2	0.95
C3-C4	1.386(5)	C3-H3	0.95
C4-C5	1.369(5)	C4-H4	0.95
C5-C6	1.380(5)	C5-H5	0.95
C7-C8	1.371(5)	C7-H7	0.95
C8-C9	1.471(4)	C9-C10	1.375(5)
C9-C14	1.412(5)	C10-C11	1.416(4)
C10-H10	0.95	C11-C15	1.411(5)
C11-C12	1.420(4)	C12-C13	1.404(5)
C12-C18	1.414(5)	C13-C14	1.362(5)
C13-H13	0.95	C14-H14	0.95
C15-C16	1.365(4)	C15-H15	0.95
C16-C17	1.401(5)	C16-H16	0.95
C17-C18	1.364(5)	C17-H17	0.95
C18-H18	0.95	C19-C24	1.389(5)
C19-C20	1.390(4)	C20-C21	1.380(5)
C20-H20	0.95	C21-C22	1.380(5)
C21-H21	0.95	C22-C23	1.371(5)
C22-H22	0.95	C23-C24	1.385(4)

C23-H23	0.95	C25-C26	1.373(5)
C25-H25	0.95	C26-C27	1.464(5)
C27-C28	1.371(5)	C27-C32	1.412(4)
C28-C29	1.416(4)	C28-H28	0.95
C29-C30	1.416(4)	C29-C33	1.417(4)
C30-C36	1.404(5)	C30-C31	1.410(5)
C31-C32	1.365(4)	C31-H31	0.95
C32-H32	0.95	C33-C34	1.362(4)
C33-H33	0.95	C34-C35	1.405(5)
C34-H34	0.95	C35-C36	1.365(5)
C35-H35	0.95	C36-H36	0.95

Table S5. Bond angles (°) for NpTP.

C1-O1-H1	109.5	C19-O2-H2A	109.5
N2-N1-C7	110.4(3)	N2-N1-C6	118.1(3)
C7-N1-C6	131.2(3)	N3-N2-N1	107.0(3)
N2-N3-C8	109.7(3)	N5-N4-C25	111.0(3)
N5-N4-C24	118.2(3)	C25-N4-C24	130.5(3)
N6-N5-N4	106.6(3)	N5-N6-C26	110.0(3)
O1-C1-C6	119.0(3)	O1-C1-C2	122.5(3)
C6-C1-C2	118.5(3)	C3-C2-C1	120.7(3)
C3-C2-H2	119.7	C1-C2-H2	119.7
C2-C3-C4	119.8(3)	C2-C3-H3	120.1
C4-C3-H3	120.1	C5-C4-C3	119.6(3)
C5-C4-H4	120.2	C3-C4-H4	120.2
C4-C5-C6	120.8(3)	C4-C5-H5	119.6
C6-C5-H5	119.6	C5-C6-C1	120.5(3)
C5-C6-N1	118.5(3)	C1-C6-N1	120.9(3)
N1-C7-C8	105.1(3)	N1-C7-H7	127.5
C8-C7-H7	127.5	N3-C8-C7	107.8(3)
N3-C8-C9	122.5(3)	C7-C8-C9	129.7(3)
C10-C9-C14	119.4(3)	C10-C9-C8	120.0(3)
C14-C9-C8	120.6(3)	C9-C10-C11	121.2(3)
C9-C10-H10	119.4	C11-C10-H10	119.4
C15-C11-C10	122.3(3)	C15-C11-C12	118.8(3)
C10-C11-C12	118.8(3)	C13-C12-C18	122.9(3)
C13-C12-C11	118.5(3)	C18-C12-C11	118.6(3)
C14-C13-C12	121.8(3)	C14-C13-H13	119.1
C12-C13-H13	119.1	C13-C14-C9	120.3(3)
C13-C14-H14	119.9	C9-C14-H14	119.9

C16-C15-C11	121.0(3)	C16-C15-H15	119.5
C11-C15-H15	119.5	C15-C16-C17	120.3(3)
C15-C16-H16	119.8	C17-C16-H16	119.8
C18-C17-C16	120.2(3)	C18-C17-H17	119.9
C16-C17-H17	119.9	C17-C18-C12	121.1(3)
C17-C18-H18	119.4	C12-C18-H18	119.4
O2-C19-C24	118.6(3)	O2-C19-C20	123.2(3)
C24-C19-C20	118.2(3)	C21-C20-C19	120.7(3)
C21-C20-H20	119.7	C19-C20-H20	119.7
C22-C21-C20	120.4(3)	C22-C21-H21	119.8
C20-C21-H21	119.8	C23-C22-C21	119.6(3)
C23-C22-H22	120.2	C21-C22-H22	120.2
C22-C23-C24	120.3(3)	C22-C23-H23	119.9
C24-C23-H23	119.9	C23-C24-C19	120.8(3)
C23-C24-N4	118.5(3)	C19-C24-N4	120.7(3)
N4-C25-C26	105.2(3)	N4-C25-H25	127.4
C26-C25-H25	127.4	N6-C26-C25	107.2(3)
N6-C26-C27	122.8(3)	C25-C26-C27	130.0(3)
C28-C27-C32	119.4(3)	C28-C27-C26	121.5(3)
C32-C27-C26	119.1(3)	C27-C28-C29	121.1(3)
C27-C28-H28	119.5	C29-C28-H28	119.5
C28-C29-C30	119.5(3)	C28-C29-C33	122.0(3)
C30-C29-C33	118.5(3)	C36-C30-C31	123.0(3)
C36-C30-C29	119.3(3)	C31-C30-C29	117.7(3)
C32-C31-C30	122.1(3)	C32-C31-H31	119.0
C30-C31-H31	119.0	C31-C32-C27	120.1(3)
C31-C32-H32	119.9	C27-C32-H32	119.9
C34-C33-C29	120.6(3)	C34-C33-H33	119.7
C29-C33-H33	119.7	C33-C34-C35	120.7(3)
C33-C34-H34	119.7	C35-C34-H34	119.7
C36-C35-C34	119.9(3)	C36-C35-H35	120.0
C34-C35-H35	120.0	C35-C36-C30	121.0(3)
C35-C36-H36	119.5	C30-C36-H36	119.5

Table S6. Anisotropic atomic displacement parameters (Å²) for NpTP.

The anisotropic atomic 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}
O1	0.0522(18)	0.0143(13)	0.0280(15)	-0.0006(11)	0.0127(12)	0.0045(12)
O2	0.0554(18)	0.0137(13)	0.0288(15)	-0.0015(11)	0.0100(13)	0.0034(12)
N1	0.0267(17)	0.0137(15)	0.0245(17)	0.0017(12)	0.0001(13)	-0.0011(13)
N2	0.0405(19)	0.0111(15)	0.0269(17)	0.0006(13)	-0.0006(14)	0.0009(14)
N3	0.0377(19)	0.0155(15)	0.0227(16)	0.0018(13)	0.0004(14)	-0.0005(14)
N4	0.0279(17)	0.0152(16)	0.0238(17)	-0.0002(12)	-0.0025(13)	-0.0018(13)
N5	0.040(2)	0.0143(16)	0.0247(16)	0.0009(13)	-0.0013(14)	-0.0010(14)
N6	0.0353(18)	0.0181(16)	0.0227(17)	-0.0002(13)	-0.0026(14)	-0.0029(14)
C1	0.026(2)	0.0190(19)	0.0234(19)	-0.0015(15)	-0.0018(16)	0.0016(16)
C2	0.030(2)	0.0132(19)	0.029(2)	0.0006(15)	-0.0003(16)	0.0030(16)
C3	0.032(2)	0.023(2)	0.0244(19)	0.0034(16)	-0.0021(17)	-0.0021(17)
C4	0.029(2)	0.029(2)	0.025(2)	-0.0006(17)	0.0050(16)	0.0034(17)
C5	0.035(2)	0.0162(19)	0.0245(18)	-0.0016(15)	-0.0008(16)	0.0001(18)
C6	0.024(2)	0.0173(19)	0.0219(19)	0.0013(15)	-0.0025(15)	-0.0013(16)
C7	0.033(2)	0.0151(19)	0.0242(19)	-0.0032(15)	-0.0002(16)	0.0012(16)
C8	0.022(2)	0.019(2)	0.024(2)	-0.0005(15)	-0.0027(15)	0.0010(16)
C9	0.0207(19)	0.0187(19)	0.025(2)	0.0017(15)	-0.0006(15)	-0.0021(15)
C10	0.0209(19)	0.020(2)	0.0234(19)	-0.0035(15)	0.0016(15)	-0.0016(15)
C11	0.0181(19)	0.0191(19)	0.0261(19)	0.0007(15)	0.0007(15)	-0.0039(15)
C12	0.0174(19)	0.023(2)	0.027(2)	-0.0018(15)	0.0031(15)	-0.0046(16)
C13	0.025(2)	0.020(2)	0.035(2)	-0.0070(17)	0.0058(16)	0.0014(16)
C14	0.028(2)	0.0198(19)	0.030(2)	0.0018(16)	0.0017(17)	0.0016(17)
C15	0.023(2)	0.024(2)	0.0274(19)	0.0007(16)	0.0013(15)	0.0050(16)
C16	0.027(2)	0.025(2)	0.032(2)	0.0086(17)	-0.0023(17)	0.0015(17)

C17	0.028(2)	0.035(2)	0.024(2)	0.0077(17)	0.0003(16)	-0.0060(18)
C18	0.023(2)	0.031(2)	0.026(2)	-0.0036(16)	0.0057(16)	-0.0043(18)
C19	0.030(2)	0.0182(19)	0.0222(19)	-0.0021(15)	-0.0017(16)	0.0003(16)
C20	0.029(2)	0.0157(19)	0.027(2)	0.0017(15)	-0.0014(16)	0.0001(16)
C21	0.036(2)	0.028(2)	0.0225(19)	0.0053(16)	-0.0034(16)	-0.0064(18)
C22	0.033(2)	0.030(2)	0.0242(19)	-0.0011(17)	0.0043(17)	-0.0019(18)
C23	0.029(2)	0.022(2)	0.025(2)	-0.0026(16)	-0.0003(16)	-0.0004(17)
C24	0.025(2)	0.0173(19)	0.0209(19)	0.0020(15)	-0.0020(15)	-0.0007(16)
C25	0.031(2)	0.0188(19)	0.0208(19)	-0.0007(15)	0.0008(16)	0.0010(16)
C26	0.0196(19)	0.0184(19)	0.0258(19)	0.0016(15)	-0.0017(15)	-0.0016(16)
C27	0.0200(19)	0.0182(19)	0.0242(18)	-0.0004(15)	-0.0011(15)	0.0028(15)
C28	0.0206(19)	0.0203(19)	0.0206(18)	-0.0007(15)	-0.0025(15)	-0.0006(16)
C29	0.0142(18)	0.0218(19)	0.0268(19)	-0.0007(15)	0.0015(15)	-0.0004(15)
C30	0.0143(19)	0.023(2)	0.0254(19)	-0.0007(15)	-0.0007(15)	0.0045(16)
C31	0.025(2)	0.023(2)	0.025(2)	-0.0065(15)	-0.0053(16)	-0.0006(16)
C32	0.028(2)	0.0163(19)	0.028(2)	0.0009(15)	-0.0021(16)	-0.0035(16)
C33	0.024(2)	0.023(2)	0.030(2)	0.0004(16)	-0.0026(16)	-0.0031(17)
C34	0.025(2)	0.025(2)	0.035(2)	0.0088(18)	0.0009(17)	-0.0035(18)
C35	0.025(2)	0.038(2)	0.026(2)	0.0089(17)	0.0030(16)	0.0084(18)
C36	0.023(2)	0.029(2)	0.025(2)	-0.0018(16)	-0.0014(15)	0.0047(17)

Table S7. Hydrogen bond distances (Å) and angles (°) for NpTP.

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O1-H1···N3	0.84	1.89	2.705(3)	163.2
O2-H2A···N6	0.84	1.90	2.728(4)	168.5
C2-H2···N2	0.95	2.39	3.265(4)	153.6
C20-H20···N5	0.95	2.45	3.325(4)	153.7