Electronic Supplementary Material (ESI) for RSC Advances.

Organic Polymorphs based on An AEE-active Tetraphenylethene Salicylaldehyde Schiff-base Derivative: The Effect of Molecular Conformation on Luminescence Properties

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(Electronic Supplementary Information)

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Å).

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Table S3. Bond lengths [Å] and angels [deg] for **TPE-Nap-O**.

Figure S1. ^{1}H NMR spectrum of **TPE-NH_2** in $CDCl_3$.

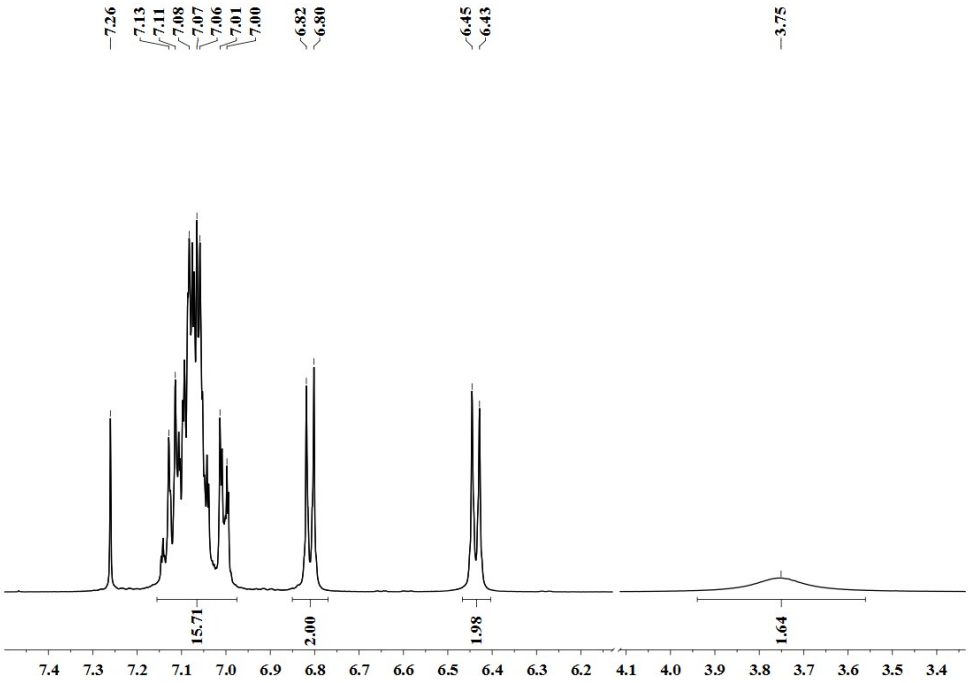

Figure S2. ^{13}C NMR spectrum of **TPE-NH_2** in $CDCl_3$.

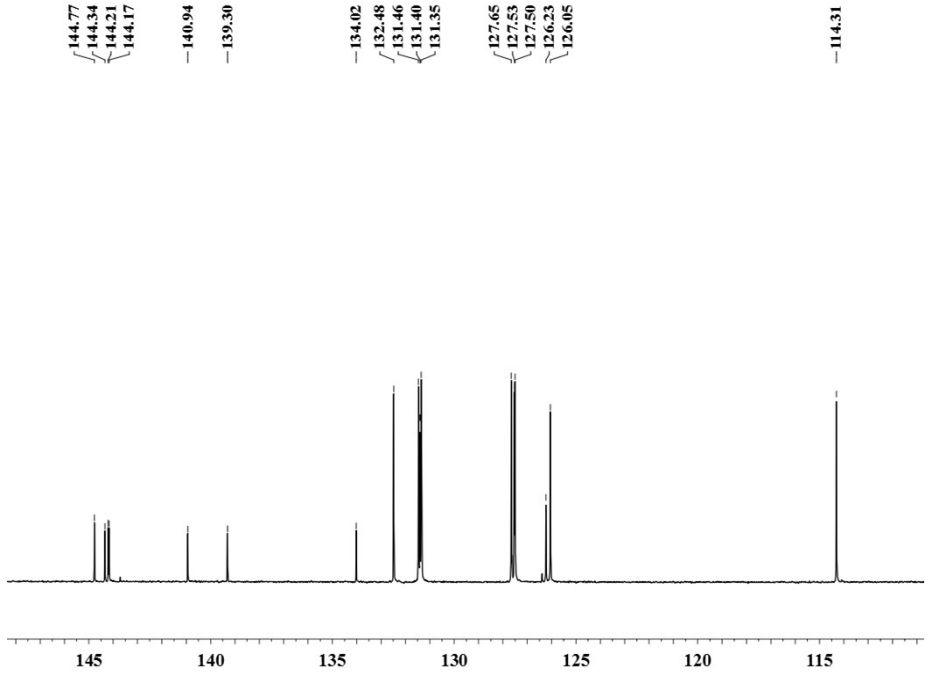

Figure S3. Mass spectrum of **TPE-NH_2** by Maldi-Tof.

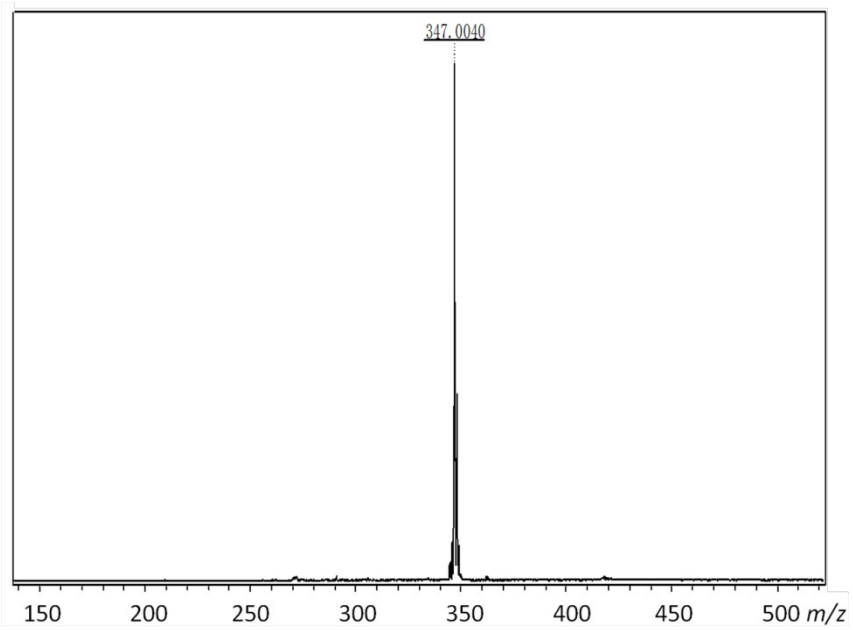

Figure S4. The FT-IR spectrum of **TPE-NH_2**.

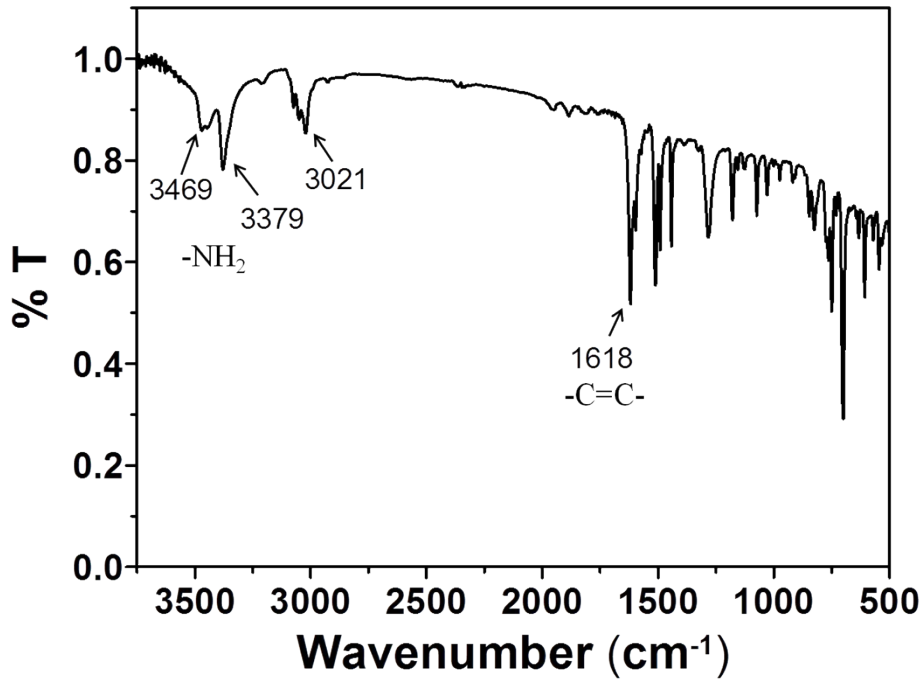

Figure S5. ^{1}H NMR spectrum of **TPE-Nap** in $CDCl_3$.

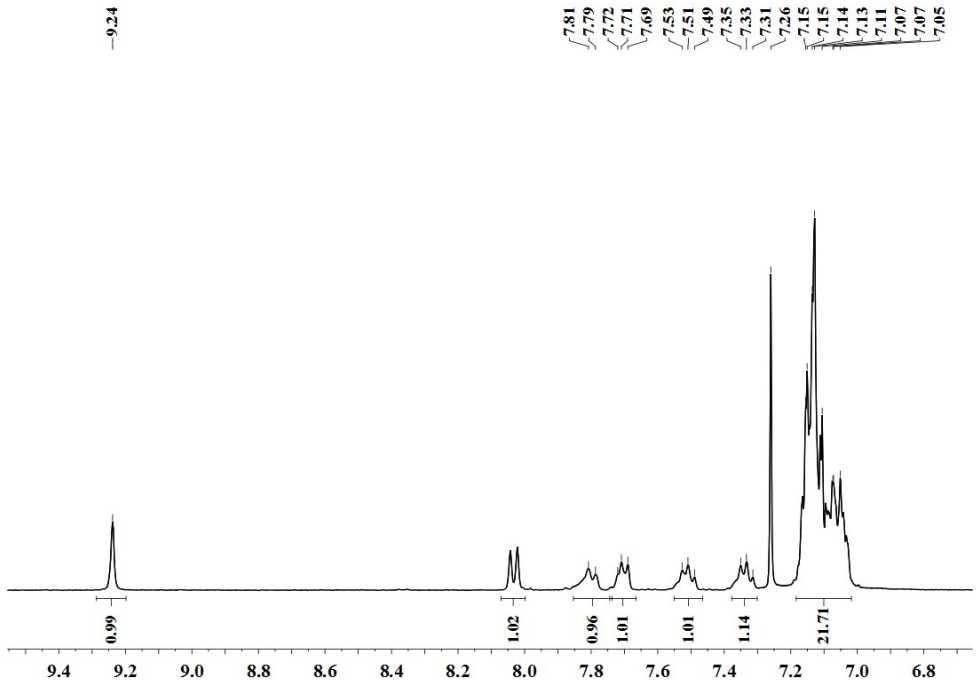

Figure S6. ^{13}C NMR spectrum of **TPE-Nap** in $CDCl_3$.

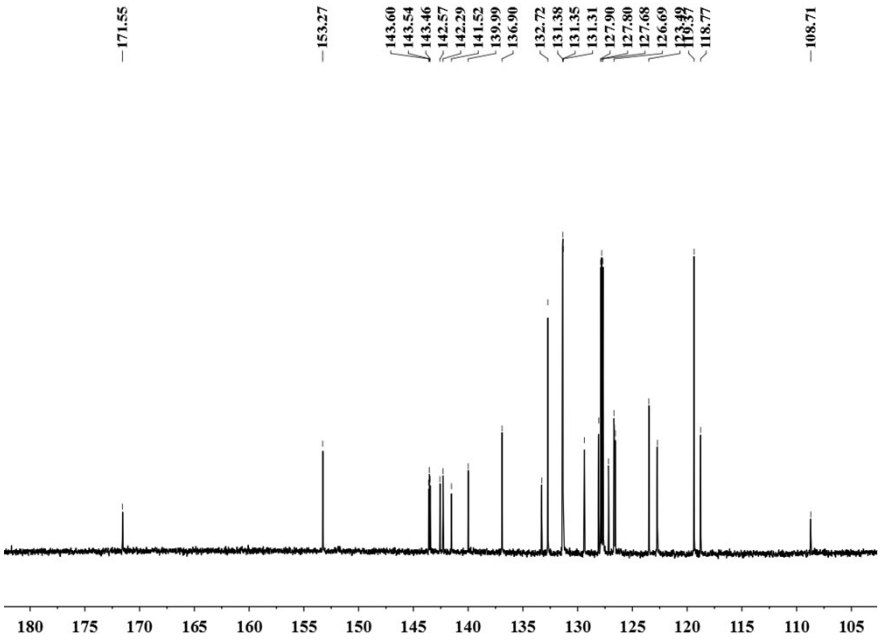

Figure S7. Mass spectrum of **TPE-Nap** by Maldi-Tof.

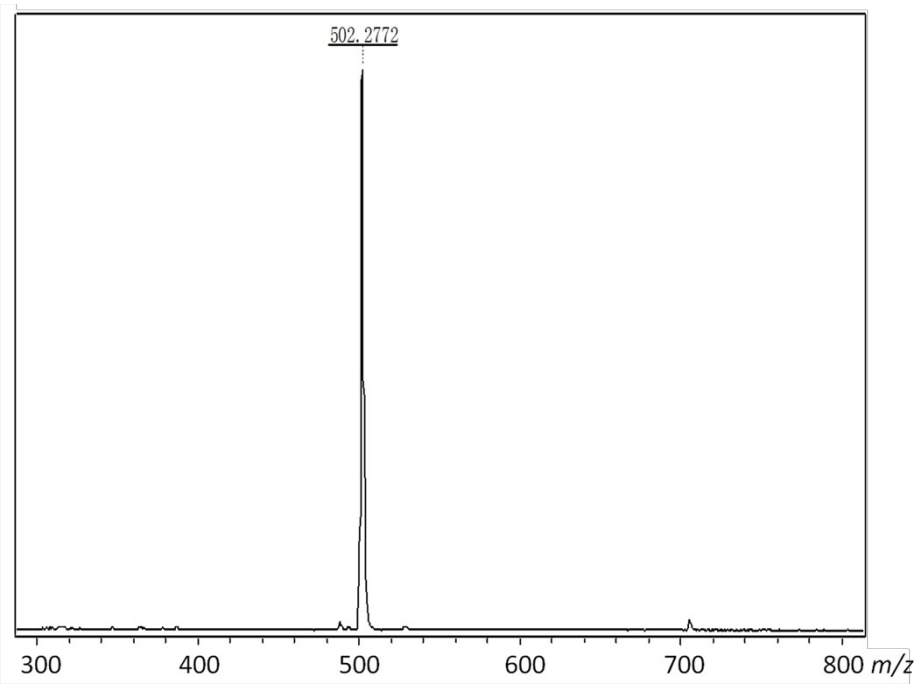

Figure S8. The FT-IR spectrum of **TPE-Nap**.

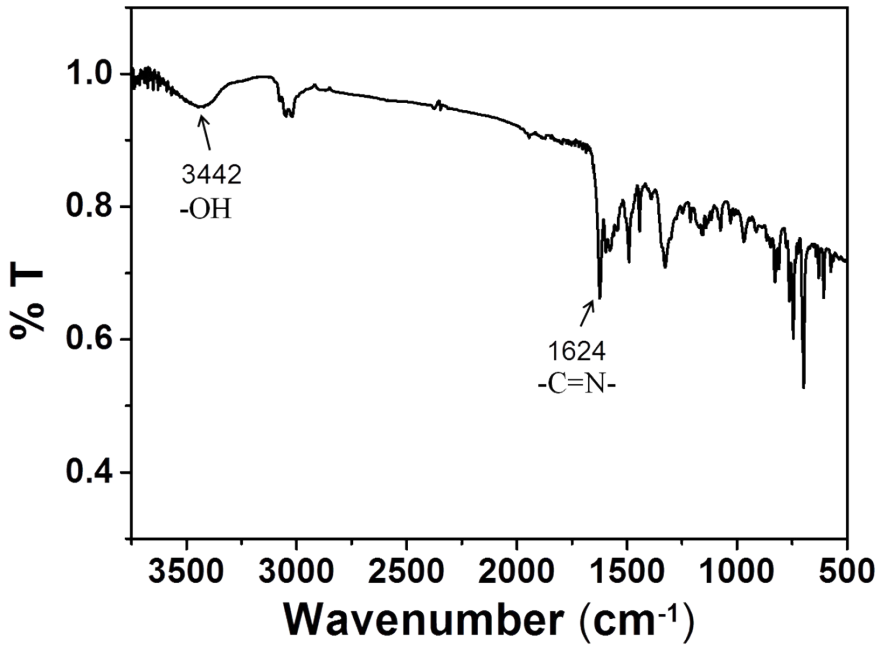

Figure S9. (a) Photograph taken under daylight; (b, c) absorption spectra of **TPE-Nap** (50 μM) in THF/H_2O mixtures with different water fraction (b: 0% - 60%; c: 60% - 90%).

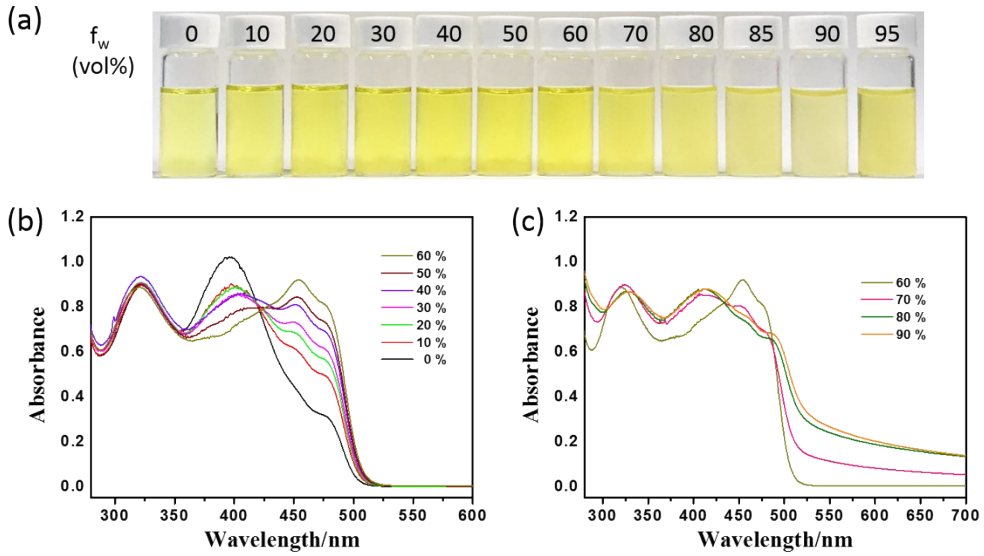

Figure S10. DLS result of **TPE-Nap** in aqueous solution of 90% H_2O/THF (*v*/*v*), the polydispersity index is 0.016. Conditions: The concentration of **TPE-Nap** is 50 μM.

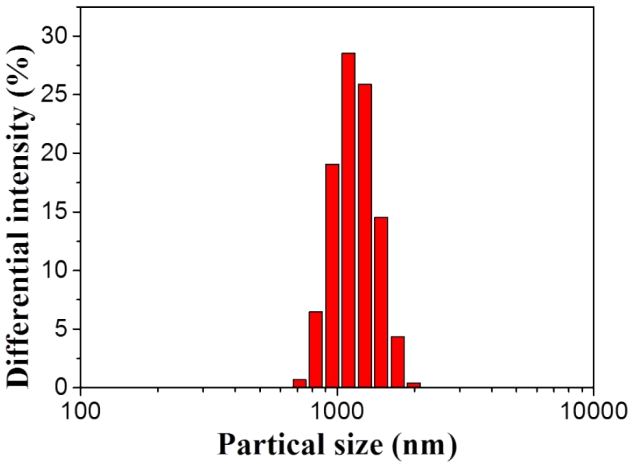

Figure S11. Crystal cell structure of (a) **TPE-Nap-Y** and (b) **TPE-Nap-O** view down the *a*-axis, *b*-axis and *c*-axis, respectively.

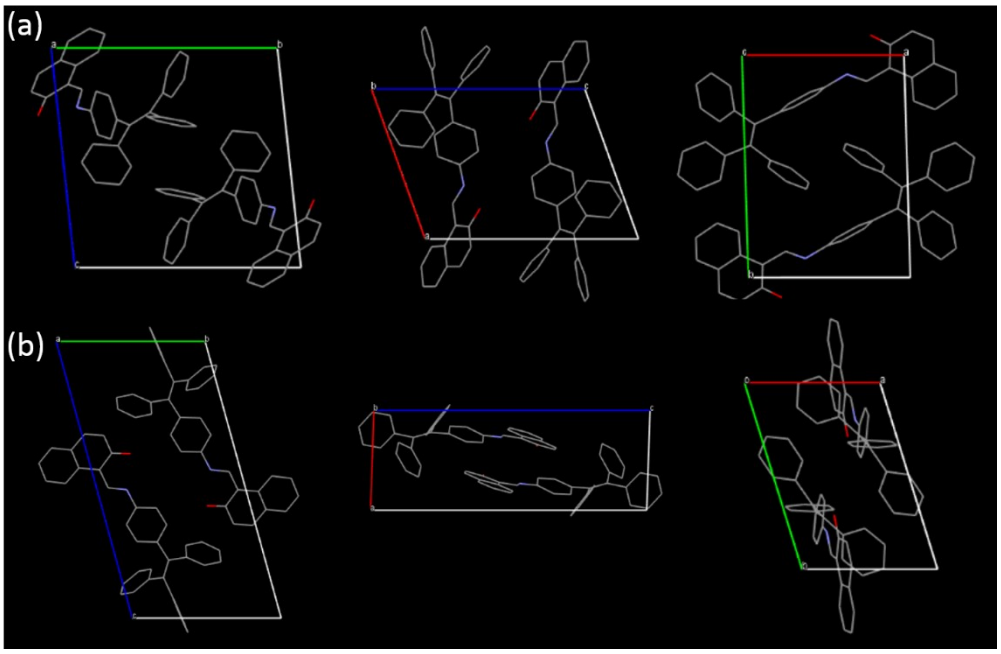

Figure S12. Crystal packing structure of **TPE-Nap-Y** view down the (a) *a*-axis, (b) *b*-axis, and (c) *c*-axis, respectively.

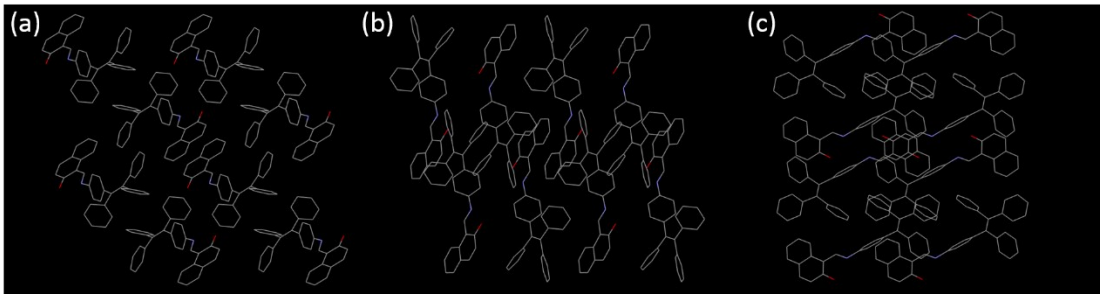

Figure S13. Crystal packing structure of **TPE-Nap-O** view down the (a) *a*-axis, (b) *b*-axis, and (c) *c*-axis, respectively.

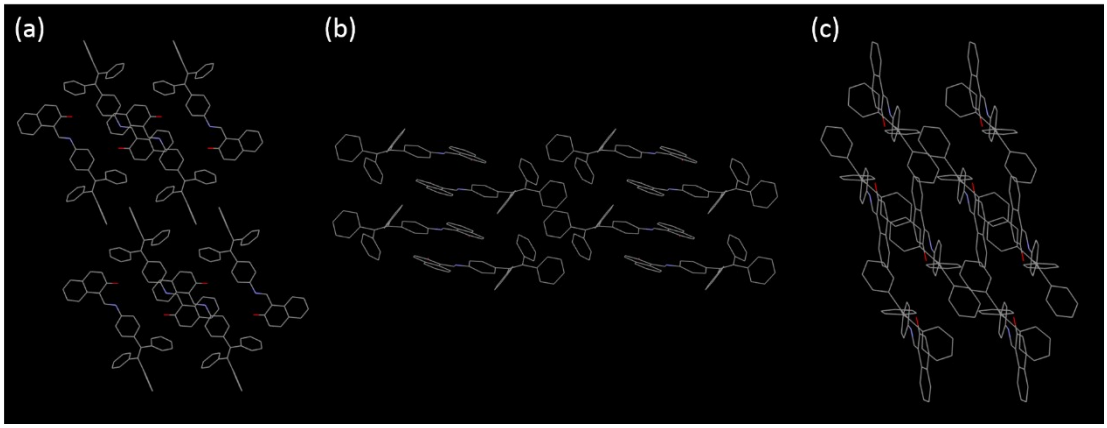

Figure S14. Normalized fluorescence emission spectra of **TPE-Nap**, **TPE-Nap-Y** and **TPE-Nap-O** at room temperature (λ_{ex} = 466 nm).

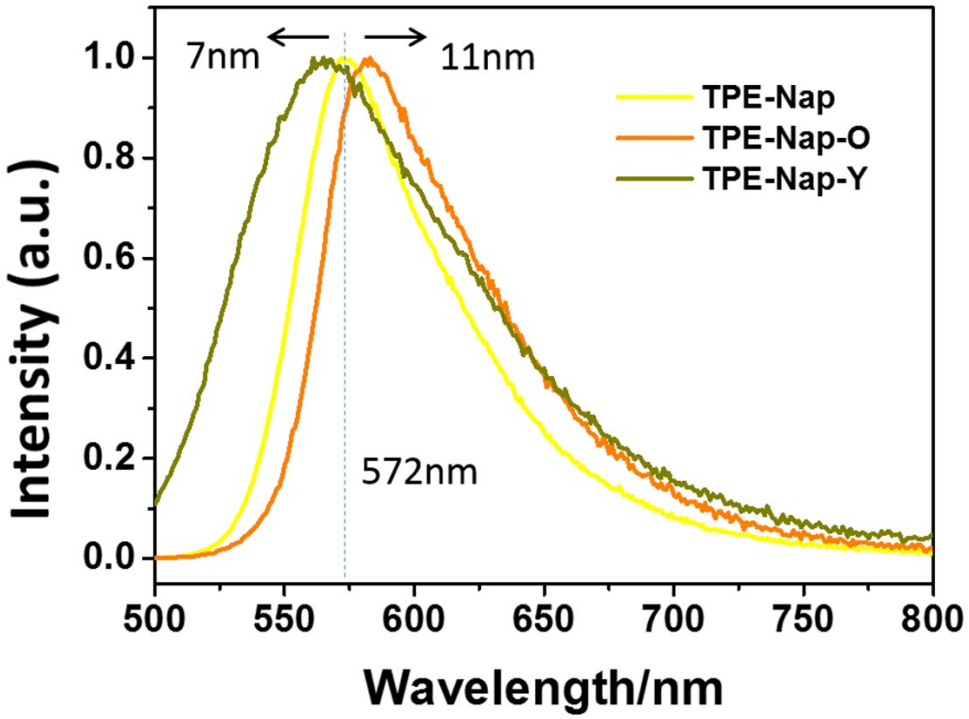

Figure S15. The dihedral angle of (a) **TPE-Nap-Y** and (b) **TPE-Nap-O** between the Nap unit and connected benzene ring of TPE unit.

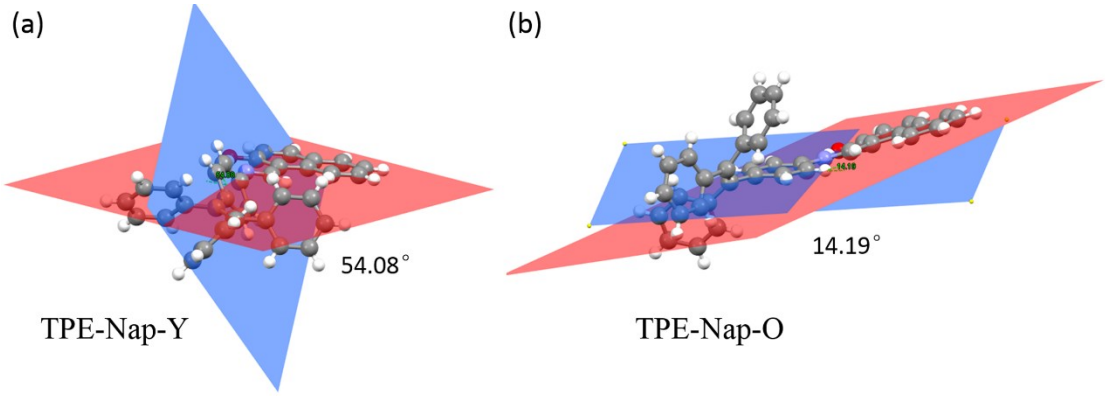

Figure S16. The weak intermolecular interactions (measured distances: Å) existed in crystals (a) **TPE-Nap-Y** and (b) **TPE-Nap-O**.

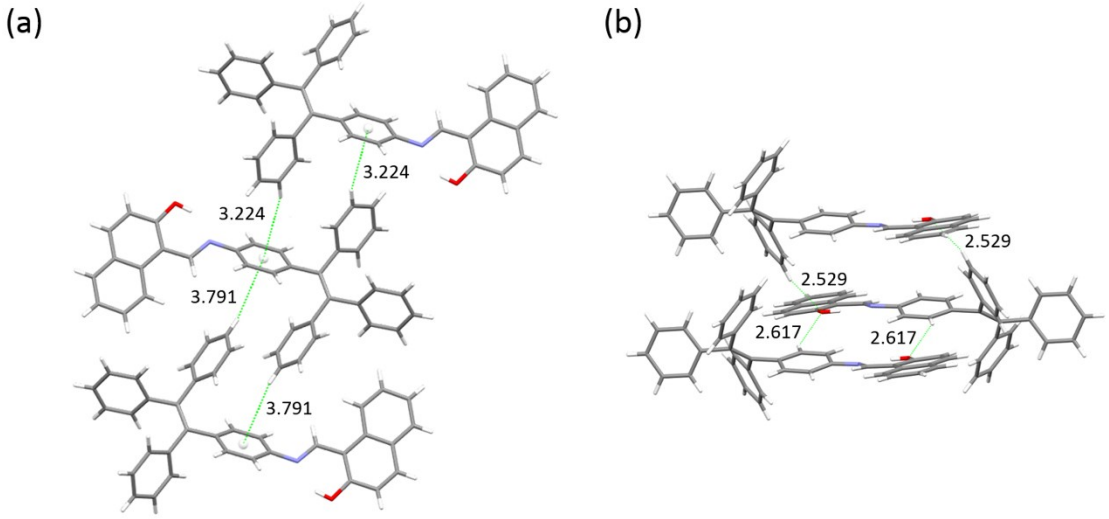

Figure S17. PXRD patterns of (a) **TPE-Nap-Y** and (b) **TPE-Nap-O**. Patterns represent calculations from single-crystal data (bottom) and experimental data (top).

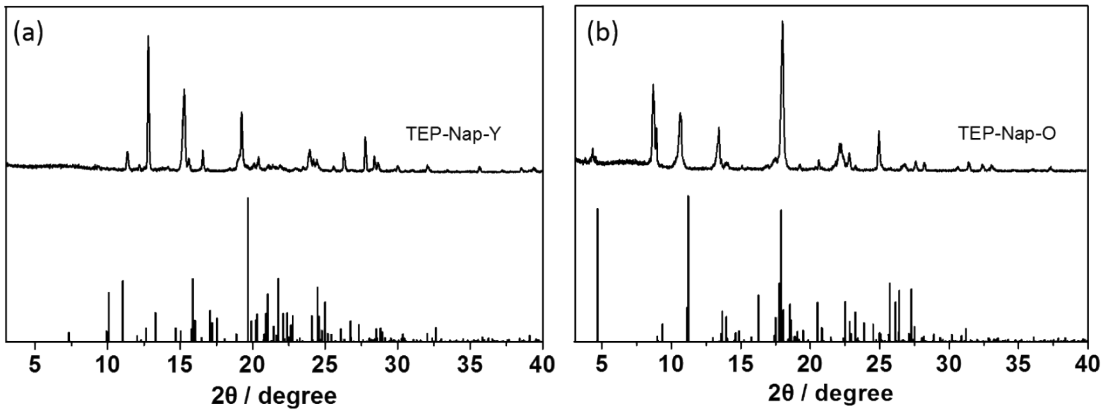

Table S1. Single crystal data of **TPE-Nap-Y** and **TPE-Nap-O** (Wavelength: 0.71073 Å).

	TPE-Nap-Y	**TPE-Nap-O**
CCDC Number	1954666	1954667
Empirical formula	$C_{37}H_{27}NO$	$C_{37}H_{27}NO$
Formula weight / g • mol^{-1}	501.59	501.59
Temperature / K	300(2)	299(2)
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
Z	2	2
a / Å	9.3440	7.1407
b / Å	12.1505	10.6510
c / Å	12.6030	19.6362
α / °	82.8769	74.5060
β / °	69.9436	87.2020
γ / °	86.0352	72.7310
Volume / $Å^3$	1333.18	1373.5
Density (calculated) / Mg • m^{-3}	1.250	1.213
Absorption coefficient / mm^{-1}	0.074	0.072
F(000)	528	528
Reflections collected	15184 / 5367 [R(int) = 0.0172]	13742 / 4807 [R(int) = 0.0494]
Data / restrains / parameters	5367 / 0 / 353	4807 / 0 / 354
Goodness-of-fit on F^2	1.067	1.009
final R indices [I > 2(I)]	R_1= 0.0437 wR_2= 0.1167	R_1= 0.0515 wR_2= 0.1222
R indices (all data)	R_1= 0.0525 wR_2= 0.1241	R_1= 0.1180 wR_2= 0.1601

Table S2. Bond lengths [Å] and angels [deg] for **TPE-Nap-Y**.

C(1)-C(2)	1.380(2)
C(1)-C(6)	1.3864(18)
C(1)-H(1)	0.9300
C(2)-C(3)	1.377(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.372(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.3846(19)
C(4)-H(4)	0.9300
C(5)-C(6)	1.3813(18)
C(5)-H(5)	0.9300
C(6)-C(7)	1.4947(16)
C(7)-C(8)	1.3512(17)
C(7)-C(21)	1.4921(16)
C(8)-C(15)	1.4893(17)
C(8)-C(9)	1.4951(17)
C(9)-C(10)	1.3851(18)
C(9)-C(14)	1.3883(19)
C(10)-C(11)	1.376(2)
C(10)-H(10)	0.9300
C(11)-C(12)	1.368(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.371(2)
C(12)-H(12)	0.9300
C(13)-C(14)	1.381(2)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(20)	1.383(2)
C(15)-C(16)	1.389(2)
C(16)-C(17)	1.385(2)
C(16)-H(16)	0.9300
C(17)-C(18)	1.380(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.358(3)
C(18)-H(18)	0.9300
C(19)-C(20)	1.382(2)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
C(21)-C(22)	1.3907(17)
C(21)-C(26)	1.3943(18)
C(22)-C(23)	1.3879(17)
C(22)-H(22)	0.9300

C(23)-C(24)	1.3872(19)
C(23)-H(23)	0.9300
C(24)-C(25)	1.3883(18)
C(24)-N(1)	1.4169(16)
C(25)-C(26)	1.3795(17)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-N(1)	1.2831(16)
C(27)-C(28)	1.4475(17)
C(27)-H(27)	0.9300
C(28)-C(37)	1.3967(19)
C(28)-C(29)	1.4397(18)
C(29)-C(30)	1.410(2)
C(29)-C(34)	1.4170(18)
C(30)-C(31)	1.369(2)
C(30)-H(30)	0.9300
C(31)-C(32)	1.398(3)
C(31)-H(31)	0.9300
C(32)-C(33)	1.342(3)
C(32)-H(32)	0.9300
C(33)-C(34)	1.419(2)
C(33)-H(33)	0.9300
C(34)-C(35)	1.410(2)
C(35)-C(36)	1.353(2)
C(35)-H(35)	0.9300
C(36)-C(37)	1.412(2)
C(36)-H(36)	0.9300
C(37)-O(1)	1.3338(17)
O(1)-H(1A)	0.8200
C(2)-C(1)-C(6)	120.67(14)
C(2)-C(1)-H(1)	119.7
C(6)-C(1)-H(1)	119.7
C(3)-C(2)-C(1)	120.24(14)
C(3)-C(2)-H(2)	119.9
C(1)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	119.48(14)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	120.46(15)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
C(6)-C(5)-C(4)	120.47(13)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8

C(5)-C(6)-C(1)	118.60(12)
C(5)-C(6)-C(7)	122.52(11)
C(1)-C(6)-C(7)	118.88(11)
C(8)-C(7)-C(21)	123.75(11)
C(8)-C(7)-C(6)	121.83(11)
C(21)-C(7)-C(6)	114.40(10)
C(7)-C(8)-C(15)	123.32(11)
C(7)-C(8)-C(9)	122.32(11)
C(15)-C(8)-C(9)	114.36(10)
C(10)-C(9)-C(14)	117.91(12)
C(10)-C(9)-C(8)	121.97(11)
C(14)-C(9)-C(8)	120.11(11)
C(11)-C(10)-C(9)	120.99(14)
C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
C(12)-C(11)-C(10)	120.22(15)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	120.01(14)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(12)-C(13)-C(14)	119.92(14)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(13)-C(14)-C(9)	120.88(13)
C(13)-C(14)-H(14)	119.6
C(9)-C(14)-H(14)	119.6
C(20)-C(15)-C(16)	118.43(13)
C(20)-C(15)-C(8)	121.94(12)
C(16)-C(15)-C(8)	119.60(13)
C(17)-C(16)-C(15)	120.41(18)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	119.87(18)
C(18)-C(17)-H(17)	120.1
C(16)-C(17)-H(17)	120.1
C(19)-C(18)-C(17)	120.20(16)
C(19)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
C(18)-C(19)-C(20)	120.27(19)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(19)-C(20)-C(15)	120.81(16)
C(19)-C(20)-H(20)	119.6

C(15)-C(20)-H(20)	119.6
C(22)-C(21)-C(26)	117.84(11)
C(22)-C(21)-C(7)	122.36(11)
C(26)-C(21)-C(7)	119.64(11)
C(23)-C(22)-C(21)	120.87(12)
C(23)-C(22)-H(22)	119.6
C(21)-C(22)-H(22)	119.6
C(24)-C(23)-C(22)	120.52(12)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	119.06(11)
C(23)-C(24)-N(1)	122.60(11)
C(25)-C(24)-N(1)	118.26(11)
C(26)-C(25)-C(24)	120.11(12)
C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9
C(25)-C(26)-C(21)	121.56(11)
C(25)-C(26)-H(26)	119.2
C(21)-C(26)-H(26)	119.2
N(1)-C(27)-C(28)	122.55(12)
N(1)-C(27)-H(27)	118.7
C(28)-C(27)-H(27)	118.7
C(37)-C(28)-C(29)	119.13(12)
C(37)-C(28)-C(27)	119.56(12)
C(29)-C(28)-C(27)	121.29(11)
C(30)-C(29)-C(34)	117.00(13)
C(30)-C(29)-C(28)	123.65(12)
C(34)-C(29)-C(28)	119.35(13)
C(31)-C(30)-C(29)	121.92(15)
C(31)-C(30)-H(30)	119.0
C(29)-C(30)-H(30)	119.0
C(30)-C(31)-C(32)	120.54(17)
C(30)-C(31)-H(31)	119.7
C(32)-C(31)-H(31)	119.7
C(33)-C(32)-C(31)	119.23(15)
C(33)-C(32)-H(32)	120.4
C(31)-C(32)-H(32)	120.4
C(32)-C(33)-C(34)	122.12(15)
C(32)-C(33)-H(33)	118.9
C(34)-C(33)-H(33)	118.9
C(35)-C(34)-C(29)	118.93(14)
C(35)-C(34)-C(33)	121.91(14)
C(29)-C(34)-C(33)	119.15(15)
C(36)-C(35)-C(34)	121.69(14)

C(36)-C(35)-H(35)	119.2
C(34)-C(35)-H(35)	119.2
C(35)-C(36)-C(37)	120.70(15)
C(35)-C(36)-H(36)	119.7
C(37)-C(36)-H(36)	119.7
O(1)-C(37)-C(28)	122.36(12)
O(1)-C(37)-C(36)	117.48(13)
C(28)-C(37)-C(36)	120.16(14)
C(27)-N(1)-C(24)	120.16(11)
C(37)-O(1)-H(1A)	109.5

Table S3. Bond lengths [Å] and angels [deg] for **TPE-Nap-O**.

C(1)-C(2)	1.380(4)
C(1)-C(6)	1.385(4)
C(1)-H(1)	0.9300
C(2)-C(3)	1.374(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.364(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.380(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.375(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.503(3)
C(7)-C(8)	1.341(3)
C(7)-C(21)	1.493(3)
C(8)-C(15)	1.495(3)
C(8)-C(9)	1.500(3)
C(9)-C(14)	1.377(4)
C(9)-C(10)	1.387(4)
C(10)-C(11)	1.381(4)
C(10)-H(10)	0.9300
C(11)-C(12)	1.374(6)
C(11)-H(11)	0.9300
C(12)-C(13)	1.350(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.374(5)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(20)	1.378(4)
C(15)-C(16)	1.386(4)
C(16)-C(17)	1.385(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.360(5)
C(17)-H(17)	0.9300
C(18)-C(19)	1.369(4)
C(18)-H(18)	0.9300
C(19)-C(20)	1.373(4)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
C(21)-C(26)	1.385(3)
C(21)-C(22)	1.390(3)
C(22)-C(23)	1.380(3)
C(22)-H(22)	0.9300

C(23)-C(24)	1.386(3)
C(23)-H(23)	0.9300
C(24)-C(25)	1.379(3)
C(24)-N(1)	1.414(3)
C(25)-C(26)	1.373(3)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-N(1)	1.300(3)
C(27)-C(28)	1.413(3)
C(27)-H(27)	0.9300
C(28)-C(37)	1.412(3)
C(28)-C(29)	1.444(3)
C(29)-C(30)	1.404(3)
C(29)-C(34)	1.415(3)
C(30)-C(31)	1.366(4)
C(30)-H(30)	0.9300
C(31)-C(32)	1.385(4)
C(31)-H(31)	0.9300
C(32)-C(33)	1.357(4)
C(32)-H(32)	0.9300
C(33)-C(34)	1.398(4)
C(33)-H(33)	0.9300
C(34)-C(35)	1.424(4)
C(35)-C(36)	1.344(4)
C(35)-H(35)	0.9300
C(36)-C(37)	1.417(4)
C(36)-H(36)	0.9300
C(37)-O(1)	1.303(3)
O(1)-H(1A)	0.8200
C(2)-C(1)-C(6)	121.4(3)
C(2)-C(1)-H(1)	119.3
C(6)-C(1)-H(1)	119.3
C(3)-C(2)-C(1)	119.3(3)
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(4)-C(3)-C(2)	120.3(3)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	119.8(3)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(6)-C(5)-C(4)	121.4(3)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3

C(5)-C(6)-C(1)	117.7(3)
C(5)-C(6)-C(7)	121.7(3)
C(1)-C(6)-C(7)	120.4(2)
C(8)-C(7)-C(21)	121.6(2)
C(8)-C(7)-C(6)	123.1(2)
C(21)-C(7)-C(6)	115.4(2)
C(7)-C(8)-C(15)	121.8(2)
C(7)-C(8)-C(9)	123.9(2)
C(15)-C(8)-C(9)	114.3(2)
C(14)-C(9)-C(10)	118.0(3)
C(14)-C(9)-C(8)	119.8(3)
C(10)-C(9)-C(8)	122.2(3)
C(11)-C(10)-C(9)	120.3(4)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(12)-C(11)-C(10)	120.4(4)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(13)-C(12)-C(11)	119.5(4)
C(13)-C(12)-H(12)	120.2
C(11)-C(12)-H(12)	120.2
C(12)-C(13)-C(14)	120.7(4)
C(12)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6
C(13)-C(14)-C(9)	121.1(4)
C(13)-C(14)-H(14)	119.4
C(9)-C(14)-H(14)	119.4
C(20)-C(15)-C(16)	118.0(3)
C(20)-C(15)-C(8)	120.3(2)
C(16)-C(15)-C(8)	121.6(3)
C(17)-C(16)-C(15)	119.9(3)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(18)-C(17)-C(16)	120.9(3)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	119.9(3)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-C(20)	119.4(3)
C(18)-C(19)-H(19)	120.3
C(20)-C(19)-H(19)	120.3
C(19)-C(20)-C(15)	121.9(3)
C(19)-C(20)-H(20)	119.1

C(15)-C(20)-H(20)	119.1
C(26)-C(21)-C(22)	117.5(2)
C(26)-C(21)-C(7)	120.2(2)
C(22)-C(21)-C(7)	122.2(2)
C(23)-C(22)-C(21)	121.8(2)
C(23)-C(22)-H(22)	119.1
C(21)-C(22)-H(22)	119.1
C(22)-C(23)-C(24)	119.7(2)
C(22)-C(23)-H(23)	120.2
C(24)-C(23)-H(23)	120.2
C(25)-C(24)-C(23)	118.9(2)
C(25)-C(24)-N(1)	117.4(2)
C(23)-C(24)-N(1)	123.7(2)
C(26)-C(25)-C(24)	121.1(2)
C(26)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	121.0(2)
C(25)-C(26)-H(26)	119.5
C(21)-C(26)-H(26)	119.5
N(1)-C(27)-C(28)	122.7(2)
N(1)-C(27)-H(27)	118.6
C(28)-C(27)-H(27)	118.6
C(37)-C(28)-C(27)	118.6(2)
C(37)-C(28)-C(29)	119.4(2)
C(27)-C(28)-C(29)	121.9(2)
C(30)-C(29)-C(34)	117.1(2)
C(30)-C(29)-C(28)	123.5(2)
C(34)-C(29)-C(28)	119.4(2)
C(31)-C(30)-C(29)	121.2(3)
C(31)-C(30)-H(30)	119.4
C(29)-C(30)-H(30)	119.4
C(30)-C(31)-C(32)	121.2(3)
C(30)-C(31)-H(31)	119.4
C(32)-C(31)-H(31)	119.4
C(33)-C(32)-C(31)	119.3(3)
C(33)-C(32)-H(32)	120.3
C(31)-C(32)-H(32)	120.3
C(32)-C(33)-C(34)	121.1(3)
C(32)-C(33)-H(33)	119.5
C(34)-C(33)-H(33)	119.5
C(33)-C(34)-C(29)	120.2(3)
C(33)-C(34)-C(35)	121.5(3)
C(29)-C(34)-C(35)	118.3(2)
C(36)-C(35)-C(34)	122.6(3)

C(36)-C(35)-H(35)	118.7
C(34)-C(35)-H(35)	118.7
C(35)-C(36)-C(37)	120.5(3)
C(35)-C(36)-H(36)	119.7
C(37)-C(36)-H(36)	119.7
O(1)-C(37)-C(28)	122.8(2)
O(1)-C(37)-C(36)	117.6(3)
C(28)-C(37)-C(36)	119.7(2)
C(27)-N(1)-C(24)	124.8(2)
C(37)-O(1)-H(1A)	109.5