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Supporting Information

How explosive TNP interacts with small tritopic receptor: a combined crystallographic and thermodynamic approach

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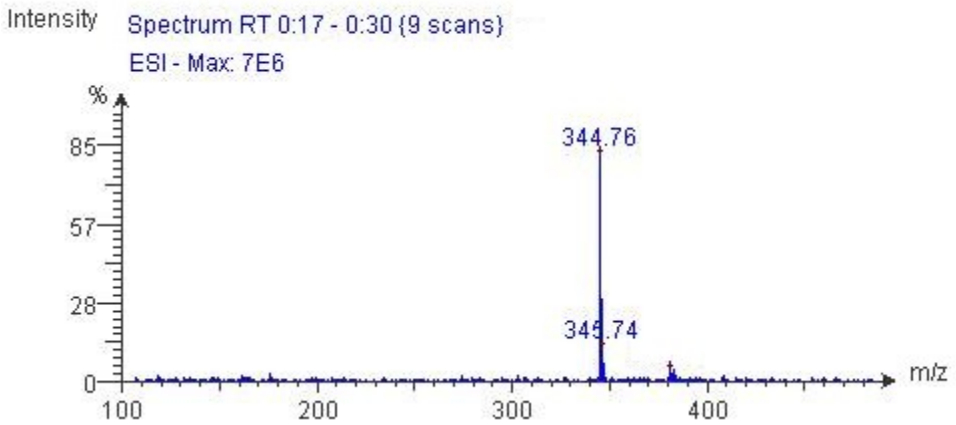

Fig. S1 ESI-MS of **PrPr.**

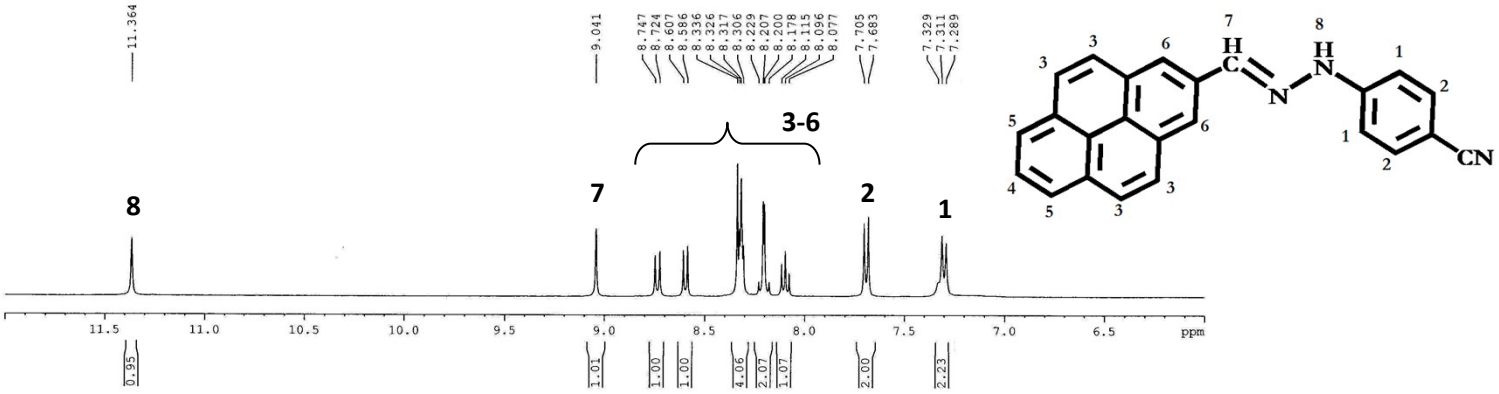

Fig. S2 ^{1}H NMR spectrum of **PrPr**.

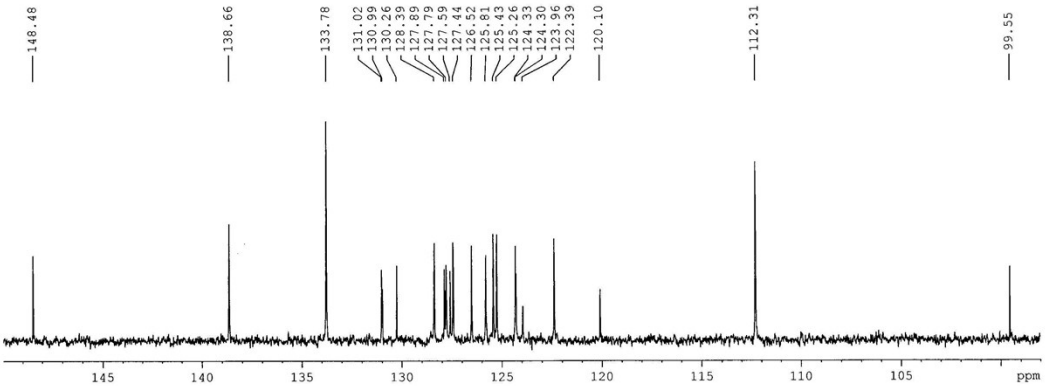

Fig. S3 ^{13}C NMR spectrum of **PrPr.**

Table S1. Crystallographic data of **PrPr**.

Crystal Data	
Formula	$C_{24}H_{15}N_3$
Formula Weight	345.39
Crystal System	Triclinic
Space group	P-1 (No. 2)
a, b, c [Angstrom]	7.1405(3) 15.6868(6) 16.3204(6)
alpha, beta, gamma [deg]	74.238(2) 86.018(2) 83.354(2)
V [Ang**3]	1746.13(12)
Z	4
D(calc) [g/cm**3]	1.314
Mu(MoKa) [/mm]	0.079
F(000)	720
Crystal Size [mm]	0.18 x 0.20 x 0.30
Data Collection	
Temperature (K)	296
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	3.3, 28.3
Dataset	-9: 9 ; -20: 20 ; -21: 21
Tot., Uniq. Data, R(int)	31478, 8539, 0.027
Observed Data [I > 2.0 sigma(I)]	5830
Refinement	
Nref, Npar	8539, 488
R, wR2, S	0.0559, 0.1556, 1.05
Min. and Max. Resd. Dens. [e/Ang^3]	-0.26, 0.24

Table S2. Bond distances of **PrPr** (Angstrom).

N001	-N003	1.356(2)	C00R	-C011	1.360(3)
N001	-C00H	1.274(2)	C00S	-C01B	1.370(3)
N003	-C007	1.362(2)	C00W	-C010	1.368(3)
N01I	-C01H	1.132(3)	C011	-C019	1.378(3)
N003	-H003	0.8600	C013	-C017	1.328(3)
N002	-C00M	1.276(2)	C018	-C01F	1.371(3)
N002	-N004	1.359(2)	C019	-C01H	1.425(3)
N004	-C006	1.360(2)	C019	-C01B	1.384(3)
N015	-C01A	1.136(3)	C01D	-C01F	1.377(3)
N004	-H004	0.8600	C00G	-H00G	0.9300
C005	-C00G	1.440(2)	C00H	-H00H	0.9300
C005	-C009	1.419(2)	C00J	-H00J	0.9300
C005	-C008	1.405(2)	C00R	-H00R	0.9300
C007	-C00S	1.383(2)	C00S	-H00S	0.9300
C007	-C00R	1.391(3)	C00W	-H00W	0.9300
C008	-C00H	1.444(2)	C010	-H010	0.9300
C008	-C00W	1.397(2)	C011	-H011	0.9300

C009	-C00K	1.419(2)	C013	-H013	0.9300
C009	-C00D	1.420(2)	C017	-H017	0.9300
C00D	-C00N	1.421(2)	C018	-H018	0.9300
C00D	-C00P	1.414(2)	C01B	-H01B	0.9300
C00G	-C00J	1.343(2)	C01D	-H01D	0.9300
C00J	-C00P	1.419(3)	C01F	-H01F	0.9300
C00K	-C017	1.432(3)	C006	-C00I	1.389(2)
C00K	-C010	1.388(3)	C006	-C00X	1.395(2)
C00N	-C018	1.392(3)	C00A	-C00M	1.446(2)
C00N	-C013	1.420(3)	C00A	-C00U	1.395(3)
C00P	-C01D	1.388(3)	C00A	-C00E	1.406(2)
C00B	-C00E	1.417(2)	C014	-C016	1.424(3)
C00B	-C00F	1.422(2)	C016	-C01C	1.397(3)
C00B	-C00C	1.417(2)	C01C	-C01G	1.370(4)
C00C	-C00L	1.389(3)	C01E	-C01G	1.377(3)
C00C	-C012	1.428(3)	C00I	-H00I	0.9300
C00E	-C00O	1.439(2)	C00L	-H00L	0.9300
C00F	-C00Q	1.413(3)	C00M	-H00M	0.9300
C00F	-C016	1.418(3)	C00O	-H00O	0.9300
C00I	-C00T	1.371(3)	C00T	-H00T	0.9300
C00L	-C00U	1.363(3)	C00U	-H00U	0.9300
C00O	-C00Z	1.341(3)	C00X	-H00X	0.9300
C00Q	-C00Z	1.425(3)	C00Y	-H00Y	0.9300
C00Q	-C01E	1.393(3)	C00Z	-H00Z	0.9300
C00T	-C00V	1.386(3)	C012	-H012	0.9300
C00V	-C00Y	1.382(3)	C014	-H014	0.9300
C00V	-C01A	1.428(3)	C01C	-H01C	0.9300
C00X	-C00Y	1.365(3)	C01E	-H01E	0.9300
C012	-C014	1.338(3)	C01G	-H01G	0.9300

Table S3 - Bond Angles of **PrPr** (Degrees).

N003	-N001	-C00H	115.65(15)	C009	-C00K	-C017	118.31(16)
N001	-N003	-C007	121.56(15)	C00D	-C00N	-C013	118.33(17)
N001	-N003	-H003	119.00	C013	-C00N	-C018	122.96(19)
C007	-N003	-H003	119.00	C00D	-C00N	-C018	118.70(17)
N004	-N002	-C00M	114.82(15)	C00D	-C00P	-C01D	119.31(16)
N002	-N004	-C006	122.41(15)	C00D	-C00P	-C00J	118.19(15)

N002	-N004	-H004	119.00	C00J	-C00P	-C01D	122.49(16)
C006	-N004	-H004	119.00	C007	-C00R	-C011	120.72(18)
C009	-C005	-C00G	117.27(14)	C007	-C00S	-C01B	119.50(16)
C008	-C005	-C009	119.53(14)	C008	-C00W	-C010	121.52(17)
C008	-C005	-C00G	123.20(15)	C00K	-C010	-C00W	121.55(16)
C00R	-C007	-C00S	119.24(16)	C00R	-C011	-C019	120.29(19)
N003	-C007	-C00R	118.76(16)	C00N	-C013	-C017	121.5(2)
N003	-C007	-C00S	122.00(15)	C00K	-C017	-C013	122.16(18)
C005	-C008	-C00H	121.14(14)	C00N	-C018	-C01F	121.22(19)
C00H	-C008	-C00W	119.99(16)	C011	-C019	-C01H	120.87(19)
C005	-C008	-C00W	118.88(16)	C011	-C019	-C01B	119.10(18)
C00D	-C009	-C00K	119.23(15)	C01B	-C019	-C01H	120.03(19)
C005	-C009	-C00K	120.15(15)	C00S	-C01B	-C019	121.13(18)
C005	-C009	-C00D	120.62(14)	C00P	-C01D	-C01F	120.79(19)
C00N	-C00D	-C00P	119.45(15)	C018	-C01F	-C01D	120.5(2)
C009	-C00D	-C00P	120.13(15)	N01I	-C01H	-C019	179.0(3)
C009	-C00D	-C00N	120.42(15)	C00J	-C00G	-H00G	119.00
C005	-C00G	-C00J	121.67(16)	C005	-C00G	-H00G	119.00
N001	-C00H	-C008	122.25(16)	C008	-C00H	-H00H	119.00
C00G	-C00J	-C00P	122.10(16)	N001	-C00H	-H00H	119.00
C009	-C00K	-C010	118.37(17)	C00P	-C00J	-H00J	119.00
C010	-C00K	-C017	123.32(16)	C00G	-C00J	-H00J	119.00
C011	-C00R	-H00R	120.00	C00C	-C00B	-C00F	119.41(15)
C007	-C00R	-H00R	120.00	C00C	-C00B	-C00E	119.84(15)
C007	-C00S	-H00S	120.00	C00E	-C00B	-C00F	120.76(15)
C01B	-C00S	-H00S	120.00	C00B	-C00C	-C012	118.65(17)

C008 -C00W -H00W 119.00 C00B -C00C -C00L 118.92(17)

C010 -C00W -H00W 119.00 C00L -C00C -C012 122.43(17)

C00W -C010 -H010 119.00 C00B -C00E -C00O 117.23(15)

C00K -C010 -H010 119.00 C00A -C00E -C00B 119.34(14)

C019 -C011 -H011 120.00 C00A -C00E -C00O 123.43(15)

C00R -C011 -H011 120.00 C00B -C00F -C016 120.26(16)

C017 -C013 -H013 119.00 C00B -C00F -C00Q 120.13(15)

C00N -C013 -H013 119.00 C00Q -C00F -C016 119.62(16)

C00K -C017 -H017 119.00 C006 -C00I -C00T 119.49(16)

C013 -C017 -H017 119.00 C00C -C00L -C00U 121.20(18)

C00N -C018 -H018 119.00 N002 -C00M -C00A 122.51(16)

C01F -C018 -H018 119.00 C00E -C00O -C00Z 121.77(17)

C019 -C01B -H01B 119.00 C00F -C00Q -C01E 119.25(18)

C00S -C01B -H01B 119.00 C00F -C00Q -C00Z 118.00(18)

C00P -C01D -H01D 120.00 C00Z -C00Q -C01E 122.75(18)

C01F -C01D -H01D 120.00 C00I -C00T -C00V 121.10(18)

C018 -C01F -H01F 120.00 C00A -C00U -C00L 121.50(18)

C01D -C01F -H01F 120.00 C00Y -C00V -C01A 119.51(18)

N004 -C006 -C00I 123.08(15) C00T -C00V -C01A 121.00(18)

N004 -C006 -C00X 117.85(16) C00T -C00V -C00Y 119.47(19)

C00I -C006 -C00X 119.06(15) C006 -C00X -C00Y 121.11(18)

C00E -C00A -C00M 121.09(15) C00V -C00Y -C00X 119.74(18)

C00M -C00A -C00U 119.70(15) C00O -C00Z -C00Q 122.12(18)

C00E -C00A -C00U 119.21(15) C00C -C012 -C014 121.71(19)

C012 -C014 -C016 121.50(19) C00A -C00U -H00U 119.00

C014 -C016 -C01C 122.88(19) C00L -C00U -H00U 119.00

C00F	-C016	-C014	118.46(18)	C006	-C00X	-H00X	119.00
C00F	-C016	-C01C	118.66(18)	C00Y	-C00X	-H00X	119.00
N015	-C01A	-C00V	177.9(2)	C00V	-C00Y	-H00Y	120.00
C016	-C01C	-C01G	121.1(2)	C00X	-C00Y	-H00Y	120.00
C00Q	-C01E	-C01G	120.6(2)	C00O	-C00Z	-H00Z	119.00
C01C	-C01G	-C01E	120.8(2)	C00Q	-C00Z	-H00Z	119.00
C006	-C00I	-H00I	120.00	C00C	-C012	-H012	119.00
C00T	-C00I	-H00I	120.00	C014	-C012	-H012	119.00
C00C	-C00L	-H00L	119.00	C012	-C014	-H014	119.00
C00U	-C00L	-H00L	119.00	C016	-C014	-H014	119.00
N002	-C00M	-H00M	119.00	C016	-C01C	-H01C	119.00
C00A	-C00M	-H00M	119.00	C01G	-C01C	-H01C	119.00
C00E	-C00O	-H00O	119.00	C00Q	-C01E	-H01E	120.00
C00Z	-C00O	-H00O	119.00	C01G	-C01E	-H01E	120.00
C00I	-C00T	-H00T	119.00	C01C	-C01G	-H01G	120.00
C00V	-C00T	-H00T	119.00	C01E	-C01G	-H01G	120.00

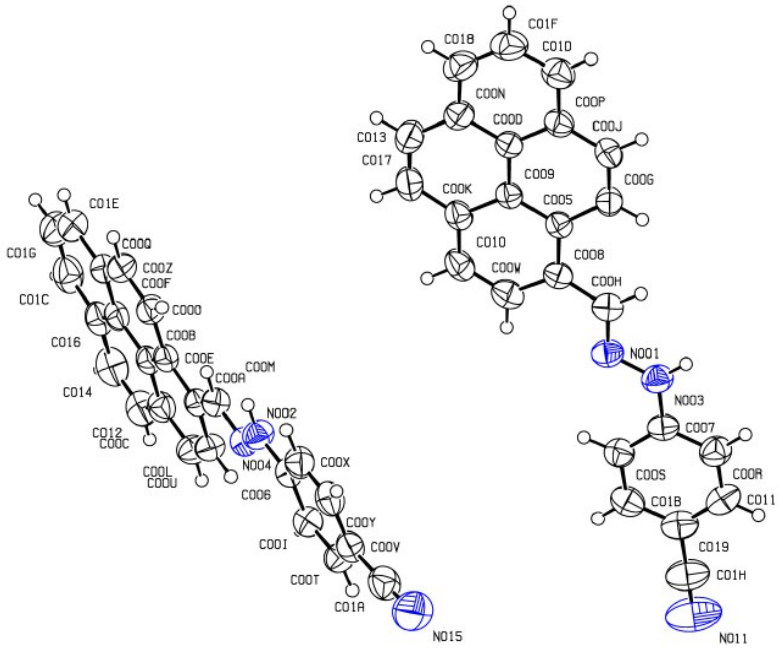

Fig. S4 ORTEP of **PrPr** (probability: 50%).

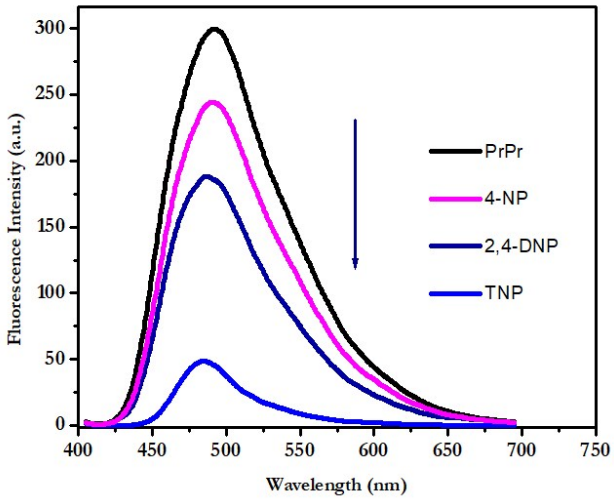

Fig. S5 Effect of 4-NP, 2,4-DNP and 2,4,6-TNP with the emission of **PrPr**.

Detection limit (DL) has been calculated through the following equation[ref1]:
DL= CL × ET
CL = Conc. of **PrPr**; ET = Conc. of titrant at which change observed.
Thus; detection limit for TNP:
DL = $1 \times 10^{-5} \times 0.13$ equiv = 1.3×10^{-6} or = 13 μM
Detection limit for Cu^{2+}:
DL = $1 \times 10^{-5} \times 0.006$ equiv = 60×10^{-9} or = 60 nM
Detection limit for F^{-}:
DL = $1 \times 10^{-5} \times 0.16$ equiv = 16×10^{-7} or = 1.6 μM

Necessary data for TCSPC of PrPr and PrPr···TNP:
PrPr
T1 = 2.394484 ch
6.69084E-11 sec
S.Dev = 1.191546E-11 sec
T2 = 94.2676 ch
2.634093E-09 sec
S.Dev = 6.410635E-11 sec
A = 0.8371606
S.Dev = 0.0900224
B1 = 0.5174316

[90.36 Rel.Ampl]
S.Dev = 0.0037282
B2 = 1.401437E-03
[9.64 Rel.Ampl]
S.Dev = 2.011166E-05
CHISQ = 1.144081

PrPr···TNP
T1 = 2.8359 ch
7.924276E-11 sec
S.Dev = 1.11131E-11 sec
T2 = 117.9392 ch
3.295543E-09 sec
S.Dev = 4.563889E-11 sec
A = 1.061588
S.Dev = 7.768673E-02
B1 = 0.4145315
[78.70 Rel.Ampl]
S.Dev = 1.635282E-03
B2 = 2.698298E-03
[21.30 Rel.Ampl]
S.Dev = 2.186206E-05
CHISQ = 1.353322

Table S4. Crystallographic data of **PrPr···TNP**.

Crystal Data	
Formula	$C_{24}H_{15}N_3,C_6H_3N_3O_7,C_2H_3N$
Formula Weight	615.56
Crystal System	triclinic
Space group	P-1 (No. 2)
a, b, c [Angstrom]	7.0879(6) 8.6017(7) 23.632(2)
alpha, beta, gamma [deg]	82.192(6) 85.543(6) 81.563(6)
V [Ang**3]	1409.5(2)
Z	2
D(calc) [g/cm**3]	1.450
Mu(MoKa) [/mm]	0.106
F(000)	636
Crystal Size [mm]	0.10 x 0.15 x 0.30
Data Collection	
Temperature (K)	293
Radiation [Angstrom]	MoKa 0.71073

Theta Min-Max [Deg]	0.9, 28.6
Dataset	-9: 9 ; -11: 11 ; -31: 23
Tot., Uniq. Data, R(int)	23305, 7093, 0.047
Observed Data [I > 2.0 sigma(I)]	3031
Refinement	
Nref, Npar	7093, 417
R, wR2, S	0.0620, 0.2227, 1.03
Min. and Max. Resd. Dens. [e/Ang^3]	-0.53, 0.38

Table S5 - Bond Distances **PrPr---TNP** adduct (Angstrom).

O1	-N1	1.188(4)	C00I	-C00P	1.363(4)
O001	-C00U	1.323(3)	C00J	-C013	1.397(4)
O2	-N2	1.220(4)	C00J	-C00R	1.384(4)
O004	-N3	1.205(4)	C00J	-C014	1.432(4)
O3	-N3	1.230(3)	C00K	-C016	1.391(4)

O008	-N1	1.212(4)	C00K	-C012	1.432(4)
O009	-N2	1.214(4)	C00L	-C011	1.426(5)
O001	-H001	0.8200	C00L	-C017	1.398(4)
N002	-N005	1.353(3)	C00M	-C00R	1.366(4)
N002	-C00O	1.285(3)	C00N	-C00O	1.459(4)
N005	-C00F	1.368(3)	C00N	-C00P	1.390(4)
N00Z	-C014	1.133(4)	C00V	-C011	1.340(4)
N005	-H005	0.8600	C00Y	-C013	1.372(4)
N1	-C00T	1.470(4)	C010	-C012	1.342(4)
N2	-C00S	1.465(4)	C016	-C018	1.373(5)
N3	-C00Q	1.466(4)	C017	-C018	1.374(5)
N015	-C019	1.119(5)	C00I	-H00I	0.9300
C00C	-C00E	1.417(4)	C00M	-H00M	0.9300
C00C	-C00G	1.428(3)	C00O	-H00O	0.9300
C00C	-C00D	1.424(3)	C00P	-H00P	0.9300
C00D	-C00K	1.424(4)	C00R	-H00R	0.9300
C00D	-C00L	1.411(4)	C00V	-H00V	0.9300
C00E	-C00V	1.427(4)	C00Y	-H00Y	0.9300
C00E	-C00I	1.391(4)	C010	-H010	0.9300
C00F	-C00Y	1.387(4)	C011	-H011	0.9300
C00F	-C00M	1.399(4)	C012	-H012	0.9300
C00G	-C010	1.436(4)	C013	-H013	0.9300
C00G	-C00N	1.409(4)	C016	-H016	0.9300
C017	-H017	0.9300	C00T	-C00X	1.369(4)
C018	-H018	0.9300	C00W	-H00W	0.9300
C00Q	-C00W	1.372(4)	C00X	-H00X	0.9300

C00Q	-C00U	1.400(4)	C019	-C01A	1.434(6)
C00S	-C00X	1.374(4)	C01A	-H01A	0.9600
C00S	-C00W	1.367(4)	C01A	-H01B	0.9600
C00T	-C00U	1.409(4)	C01A	-H01C	0.9600

Table S6 - Bond angles of **PrPr**---TNP (Degrees).

C00U	-O001	-H001	109.00	C00C	-C00G	-C00N	119.0(2)
N005	-N002	-C00O	116.5(2)	C00E	-C00I	-C00P	121.2(2)
N002	-N005	-C00F	120.2(2)	C013	-C00J	-C014	120.4(3)
C00F	-N005	-H005	120.00	C00R	-C00J	-C013	119.6(2)
N002	-N005	-H005	120.00	C00R	-C00J	-C014	119.9(3)
O1	-N1	-C00T	120.5(3)	C012	-C00K	-C016	122.9(3)
O008	-N1	-C00T	116.6(3)	C00D	-C00K	-C016	118.6(3)
O1	-N1	-O008	122.9(3)	C00D	-C00K	-C012	118.5(2)
O009	-N2	-C00S	117.6(3)	C00D	-C00L	-C011	118.7(3)
O2	-N2	-O009	124.9(3)	C011	-C00L	-C017	122.5(3)
O2	-N2	-C00S	117.5(3)	C00D	-C00L	-C017	118.8(3)
O004	-N3	-O3	123.4(3)	C00F	-C00M	-C00R	119.7(2)
O3	-N3	-C00Q	118.1(2)	C00G	-C00N	-C00P	119.0(2)
O004	-N3	-C00Q	118.5(3)	C00G	-C00N	-C00O	121.1(2)
C00D	-C00C	-C00E	119.1(2)	C00O	-C00N	-C00P	119.9(2)
C00D	-C00C	-C00G	120.8(2)	N002	-C00O	-C00N	120.3(2)
C00E	-C00C	-C00G	120.1(2)	C00I	-C00P	-C00N	122.1(2)
C00K	-C00D	-C00L	119.8(2)	C00J	-C00R	-C00M	120.9(2)
C00C	-C00D	-C00L	120.5(2)	C00E	-C00V	-C011	121.8(3)
C00C	-C00D	-C00K	119.7(2)	C00F	-C00Y	-C013	120.8(2)
C00I	-C00E	-C00V	122.7(2)	C00G	-C010	-C012	122.4(3)

C00C	-C00E	-C00I	118.5(2)	C00L	-C011	-C00V	121.1(3)
C00C	-C00E	-C00V	118.8(2)	C00K	-C012	-C010	121.4(2)
N005	-C00F	-C00M	121.5(2)	C00J	-C013	-C00Y	119.5(2)
C00M	-C00F	-C00Y	119.4(2)	N00Z	-C014	-C00J	179.3(4)
N005	-C00F	-C00Y	119.1(2)	C00K	-C016	-C018	121.2(3)
C00N	-C00G	-C010	123.8(2)	C00L	-C017	-C018	121.0(3)
C00C	-C00G	-C010	117.2(2)	C016	-C018	-C017	120.6(3)
C00E	-C00I	-H00I	119.00	C017	-C018	-H018	120.00
C00P	-C00I	-H00I	119.00	N3	-C00Q	-C00W	116.3(2)
C00F	-C00M	-H00M	120.00	C00U	-C00Q	-C00W	122.8(2)
C00R	-C00M	-H00M	120.00	N3	-C00Q	-C00U	120.8(2)
N002	-C00O	-H00O	120.00	N2	-C00S	-C00W	118.7(3)
C00N	-C00O	-H00O	120.00	C00W	-C00S	-C00X	122.0(3)
C00N	-C00P	-H00P	119.00	N2	-C00S	-C00X	119.3(2)
C00I	-C00P	-H00P	119.00	N1	-C00T	-C00U	121.6(2)
C00J	-C00R	-H00R	120.00	C00U	-C00T	-C00X	121.6(3)
C00M	-C00R	-H00R	120.00	N1	-C00T	-C00X	116.9(2)
C00E	-C00V	-H00V	119.00	O001	-C00U	-C00Q	122.5(2)
C011	-C00V	-H00V	119.00	O001	-C00U	-C00T	121.3(2)
C00F	-C00Y	-H00Y	120.00	C00Q	-C00U	-C00T	116.2(2)
C013	-C00Y	-H00Y	120.00	C00Q	-C00W	-C00S	118.2(3)
C00G	-C010	-H010	119.00	C00S	-C00X	-C00T	119.3(2)
C012	-C010	-H010	119.00	C00Q	-C00W	-H00W	121.00
C00L	-C011	-H011	119.00	C00S	-C00W	-H00W	121.00
C00V	-C011	-H011	119.00	C00S	-C00X	-H00X	120.00
C010	-C012	-H012	119.00	C00T	-C00X	-H00X	120.00

C00K	-C012	-H012	119.00	N015	-C019	-C01A	178.9(4)
C00J	-C013	-H013	120.00	C019	-C01A	-H01A	109.00
C00Y	-C013	-H013	120.00	C019	-C01A	-H01B	109.00
C018	-C016	-H016	119.00	C019	-C01A	-H01C	110.00
C00K	-C016	-H016	119.00	H01A	-C01A	-H01B	109.00
C00L	-C017	-H017	120.00	H01A	-C01A	-H01C	109.00
C018	-C017	-H017	120.00	H01B	-C01A	-H01C	109.00
C016	-C018	-H018	120.00				

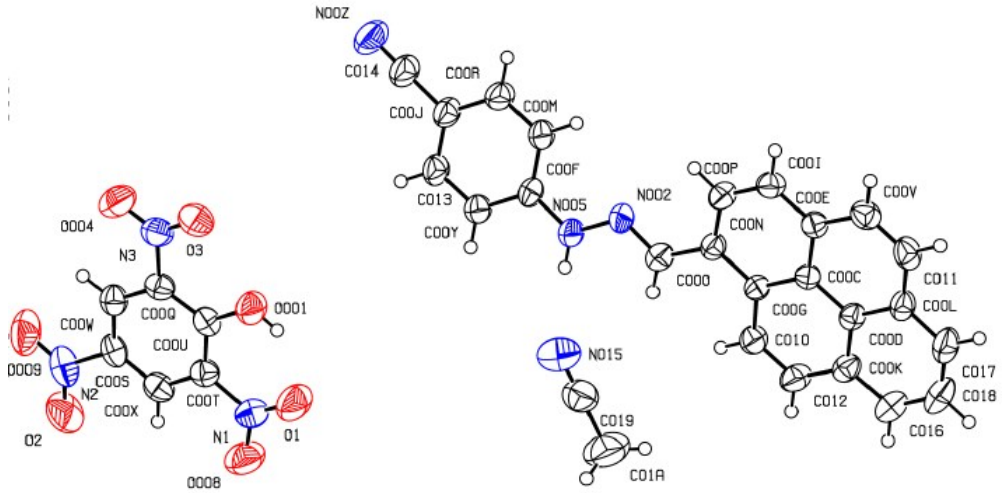

Fig. S6 ORTEP of **PrPr**---TNP (probability: 50%).

Table S7 – Geometry optimized coordinates of **PrPr**.

N	7.3551597	15.1588825	14.1908431
N	8.2595806	15.6291894	13.3235383
C	9.4112033	14.9400964	13.0134195
C	5.2651401	15.4398885	15.3554615
C	3.1174879	15.7608867	16.5323080
C	3.2972049	14.5097161	17.2034796
C	4.1040693	16.2344218	15.6006060
C	1.9422023	16.5358844	16.8007165
C	9.7120229	13.6845826	13.5896581
C	4.4570608	13.7540478	16.9324851
C	6.3038774	15.8734612	14.4206816
C	3.8614098	17.5024995	14.9577664

C	1.7393017	17.7895513	16.1420398
C	10.8851533	13.0258160	13.2483729
C	5.4093818	14.2098897	16.0348075
C	11.7915670	13.5943008	12.3264276
C	10.3175655	15.5108897	12.0893929
C	11.4883606	14.8488924	11.7516877
C	2.7403455	18.2397620	15.2143032
C	2.2971040	14.0580957	18.1313502
C	1.1778751	14.7994392	18.3855934
N	13.9811394	12.3539043	11.6977523
C	0.9603281	16.0618930	17.7311984
C	12.9983066	12.9104543	11.9797941
C	-0.1861400	16.8434494	17.9775044
C	0.5782790	18.5369449	16.4187850
C	-0.3725900	18.0657901	17.3277954
H	8.1004816	16.5319631	12.8702441
H	9.0163232	13.2415338	14.3013418
H	4.6007128	12.7969472	17.4415075
H	6.1821665	16.8362076	13.9028135
H	4.5861445	17.8947682	14.2440703
H	11.1083139	12.0562495	13.6992216
H	6.3012387	13.6123950	15.8382780
H	10.0913411	16.4812981	11.6398795
H	12.1791175	15.3016792	11.0371932
H	2.5893899	19.1972735	14.7080130
H	2.4519683	13.0996430	18.6346770
H	0.4258127	14.4421918	19.0946442
H	-0.9337382	16.4798979	18.6880051
H	0.4280617	19.4944933	15.9124020
H	-1.2687308	18.6578289	17.5319405

Table S8 Geometry optimized coordinates of **PrPr**---TNP.

O	1.1740144	4.7740753	6.0807141
O	1.2059083	2.7201911	4.4320826
O	2.5297906	2.9608063	2.7412351
N	1.0121972	7.6425346	6.2089787
N	1.8385712	3.4037934	3.6466448
O	0.9797938	8.8540242	6.1812001
O	2.6138756	7.1734181	0.4790131
O	2.1805248	8.9988451	1.5559683
N	2.2737502	7.7835125	1.4804928
O	0.7804252	6.9826692	7.2335648
C	1.7558845	4.8685843	3.7695167
C	1.9633008	7.0007754	2.6820014
C	1.3449017	6.9133865	4.9911636
C	1.4005589	5.4841473	5.0050306
C	2.0436856	5.6095934	2.6326585
C	1.6118998	7.6631826	3.8500608
N	3.7509169	6.6133791	9.2280285
N	3.4696376	5.9679275	10.3634759

C	5.2347625	6.4640349	4.5851229
C	5.6552308	5.7189547	3.4351739
C	5.1115446	7.8870399	4.4892530
C	2.9877527	6.6182152	11.4793352
C	4.9292951	5.7890571	5.8167990
C	4.6998826	8.6111833	5.6283284
C	2.0023935	7.8741459	13.8018033
C	5.7803309	4.2957614	3.5041872
C	5.9490857	6.3929193	2.2049828
C	2.7452947	8.0106624	11.4873782
C	4.5087917	6.5580050	6.9450087
C	4.1737286	5.9242438	8.2207027
C	4.4112327	7.9618357	6.8184372
C	2.2601112	8.6249752	12.6336520
C	5.4041542	8.5364461	3.2408310
C	2.7295425	5.8642124	12.6474247
N	1.0930836	9.0339105	15.9364649
C	5.0579242	4.3528718	5.8415538
C	5.8043570	7.8227764	2.1463624
C	5.4633902	3.6452896	4.7449650
C	2.2445748	6.4824340	13.7903868
C	1.5014803	8.5133701	14.9786867
C	6.1999462	3.5817481	2.3656022
C	6.3641871	5.6379592	1.0905044
C	6.4906157	4.2493422	1.1736159
H	0.9456126	5.4130106	6.8117748
H	2.3266903	5.1004900	1.7130295
H	1.5486959	8.7491377	3.8835769
H	3.6046961	4.9553997	10.4157244
H	4.6084532	9.6988508	5.5647721
H	2.9391032	8.5923155	10.5869096
H	4.2881825	4.8347866	8.3193432
H	4.0955857	8.5377854	7.6899284
H	2.0747515	9.7014035	12.6300237
H	5.2946472	9.6226628	3.1827652
H	2.9146212	4.7868813	12.6474199
H	4.8298994	3.8045027	6.7555610
H	6.0182686	8.3309203	1.2021689
H	5.5505243	2.5567753	4.8005472
H	2.0498156	5.8883731	14.6858069
H	6.2948904	2.4940915	2.4240623
H	6.5871997	6.1544218	0.1528838
H	6.8160328	3.6809514	0.2983094

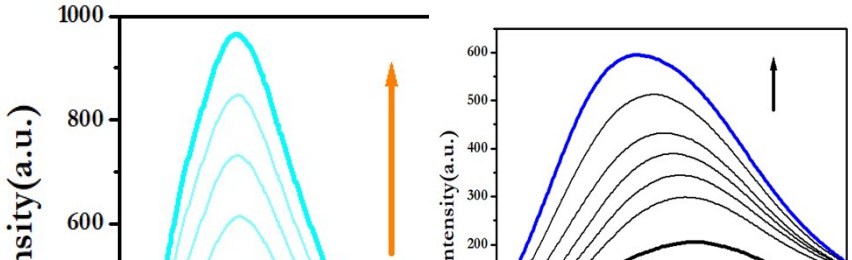

Fig. S7 Fluorescence titration of **PrPr** with Cu^{2+} and F^- (inset).

Fig. S8 Job's plot analysis of **PrPr** with (a) Cu^{2+} and (b) F^-.

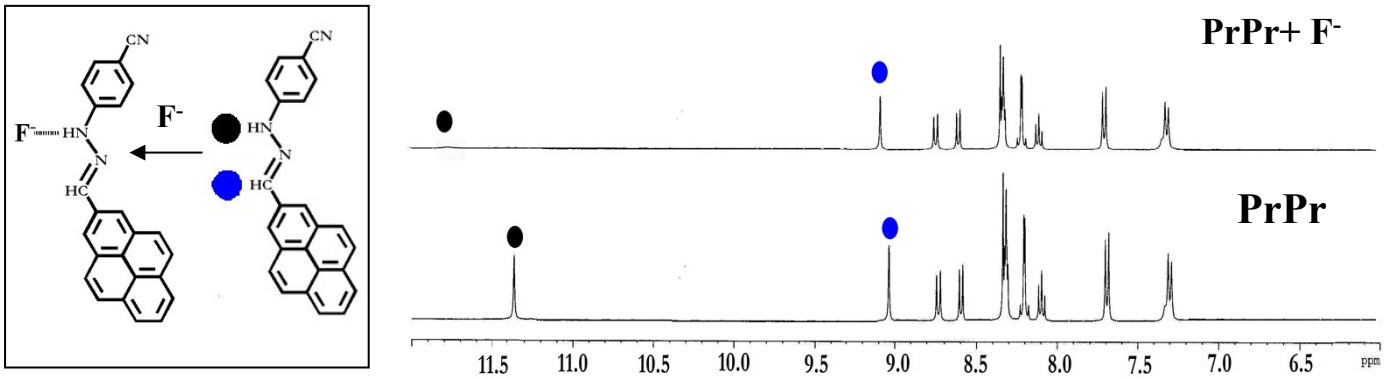

Fig. S9 ^{1}H-NMR spectra of both **PrPr** and **PrPr**···F^- adduct.

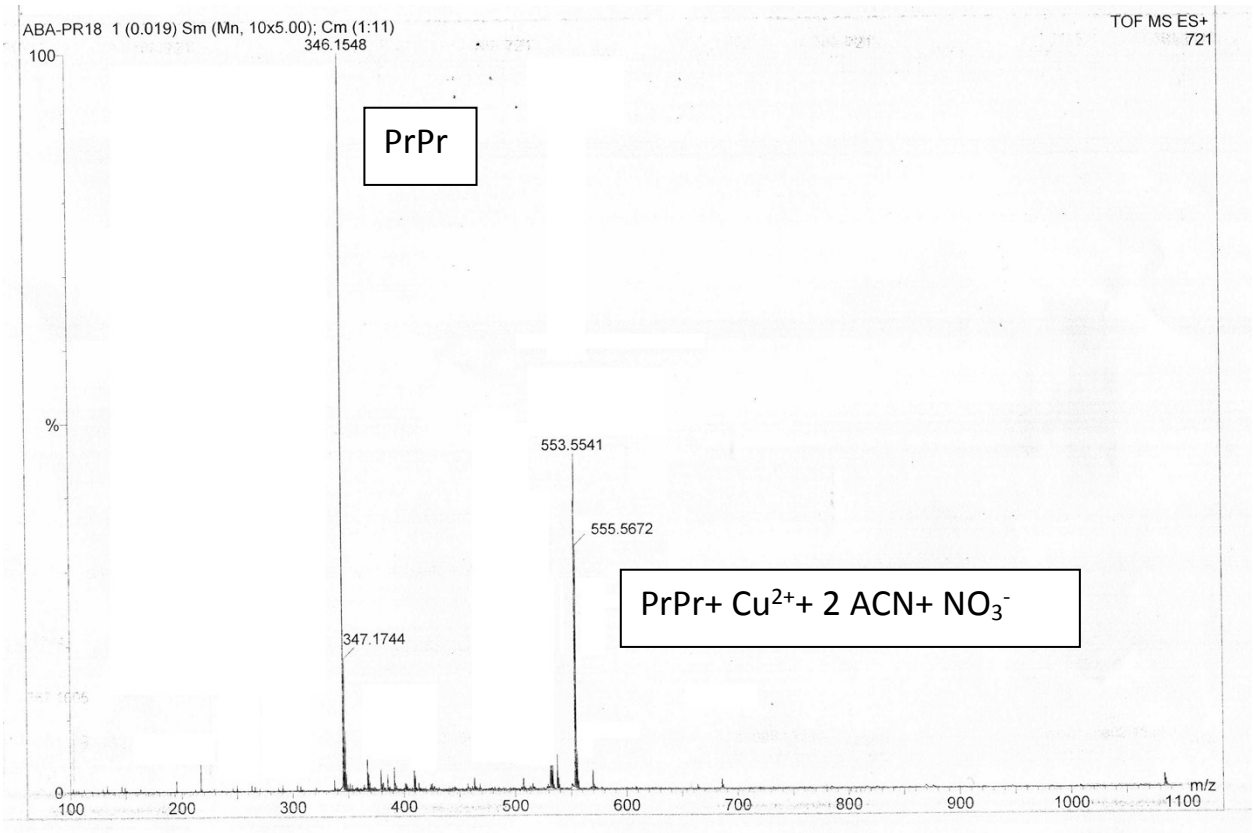

Fig. S10 ESI-MS of **PrPr** with Cu^{2+} in ACN: water medium.

References:

ref 1: J. Pan, F. Tang, A. Ding, L. Kong, L. Yang, X. Tao, Y. Tian, J. Yang, RSC Adv., 2015, 5, 191.