Electronic Supplementary Material (ESI) for Analytical Methods.

New Schiff base chromophores composed of salicylaldehyde and naphthalimide derivatives for ion sensor application

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Table S1 Crystallographic Data for **NA-N**.

Formula sum	C19 H11 N3 O5
Formula weight	361.31 g/mol
Crystal system	monoclinic
Space-group	P 1 21 1 (4)
Cell parameters	a=8.5796(8) Å b=7.6309(6) Å c=11.7149(10) Å β=94.235(4)°
Cell ratio	a/b=1.1243 b/c=0.6514 c/a=1.3654
Cell volume	764.88(11) $Å^3$
Z	2
Calc. density	1.5687 g/cm^3
Meas. density	
Melting point	
RAll	0.1078
RObs	
Pearson code	mP76
Formula type	N3O5P11Q19
Wyckoff sequence	a38
Formula sum	C14 H11 N3 O2
Formula weight	253.26 g/mol
Crystal system	triclinic
Space-group	P -1 (2)
Cell parameters	a=8.1726(7) Å b=12.0345(12) Å c=14.2401(12) Å α=110.964(3)° β=103.662(3)° γ=98.181(3)°
Cell ratio	a/b=0.6791 b/c=0.8451 c/a=1.7424
Cell volume	1230.5(2) $Å^3$
Z	4
Calc. density	1.36699 g/cm^3
Meas. density	
Melting point	
RAll	0.1254
RObs	
Pearson code	aP120
Formula type	N2O3P11Q14
Wyckoff sequence	i60

Table S2 Atomic parameters for **NA-N**.

Atom	Ox.	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å^2]
C1		2a	1		0.4082(6)	0.7547(6)	0.5731(5)	
C2		2a	1		0.2773(6)	1.0484(6)	0.5536(4)	
C3		2a	1		0.3636(6)	1.1026(7)	0.6621(4)	
C4		2a	1		0.3382(6)	1.2669(6)	0.7045(5)	
H4		2a	1		0.26730	1.34450	0.66410	0.0240
C5		2a	1		0.4176(7)	1.3195(8)	0.8077(5)	
H5		2a	1		0.39930	1.43310	0.83720	0.0320
C6		2a	1		0.5201(6)	1.2108(7)	0.8663(5)	
H6		2a	1		0.57320	1.24980	0.93570	0.0290
C7		2a	1		0.5492(6)	1.0398(7)	0.8252(4)	
C8		2a	1		0.6550(6)	0.9208(7)	0.8820(5)	
H8		2a	1		0.70990	0.95510	0.95180	0.0280
C9		2a	1		0.6798(7)	0.7587(7)	0.8392(5)	
H9		2a	1		0.75110	0.68100	0.87910	0.0310
C10		2a	1		0.5999(6)	0.7057(7)	0.7357(5)	
H10		2a	1		0.61830	0.59290	0.70520	0.0250
C11		2a	1		0.4950(6)	0.8174(7)	0.6789(4)	
C12		2a	1		0.4686(6)	0.9859(7)	0.7208(4)	
C13		2a	1		0.1541(6)	0.6743(7)	0.4124(5)	
H13		2a	1		0.15990	0.60020	0.47770	0.0240
C14		2a	1		0.0516(6)	0.7267(6)	0.2096(5)	
C15		2a	1		0.0724(5)	0.6170(7)	0.3049(4)	
C16		2a	1		0.0093(6)	0.4492(7)	0.3000(4)	
H16		2a	1		0.02400	0.37250	0.36380	0.0220
C17		2a	1		-0.0751(6)	0.3953(7)	0.2014(5)	
C18		2a	1		-0.0964(6)	0.5038(7)	0.1059(5)	
H18		2a	1		-0.15360	0.46380	0.03840	0.0280
C19		2a	1		-0.0338(6)	0.6687(7)	0.1106(5)	
H19		2a	1		-0.04850	0.74420	0.04620	0.0290
N1		2a	1		0.2960(5)	0.8709(5)	0.5229(4)	
N2		2a	1		0.2176(5)	0.8260(6)	0.4168(4)	
N3		2a	1		-0.1452(5)	0.2221(6)	0.1981(4)	
O1		2a	1		0.4278(4)	0.6101(5)	0.5322(3)	
O2		2a	1		0.1105(4)	0.8901(5)	0.2073(3)	
H2A		2a	1		0.148(6)	0.904(8)	0.275(5)	0.0340
O3		2a	1		-0.1426(4)	0.1371(5)	0.2869(3)	
O4		2a	1		-0.2070(5)	0.1698(6)	0.1056(3)	
O5		2a	1		0.1887(4)	1.1422(5)	0.4954(3)	
Atom	**Ox.**	**Wyck.**	**Site**	**S.O.F.**	**x/a**	**y/b**	**z/c**	**U [Å^2]**
C1A		2i	1		0.2879(4)	0.7515(3)	0.1079(2)	

C2A	2i	1	0.3241(3)	0.5771(3)	-0.0177(2)	
C3A	2i	1	0.2460(3)	0.5396(3)	0.05398(19)	
C4A	2i	1	0.2273(3)	0.6436(3)	0.1295(2)	
C5A	2i	1	0.1539(4)	0.6370(3)	0.2061(2)	
H5A	2i	1	0.14420	0.70880	0.25900	0.0370
C6A	2i	1	0.0954(3)	0.5217(3)	0.2025(2)	
H6A	2i	1	0.04260	0.51390	0.25330	0.0340
C7A	2i	1	0.1119(4)	0.4171(3)	0.1264(2)	
H7A	2i	1	0.06930	0.33900	0.12550	0.0370
C8A	2i	1	0.1900(4)	0.4245(3)	0.0510(2)	
H8A	2i	1	0.20410	0.35320	-0.00030	0.0320
C9A	2i	1	0.3940(4)	0.7763(3)	-0.03585(19)	
C10A	2i	1	0.5958(4)	0.8599(3)	-0.0909(2)	
C11A	2i	1	0.4712(4)	0.9012(3)	-0.1432(2)	
H11A	2i	1	0.49930	0.94570	-0.18290	0.0340
C12A	2i	1	0.3047(4)	0.8772(3)	-0.1371(2)	
C13A	2i	1	0.7794(4)	0.8843(3)	-0.0939(2)	
H13A	2i	1	0.85470	0.86740	-0.03870	0.0620
H13B	2i	1	0.81920	0.97060	-0.08160	0.0620
H13C	2i	1	0.78410	0.83110	-0.16330	0.0620
C14A	2i	1	0.1626(4)	0.9211(3)	-0.1891(2)	
H14A	2i	1	0.05350	0.85700	-0.21910	0.0610
H14B	2i	1	0.19190	0.93960	-0.24570	0.0610
H14C	2i	1	0.14890	0.99550	-0.13670	0.0610
C1B	2i	1	0.9176(4)	0.3537(3)	0.4149(2)	
C2B	2i	1	0.7271(4)	0.2676(3)	0.4832(2)	
C3B	2i	1	0.6351(3)	0.3322(3)	0.42465(19)	
C4B	2i	1	0.7483(3)	0.3823(3)	0.38329(19)	
C5B	2i	1	0.6971(4)	0.4469(3)	0.3237(2)	
H5B	2i	1	0.77520	0.48180	0.29590	0.0340
C6B	2i	1	0.5283(4)	0.4591(3)	0.3057(2)	
H6B	2i	1	0.48890	0.50200	0.26380	0.0380
C7B	2i	1	0.4147(4)	0.4098(3)	0.3480(2)	
H7B	2i	1	0.29980	0.42060	0.33550	0.0380
C8B	2i	1	0.4675(4)	0.3453(3)	0.4079(2)	
H8B	2i	1	0.39030	0.31110	0.43660	0.0340
C9B	2i	1	1.0235(3)	0.2269(3)	0.5116(2)	
C10B	2i	1	1.1818(4)	0.1898(3)	0.6447(2)	
C11B	2i	1	1.2513(4)	0.1146(3)	0.5742(2)	
H11B	2i	1	1.33390	0.07420	0.59730	0.0340
C12B	2i	1	1.1986(4)	0.0992(3)	0.4699(2)	
C13B	2i	1	1.2316(4)	0.2113(3)	0.7591(2)	

H13D	2i	1	1.27750	0.29960	0.80300	0.0640
H13E	2i	1	1.32090	0.16810	0.77380	0.0640
H13F	2i	1	1.12900	0.18030	0.77540	0.0640
C14B	2i	1	1.2658(4)	0.0195(3)	0.3874(2)	
H14D	2i	1	1.18980	0.00290	0.31690	0.0560
H14E	2i	1	1.26750	-0.05830	0.39480	0.0560
H14F	2i	1	1.38390	0.06170	0.39660	0.0560
N1A	2i	1	0.3478(3)	0.7055(2)	0.02056(16)	
N2A	2i	1	0.2631(3)	0.8114(2)	-0.08278(16)	
N3A	2i	1	0.5585(3)	0.7959(2)	-0.03427(16)	
N1B	2i	1	0.8972(3)	0.2846(2)	0.47528(16)	
N2B	2i	1	1.0810(3)	0.1559(2)	0.43747(17)	
N3B	2i	1	1.0660(3)	0.2479(2)	0.61308(17)	
O1A	2i	1	0.2907(3)	0.8575(2)	0.15381(16)	
O2A	2i	1	0.3588(3)	0.51591(18)	-0.09457(14)	
O1B	2i	1	1.0503(2)	0.3835(2)	0.39670(15)	
O2B	2i	1	0.6735(3)	0.2082(2)	0.52737(16)	

Table S3 Anisotropic displacement parameters for **NA-N**.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.013(3)	0.018(3)	0.021(3)	-0.002(2)	0.003(2)	-0.001(3)
C2	0.016(3)	0.021(3)	0.018(3)	-0.002(2)	0.004(2)	0.003(2)
C3	0.016(3)	0.020(3)	0.016(3)	-0.004(2)	0.004(2)	-0.001(2)
C4	0.022(3)	0.016(3)	0.024(3)	0.002(2)	0.003(3)	0.002(2)
C5	0.031(3)	0.017(3)	0.033(4)	-0.001(3)	0.003(3)	-0.006(3)
C6	0.022(3)	0.026(3)	0.023(3)	-0.006(3)	-0.001(3)	-0.009(3)
C7	0.018(3)	0.020(3)	0.018(3)	-0.003(2)	0.004(2)	-0.002(3)
C8	0.020(3)	0.030(3)	0.020(3)	0.000(3)	-0.004(3)	-0.002(3)
C9	0.026(3)	0.026(3)	0.025(3)	0.003(3)	-0.004(3)	0.004(3)
C10	0.023(3)	0.016(3)	0.024(3)	0.001(2)	-0.002(3)	-0.005(2)
C11	0.017(3)	0.020(3)	0.013(3)	-0.003(2)	0.000(2)	-0.001(2)
C12	0.013(3)	0.013(3)	0.019(3)	-0.003(2)	0.003(2)	0.000(2)
C13	0.016(3)	0.020(3)	0.023(3)	-0.002(2)	-0.003(2)	0.001(2)
C14	0.017(3)	0.017(3)	0.027(3)	-0.003(2)	0.002(2)	0.000(3)
C15	0.012(3)	0.020(3)	0.018(3)	0.001(2)	0.000(2)	-0.005(3)
C16	0.017(3)	0.022(3)	0.017(3)	0.002(2)	0.001(2)	0.000(2)
C17	0.019(3)	0.017(3)	0.022(3)	-0.004(2)	0.002(2)	-0.005(2)
C18	0.021(3)	0.031(3)	0.019(3)	0.000(3)	-0.001(3)	-0.004(3)
C19	0.024(3)	0.027(3)	0.019(3)	-0.001(3)	-0.004(2)	0.002(3)
N1	0.018(2)	0.018(2)	0.014(2)	-0.0040(19)	-0.0054(19)	-0.0041(19)
N2	0.021(3)	0.025(3)	0.014(2)	0.001(2)	-0.002(2)	-0.004(2)
N3	0.023(3)	0.030(3)	0.029(3)	-0.005(2)	0.000(2)	-0.006(3)
O1	0.025(2)	0.021(2)	0.022(2)	-0.0013(18)	0.0006(17)	-0.0069(18)
O2	0.037(2)	0.026(2)	0.020(2)	-0.004(2)	-0.0071(19)	0.0055(18)
O3	0.039(2)	0.024(2)	0.028(2)	-0.009(2)	0.0030(19)	0.000(2)
O4	0.064(3)	0.043(3)	0.026(2)	-0.028(3)	-0.009(2)	-0.010(2)
O5	0.028(2)	0.023(2)	0.022(2)	0.0038(19)	-0.0066(17)	0.003(2)

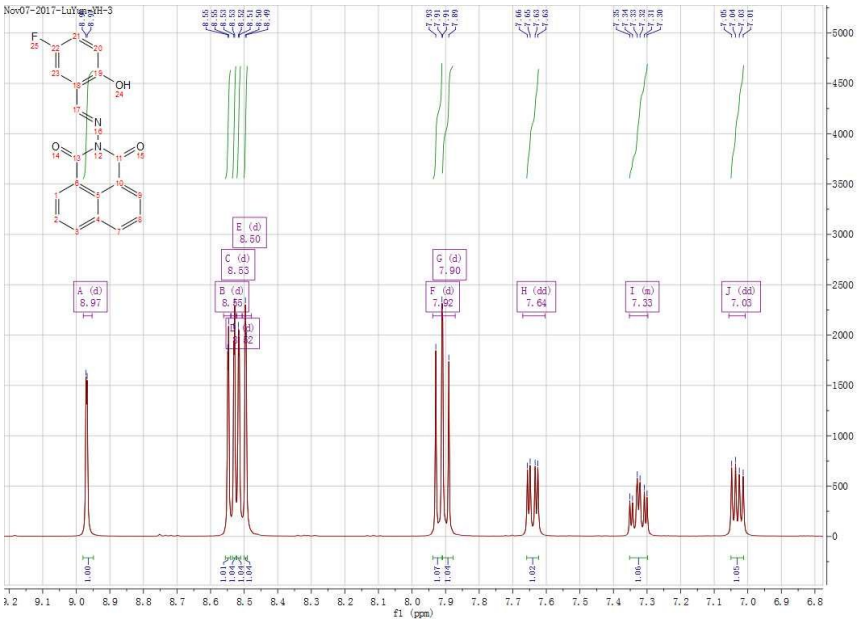

Fig. S1. The ^{1}H NMR spectrum of **NA-F**.

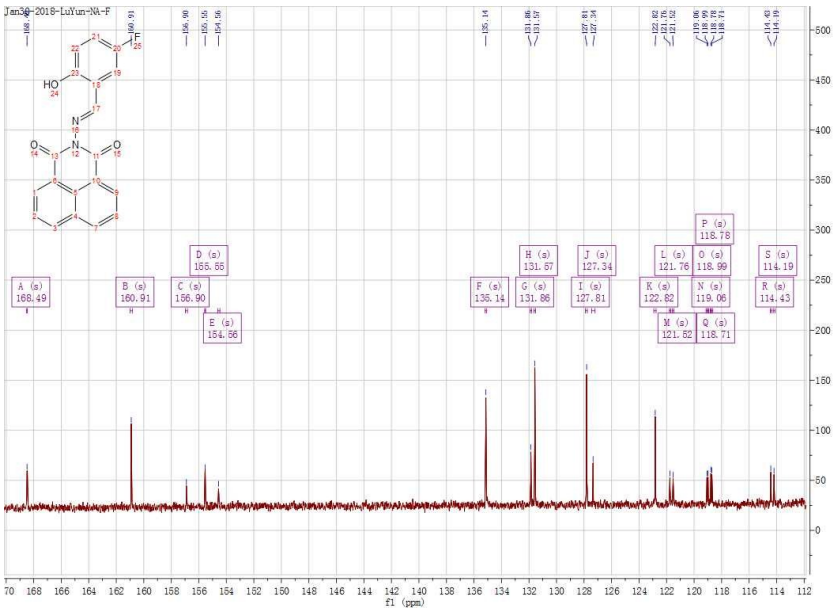

Fig. S2. The ^{13}C NMR spectrum of **NA-F**.

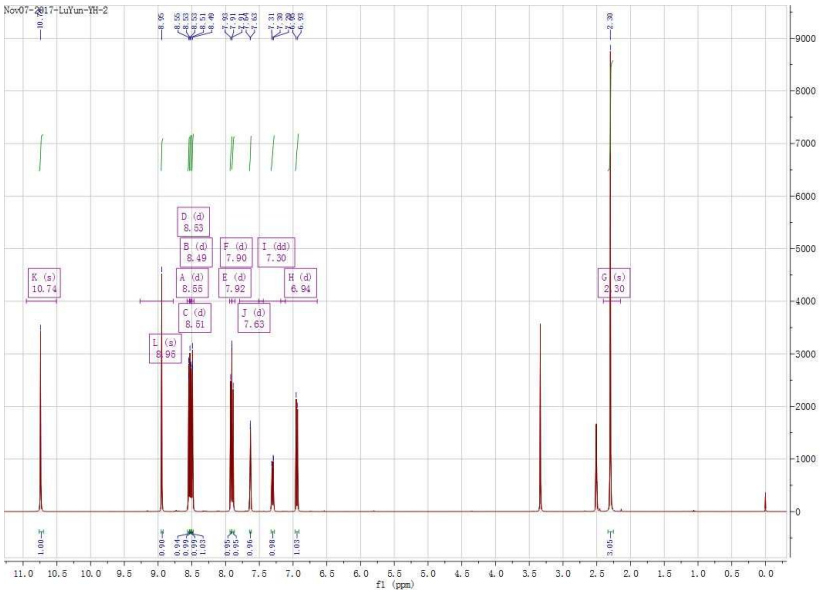

Fig. S3. The ^{1}H NMR spectrum of **NA-M**.

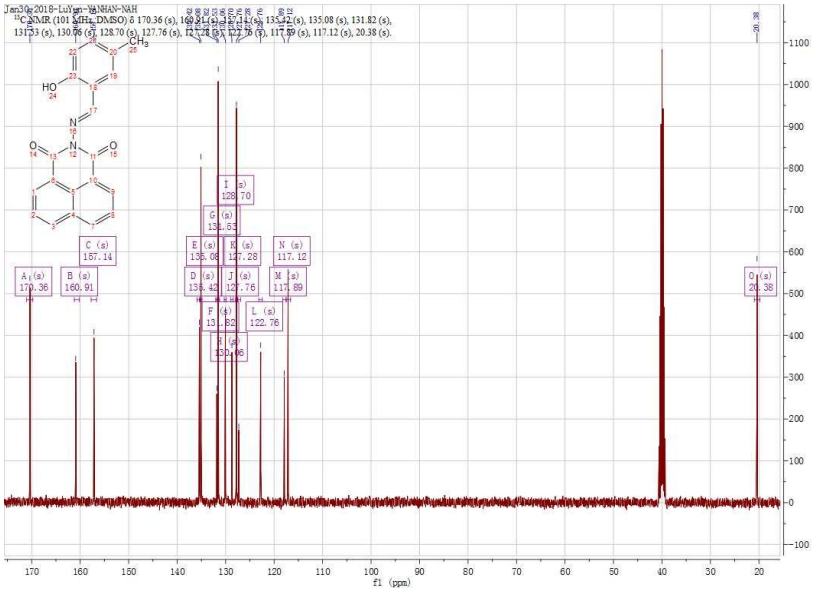

Fig. S4. The ^{13}C NMR spectrum of **NA-M**.

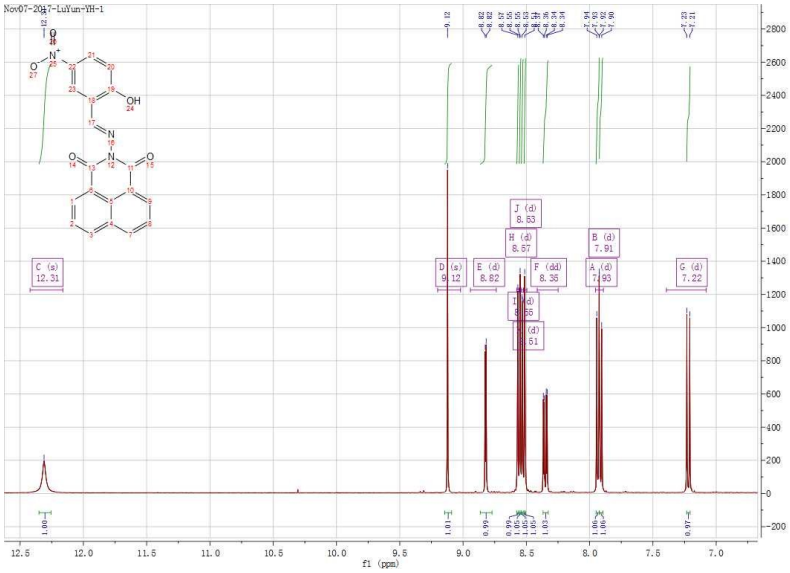

Fig. S5. The ^{1}H NMR spectrum of **NA-N**.

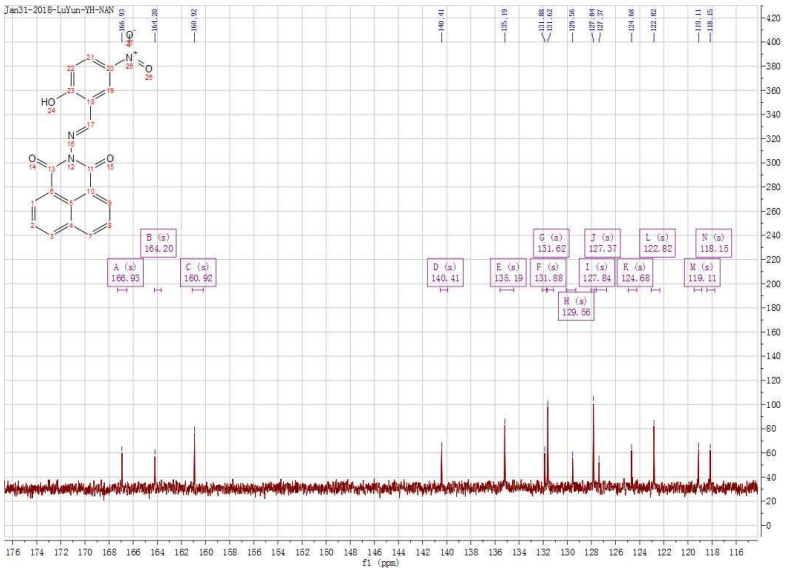

Fig. S6. The ^{13}C NMR spectrum of **NA-N**.

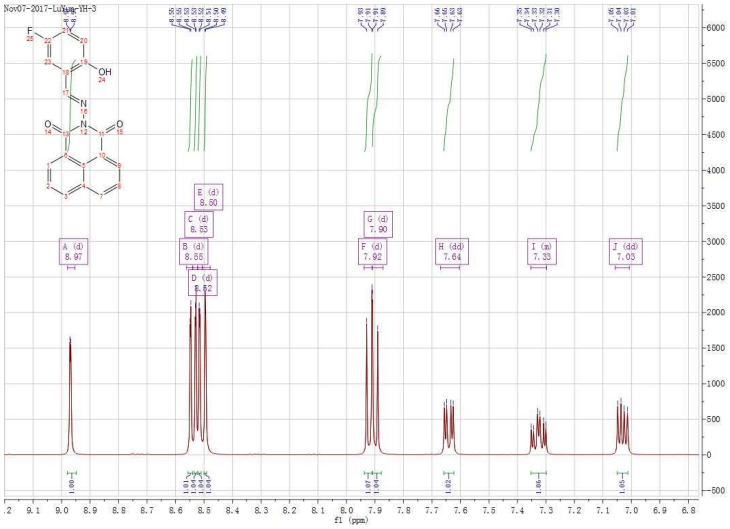

Fig. S7. The ^{1}H NMR spectrum of **NA-EF**.

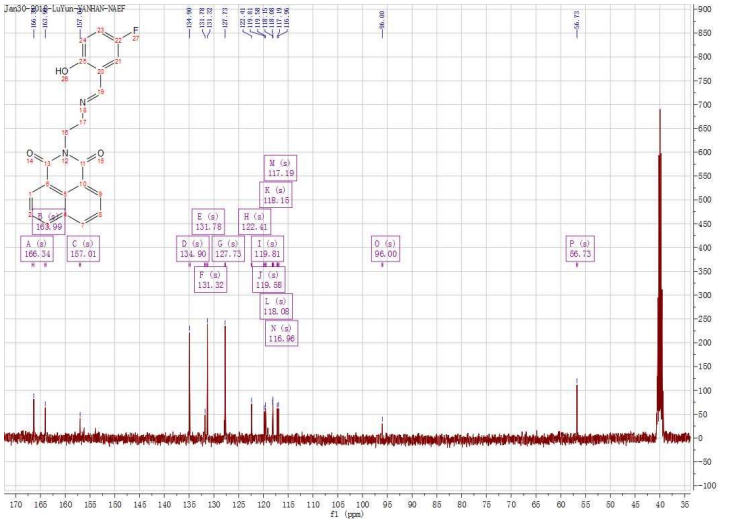

Fig. S8. The ^{13}C NMR spectrum of **NA-EF**.

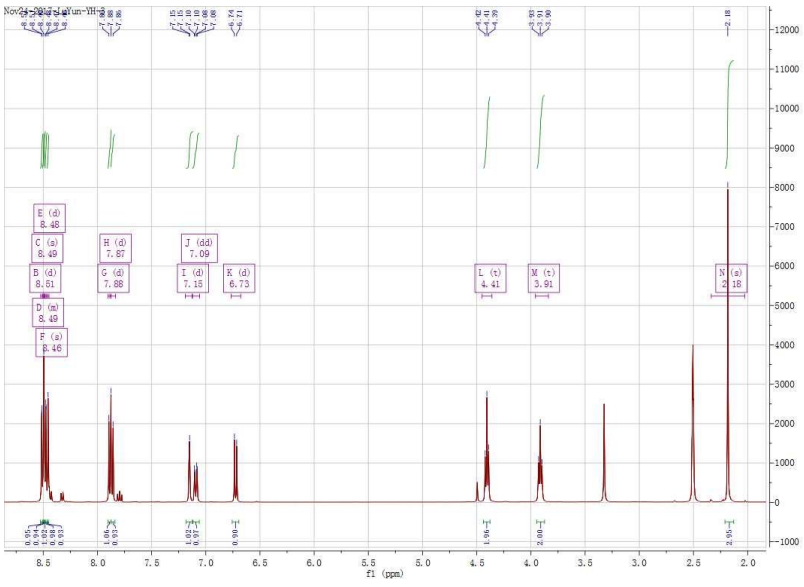

Fig. S9. The ^{1}H NMR spectrum of **NA-EM**.

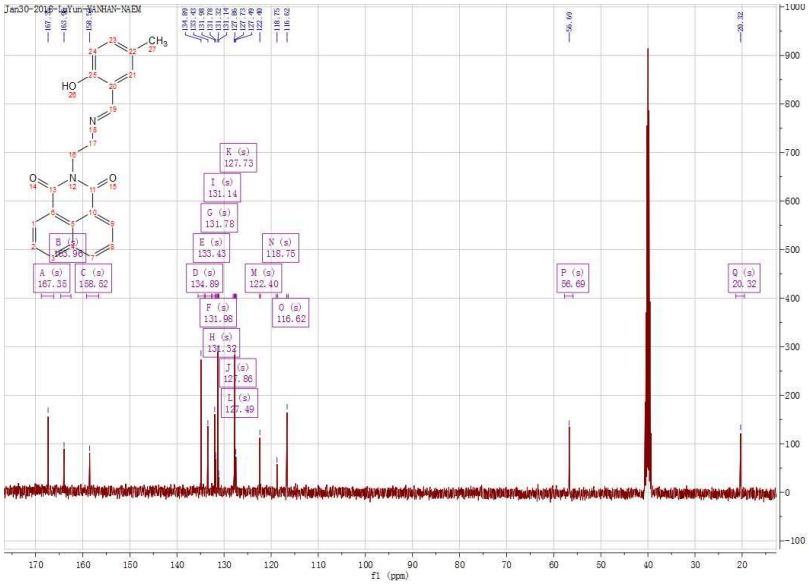

Fig. S10. The ^{13}C NMR spectrum of **NA-EM**.

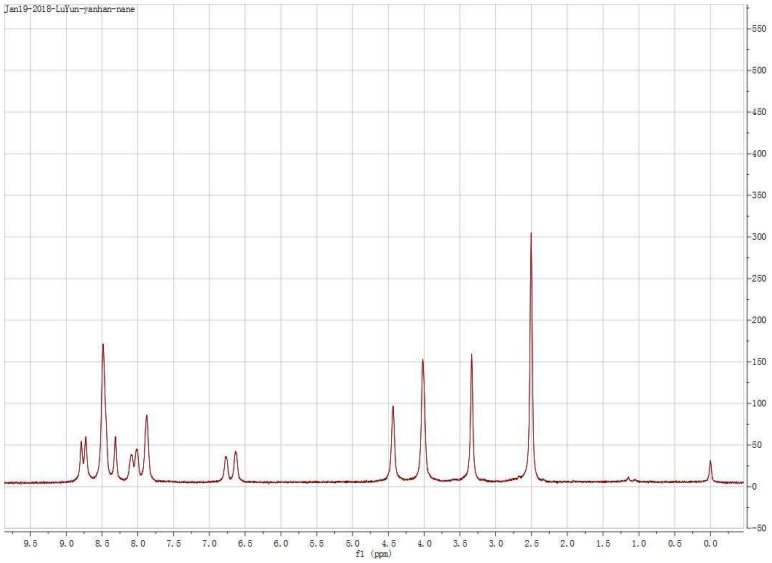

Fig. S11. The ^{1}H NMR spectrum of **NA-EN**.

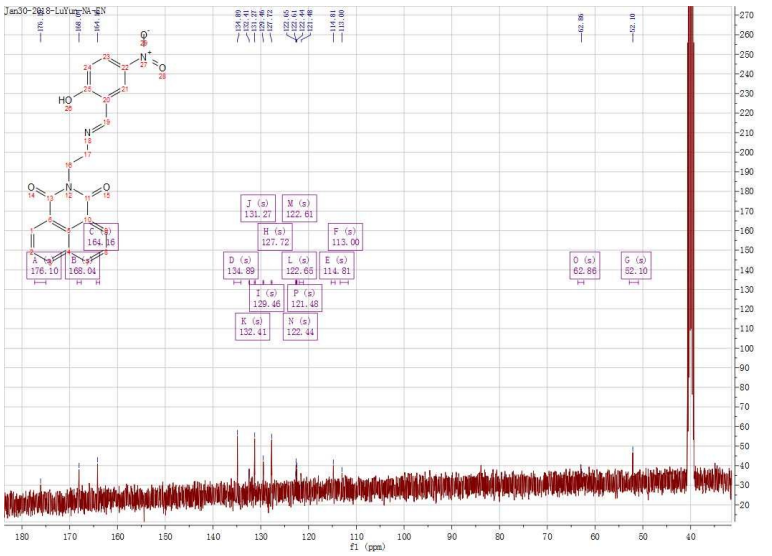

Fig. S12. The ^{13}C NMR spectrum of **NA-EN**.