Support information for

Rationally molecular design: functional quinoline derivatives for PA detection, gaseous acid/base switching and anion-controlled

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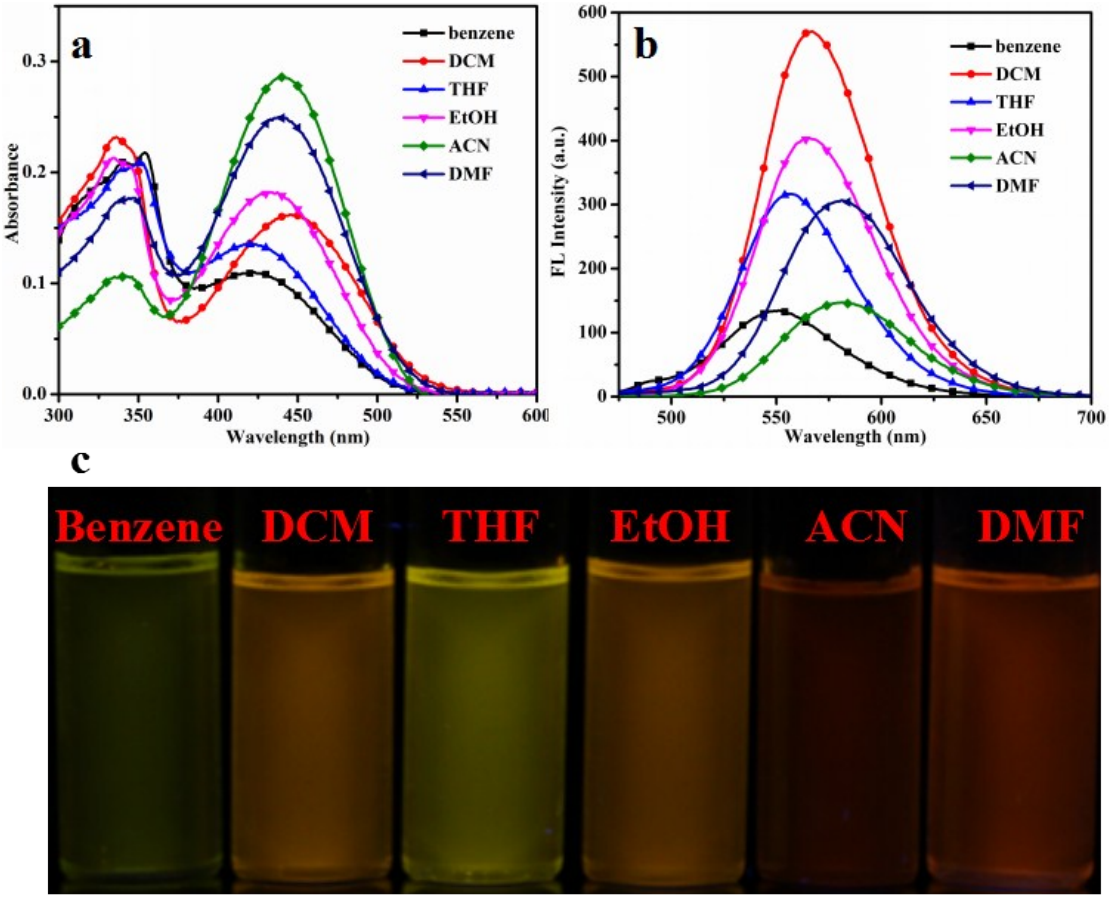

Fig. S1 (a) The UV-Vis spectra; (b) fluorescence spectra of **G2** in different solvents and (c) Photographs of compound **G2** dispersed in different solvents

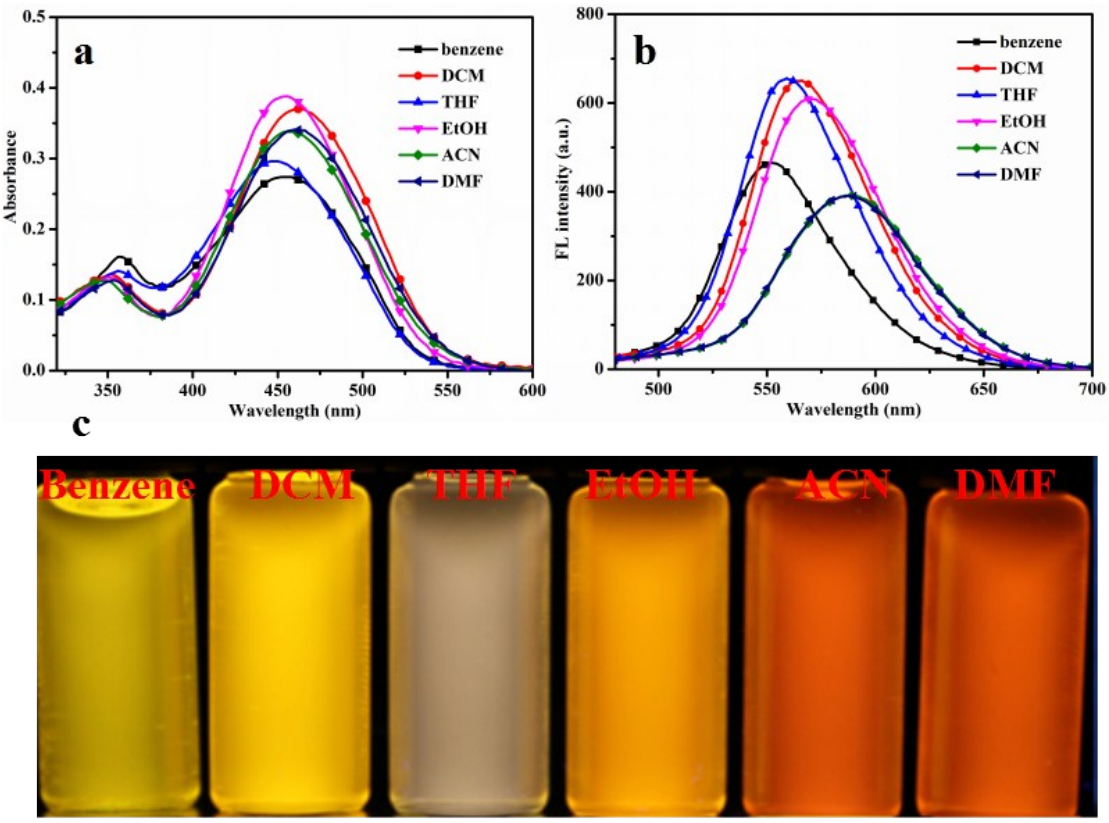

Fig. S2 (a) The UV-vis spectra; (b) fluorescence spectra of **G3** in different solvents and (c) Photographs of compound **G3** dispersed in different solvents

Table S1 The UV-vis absorption data of **G1-G3** in different solvents

		Benzene	DCM	THF	EtOH	ACN	DMF
G_1	λ_{max}(nm)	421	445	420	428	438	439
	$\varepsilon_{max}(10^4)$	1.10	1.62	1.35	1.82	2.86	2.50
G_2	λ_{max}(nm)	421	446	419	434	430	428
	$\varepsilon_{max}(10^4)$	0.72	1.30	0.84	1.34	1.51	1.43

G_3	λ_{max}(nm)	455	460	447	452	457	457
	$\varepsilon_{max}(10^4)$	2.74	3.70	2.96	3.88	3.38	3.41

Table S2 The fluorescent data of **G1-G3** in different solvents

		Benzene	DCM	THF	EtOH	ACN	DMF
G_1	λ_{max}(nm)	553	585	558	581	592	591
G_2	λ_{max}(nm)	551	567	557	565	582	581
G_3	λ_{max}(nm)	552	564	559	570	586	588

Table S3 The relative data of **G1-G3** in different solvents

	Benzene	DCM	THF	EtOH	ACN	DMF
ε	2.28	9.10	7.58	25.70	37.50	36.71
n	1.5011	1.4244	1.407	1.3614	1.3441	1.4282
Δf	0.0029	0.2184	0.2671	0.2901	0.3054	0.2752

Table S4 The Stokes' shift of **G1-G3** in different solvents

		Benzene	DCM	THF	EtOH	ACN	DMF
G_1	λ_{abs}/nm	428	448	420	430	428	428
	λ_{em}/nm	553	585	558	581	592	591
	$\Delta\nu$/cm^{-1}	5281	5227	5888	6044	6472	6444
G_2	λ_{abs}/nm	423	446	421	433	440	438
	λ_{em}/nm	551	567	557	565	582	581
	$\Delta\nu$/cm^{-1}	5492	4785	5800	5396	5545	5619
G_3	λ_{abs}/nm	454	462	448	454	456	460
	λ_{em}/nm	552	564	559	570	586	588
	$\Delta\nu$/cm^{-1}	3910	3910	4432	4482	4864	4732

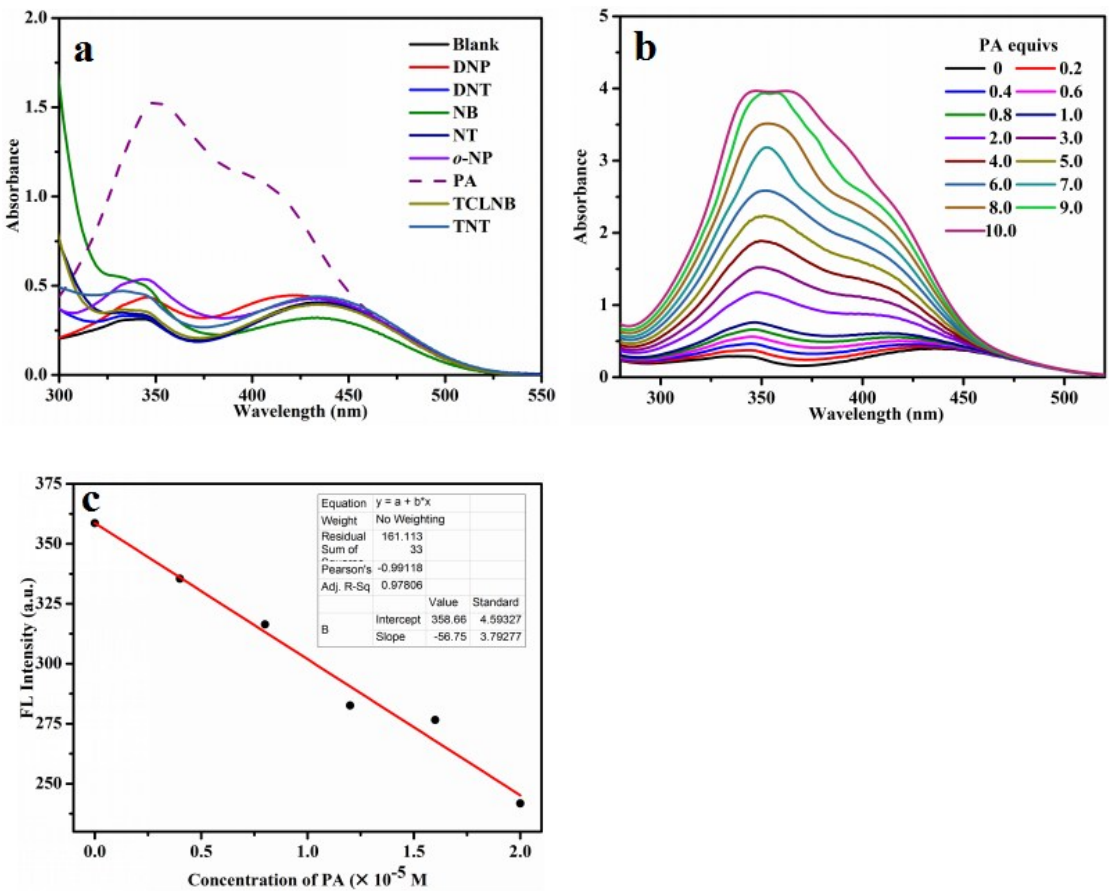

Fig. S3 (a) UV-vis absorption spectra of different nitroaromatic compounds; (b) UV-vis absorption spectra of different concentrations of PA in **G1** solution; (c) The linear relationship between the fluorescence intensity and the PA concentration in **G1** solution

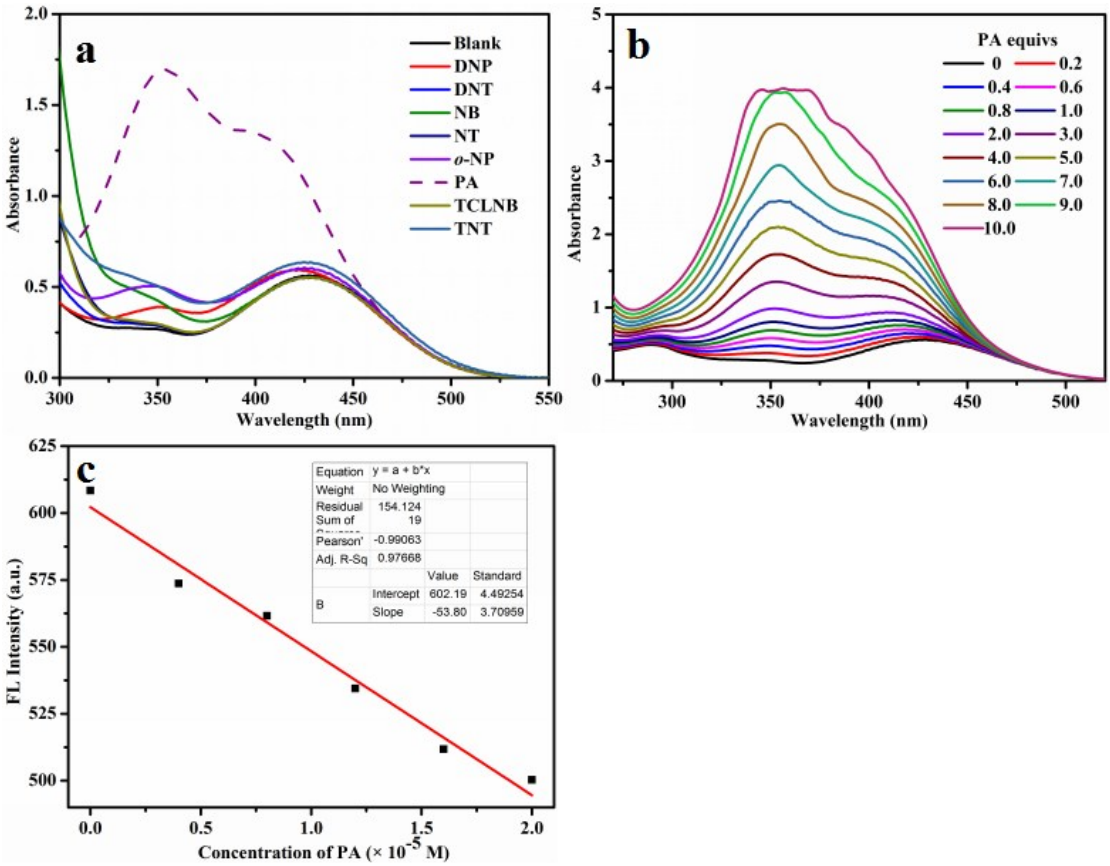

Fig. S4 (a) UV-vis absorption spectra of different nitroaromatic compounds; (b) UV-vis absorption spectra of different concentrations of PA in **G2** solution; (c) The linear relationship between the fluorescence intensity and the PA concentration in **G2** solution

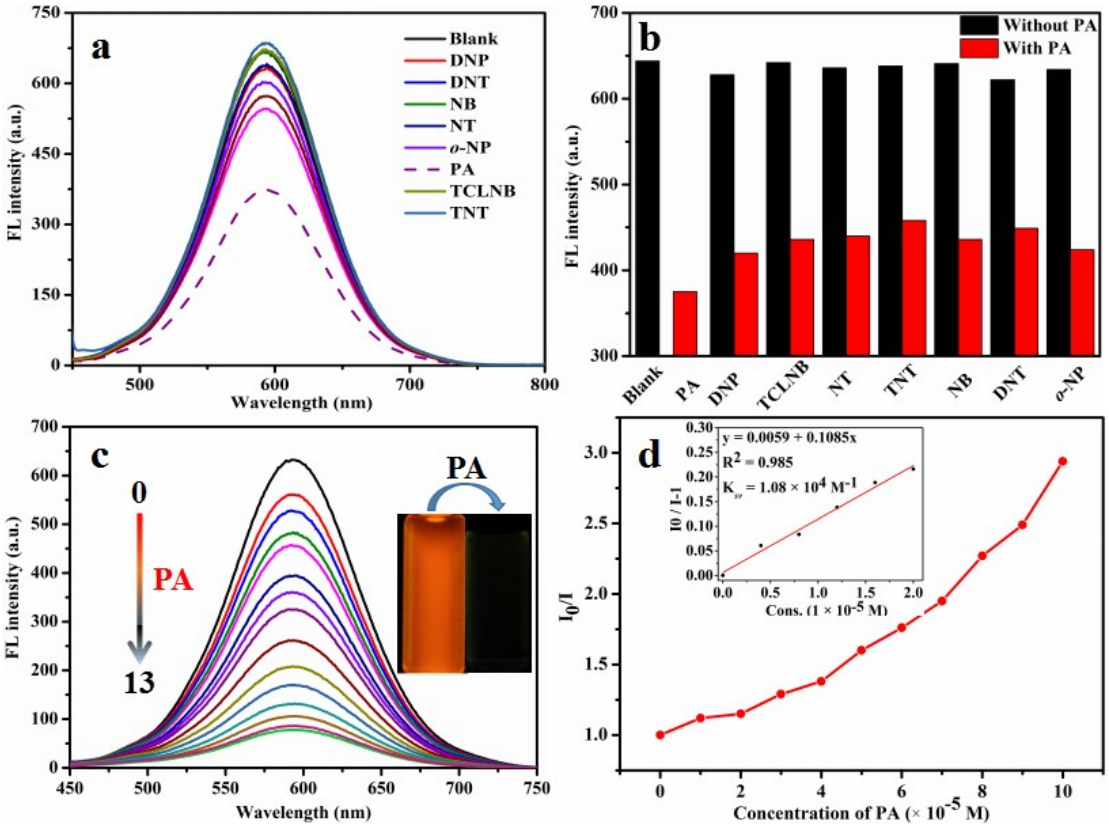

Fig. S5 (a) FL spectra obtained for different analytes (100 ppm); (b) Quenching percentage of compound **G2** (10 mM) with analytes (200 ppm) in CH_3OH/water (v/v = 90 : 10) mixtures before (black) and after (red) the addition of 100 ppm PA; (c) FL spectra of **G2** in CH_3OH/water (v/v = 90 : 10) containing different amounts of PA; (d) Corresponding Stern-Volmer plot of PA. Inset: Stern-Volmer plot obtained at lower concentration of PA

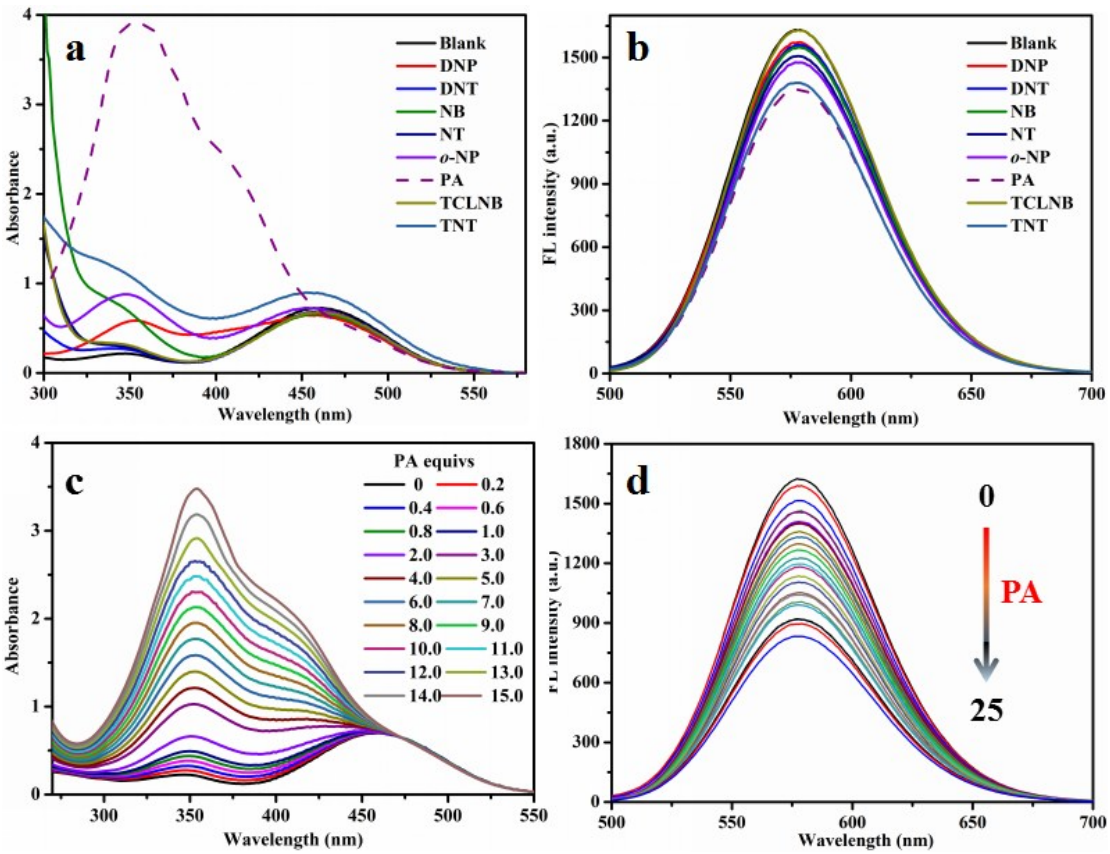

Fig. S6 (a) UV-vis absorption spectra of different nitroaromatic compounds; (B) FL spectra obtained for different analytes (300 ppm); (C) UV-vis absorption spectra of different concentrations of PA in **G3** solution; (D) FL spectra of **G3** in CH_3OH/water (v/v = 90 : 10) containing different amounts of PA

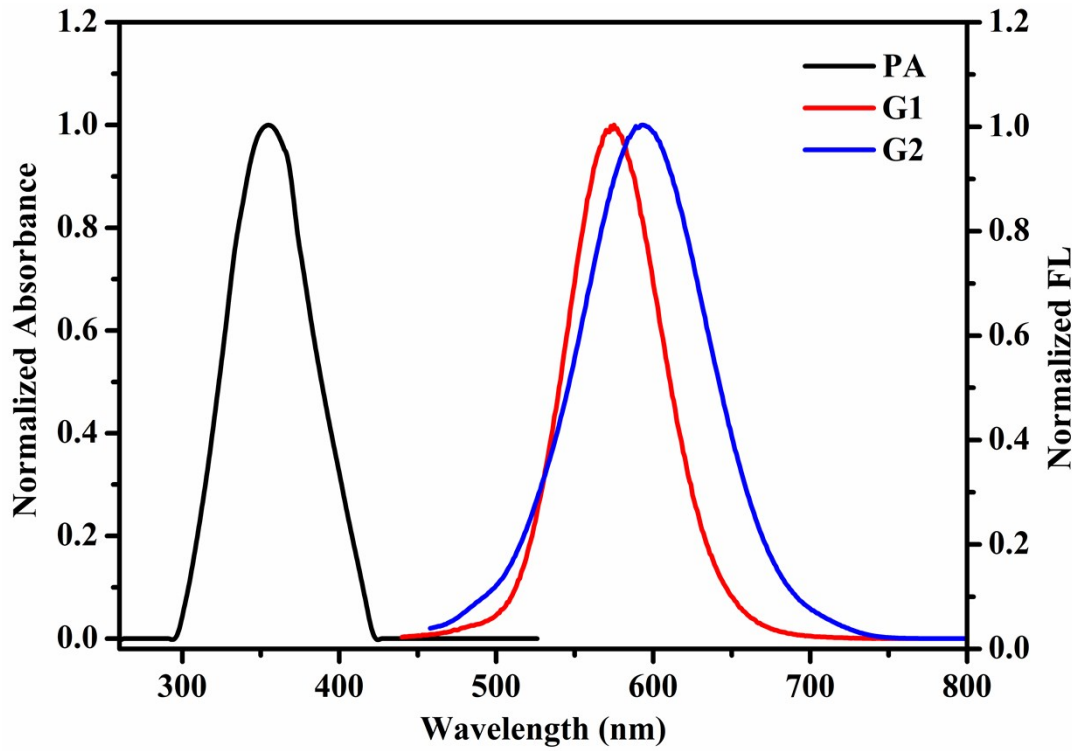

Fig. S7 UV-vis absorption spectra of PA; Normalized Fluorescence of **G1** and **G2**

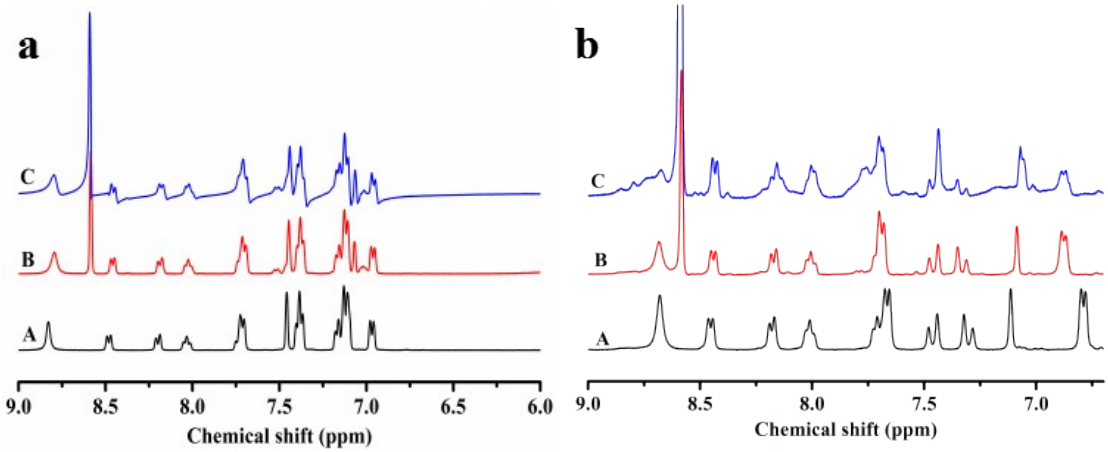

Fig. S8 (a) ^{1}H NMR spectra of **G1** in $CDCl_3$; (b) ^{1}H NMR spectra of **G2** in DMSO-d_6; (A: **G1**/**G2** samples, B: original sample + 3 equivalents PA; C: original sample + 5 equivalents PA.

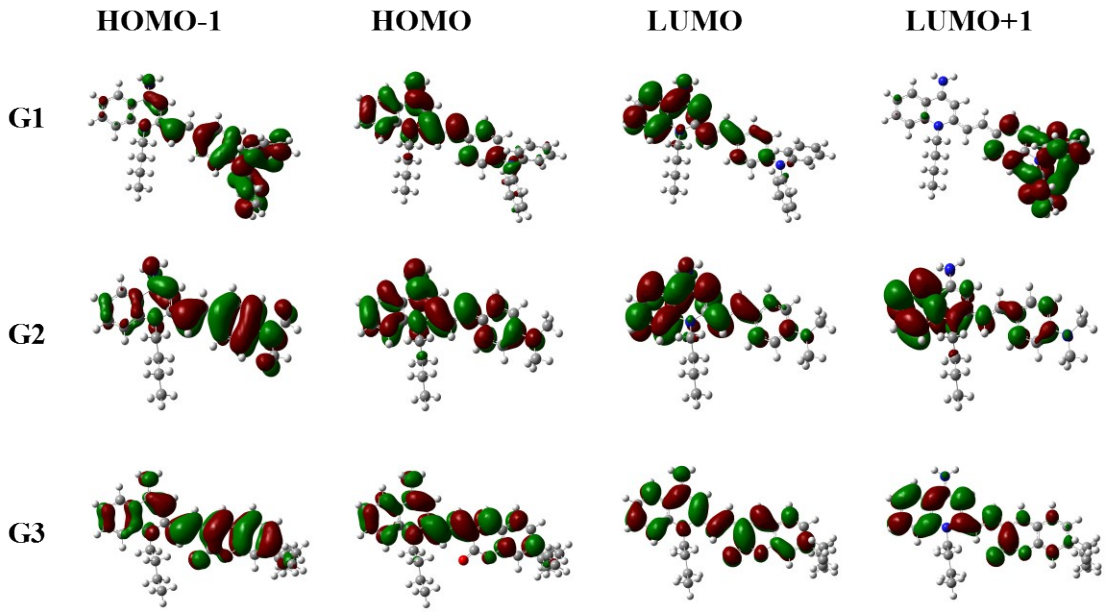

Fig. S9 Frontier orbitals of compounds **G1**, **G2** and **G3**

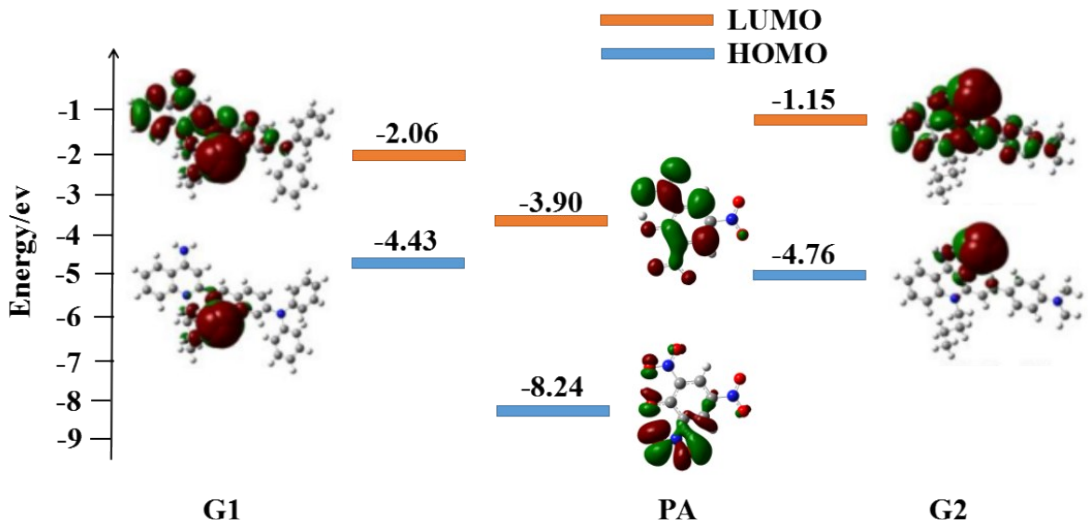

Fig. S10 HOMO and LUMO energy-level diagram of **G1**, **G2** and PA

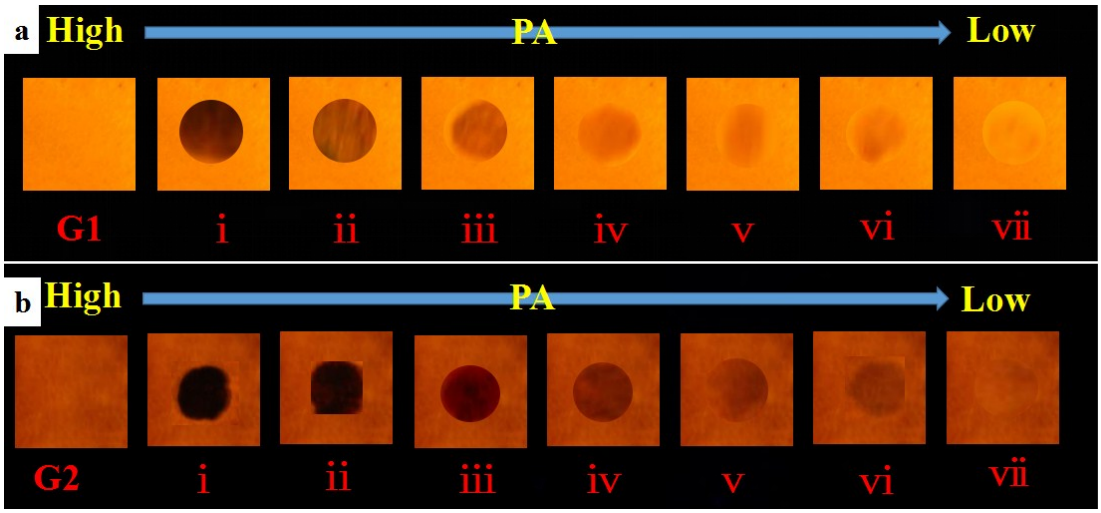

Fig. S11 Photographs of fluorescence quenching of **G1** (a) and **G2** (b)for detecting different concentrations of PA under 365 nm UV light. From left to right: blank, 5.0×10^{-2}, 1.0×10^{-2}, 5.0×10^{-3}, 1.0×10^{-3}, 5.0×10^{-4}, 1.0×10^{-4}, 5.0×10^{-5}

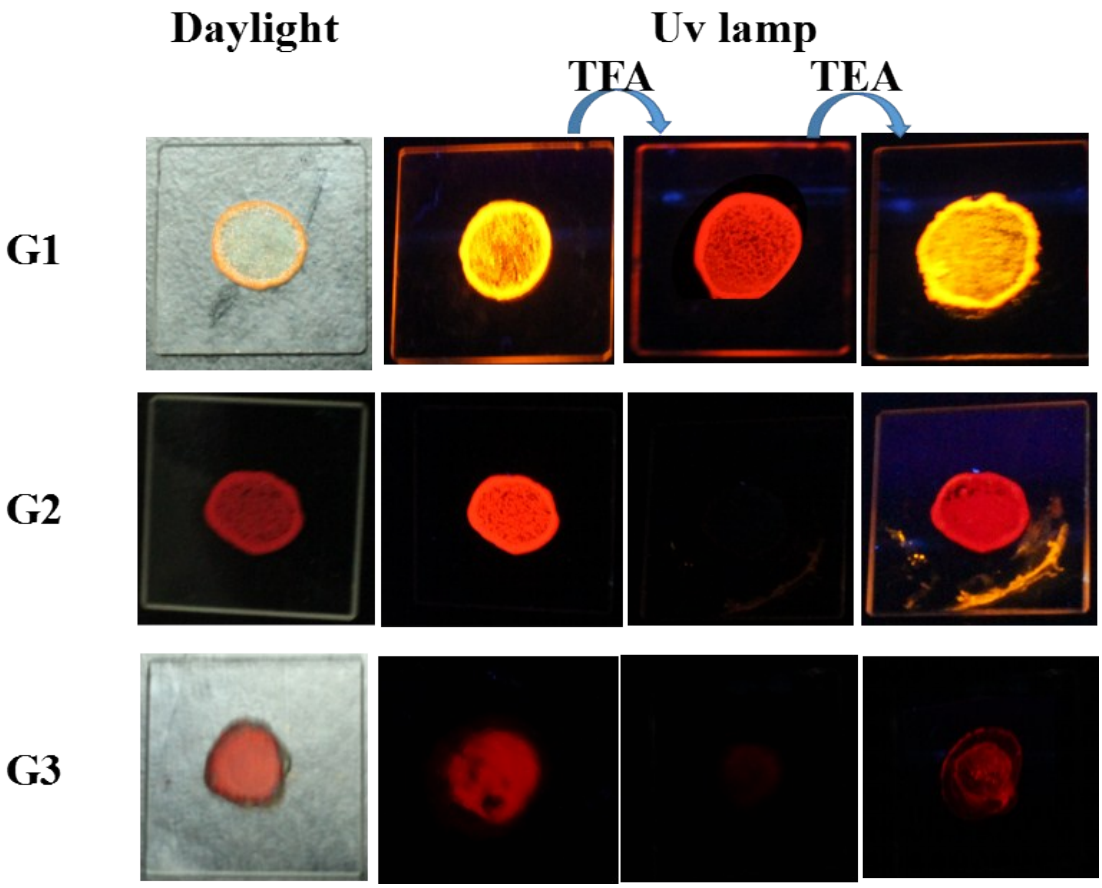

Fig. S12 Recycling of the fluorescence switching and color of **G1-G3** in solid state

upon fuming with TFA and TEA vapors under daylight (left) and 365 nm lamp (right)

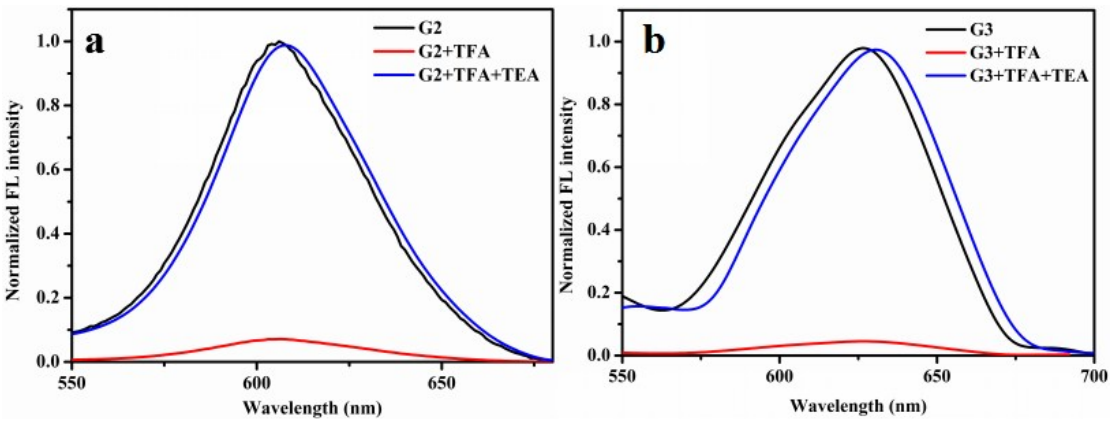

Fig. S13 The fluorescence spectra of **G2** and **G3** exposure to TFA and TEA vapors

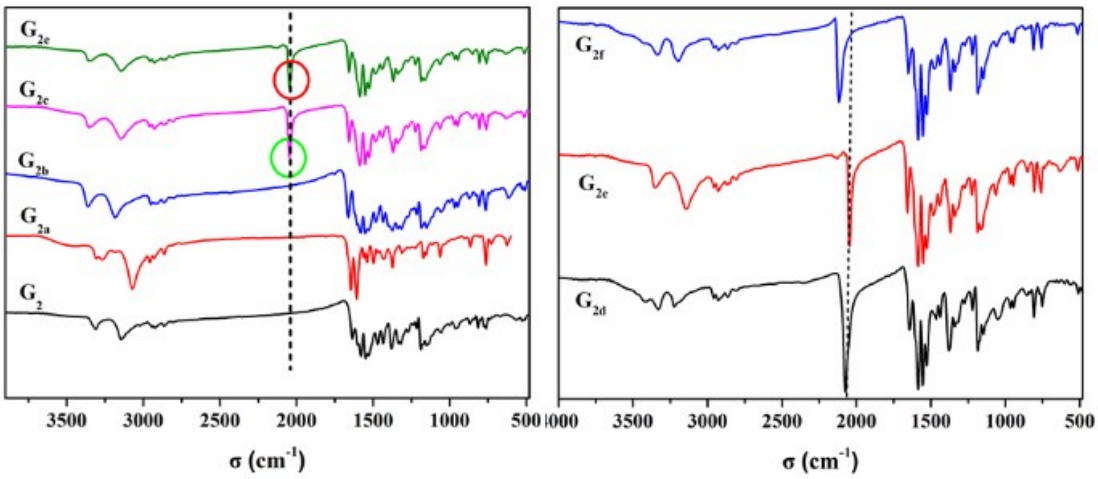

Fig. S14 FT-IR spectra of compounds $\mathbf{G_{2a}}$-$\mathbf{G_{2f}}$ with different anions

Table S5 Emission wavelength of **G2** and $\mathbf{G_{2a}}$-$\mathbf{G_{2f}}$

Compounds	**G2**	$\mathbf{G_{2a}}$	$\mathbf{G_{2b}}$	$\mathbf{G_{2c}}$	$\mathbf{G_{2d}}$	$\mathbf{G_{2e}}$	$\mathbf{G_{2f}}$

Emission wavelengt (nm)	612	571	590	631	645	628	593

Table S6 Selected bond lengths (Å) and angles (°) of compound **G_{2b}, G_{2d}** and **G_{2f}**

lengths (Å)		**angles (°)**	
Compound G_{2b}			
C(19)-C(20)	1.408(3)	C(11)-N(3)-C(19)	120.35(15)
C(18)-C(23)	1.402(3)	C(19)-N(3)-C(13)	118.73(15)
C(18)-C(19)	1.409(3)	C(7)-C(8)-C(9)	123.93(18)
C(17)-N(2)	1.336(2)	C(23)-C(18)-C(17)	122.21(18)
C(3)-N(1)	1.360(3)	N(2)-C(17)-C(18)	121.79(17)
N(3)-C(13)	1.485(2)	N(1)-C(3)-C(4)	122.25(18)
N(3)-C(19)	1.395(2)	N(3)-C(11)-C(10)	120.46(17)
N(3)-C(11)	1.371(2)	N(3)-C(19)-C(18)	120.65(17)
N(4)-O(2)	1.209(2)	O(2)-N(4)-O(1)	119.13(18)

Compound G_{2d}			
Zn(1)-N(5)	1.936(3)	N(5)-Zn(1)-N(5)	109.3(2)
Zn(1)-N(4)	1.965(3)	N(5)-Zn(1)-N(4)	108.30(13)
S(1)-C(24)	1.612(4)	N(5)-Zn(1)-N(4)	110.67(14)
S(2)-C(25)	1.610(4)	C(9)-N(2)-C(1)	120.7(2)
N(2)-C(9)	1.368(3)	C(1)-N(2)-C(20)	118.6(2)
N(2)-C(20)	1.509(4)	C(1)-C(6)-C(7)	118.7(3)
C(6)-C(1)	1.409(4)	N(1)-C(7)-C(8)	121.4(3)
C(7)-N(1)	1.346(4)	N(1)-C(7)-C(6)	z
C(17)-C(16)	1.368(4)	N(2)-C(1)-C(6)	120.0(3)
C(15)-C(14)	1.412(4)	C(9)-C(8)-H(8)	117(2)
S(1)-C(24)	1.612(4)	N(5)-Zn(1)-N(4)	110.67(14)
Compound G_{2f}			
Hg(1)-S(3)	2.4364(18)	S(3)-Hg(1)-S(2)	137.86(6)
Hg(1)-S(2)	2.4547(17)	S(2)-Hg(1)-S(1)	111.83(6)
Hg(1)-S(1)	2.5297(19)	S(3)-Hg(1)-N(4)	93.39(16)
Hg(1)-N(4)	2.563(6)	S(1)-Hg(1)-N(4)	101.92(19)
S(2)-C(24)	1.648(8)	C(26)-S(3)-Hg(1)	97.7(3)
S(3)-C(26)	1.643(9)	N(4)-C(24)-S(2)	177.4(6)
N(6)-C(26)	1.130(10)	C(9)-N(2)-C(20)	120.3(4)
N(2)-C(9))	1.374(7)	N(2)-C(9)-C(8)	120.2(5)
N(2)-C(20)	1.482(7)	N(2)-C(4)-C(5)	120.9(5)

Table S7 Crystal data collections and structure refinements of compounds **G_{2b}, G_{2d}** and **G_{2f}**

compounds	**G_{2b}**	**G_{2d}**	**G_{2f}**
empirical formula C	$C_{23}H_{28}N_4O_3$	$C_{50}H_{56}N_{10}S_4Zn$	$C_{26}H_{27}N_6S_3Hg$
formula weight	408.49	990.66	720.31
crystal system	Monoclinic	Monoclinic	Triclinic
space group	$P2_1/n$	C2/c	P^{-1}
a [Å]	13.215(5)	20.941(5)	11.226(5)
b [Å]	10.327(5)	11.461(5)	11.535(5)
c [Å]	16.162(5)	22.337(5)	11.969(5)
α [°]	90.000(5)	90.000(5)	108.012(5)
β [°]	93.560(5)	107.490(5)	100.682(5)
γ [°]	90.000(5)	90.000(5)	90.099(5)
V [Å3]	2201.4(15)	5113(3)	1445.5(11)
Z	4	4	2
T [K]	296(2)	296(2)	296(2)
D calcd [$g \cdot cm^{-3}$]	1.233	1.287	1.655
μ [mm^{-1}]	0.083	0.688	5.566

θ range [°]	2.34-24.84	2.34-20.32	2.33-23.02
total no. data	3870	4517	4711
no.unique data	2884	2736	3821
no.params refined	274	321	328
R_1	0.0471	0.0457	0.0308
wR_2	0.1356	0.1298	0.0834
Goodness-of-fit on F^2	1.001	0.999	0.997

Table S8 Hydrogen bond lengths (Å) and bond angles (°) of compounds **G_{2b}**, **G_{2d}** and **G_{2f}**

Compound **G_{2b}**				
D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠DHA
C(7)–H(7)···N(4)	0.930	2.732	3.622	160.37
C(20)–H(20)···O(2)	0.930	2.622	3.454	149.22
C(15)–H(15B)···O(2)	0.970	2.557	3.407	146.40
C(13)–H(13B)···O(2)	0.970	2.455	3.296	144.90
C(13)–H(13B)···O(3)	0.970	2.692	3.611	158.29
N(2)–H(2B)···O(1)	0.860	2.054	2.831	149.83
C(9)–H(9)···O(3)	0.930	2.709	3.600	160.86
N(2)–H(2A)···O(1)	0.860	2.068	2.894	160.
C(23)–H(23)···O(2)	0.930	2.556	3.410	152.81
Compound **G_{2d}**				
D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠DHA
C(5)–H(5)···N(1)	0.883	2.589	2.886	100.69
N(1)–H(1A)···N(4)	0.860	2.558	3.372	158.35
N(1)–H(1B)···S(2)	0.860	2.889	3.733	167.42
C(5)–H(5)···S(2)	0.883	2.923	3.738	154.27
C(3)–H(3)···N(4)	0.966	2.743	3.667	160.25
Compound **G_{2f}**				
D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠DHA
C(5)–H(5)···N(4)	0.930	2.878	3.555	130.67
C(2)–H(2)···N(1)	0.930	2.613	2.902	98.61
N(1)–H(1A)···N(6)	0.860	2.428	3.238	157.25
N(1)–H(1B)···N(5)	0.860	2.132	2.969	164.25

C(2)–H(2)···N(5)	0.930	2.559	3.475	168.59
C(19)–H(19A)···N(1)	0.960	2.657	3.537	152.61

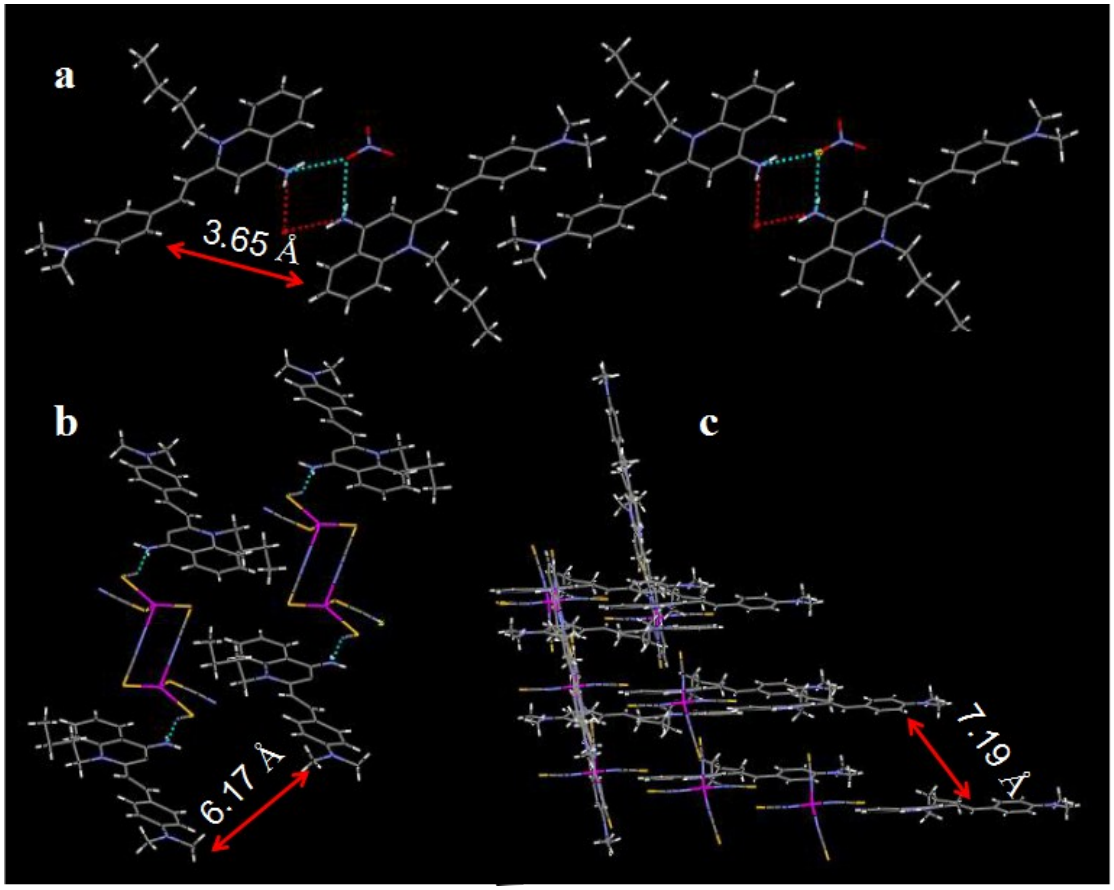

Fig. S15 Molecular arrangement of $\mathbf{G_{2b}}$ (a); $\mathbf{G_{2d}}$ (b) and $\mathbf{G_{2f}}$ (c).

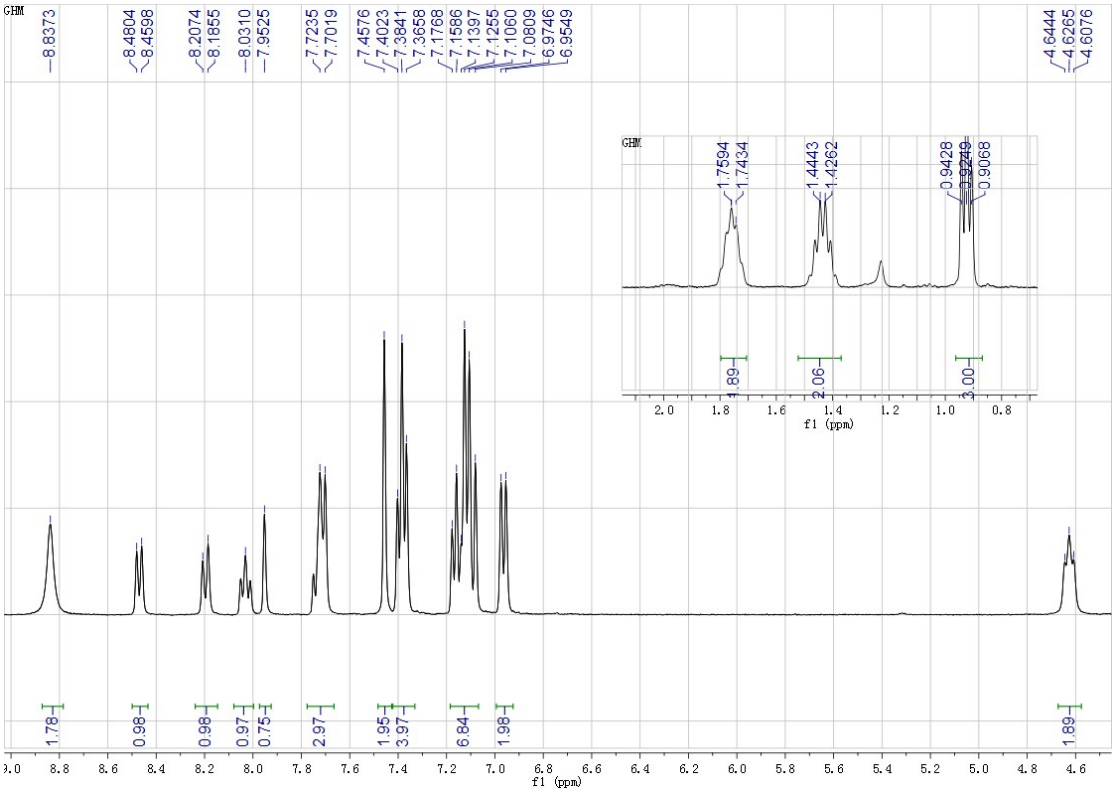

Fig. S16 ^{1}H NMR spectrum (400 MHz) of **G1** in DMSO-d_6

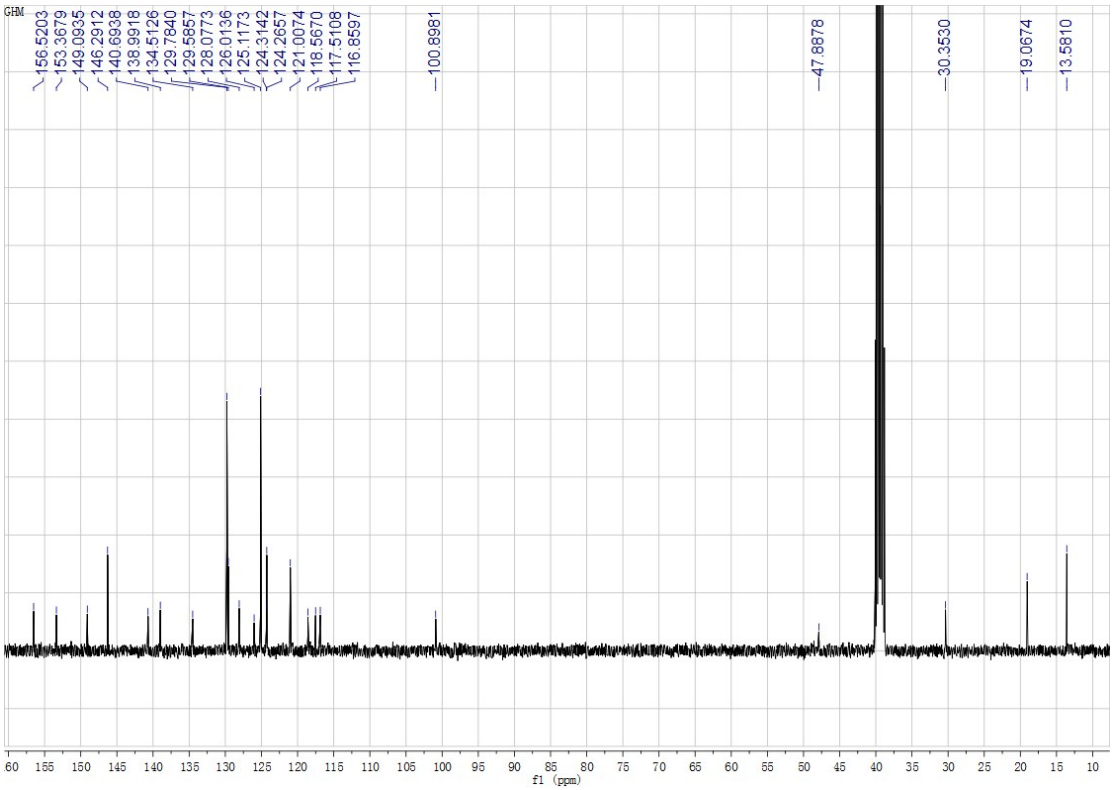

Fig. S17 ^{13}C NMR spectrum (100 MHz) of **G1** in DMSO-d_6

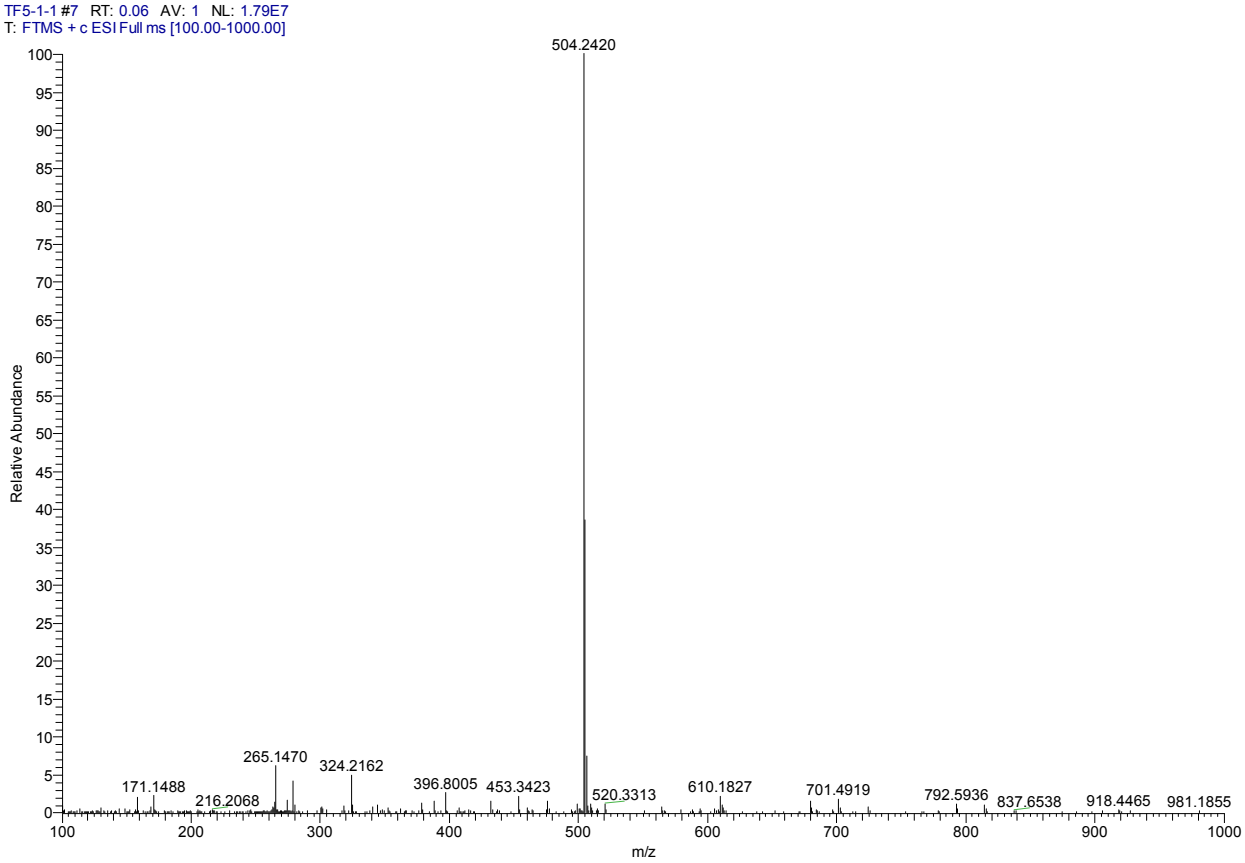

Fig. S18 ESI-MS spectrum of **G1**

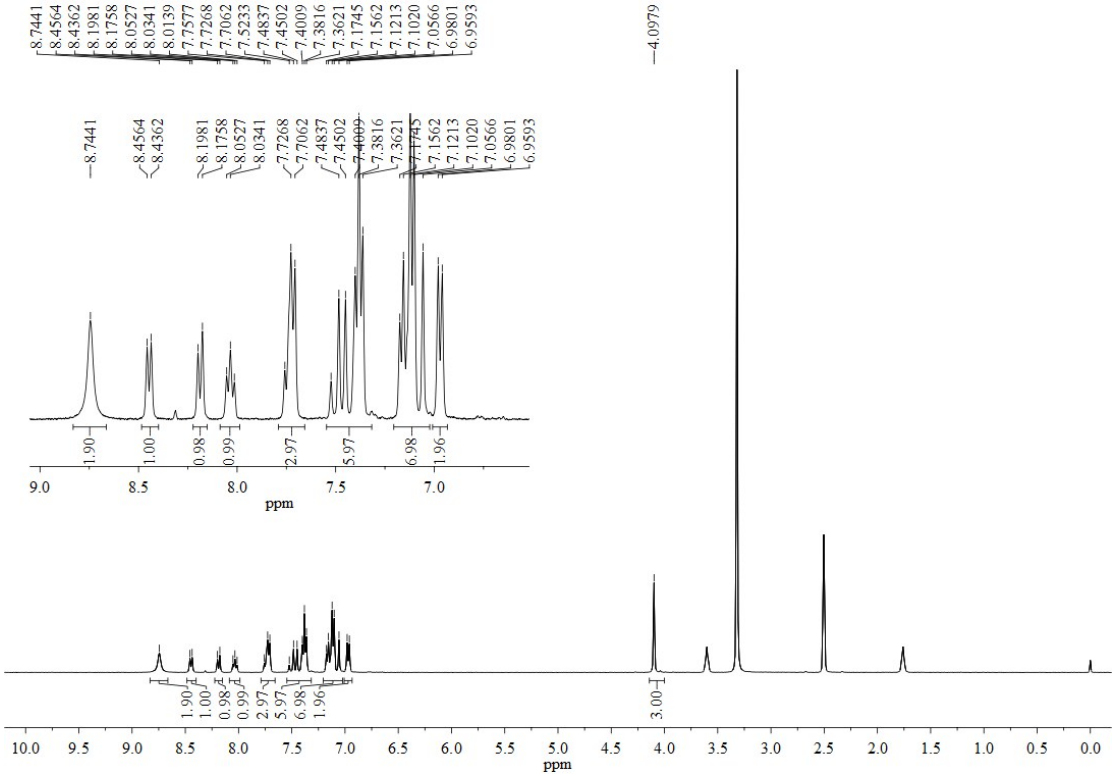

Fig. S19 ^{1}H NMR spectrum (400 MHz) of **G2** in DMSO-d_6

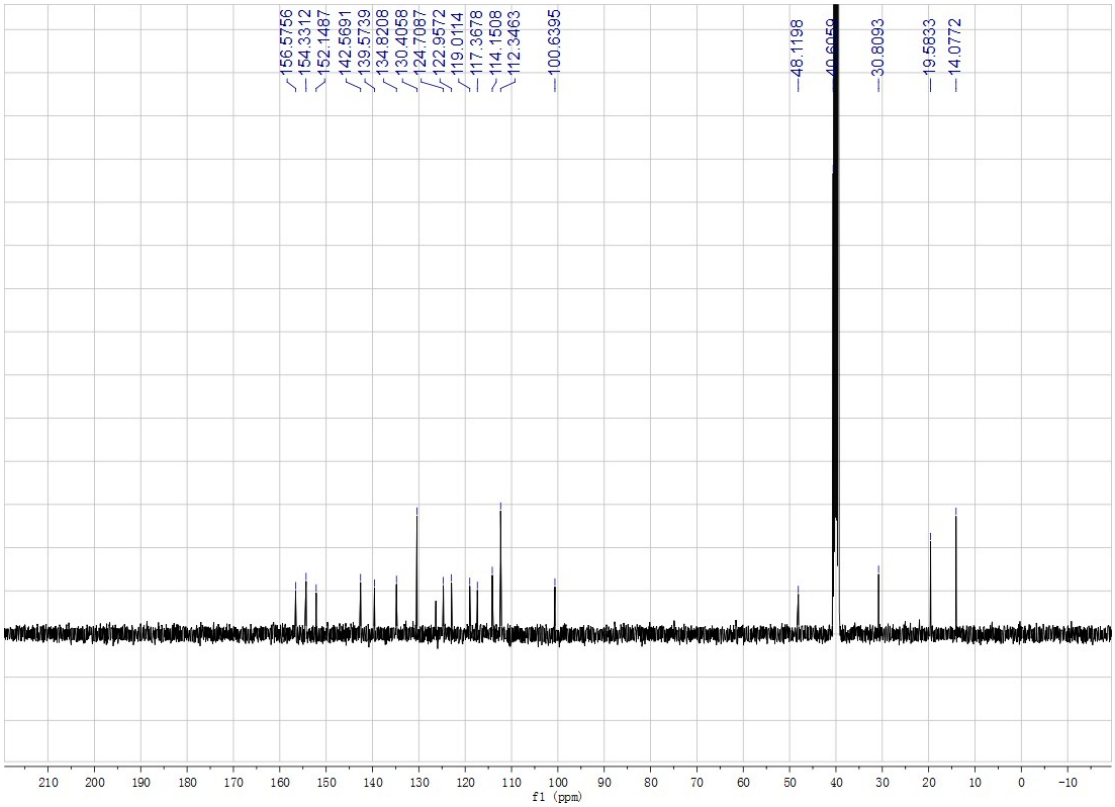

Fig. S20 ^{13}C NMR spectrum (100 MHz) of **G1** DMSO-d_6

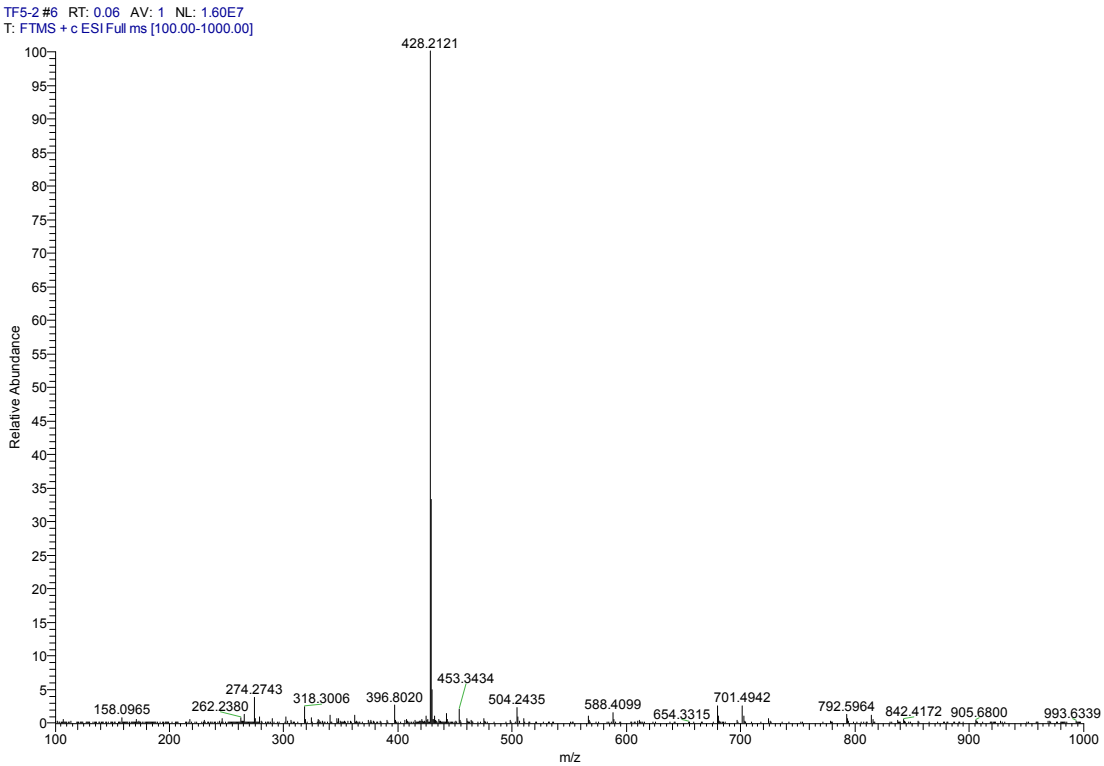

Fig. S21 ESI-MS spectrum of **G2**

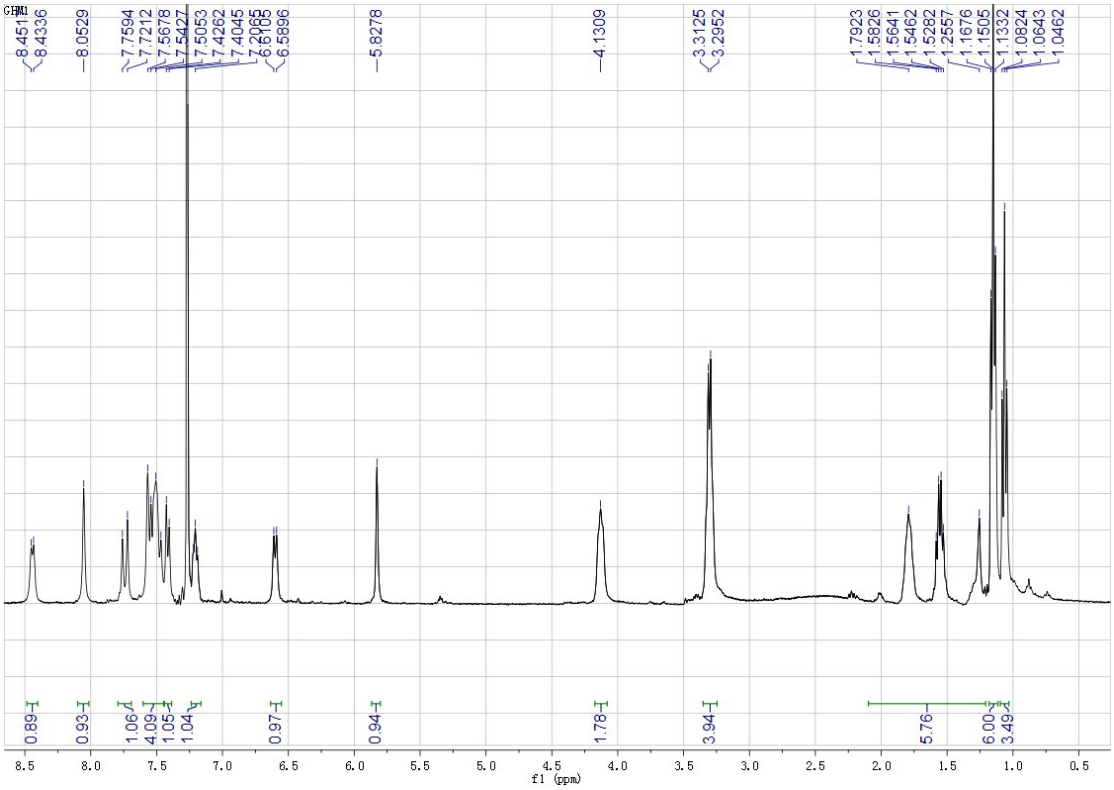

Fig. S22 ^{1}H NMR spectrum (400 MHz) of **G3** in $CDCl_3$

Fig. S23 ^{13}C NMR spectrum (100 MHz) of **G3** in $CDCl_3$

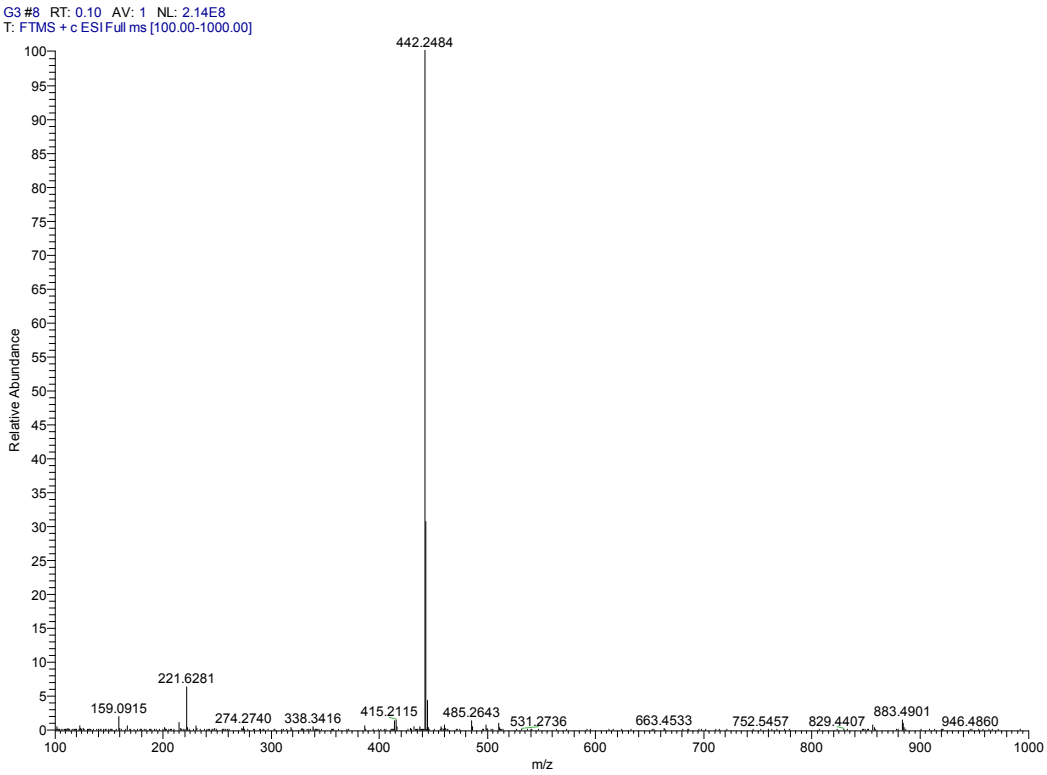

Fig. S24 ESI-MS spectrum of **G3**