Supporting Information

Donor-acceptor typed aggregation-induced emission luminophores based on 1,1-dicyanomethylene-3-indanone unit for bridge-dependent reversible mechanochromism and light-up biosensing of hypochlorite

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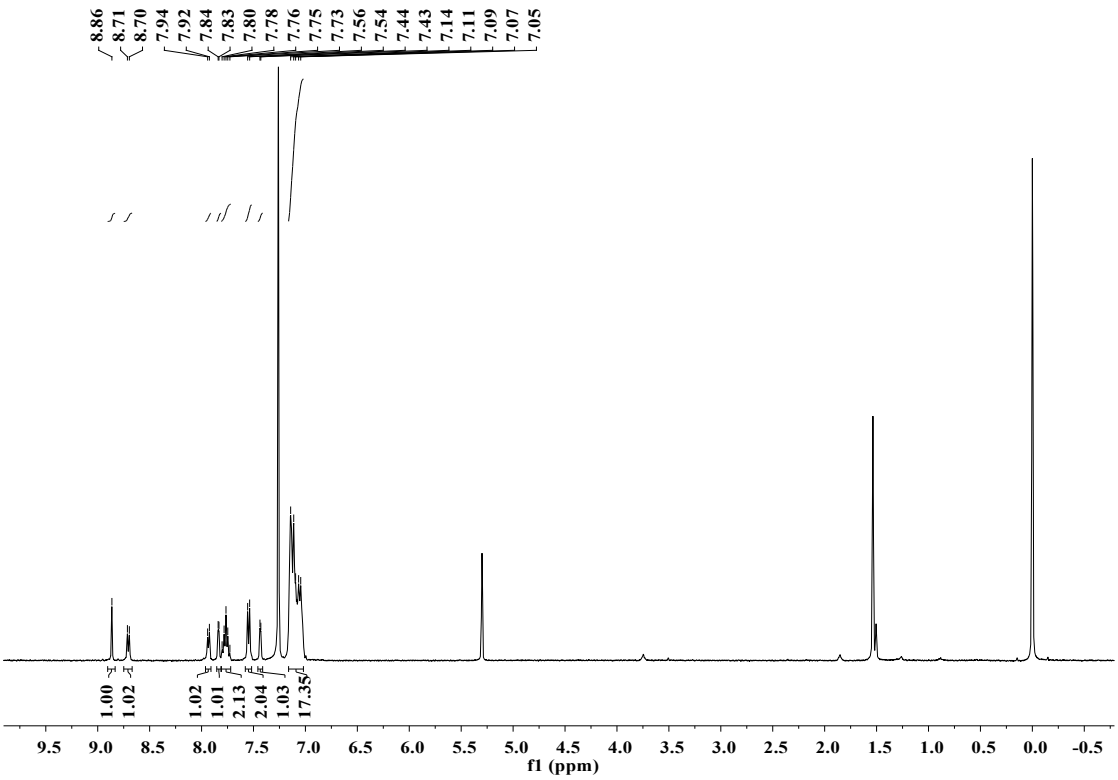


Figure S1. ^{1}H NMR spectrum (in $CDCl_3$) of **TPEThIC**.

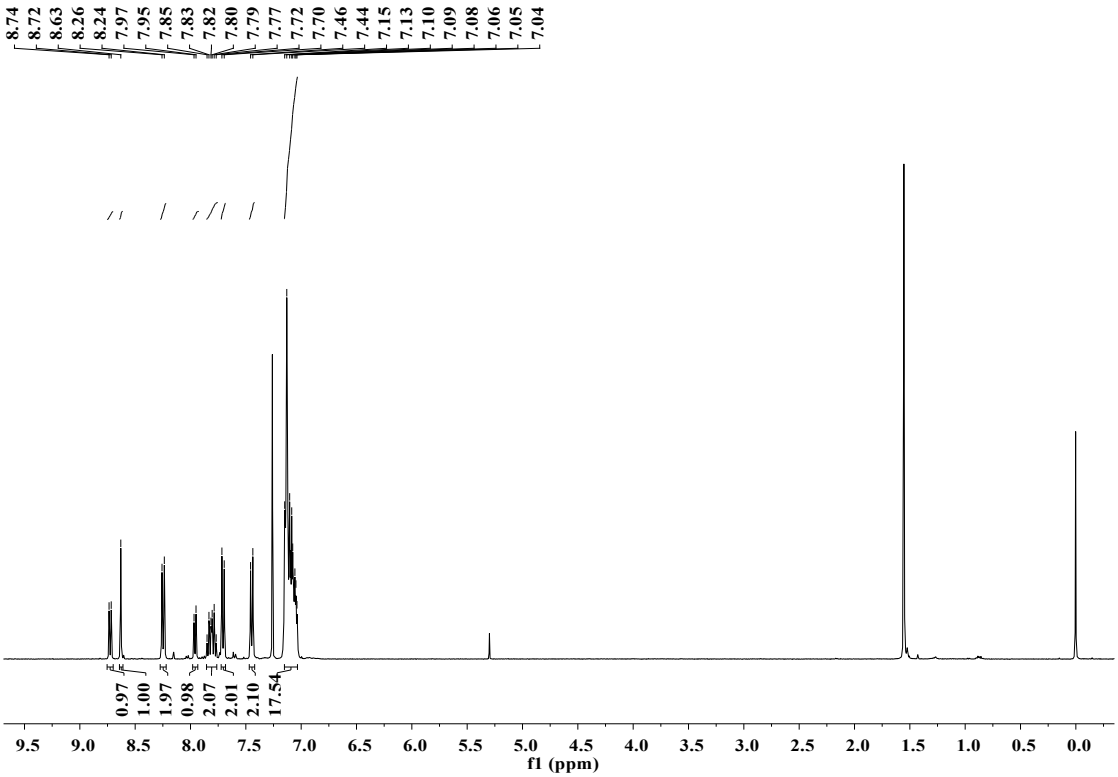


Figure S2. ^{1}H NMR spectrum (in $CDCl_3$) of **TPEPhIC**.

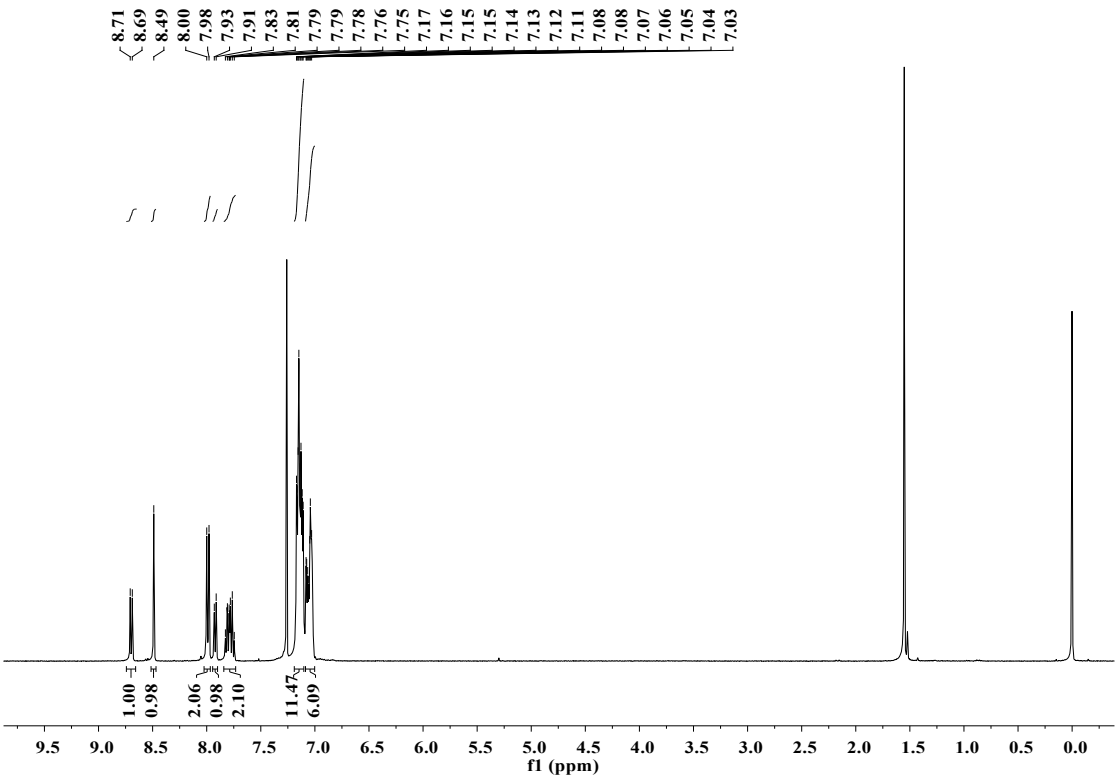


Figure S3. ^{1}H NMR spectrum (in $CDCl_3$) of **TPEIC**.

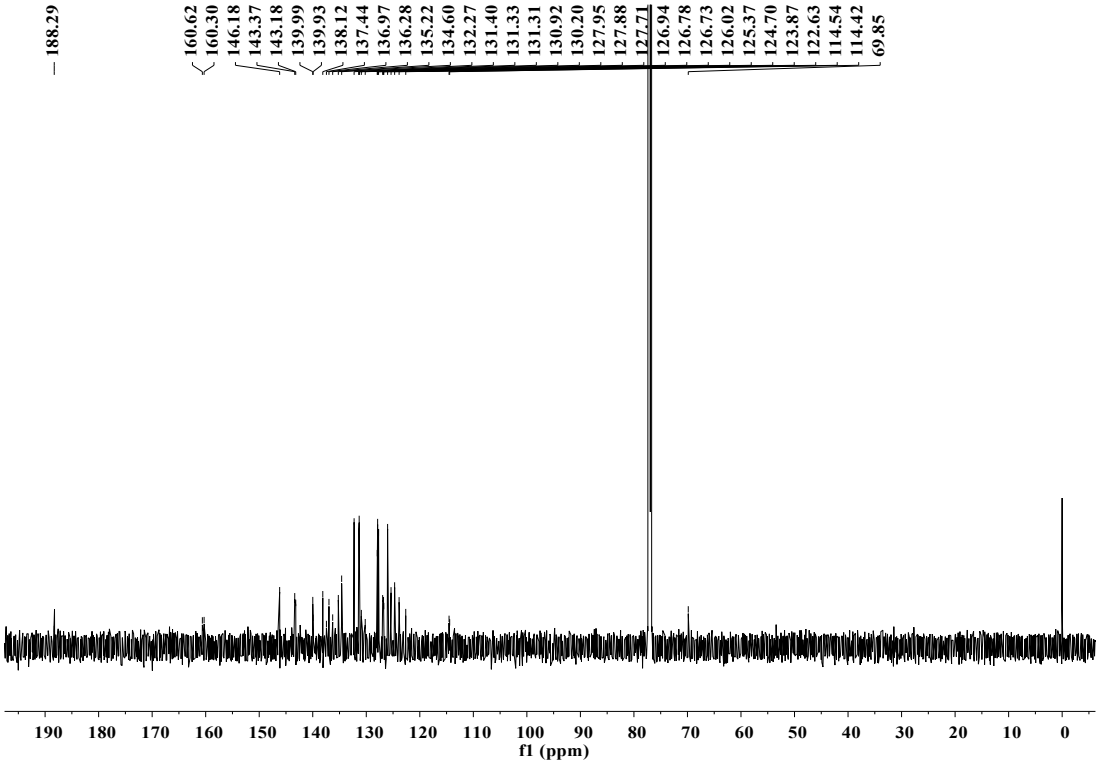


Figure S4. ^{13}C NMR spectrum (in $CDCl_3$) of **TPEThIC**.

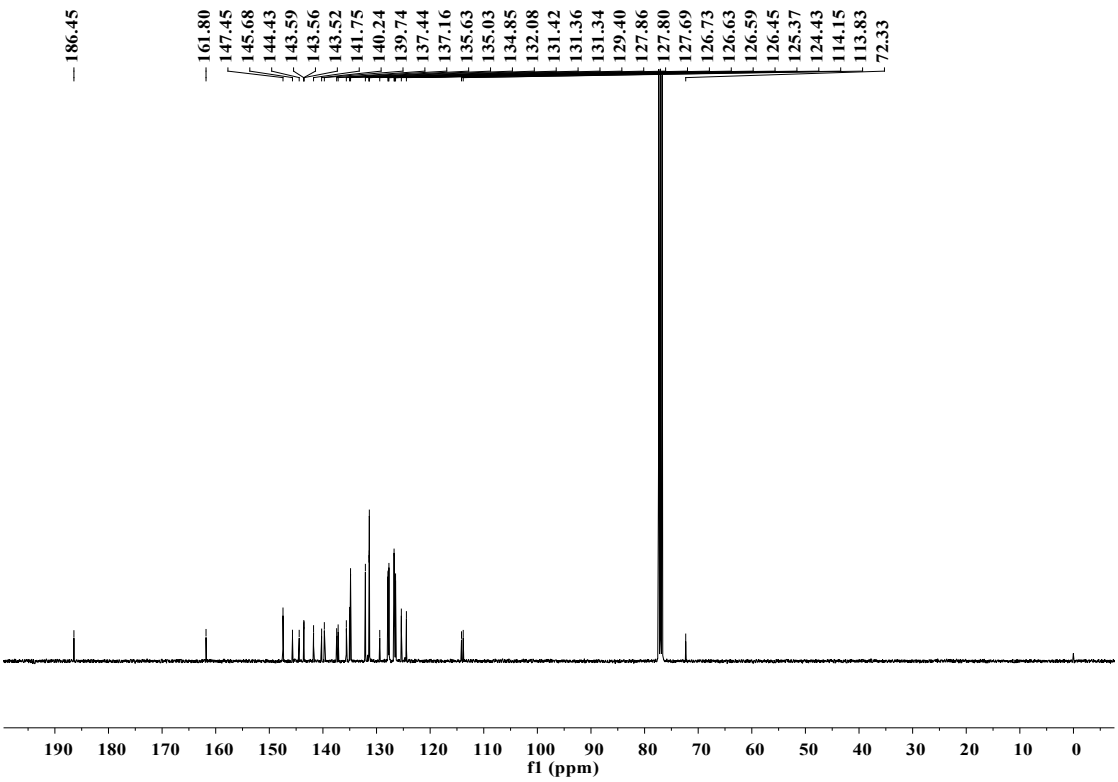


Figure S5. ^{13}C NMR spectrum (in $CDCl_3$) of **TPEPhIC**.

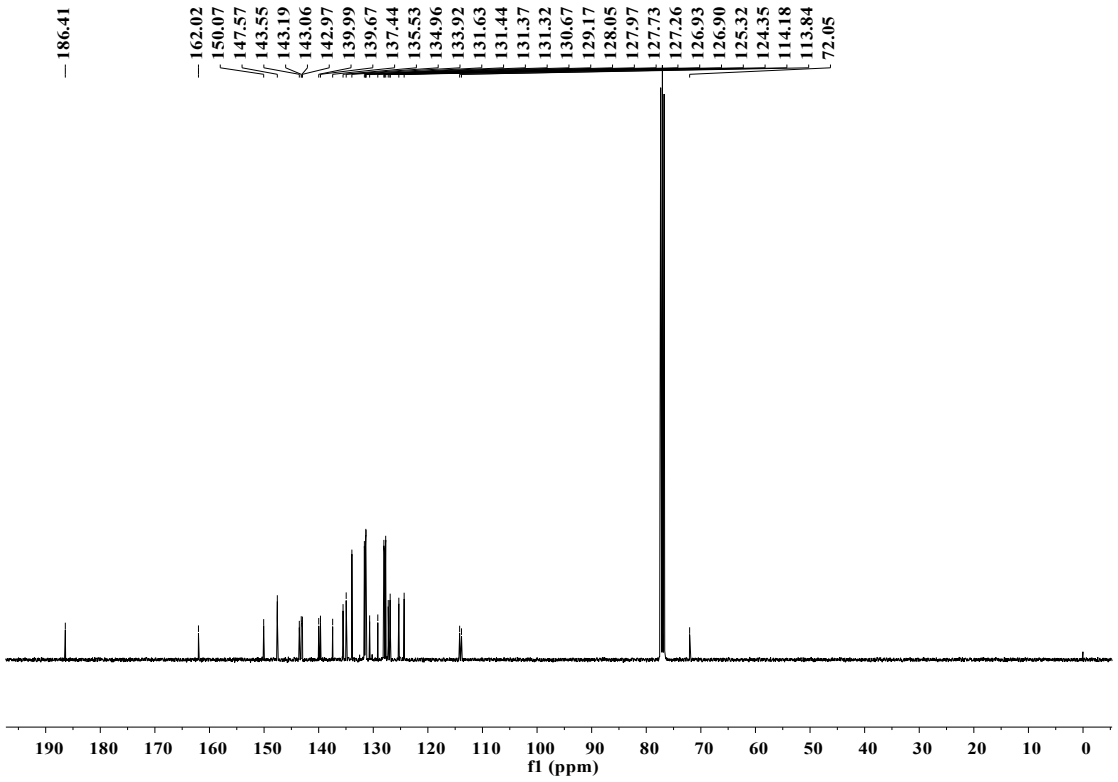
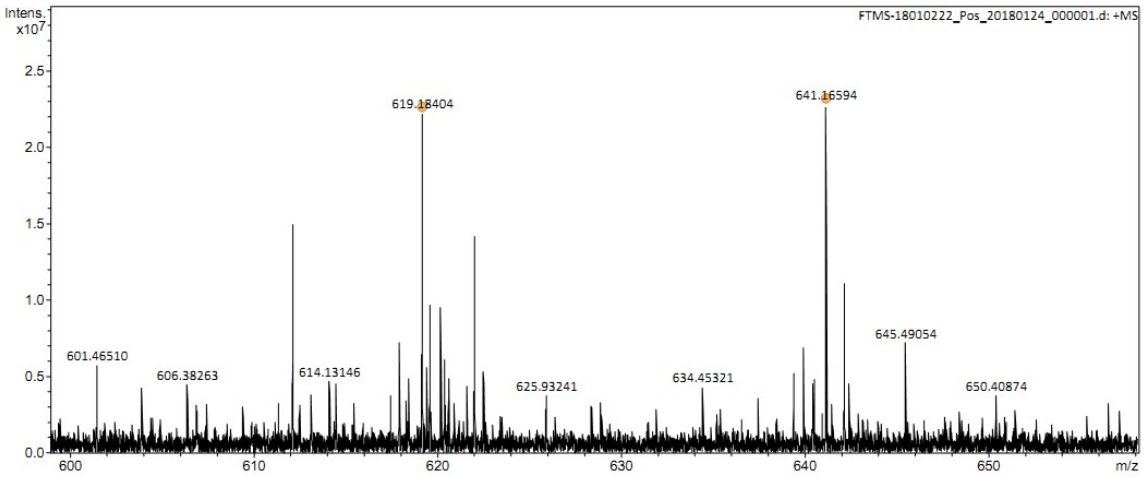
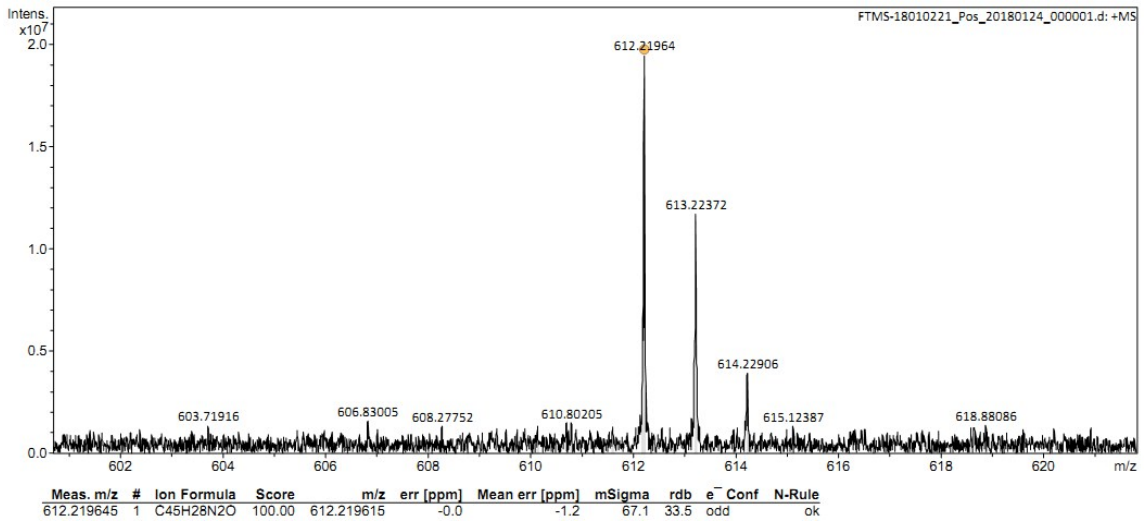


Figure S6. ^{13}C NMR spectrum (in $CDCl_3$) of **TPEIC**.



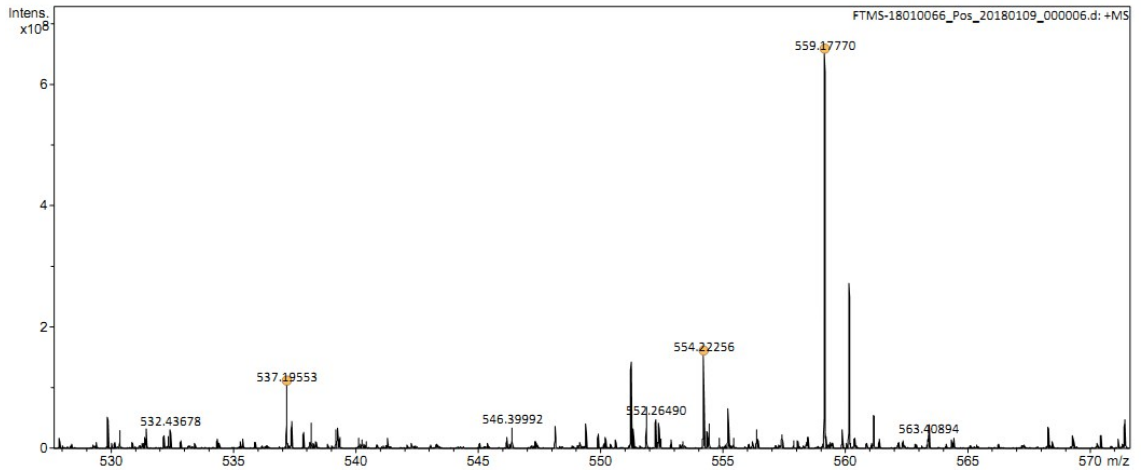
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
619.184042	1	C43H27N2OS	100.00	619.183861	-0.3	-0.3	77.7	32.0	even	ok
641.165941	1	C43H26N2NaOS	100.00	641.165805	-0.2	-0.9	35.3	32.0	even	ok

Figure S7. Mass spectrum of **TPEThIC**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
612.219645	1	C45H28N2O	100.00	612.219615	-0.0	-1.2	67.1	33.5	odd	ok

Figure S8. Mass spectrum of **TPEPhIC**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
537.195532	1	C39H25N2O	100.00	537.196140	1.1	-4.5	107.0	29.0	even	ok
554.222562	1	C39H28N3O	100.00	554.222689	0.2	-3.7	10.2	28.0	even	ok
559.177701	1	C39H24N2NaO	100.00	559.178084	0.7	-6.1	7.4	29.0	even	ok

Figure S9. Mass spectrum of **TPEIC**.

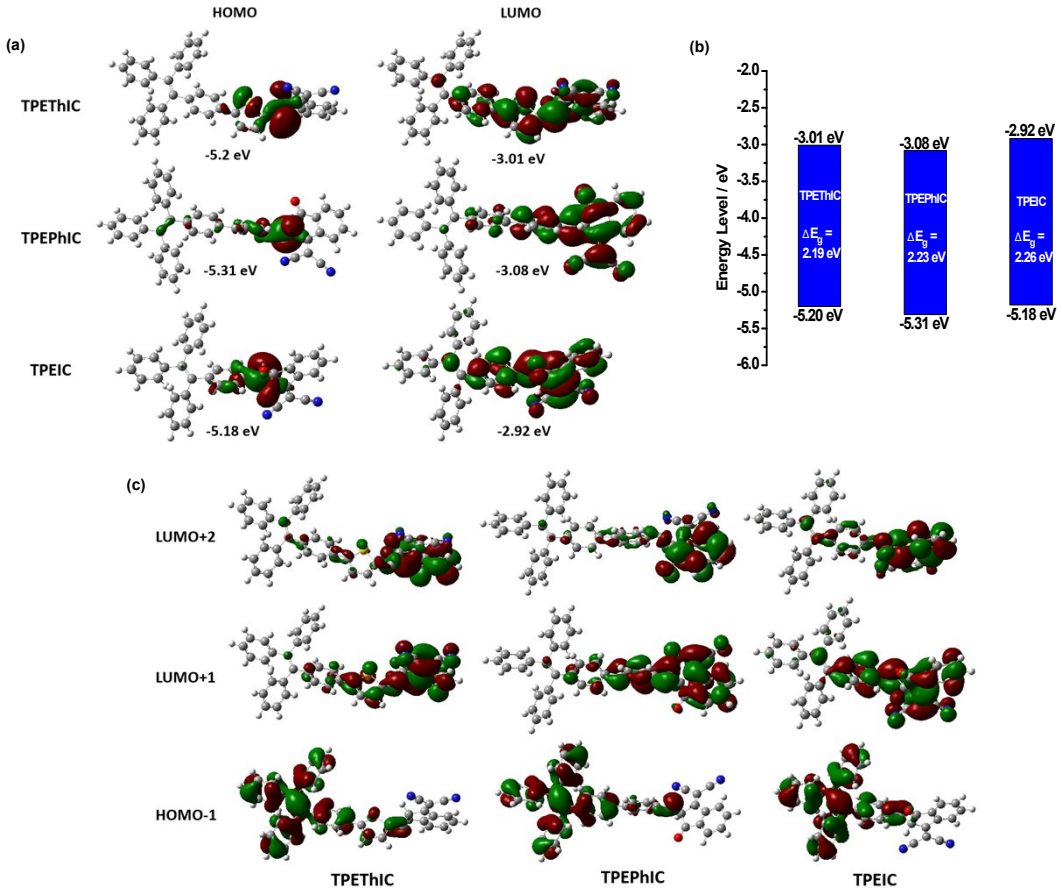


Figure S10. (a) Molecular orbital HOMO and LUMO diagram, (b) Energy level diagram of **TPEThIC**, **TPEPhIC** and **TPEIC** and (c) HOMO-1 and LUMO+1/2 molecular orbitals distributions by theoretical calculations.

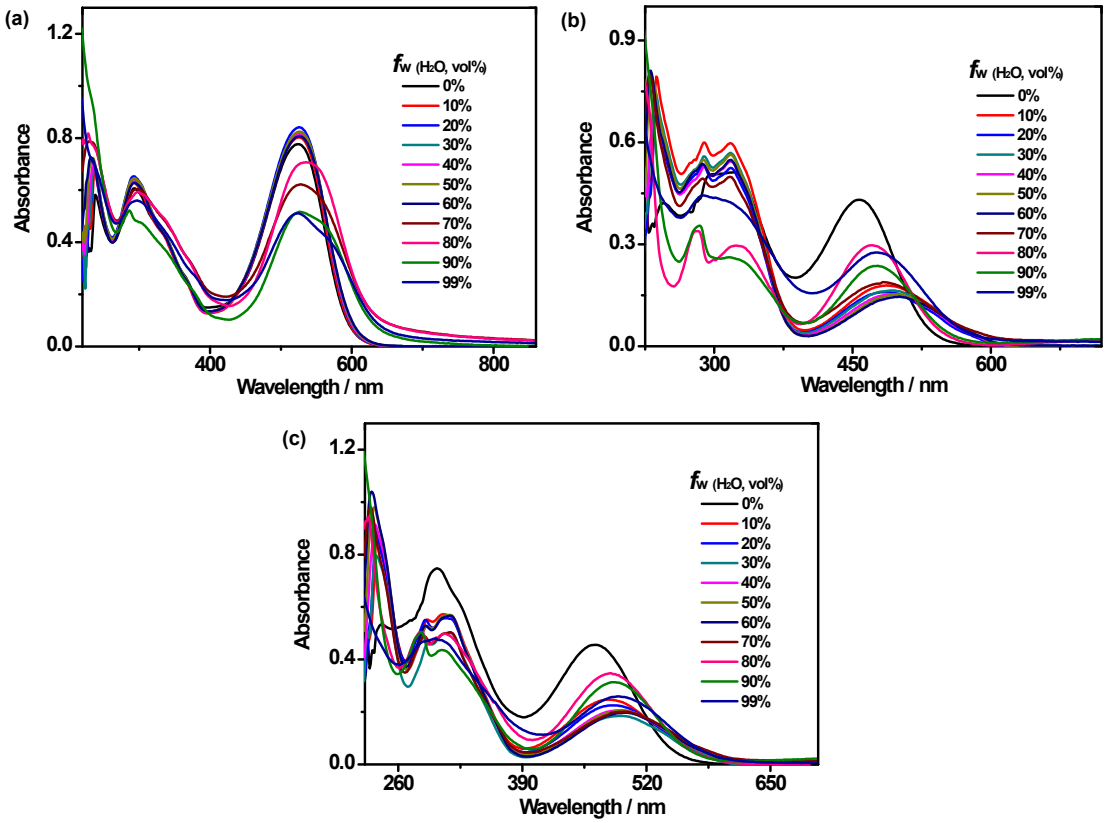


Figure S11. Absorption spectra of (a) **TPEThIC**, (b) **TPEPhIC** and (c) **TPEIC** in THF-water mixtures with various water contents (0-99%) at 296 K.

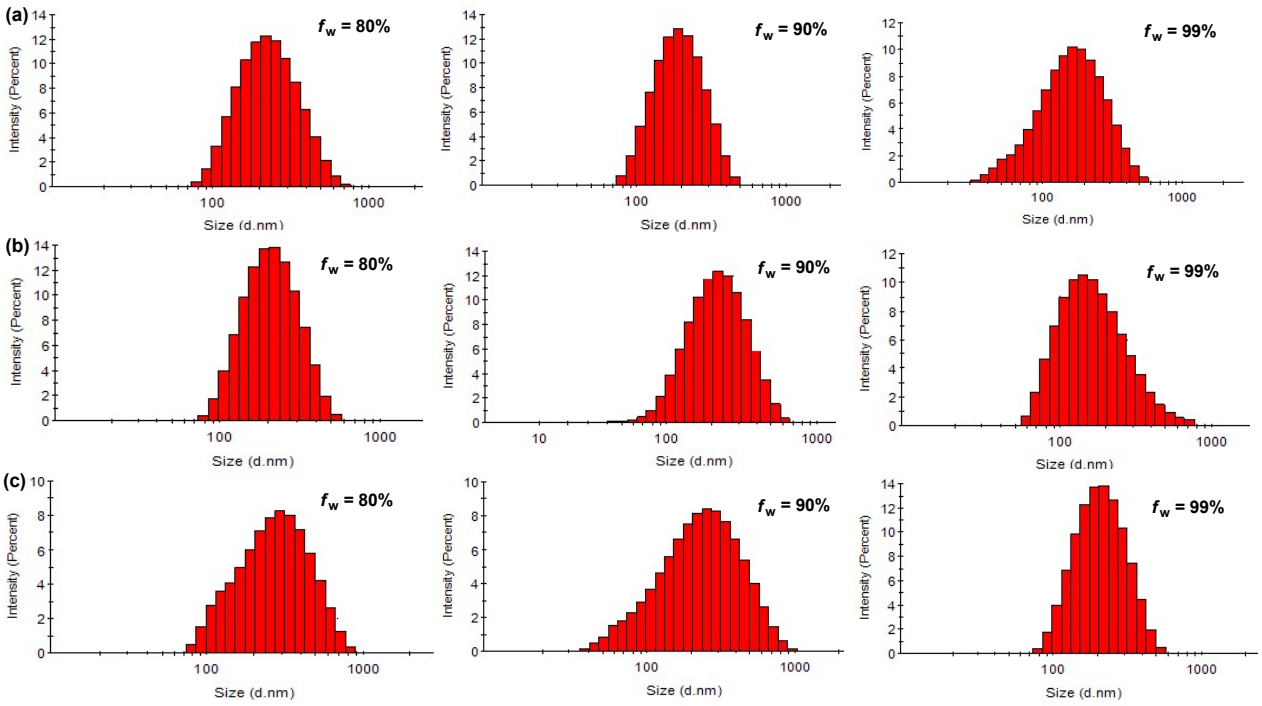


Figure S12. Particle size distributions of (a) **TPEThIC**, (b) **TPEPhIC** and (c) **TPEIC** in THF/water mixtures with water fractions of 80%, 90% and 99% by dynamic light scattering measurements.

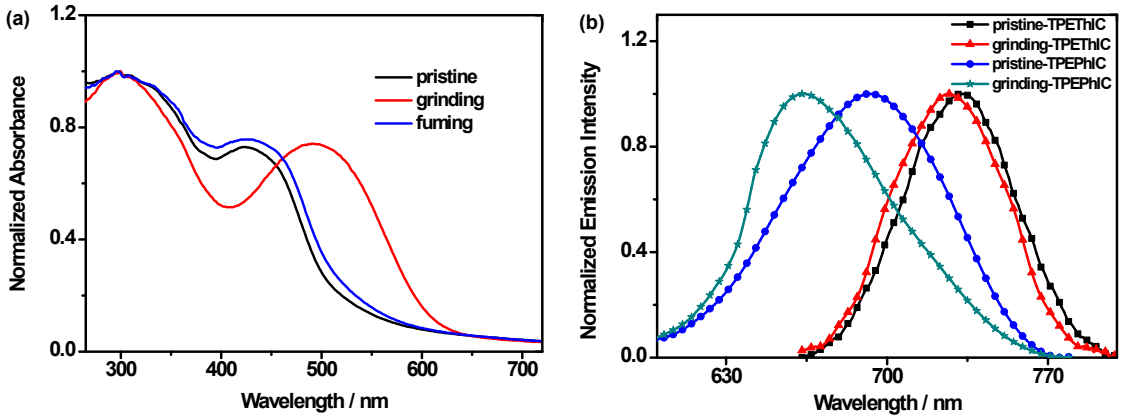


Figure S13. (a) Normalized UV-vis absorption spectra of **TPEIC** under pristine, grinding and fuming conditions and (b) Normalized fluorescence spectra of **TPEThIC** and **TPEPhIC** in the pristine and grinding states.

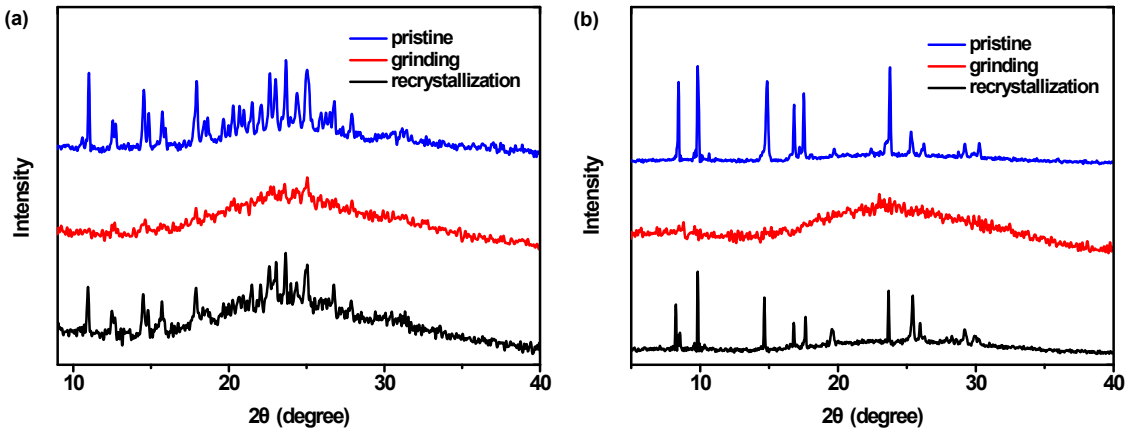


Figure S14. PXRD diffraction patterns of (a) **TPEThIC** and (b) **TPEPhIC** under the pristine, grinding conditions.

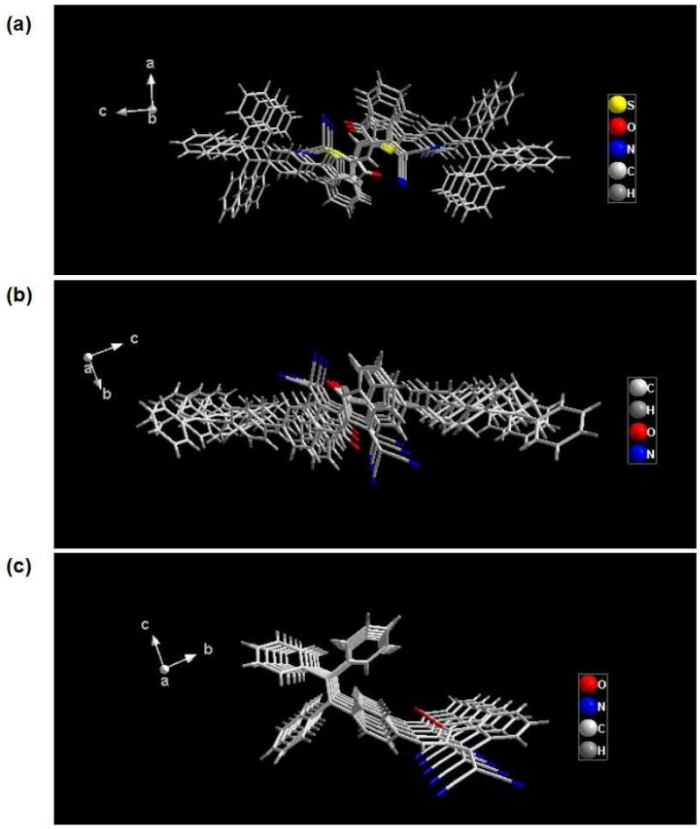


Figure S15. Single-crystal packing structures of (a) **TPEThIC**, (b) **TPEPhIC** and (c) **TPEIC**.

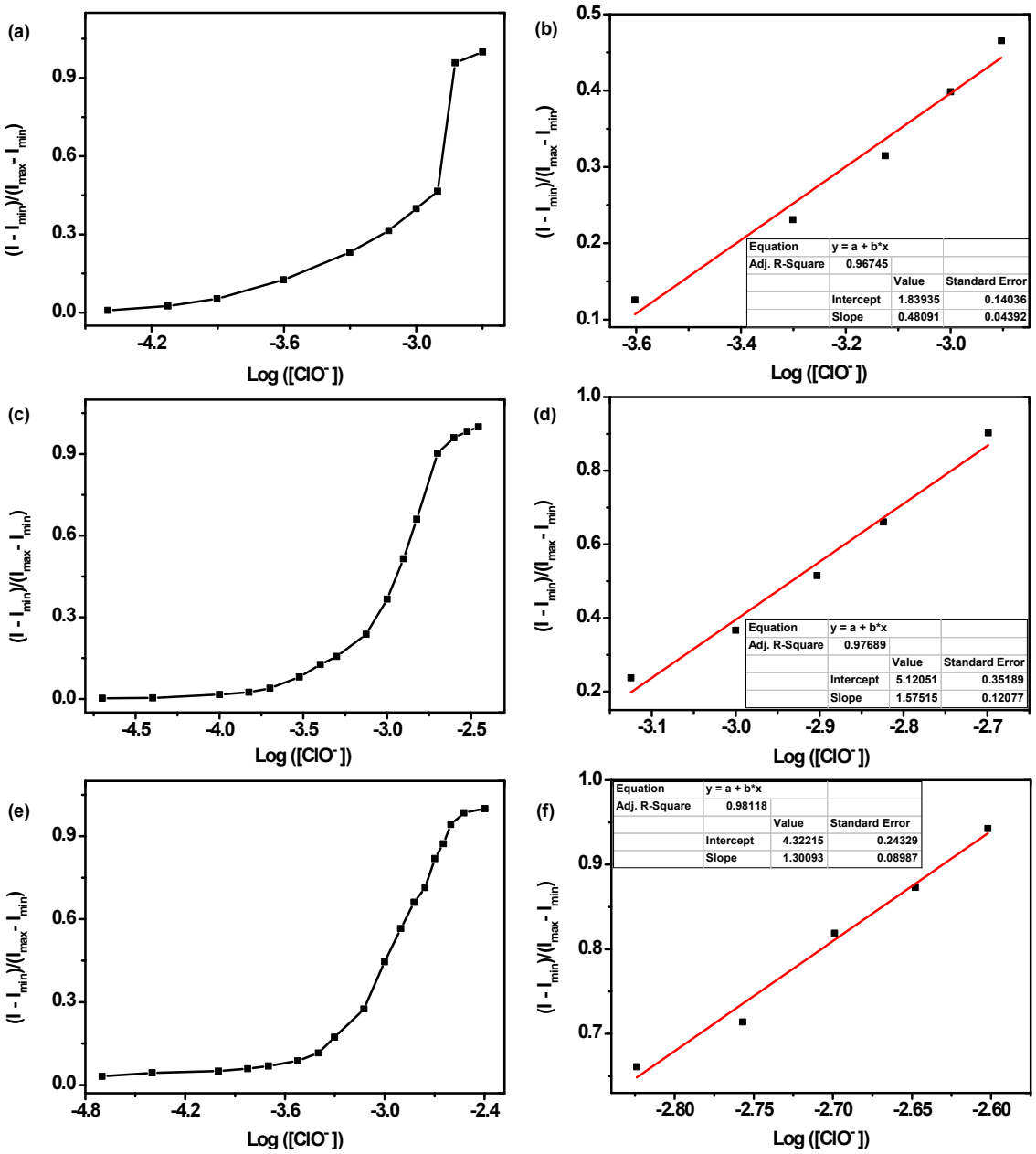


Figure S16. Linear fit plots of $(I - I_{min})/(I_{max} - I_{min})$ versus log [ClO^-] for (a,b) **TPEThIC**, (c,d) **TPEPhIC** and (e,f) **TPEIC**.

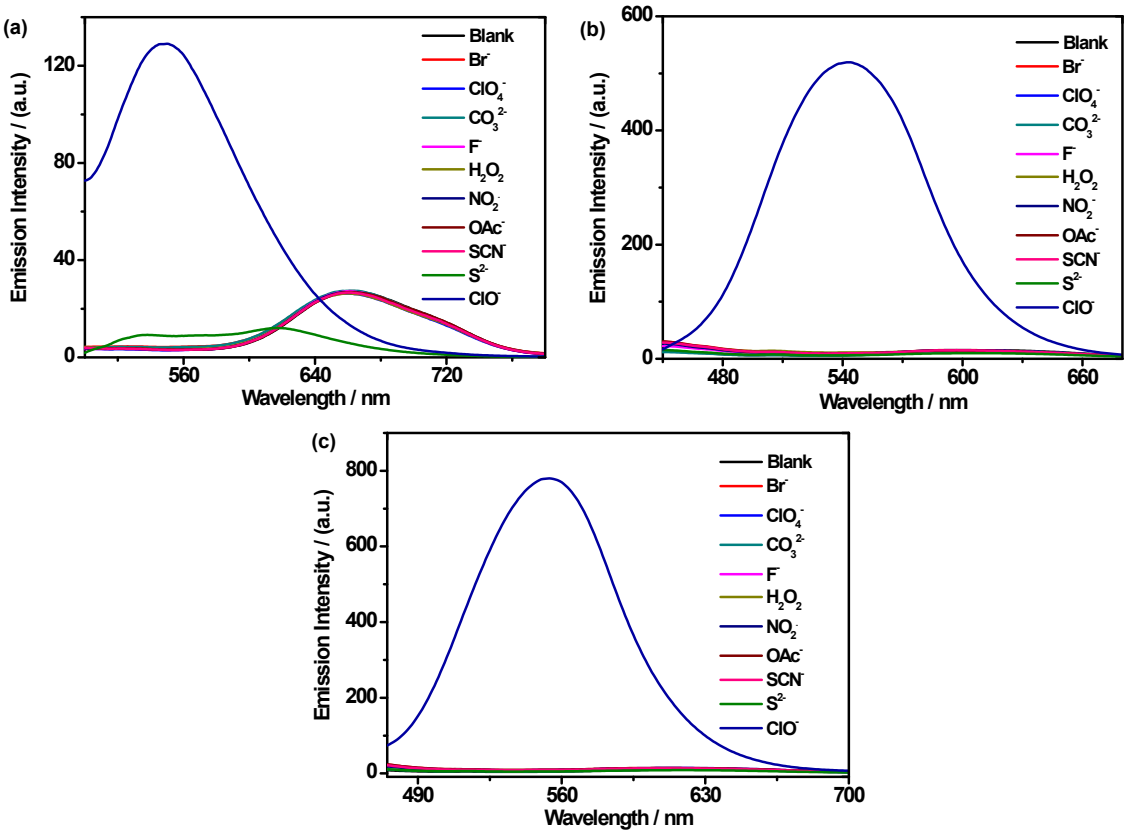


Figure S17. Fluorescence spectra of compound (a) **TPEThIC**, (b) **TPEPhIC**, (c) **TPEIC** in THF-H_2O solution at the presence of different analytes

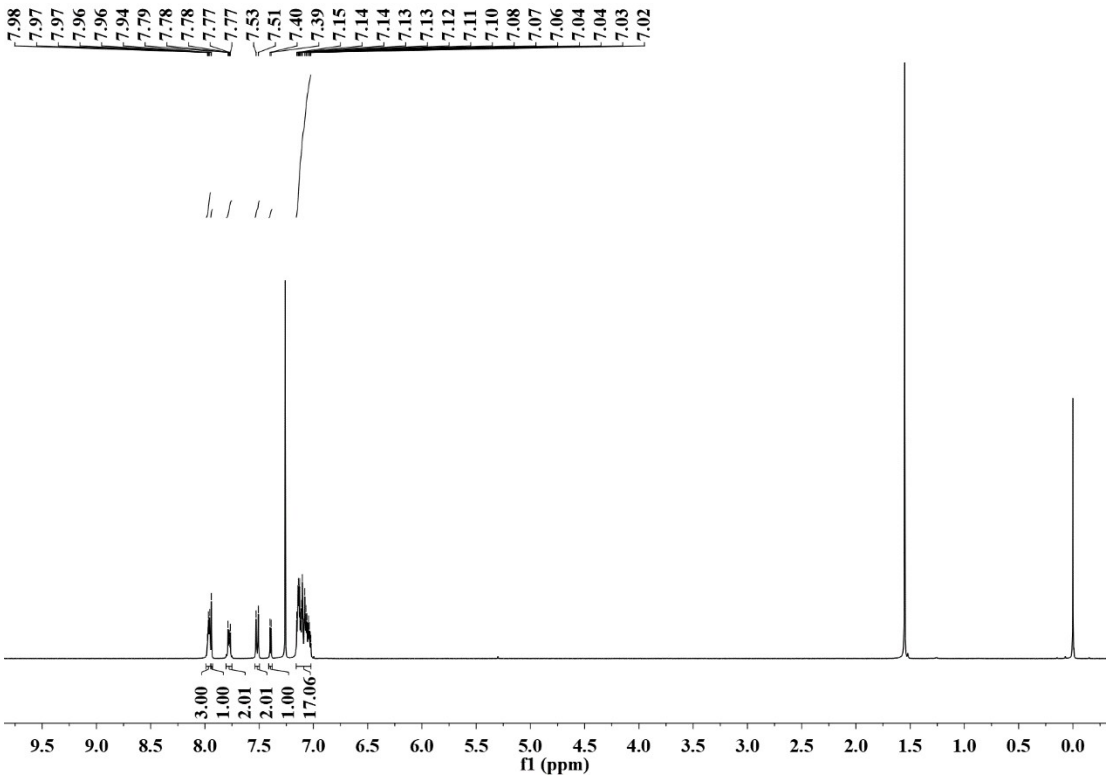


Figure S18. ^1H NMR spectrum (in $CDCl_3$) of **TPEThIC-ClO$^-$**.

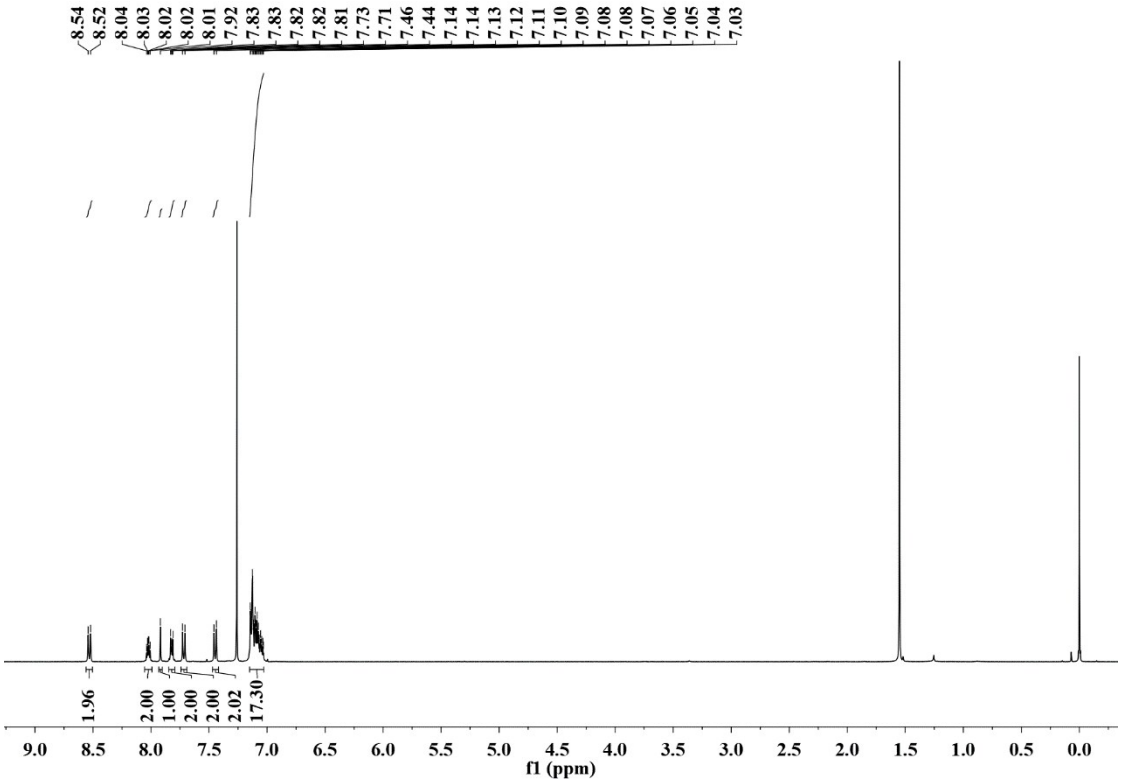


Figure S19. ^{1}H NMR spectrum (in $CDCl_3$) of **TPEPhIC-ClO^{-}**.

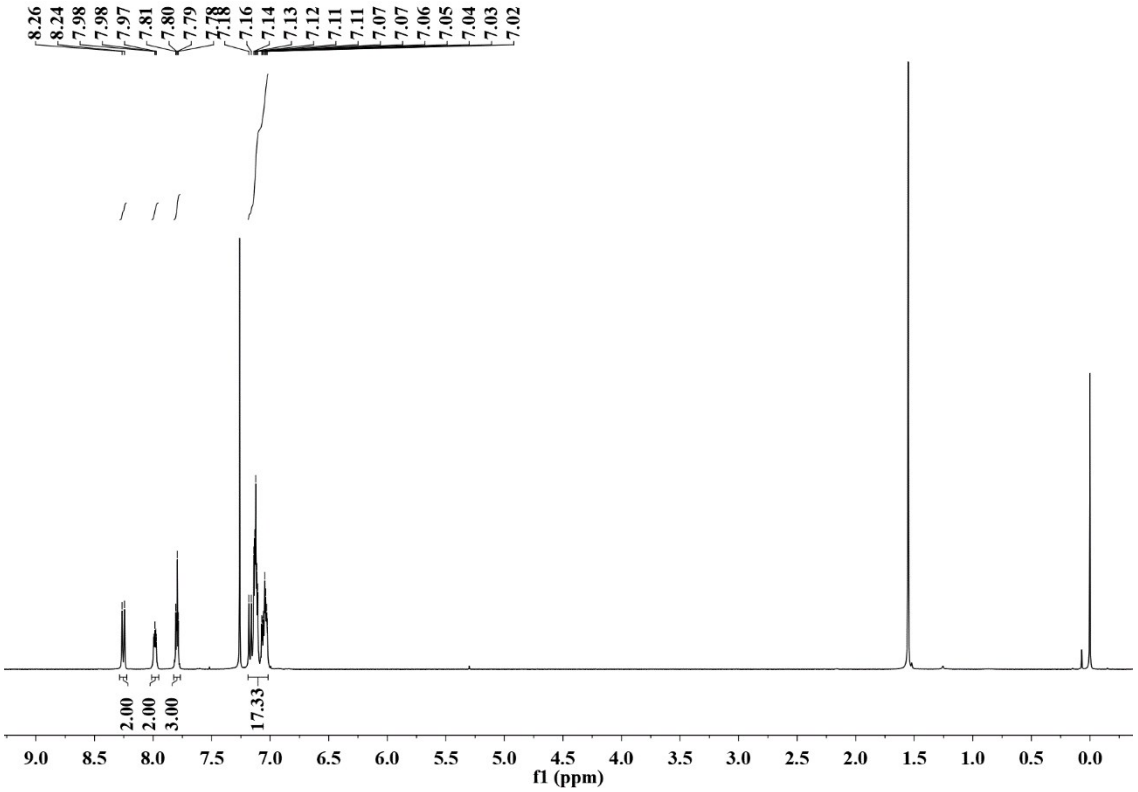


Figure S20. ^{1}H NMR spectrum (in $CDCl_3$) of **TPEIC-ClO^{-}**.

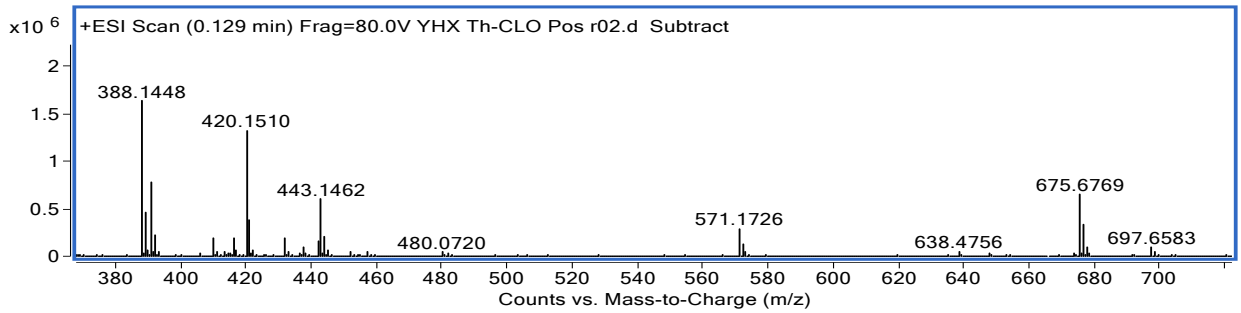


Figure S21. Mass spectrum of **TPEThIC**-ClO^-.

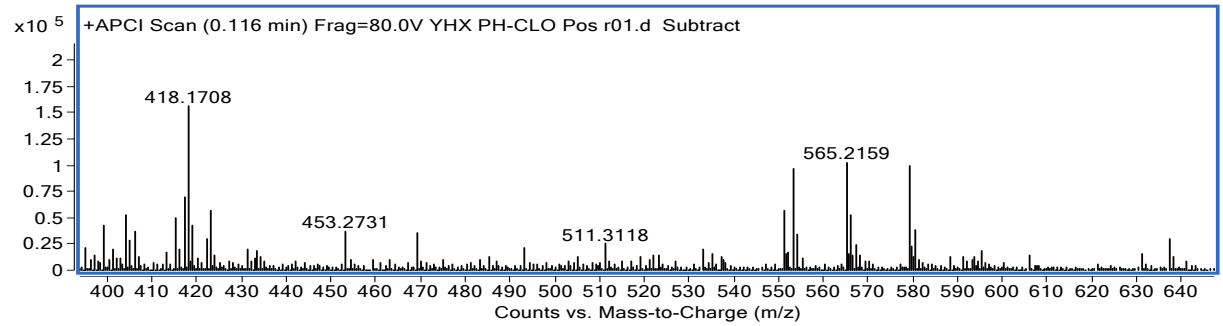


Figure S22. Mass spectrum of **TPEPhIC**-ClO^-.

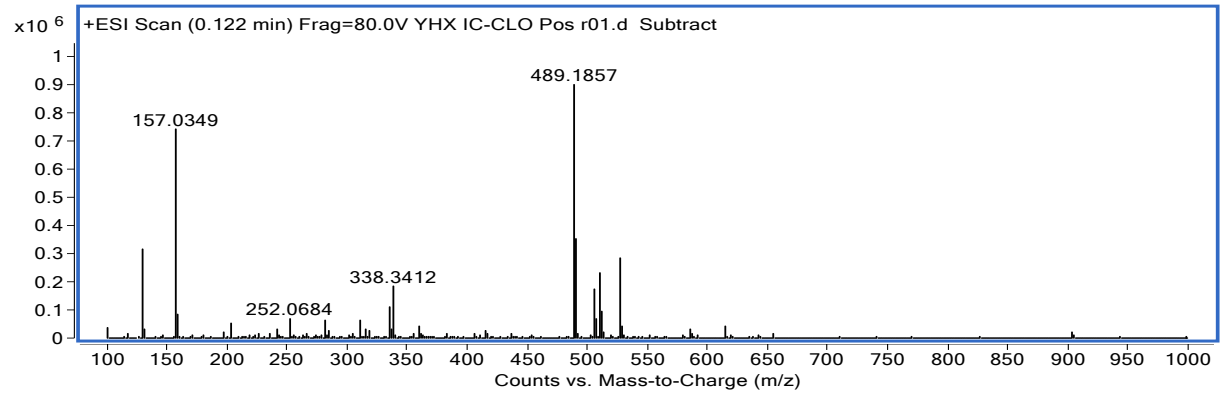


Figure S23. Mass spectrum of **TPEIC**-ClO^-.

Table S1. List of X-ray crystallographic data for **TPEThIC**, **TPEPhIC** and **TPEIC** (CCDC 1888023, 1888024 and 1888025).

Compound		**TPEThIC**	**TPEPhIC**	**TPEIC**
Temperature		150 K	296 K	150 K
Bond precision		C-C = 0.0035 Å	C-C = 0.0056 Å	C-C = 0.0059 Å
		Wavelength = 1.54178 Å	Wavelength = 0.71073 Å	Wavelength = 1.54178 Å
Cell	a (Å)	12.1544(4)	10.4273(10)	5.87(2)
	b (Å)	8.7132(3)	10.629(1)	10.236(18)
	c (Å)	33.3446(11)	15.8336(15)	25.27(5)
	α (°)	90	90.857(3)	84.03(9)
	β (°)	92.610(2)	94.538(3)	89.02(15)

γ (°)	90	100.500(3)	73.63(17)
Volume	3527.7(2)	1719.3(3)	1448(6)
Crystal system	monoclinic	triclinic	triclinic
Space group	P 21/n	P -1	P -1
Hall group	-P 2yn	-P 1	-P 1
Formula	$C_{43}H_{26}N_2OS$	$C_{45}H_{28}N_2O$	$C_{39}H_{24}N_2O$
Molecular Weight	618.74	612.69	536.60
Dx, g cm^{-3}	1.325	1.184	1.231
Z	4	2	2
μ (mm^{-1})	2.503	0.071	0.576
F000	1456.0	640.0	560.0
h, k, lmax	14, 10, 39	12, 12, 18	6, 12, 29
Data completeness	0.995	0.991	0.885
Theta(max)	65.228	24.851	67.082
R(reflections)	0.0574(5228)	0.0871(4211)	0.3111(3397)
wR2(reflections)	0.1630(6011)	0.2807(5907)	0.6943(4562)
S	1.019	1.142	1.068
Npar	451	433	381