Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Efficient orange and red thermally activated delayed fluorescence materials based on 1,8-naphthalimide derivatives

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1. Structural Characterization information

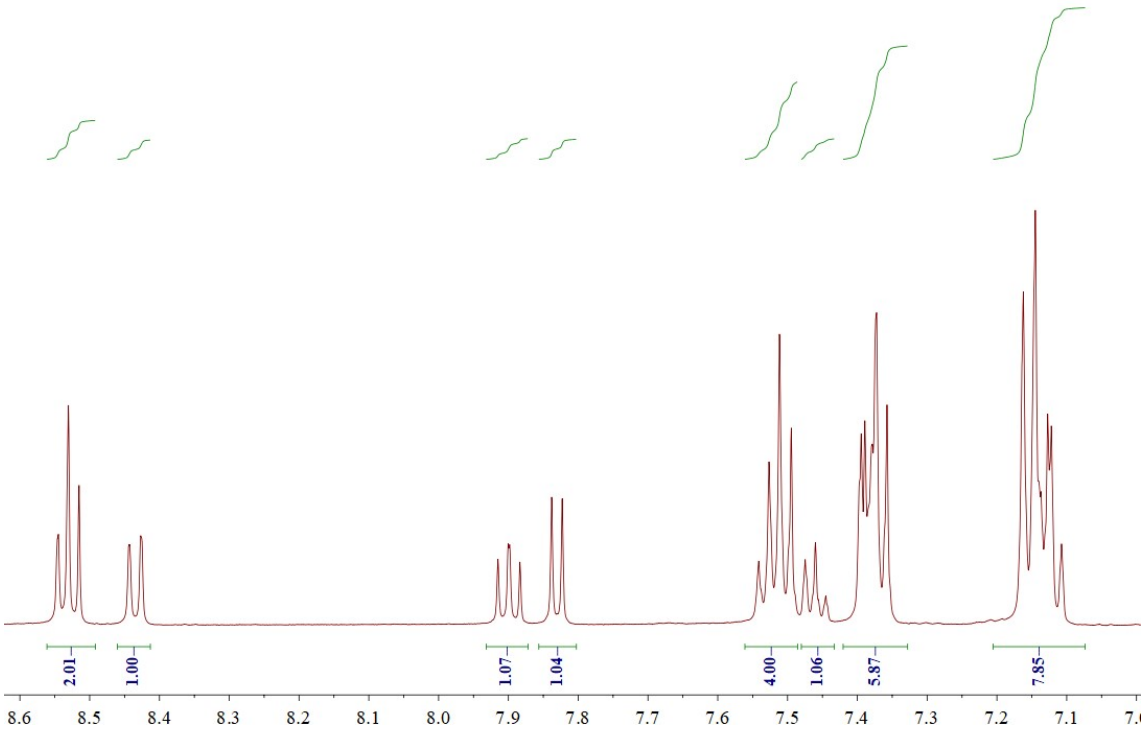

Figure S1 ^{1}H NMR spectrum of compound NI-TPA

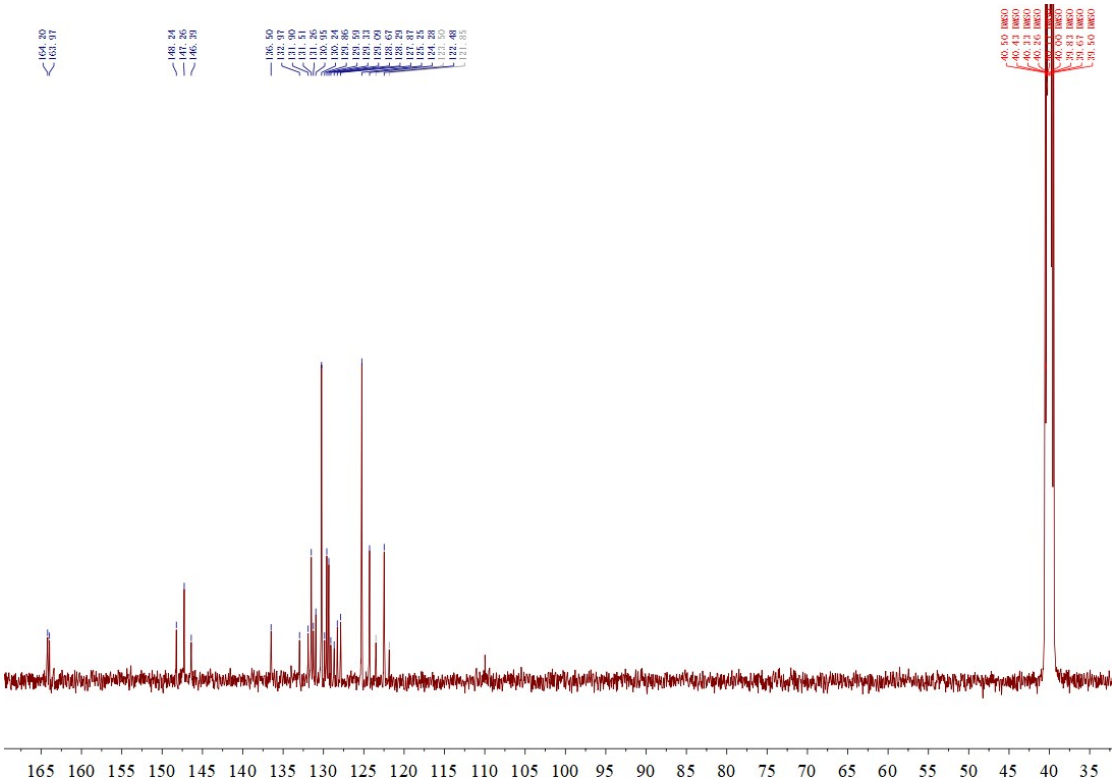

Figure S2 ^{13}C NMR spectrum of compound NI-TPA

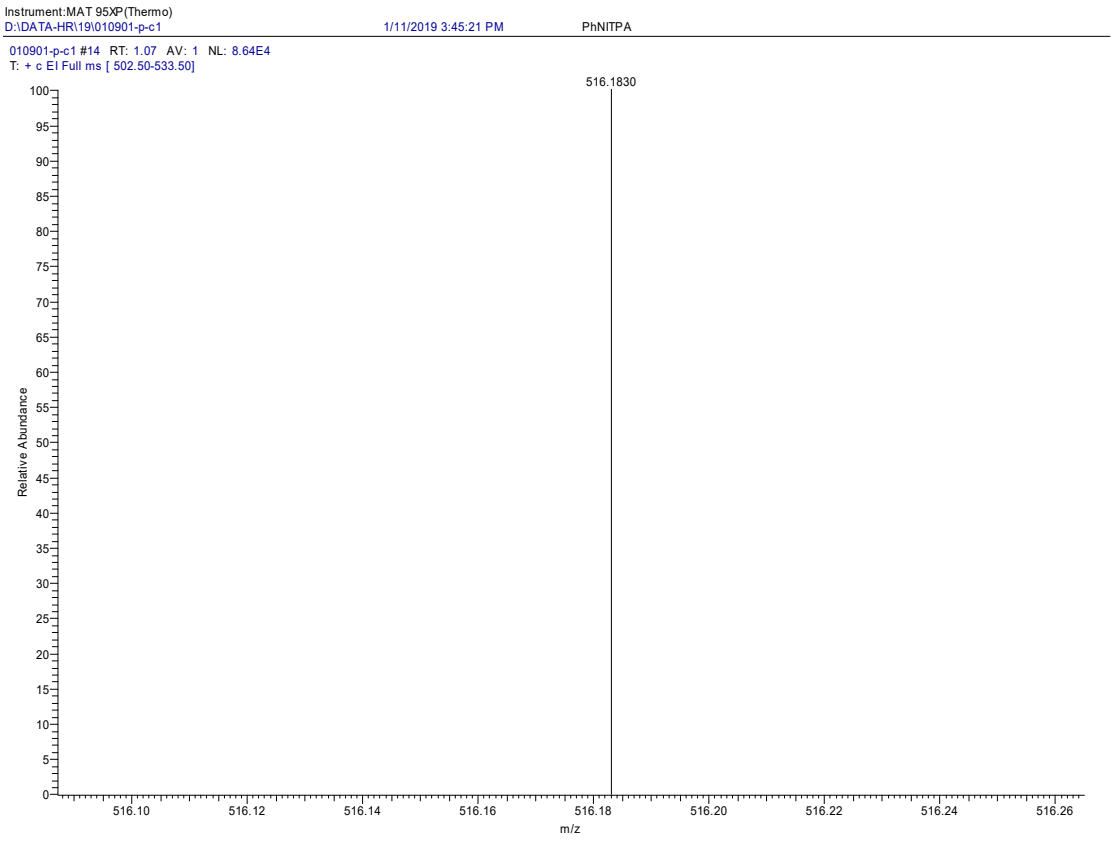

Figure S3 HRMS spectrum of compound NI-TPA.

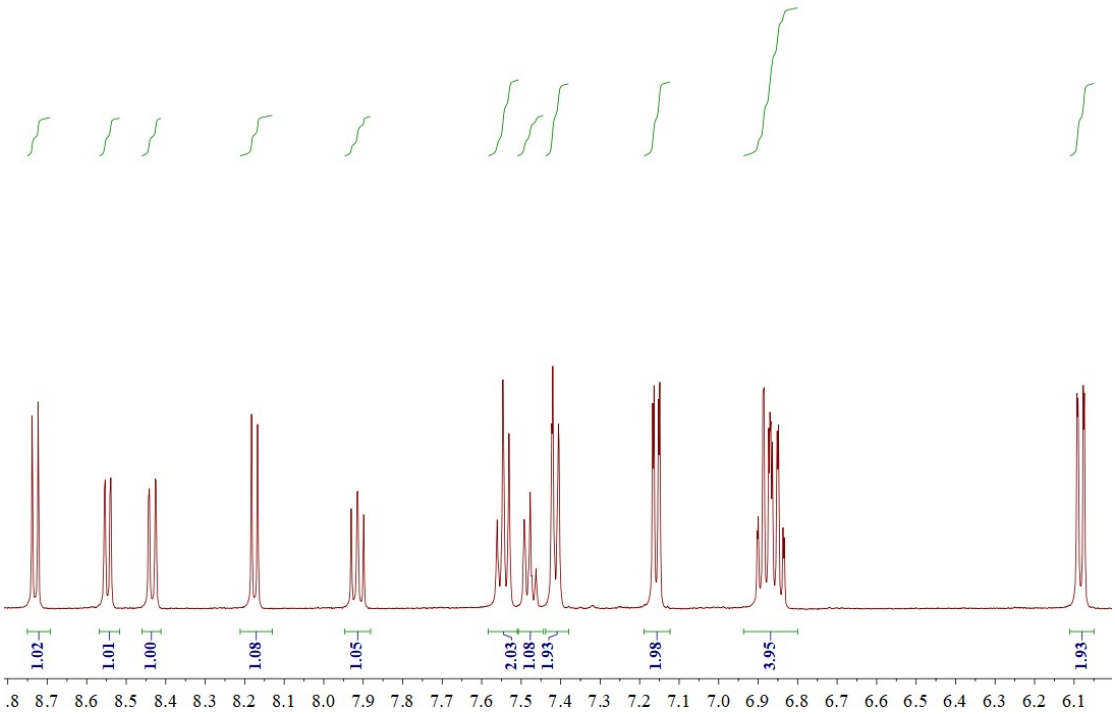

Figure S4 ^{1}H NMR spectrum of compound NI-Pz

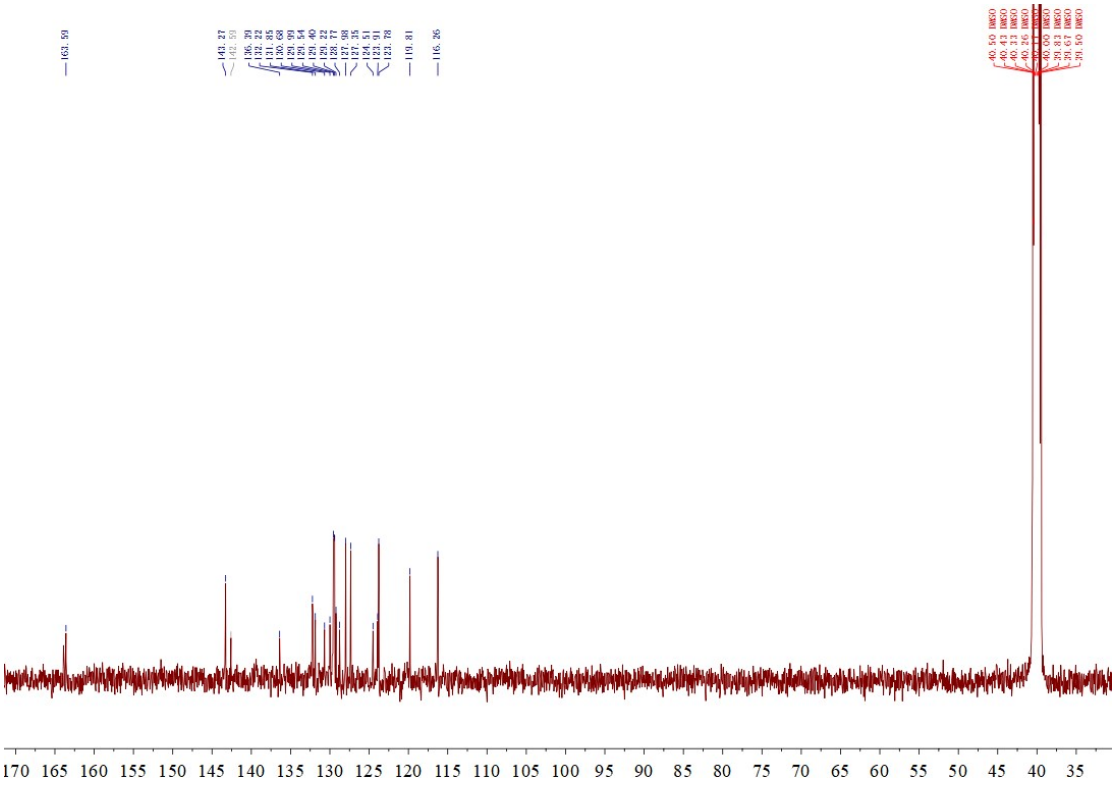

Figure S5 ^{13}C NMR spectrum of compound NI-Pz

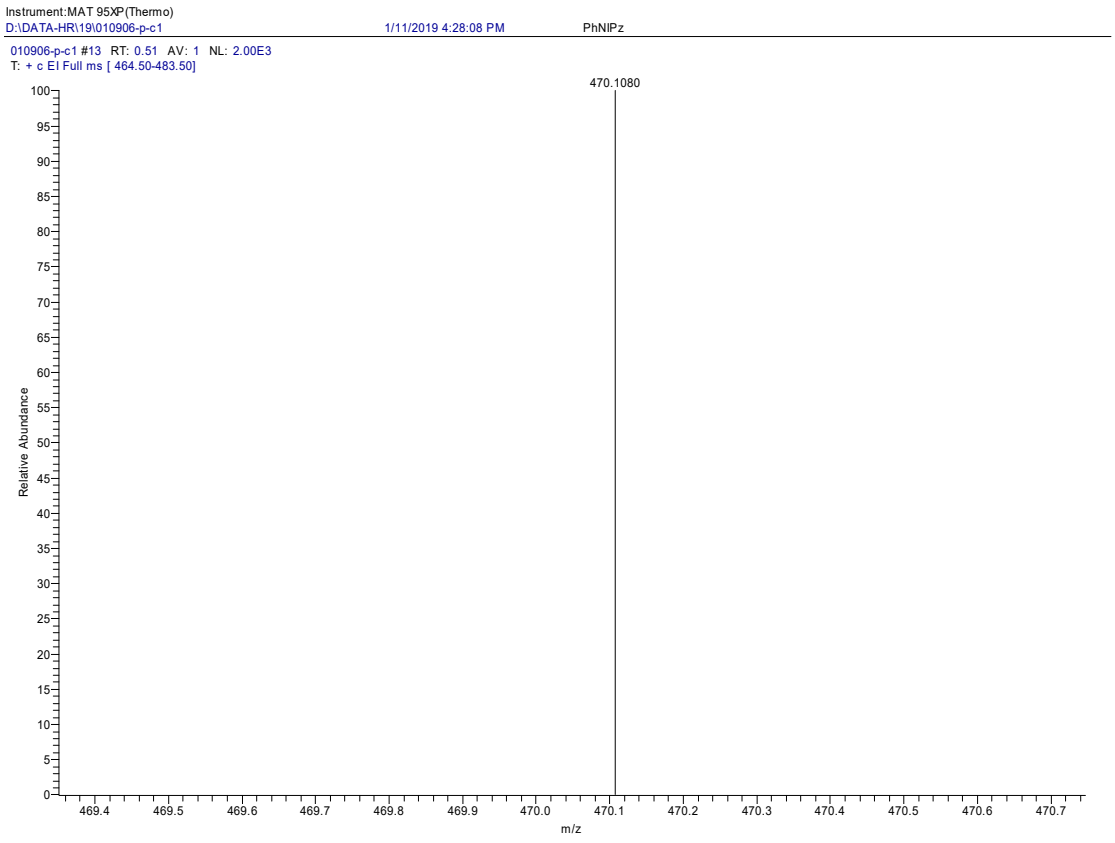

Figure S6 HRMS spectrum of compound NI-Pz.

2 Support figures

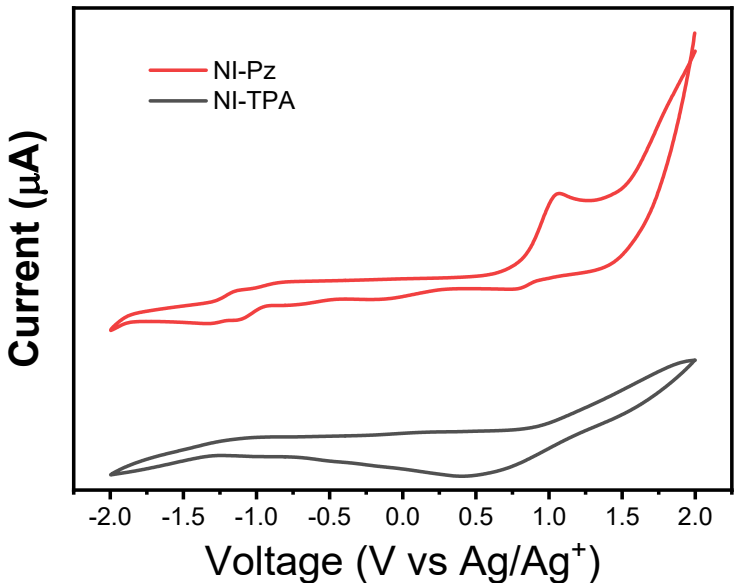

Figure S6 HRMS spectrum of compound NI-Pz.

3. Supporting Tables

Table S1 Crystal data and structure refinement for NI-TPA.

Identification code	NI-TPA
Empirical formula	$C_{216}H_{144}N_{12}O_{12}$
Formula weight	3099.42
Temperature/K	291.7(6)
Crystal system	triclinic
Space group	P1
a/Å	10.9035(4)
b/Å	16.1895(6)
c/Å	24.4187(17)
α/°	102.495(5)
β/°	95.298(4)
γ/°	105.416(3)
Volume/Å^3	4005.2(4)
Z	1
ρ_{calc}g/cm^3	1.285

μ/mm^{-1}	0.630
F(000)	1620.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.512 to 149.804
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 19, -30 ≤ l ≤ 28
Reflections collected	24159
Independent reflections	17835 [R_{int} = 0.0638, R_{sigma} = 0.0678]
Data/restraints/parameters	17835/3/2161
Goodness-of-fit on F^2	1.384
Final R indexes [I>=2σ (I)]	R_1 = 0.1377, wR_2 = 0.3838
Final R indexes [all data]	R_1 = 0.1625, wR_2 = 0.4112
Largest diff. peak/hole / e $Å^{-3}$	0.75/-0.40
Flack parameter	-1.0(6)

Table S2 Crystal data and structure refinement for NI-Pz.

Identification code	NI-Pz
Empirical formula	$C_{60}H_{34}N_4O_4S_2$
Formula weight	939.03
Temperature/K	119.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.3848(3)
b/Å	13.2196(5)
c/Å	19.2723(6)
α/°	79.837(3)
β/°	79.503(2)
γ/°	84.025(2)
Volume/$Å^3$	2307.68(14)
Z	2
$\rho_{calc}g/cm^3$	1.351
μ/mm^{-1}	1.496
F(000)	972.0
Crystal size/mm^3	0.6 × 0.05 × 0.02
Radiation	CuKα (λ = 1.54184)

2Θ range for data collection/°	7.642 to 148.492
Index ranges	$-11 \leq h \leq 8$, $-16 \leq k \leq 15$, $-23 \leq l \leq 24$
Reflections collected	16603
Independent reflections	9130 [R_{int} = 0.0269, R_{sigma} = 0.0381]
Data/restraints/parameters	9130/0/631
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.1011
Final R indexes [all data]	R_1 = 0.0425, wR_2 = 0.1048
Largest diff. peak/hole / e $Å^{-3}$	0.81/-0.26

Table S3 The fitting parameters for decay lifetimes of NI-TPA and NI-Pz neat films in Figure 5a and figure 5b.

Compounds	Tem. (K)	T_1 (μs)	A_1 (%)	T_2 (μs)	A_2 (%)	$T_{average}$
NI-TPA	100					
	200					
	300					
NI-Pz	100					
	200					
	300					

Tem., temperature; T1 and T2, lifetime components; A_1 and A_2, the ratios of lifetime components; Taverage, the average lifetime, Taverage = $T_1 \times A_1 + T_2 \times A_2$.

Table S4 Energy levels of the lowest singlet and triplet excited states of NI-TPA and NI-Pz.

Compound	S_1 (eV)	T_1 (eV)	ΔE_{ST} (eV)
NI-TPA	2.56	2.45	0.11
NI-Pz	2.27	2.15	0.12

The energy levels are calculated from the onsets of their spectra in Figure 2.