

Supporting Information

Fluorescent Electronic Tongue Based on Soluble Conjugated Polymeric Nanoparticles for the Discrimination of Heavy Metal Ions in Aqueous Solution

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Chemicals and Materials

p-Diethynylbenzene (Energy, 97%), 1,3,5-Triethynylbenzene (TCI, 98%), 1,3,5-Triiodobenzene (Aladdin, 98%), Tris(4-iodophenyl)amine (Energy, 98%), 2,2',7,7'-Tetrabromo-9,9'-spirobifluorene (Energy, 97%), 4,7-Dibromo-2,1,3-benzothiadiazole (Energy, 98%), 5,7-Dibromo-2,3-dihydro-thieno[3,4-b][1,4]dioxine (Energy, 98%), Tetrakis(4-bromophenyl)ethene (Shanghai D&B, ≥97%), diisopropylethylamine (DIPEA, Energy, 99.5%), N,N,N',N"-Pentamethyldiethylenetriamine (PMDETA, Energy, 98%), and N₃-PEG1000 (Hua Teng Pharma, 95+%) were all used without further purification. N,N-Dimethylformamide (DMF) and tetrahydrofuran (THF) were distilled with CaH₂ before use. Other chemicals were obtained from Energy Chemical (>98%, Shanghai, China).

Characterizations

UV-Vis-NIR Absorption Spectroscopy. Optical absorption spectra of dilute DMF solutions of SCPNs were recorded employing Evolution 201 UV spectrophotometer (Thermo Fisher, USA) at 25°C.

Fluorescence Spectroscopy. Fluorescence spectra of SCPN and PEGylated SCPN solutions were recorded using Fluorolog-3-P UV-Vis-NIR fluorescence spectrophotometer (Jobin Yvon, France). Both the entrance and exit slits were set at a width of 7 nm.

Nuclear Magnetic Resonance Spectroscopy. ¹H NMR (400 MHz) and ¹³C NMR (100 MHz) were obtained on a Bruker AVANCE FT NMR spectrometer in chloroform-d (CDCl₃) and tetrahydrofuran-d (d₈-THF) on an Ultra Shield 400 spectrometer (BRUKER BIOSPIN AG, Magnet System 400 MHz/54 mm).

Dynamic Light Scattering (DLS). The hydrodynamic diameters of the SCPNs and PEGylated SCPNs were analyzed using a ZetasizerNano ZS (Malvern, UK) at 25 °C with a 633 nm laser in DMF and water.

Infrared Spectroscopy (IR). Fourier transform infrared analysis (FTIR) of SCPNs and PEGylated SCPNs were recorded from KBr pallets on a Nicolet Magna 5700 FTIR spectrometer.

High-Resolution Transmission Electron Microscopy (HR-TEM). Images were obtained on a JEM-2100 microscope (JEOL, Japan) at an acceleration voltage of 200 kV. The Pd@SS-CNMs nanoreactor samples were prepared by drop-casting anhydrous ethanol dispersion on a carbon-coated 200 mesh copper grids.

Inductively Coupled Plasma Atomic Emission Spectroscopy. The palladium content of nanoreactors was measured using a Thermo Elemental IRIS 1000 instrument.

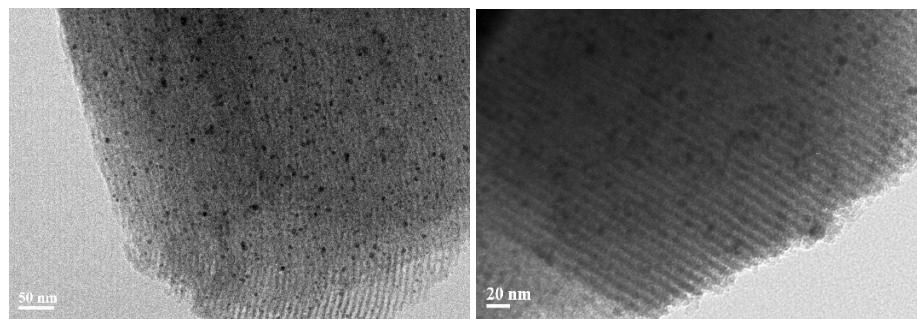


Figure S1. HR-TEM images of Pd@SS-CNMs nanoreactors.

Table S1. The structure information of the SCPNs.

| SCPN_(x) | 1 | 2 | 3 | 4 | 5 | 6 |
|---------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| $A_{(x)}+B_{(y)}$ | $A_{(1)}+B_{(2)}$ | $A_{(2)}+B_{(2)}$ | $A_{(3)}+B_{(2)}$ | $A_{(4)}+B_{(1)}$ | $A_{(5)}+B_{(1)}$ | $A_{(6)}+B_{(2)}$ |

Note: The SCPNs are prepared from the Sonogashira polycondensation between monomer $A_{(x)}$ and $B_{(y)}$ in confined nanoreactors. For the PEGylated SCPN sensors, the SCPNs are grafted with $N_3\text{-PEG}_{1000}$ via click reaction.

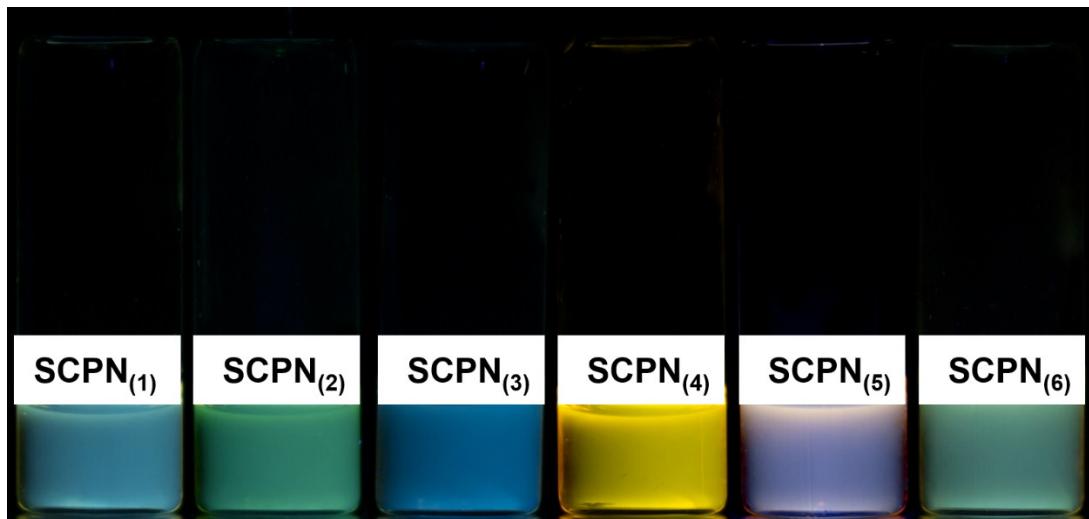


Figure S2. Fluorescent images of SCPNs in DMF solutions under the irradiation of UV light (365 nm, 1 mg/mL).

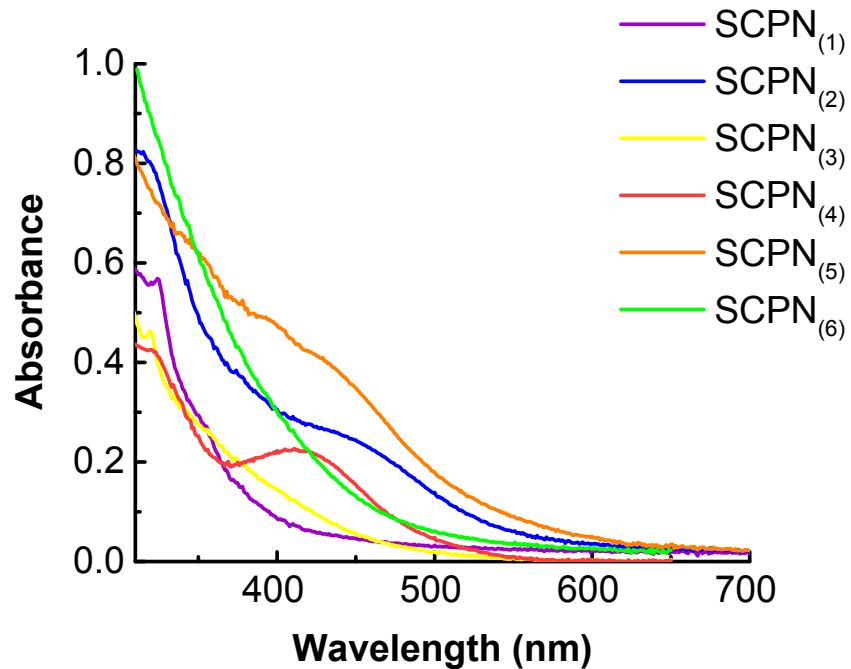


Figure S3. The UV-Vis absorption spectra of SCPNs in DMF solutions.

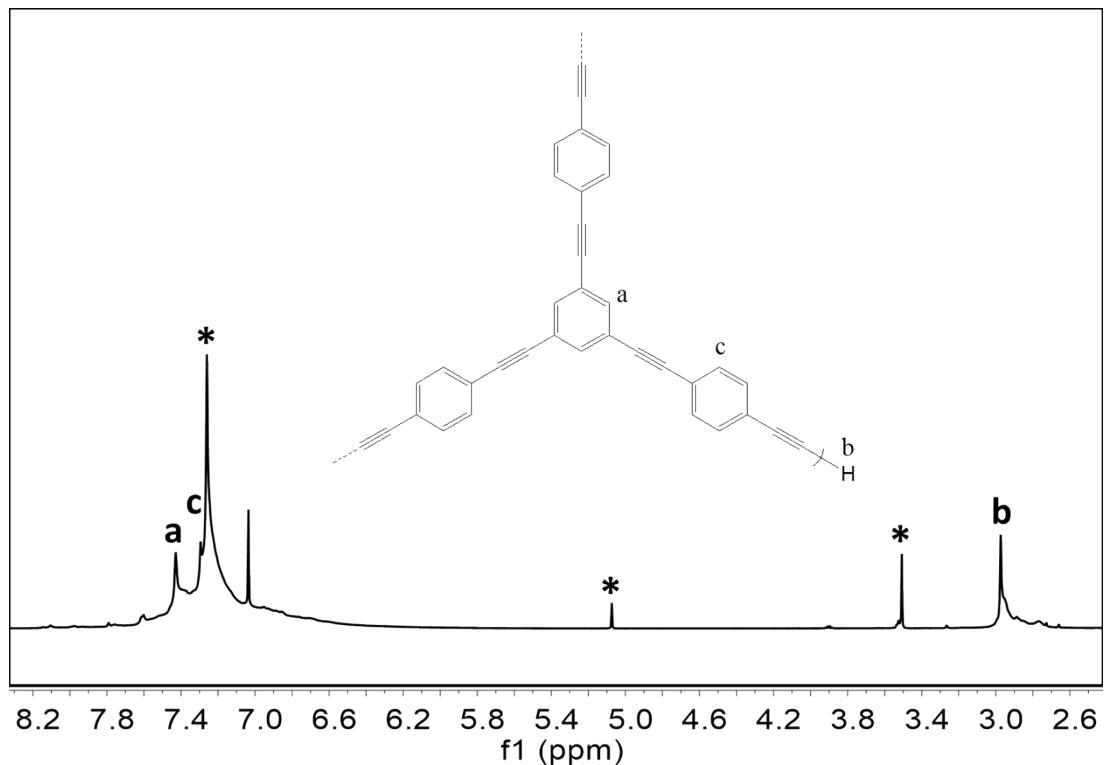


Figure S4. ¹H NMR spectrum of SCPN₍₁₎ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform, dichloromethane and methanol).

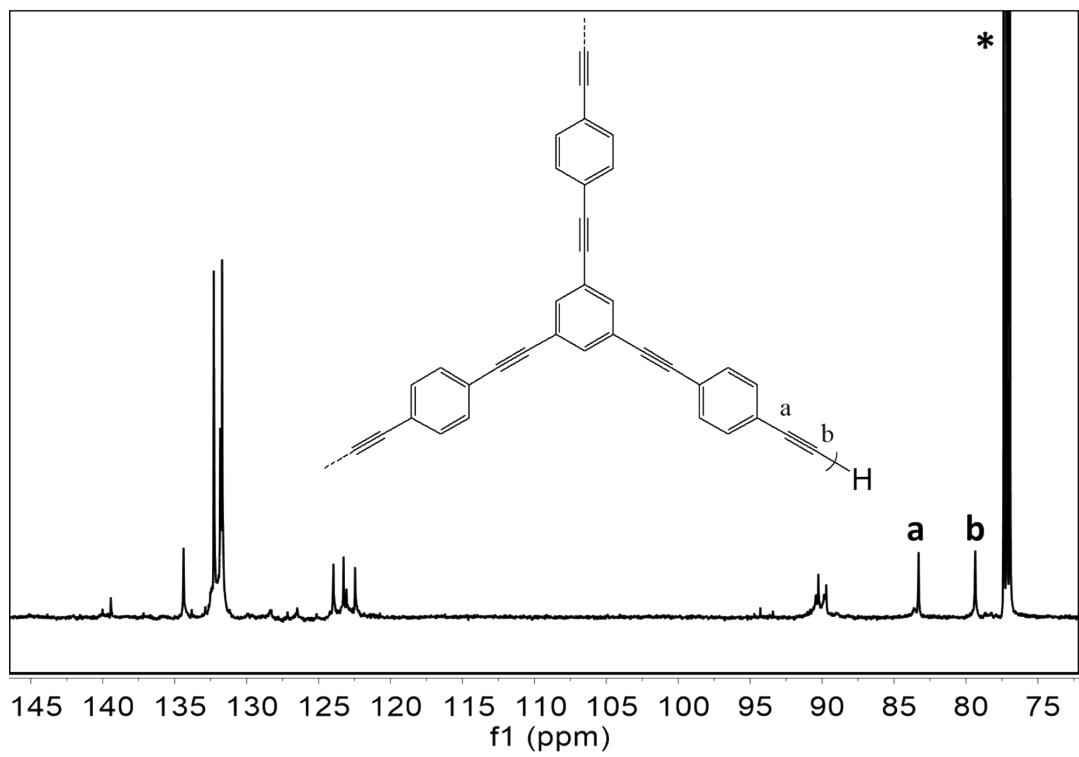


Figure S5. ^{13}C NMR spectrum of $\text{SCPN}_{(1)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform).

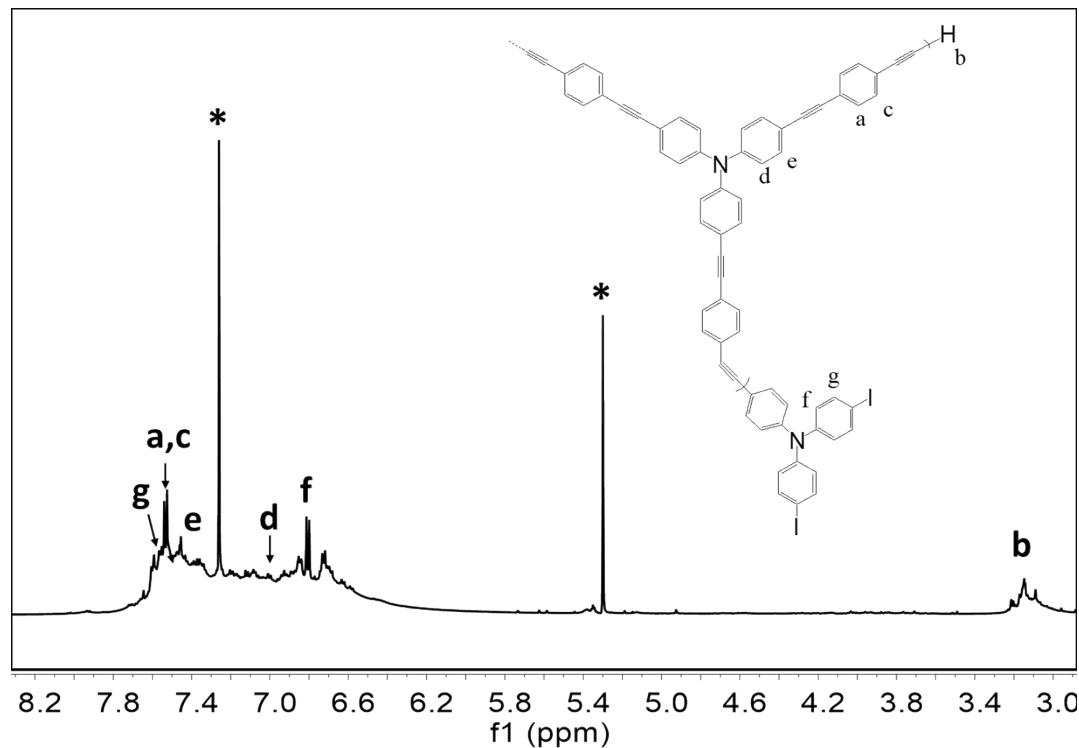


Figure S6. ^1H NMR spectrum of $\text{SCPN}_{(2)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform and dichloromethane).

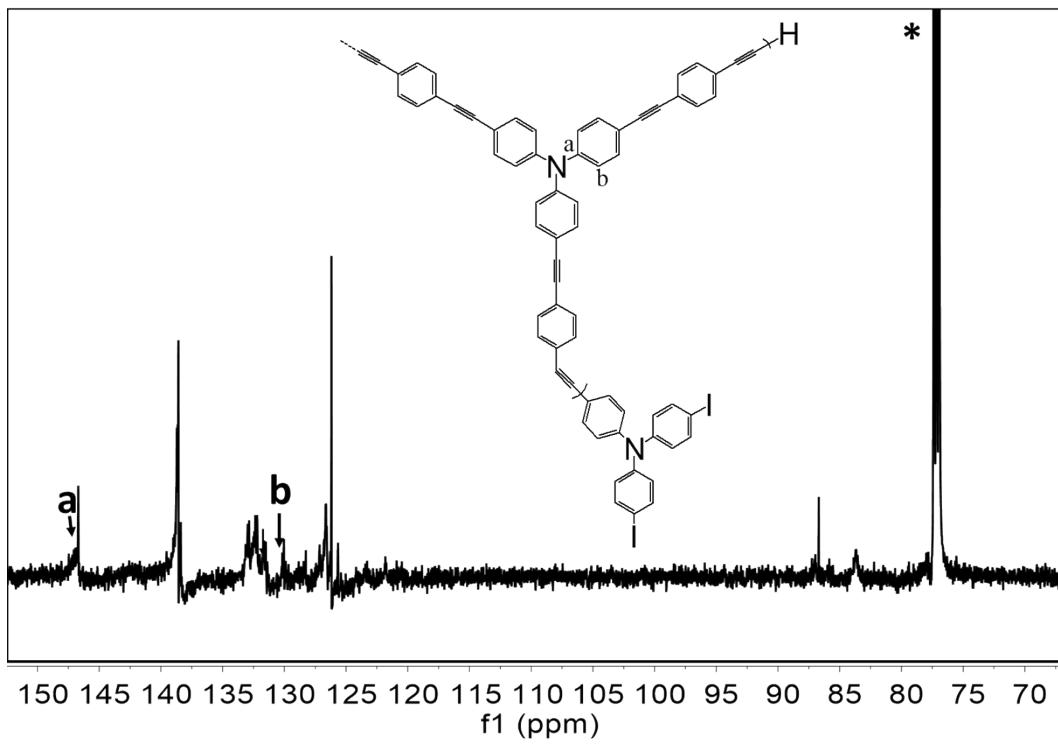


Figure S7. ^{13}C NMR spectrum of $\text{SCPN}_{(2)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform).

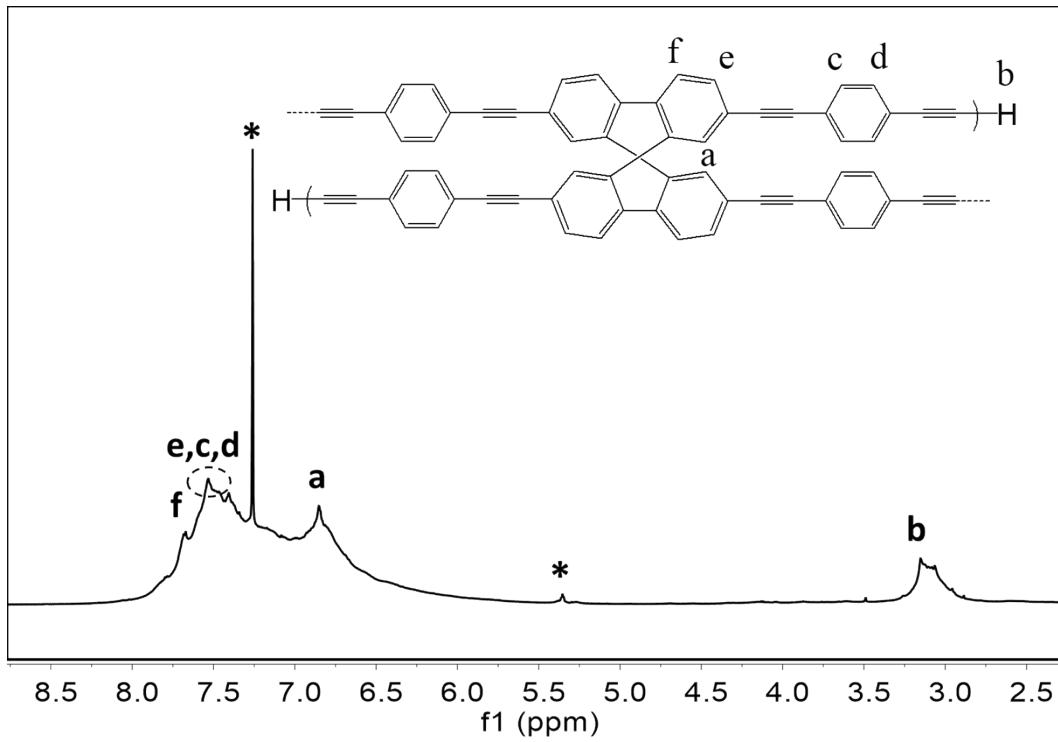


Figure S8. ^1H NMR spectrum of $\text{SCPN}_{(3)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform and dichloromethane).

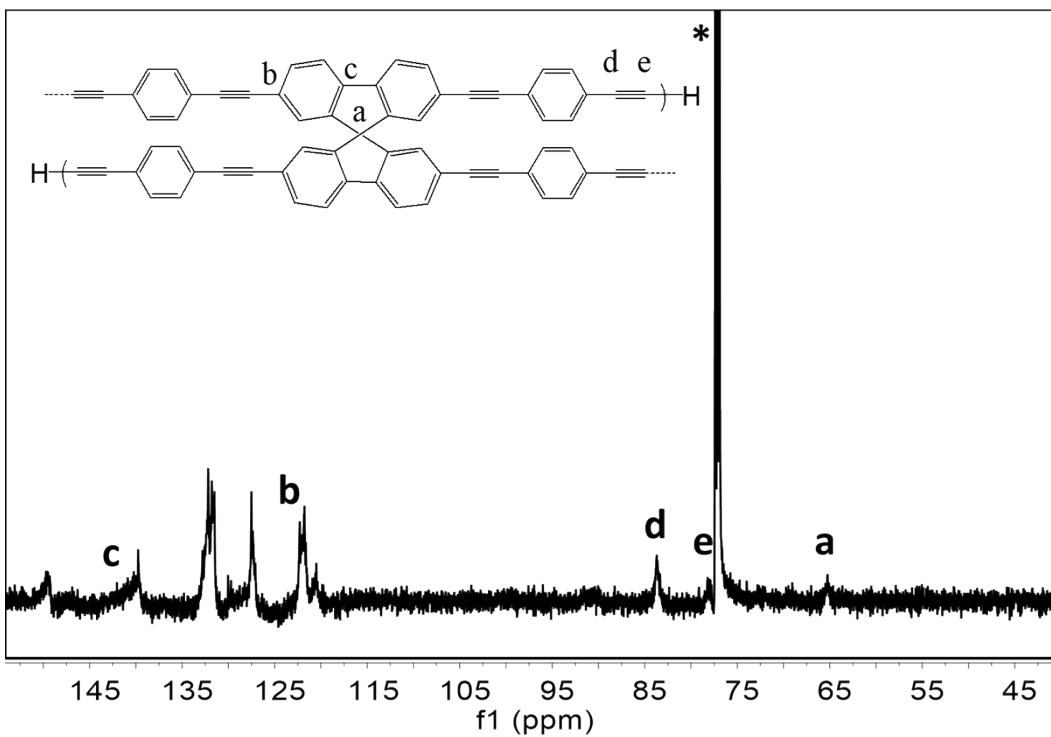


Figure S9. ^{13}C NMR spectrum of $\text{SCPN}_{(3)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform).

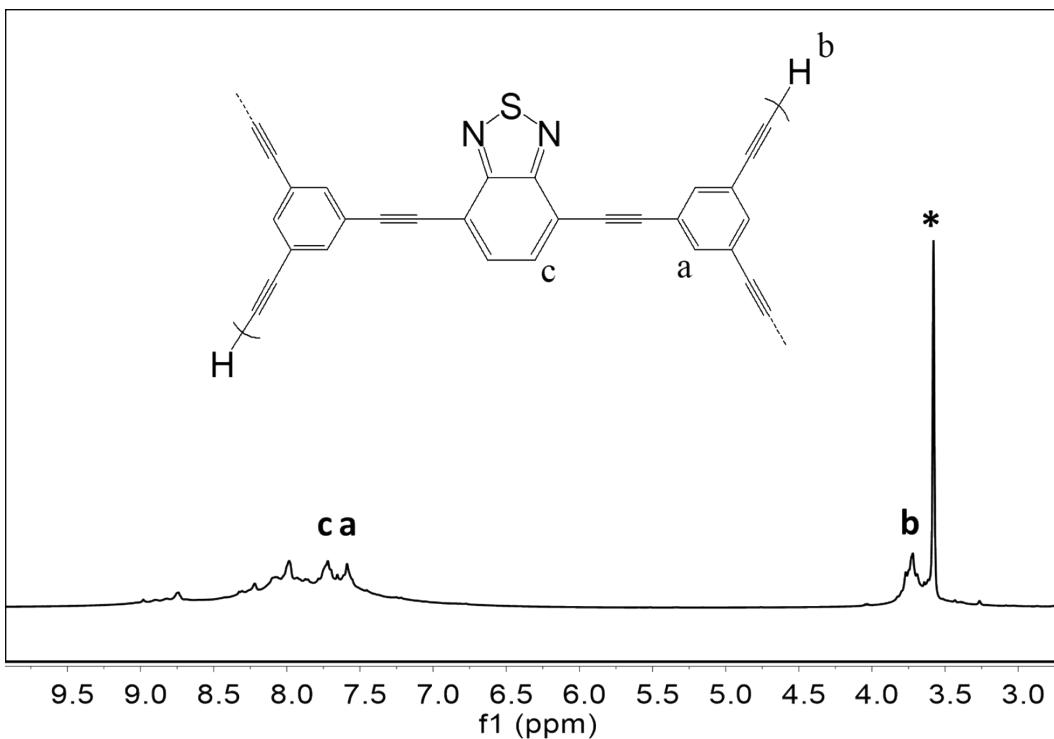


Figure S10. ^1H NMR spectrum of $\text{SCPN}_{(4)}$ in tetrahydrofuran-d₈. The asterisk (*) indicates the solvent residue(tetrahydrofuran).

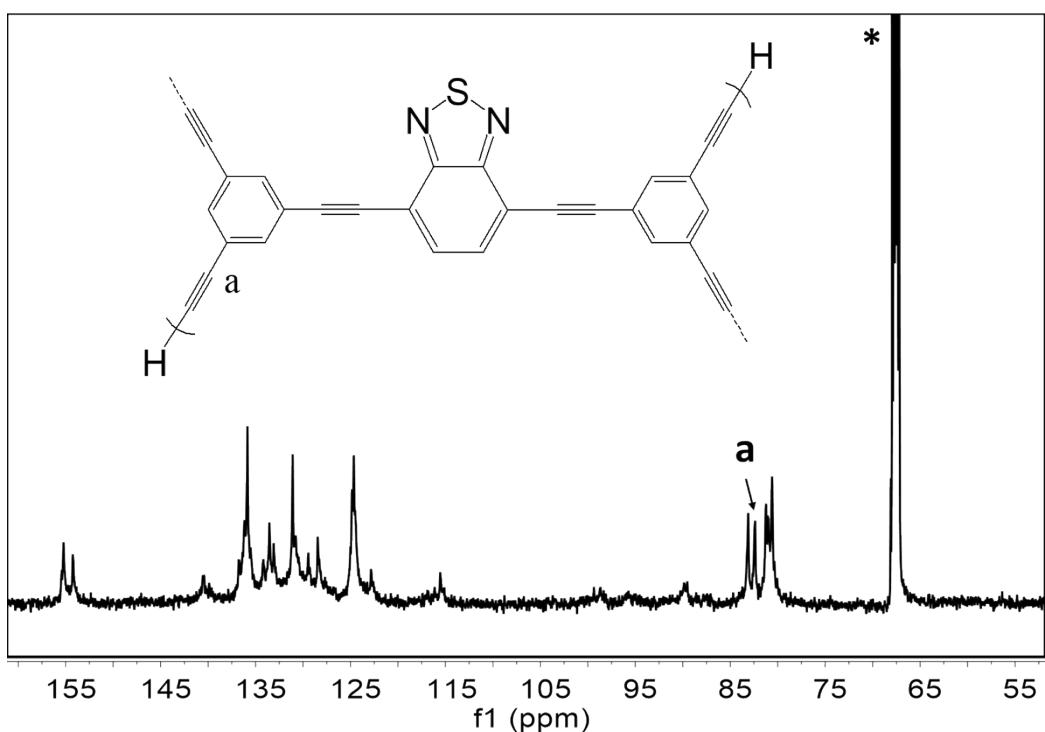


Figure S11. ^{13}C NMR spectrum of SCPN₍₄₎ in tetrahydrofuran-d₈. The asterisk (*) indicates the solvent residue(tetrahydrofuran).

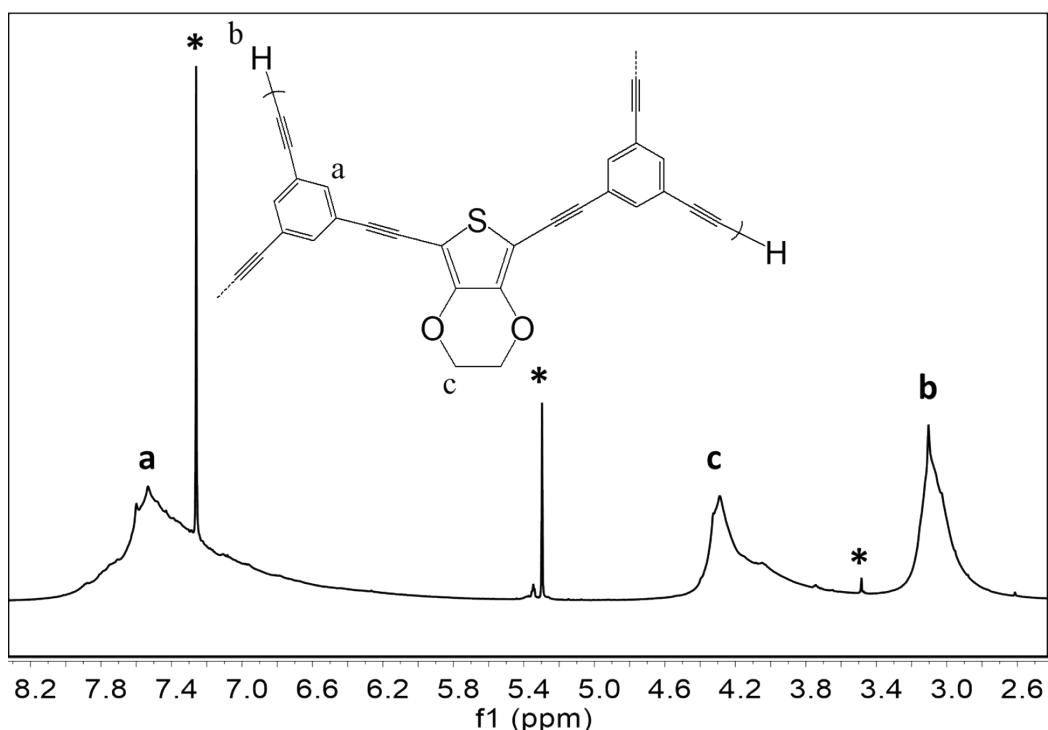


Figure S12. ^1H NMR spectrum of SCPN₍₅₎ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform).

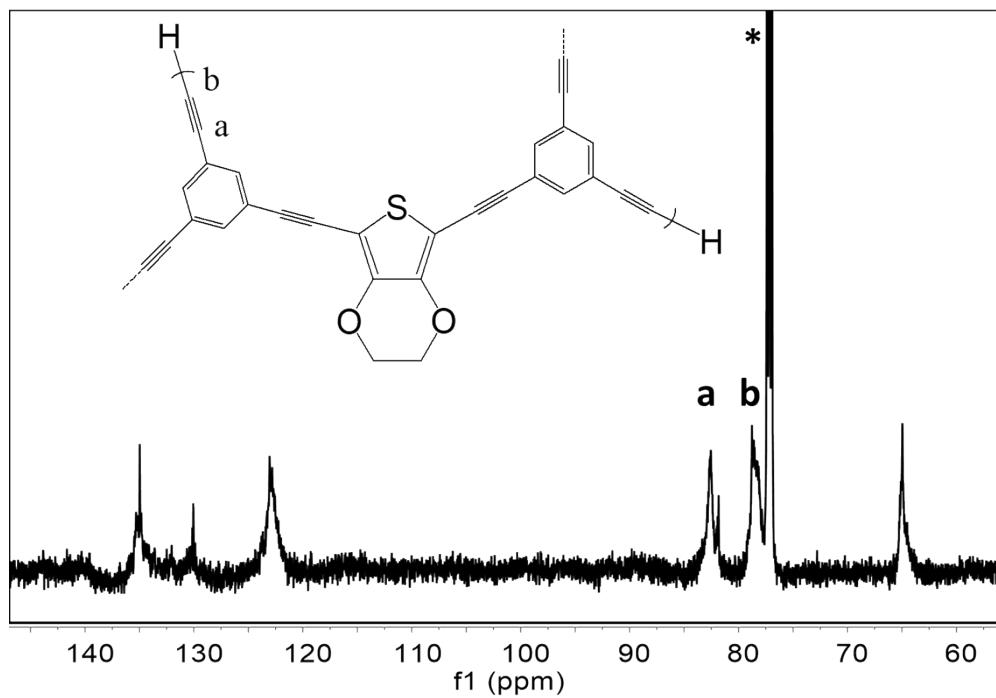


Figure S13. ^{13}C NMR spectrum of $\text{SCPN}_{(5)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform).

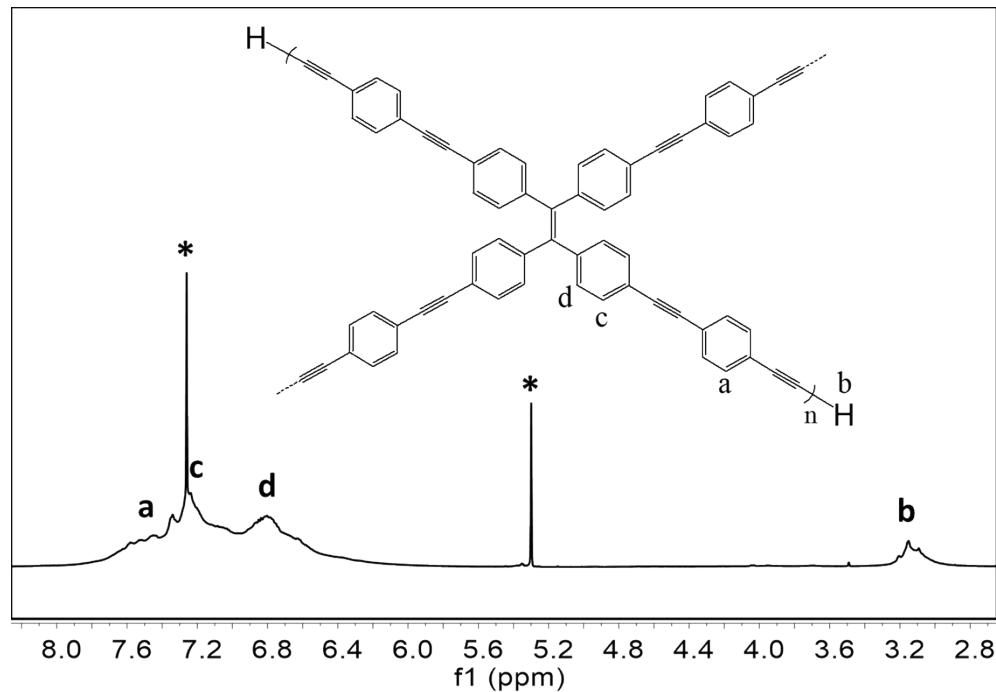


Figure S14. ^1H NMR spectrum of $\text{SCPN}_{(6)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform).

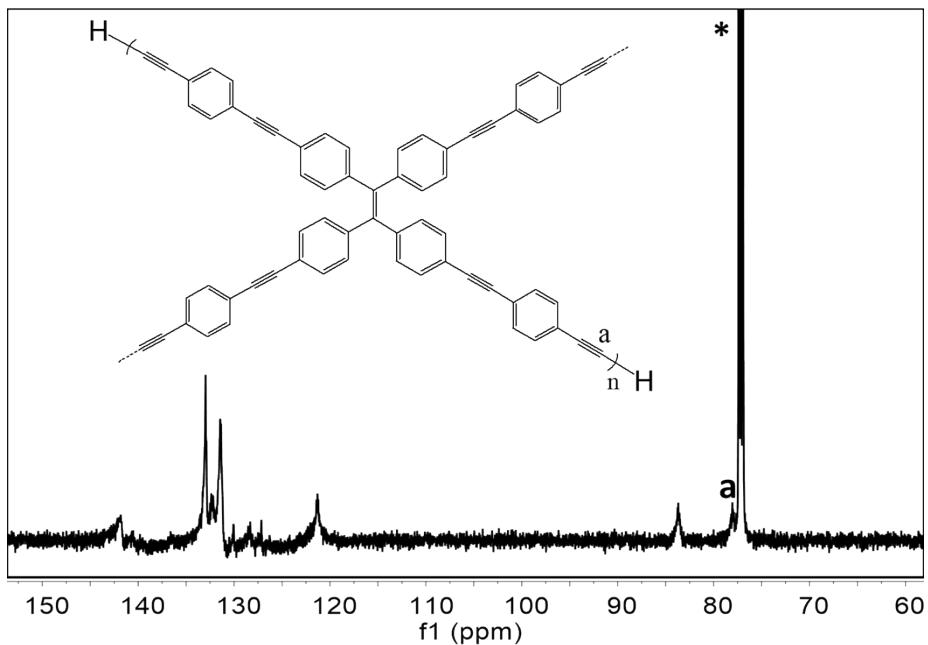


Figure S15. ^{13}C NMR spectrum of $\text{SCPN}_{(6)}$ in chloroform-d. The asterisk (*) indicates the solvent residue(chloroform).

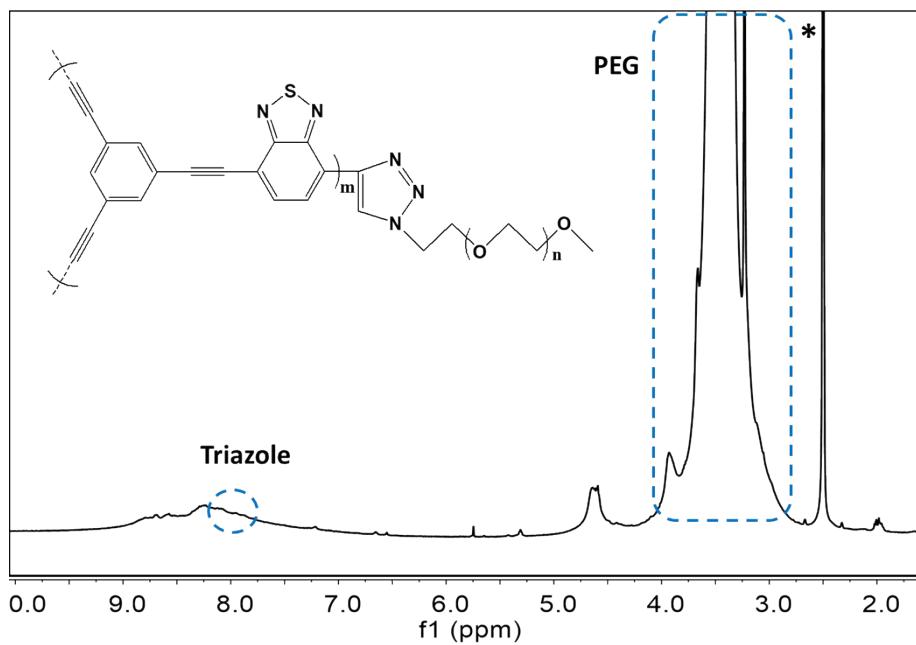


Figure S16. ^1H NMR spectrum of PEGylated $\text{SCPN}_{(4)}$ in dimethyl sulfoxide-d₆. The asterisk (*) indicates the solvent residue(dimethyl sulfoxide).

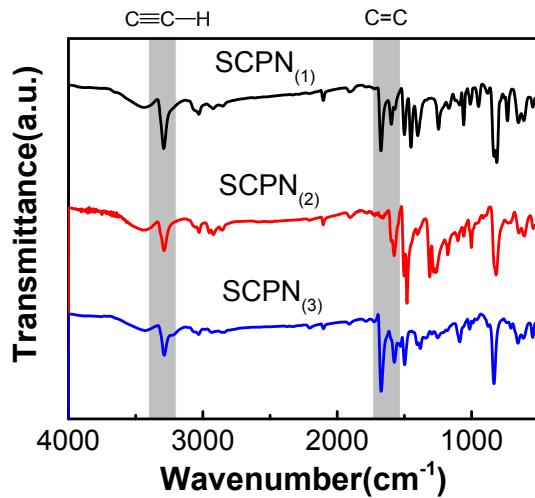


Figure S17. The FTIR spectrum of $\text{SCPN}_{(1)}$, $\text{SCPN}_{(2)}$ and $\text{SCPN}_{(3)}$.

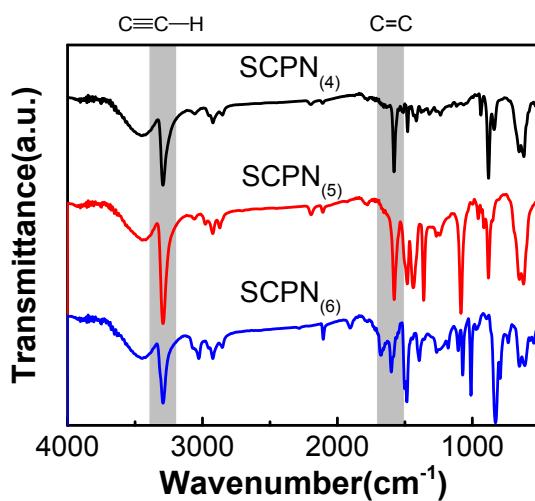


Figure S18. The FTIR spectrum of $\text{SCPN}_{(4)}$, $\text{SCPN}_{(5)}$ and $\text{SCPN}_{(6)}$.

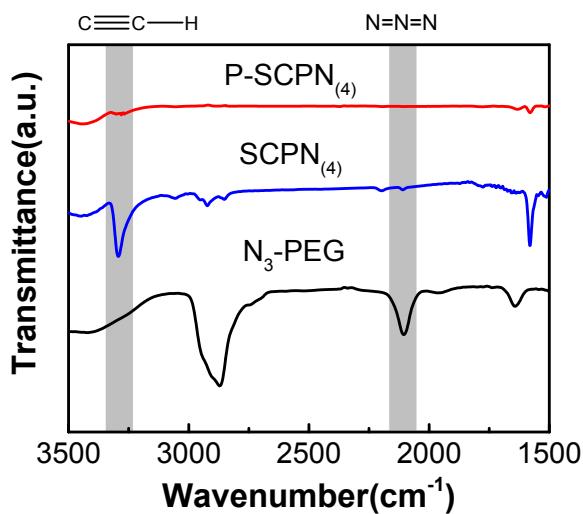
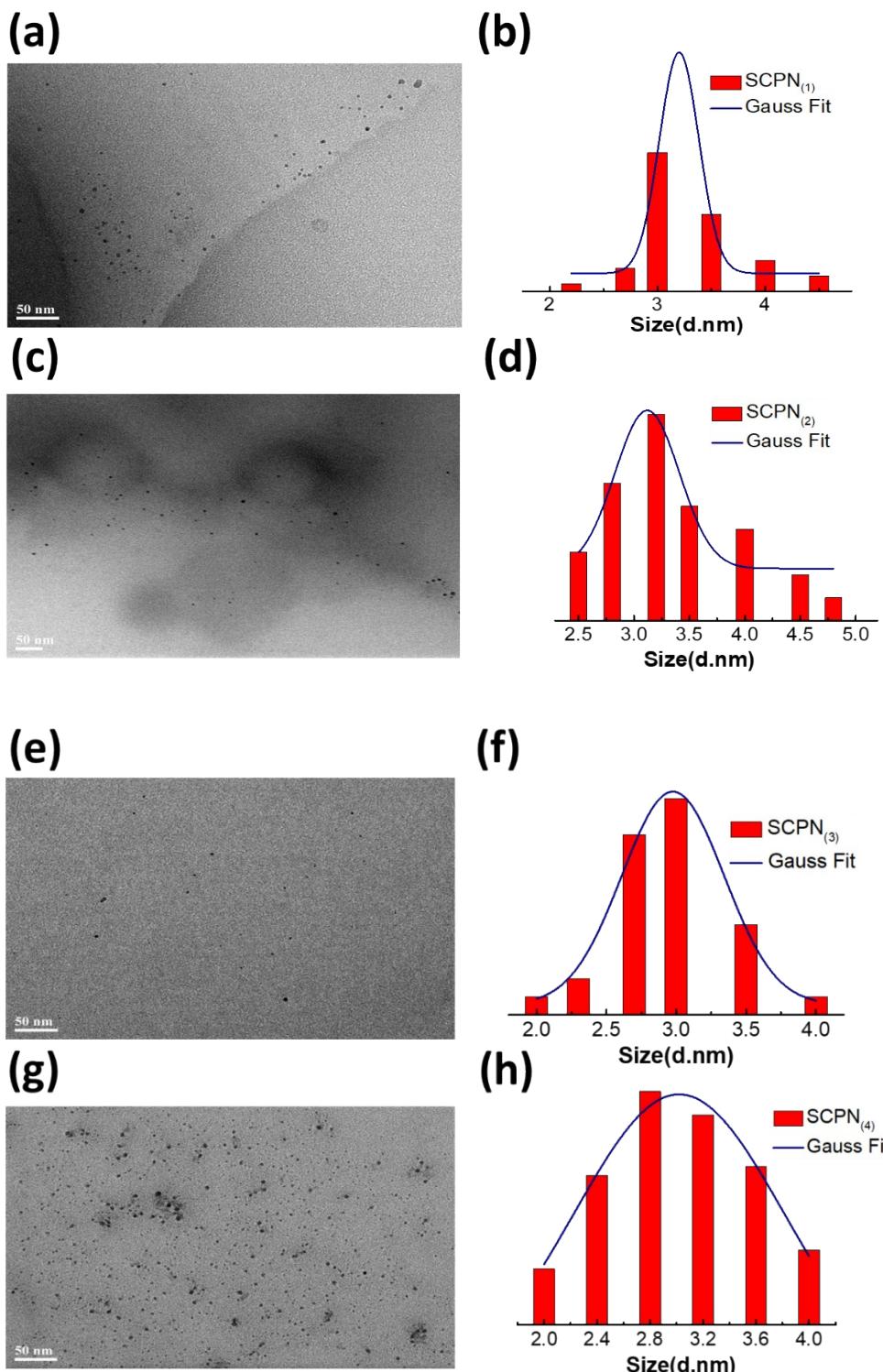


Figure S19. Comparison of the FTIR spectrum of N₃-PEG, PEGylated SCPN₍₄₎ and SCPN₍₄₎.



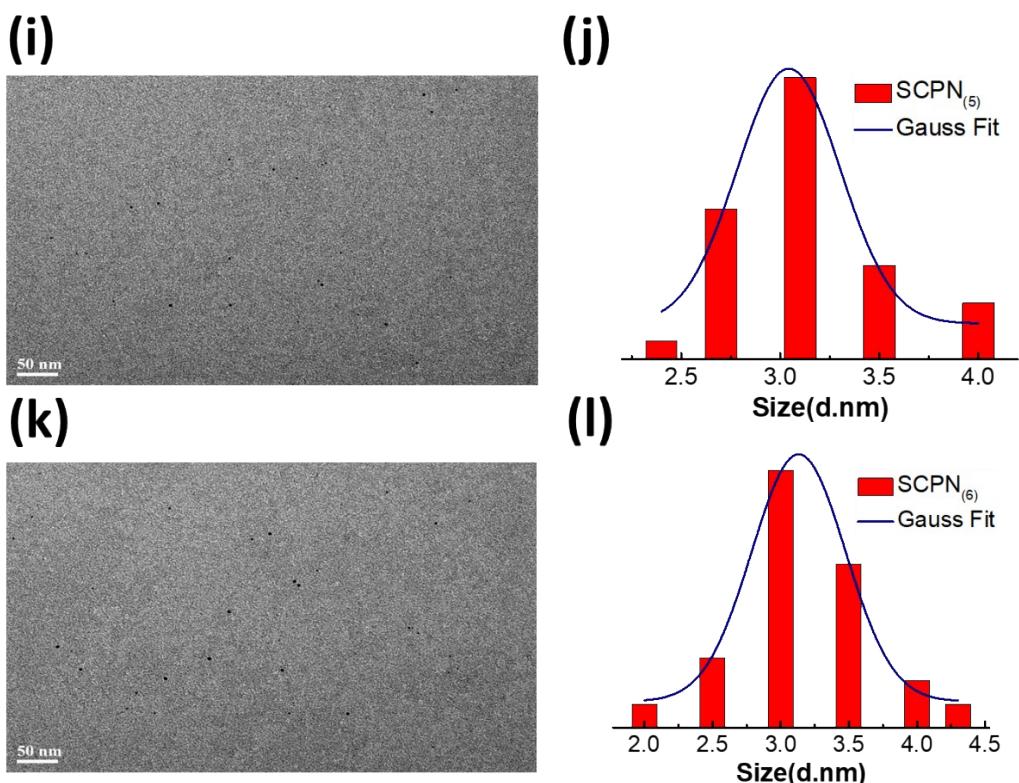


Figure S20. HR-TEM images of SCPNs nanoparticles (left) and statistical size histograms of SCPNs counted from several HR-TEM images (right). (a) and (b) SCPN₍₁₎; (c) and (d) SCPN₍₂₎; (e) and (f) SCPN₍₃₎; (g) and (h) SCPN₍₄₎; (i) and (j) SCPN₍₅₎; (k) and (l) SCPN₍₆₎.

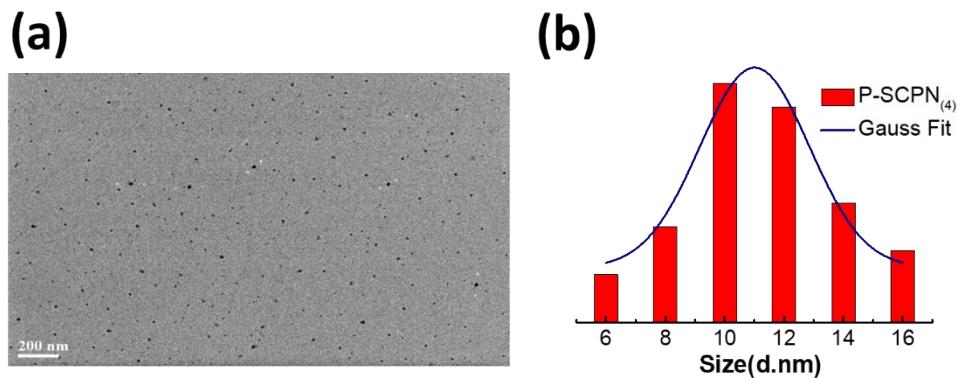


Figure S21. HR-TEM images of P-SCPN₍₄₎ nanoparticles (left) and statistical size histograms of SCPN₍₄₎ counted from several HR-TEM images (right).

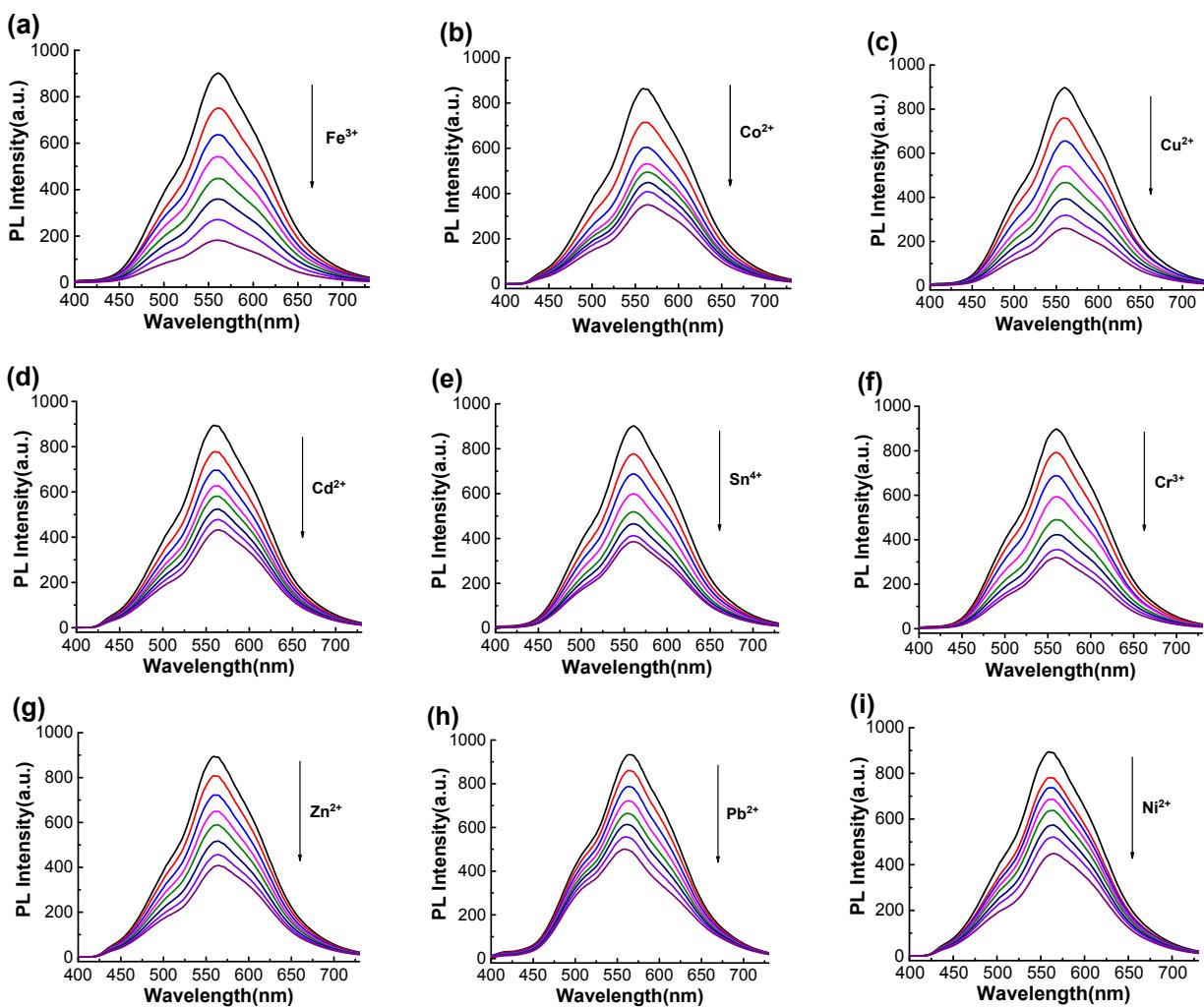


Figure S22. Fluorescence quenching titration experiments for $\text{SCPN}_{(4)}$ (as the representative SCPN) with 9 metal ions. The initial concentration of metal ions added are listed below: (a) 40 mM; (b), (c), (d), (e) and (f) 50 mM; (g), (h) and (i) 70 mM.

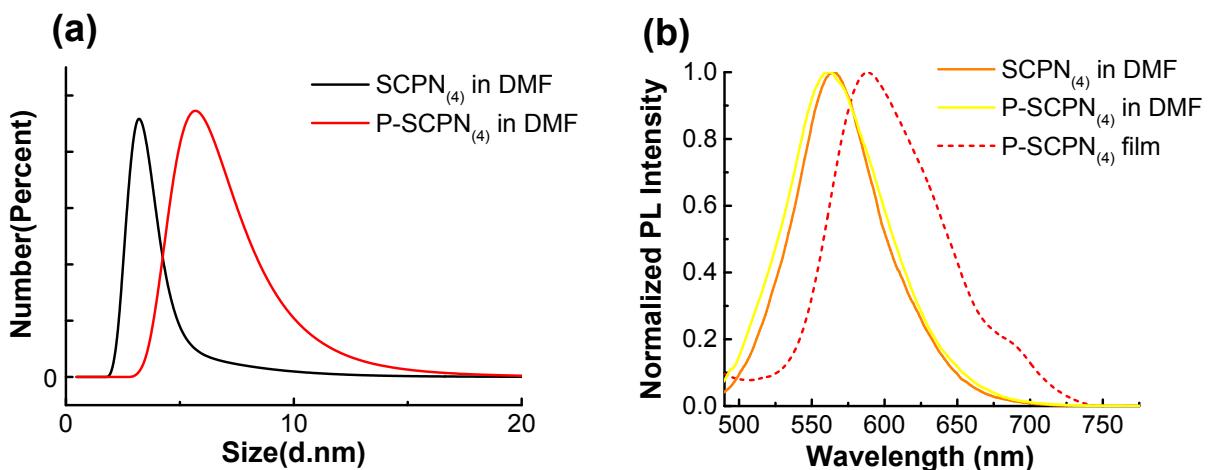
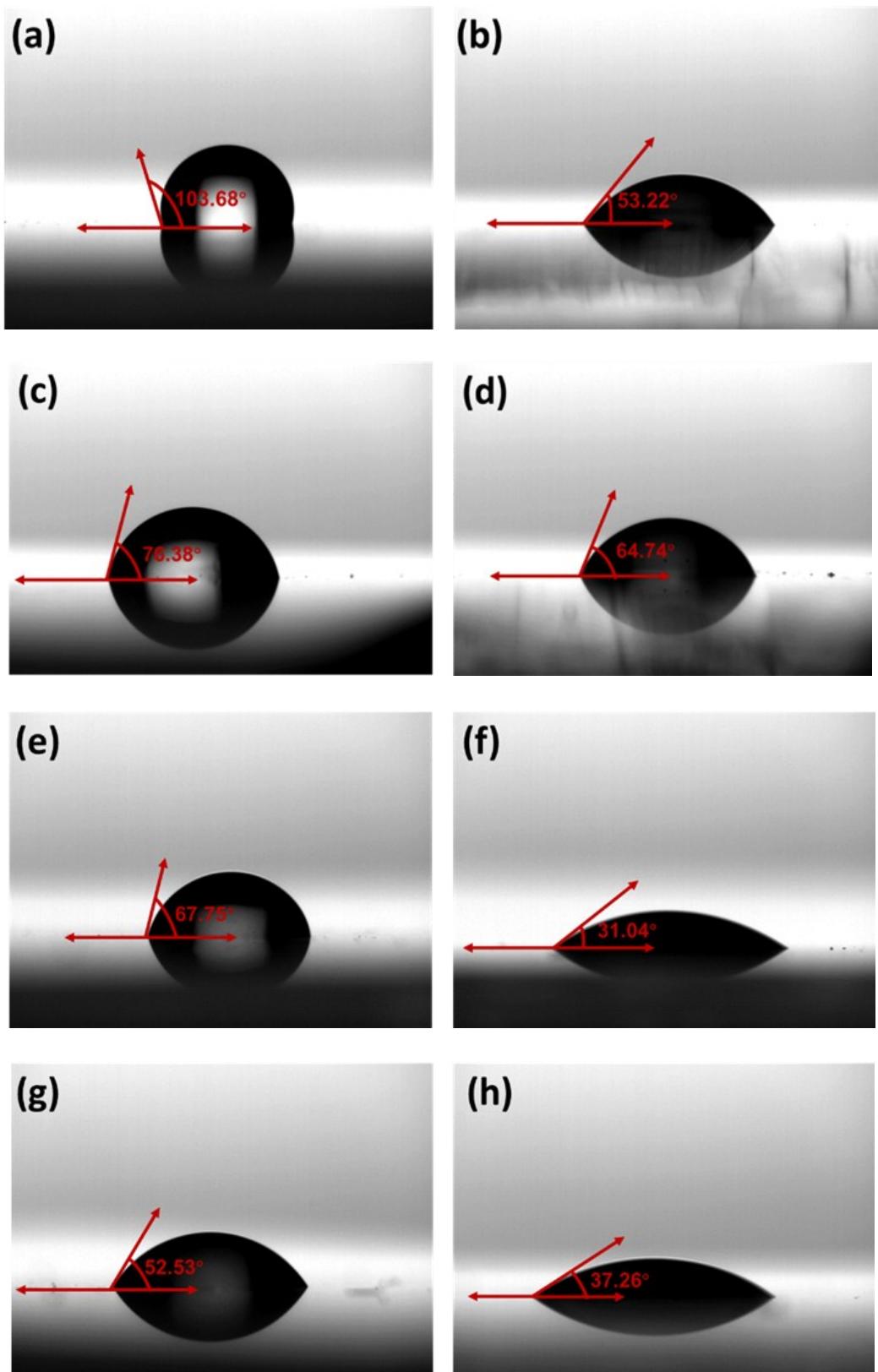


Figure S23. (a) DLS curves of $\text{SCPN}_{(4)}$ and PEGylated $\text{SCPN}_{(4)}$ (P- $\text{SCPN}_{(4)}$) in DMF solutions; (b) comparison of fluorescence emissions of $\text{SCPN}_{(4)}$ and P- $\text{SCPN}_{(4)}$ in DMF solutions (solid lines) and P- $\text{SCPN}_{(4)}$ in thin film state (dotted line).



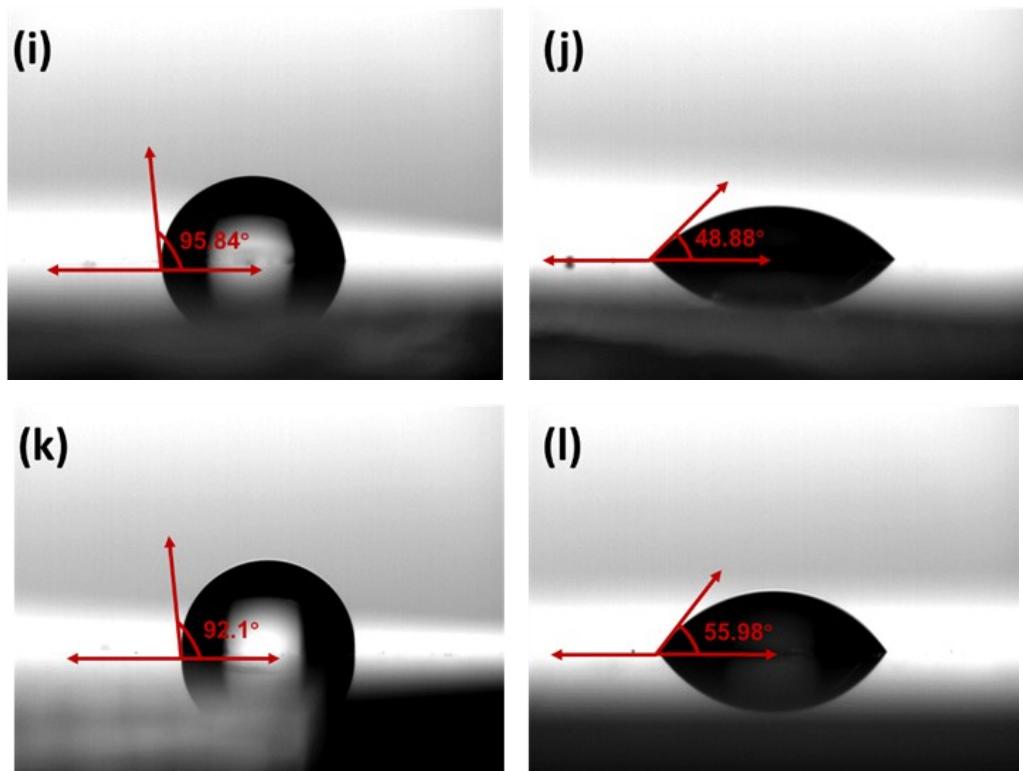


Figure S24. Profiles of a water drop on the films of the SCPNs (left) and PEGylated SCPNs (right). (a) SCPN₍₁₎; (b) PEGylated SCPN₍₁₎; (c) SCPN₍₂₎; (d) PEGylated SCPN₍₂₎; (e) SCPN₍₃₎; (f) PEGylated SCPN₍₃₎; (g) SCPN₍₄₎; (h) PEGylated SCPN₍₄₎; (i) SCPN₍₅₎; (j) PEGylated SCPN₍₅₎; (k) SCPN₍₆₎; (l) PEGylated SCPN₍₆₎.

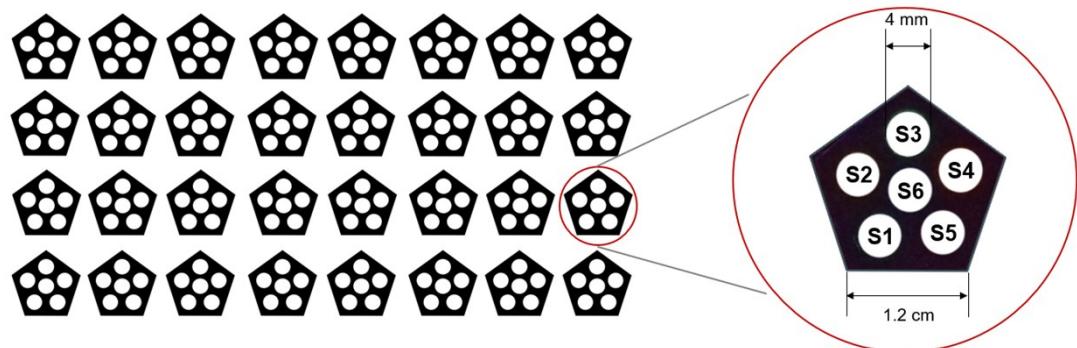


Figure S25. Ordinary array substrates cut into pentagons with all regions printed in black by a laser printer except 6 blank circles.

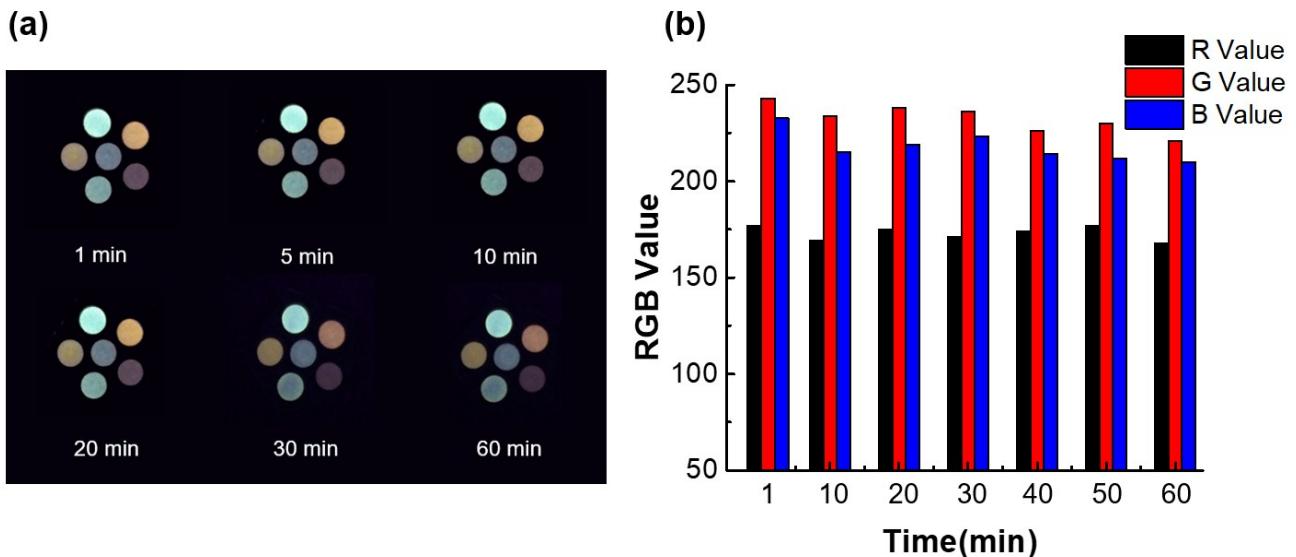


Figure S26. The stability of fluorescence sensing array in aqueous solution. (a) the fluorescence patterns of the sensing array with different exposure time; (b) the RGB value of P-SCPN₍₃₎ versus exposure time.

Table S2. Shortest response time for each metal ion (1 mM concentration).

| Metal Ions | Cd ²⁺ | Zn ²⁺ | Co ²⁺ | Sn ⁴⁺ | Pb ²⁺ | Fe ³⁺ | Cu ²⁺ | Cr ³⁺ | Ni ²⁺ | Ag ⁺ |
|------------------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|-----------------|
| Shortest Response Time (min) | 4 | 5 | 5 | 4 | 4 | 2 | 3 | 3 | 4 | 5 |

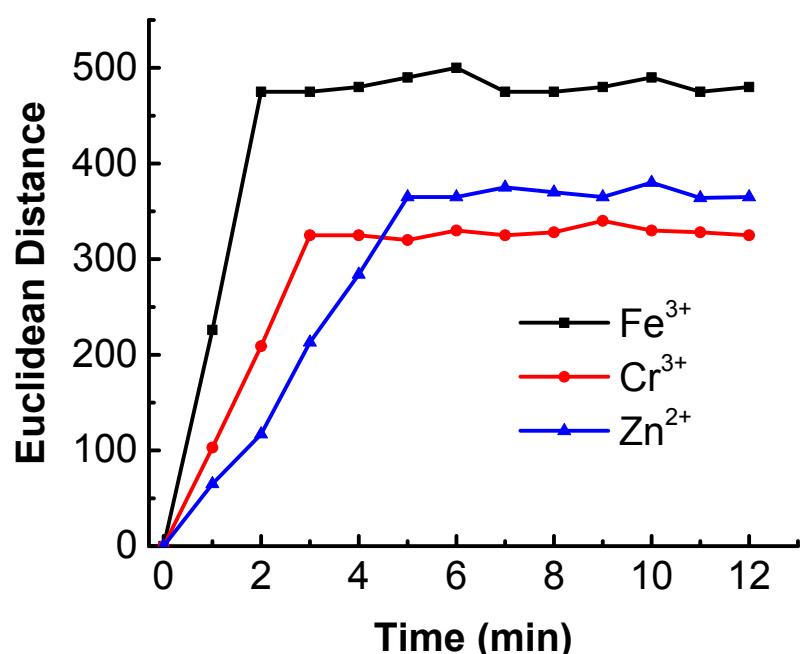


Figure S27. Euclidean distance between the representative analytes (Fe³⁺, Cr³⁺ and Zn²⁺) and the control group plotted versus exposure time at room temperature (1 mM concentration).

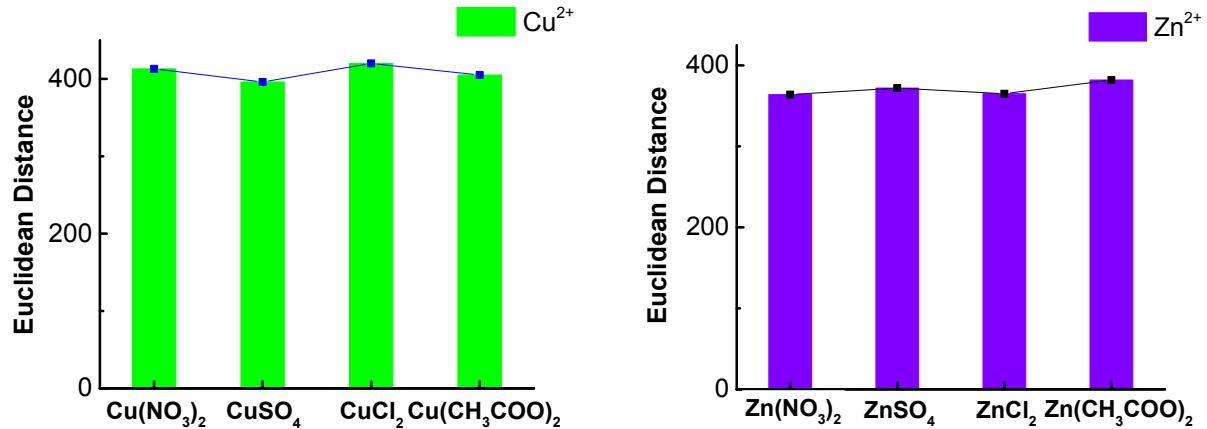


Figure S28. Euclidean distance between the representative metal salt solutions (Cu^{2+} and Zn^{2+} as cations respectively) with various anions (NO_3^- , SO_4^{2-} , Cl^- and CH_3COO^-) and the control group (1 mM concentration).

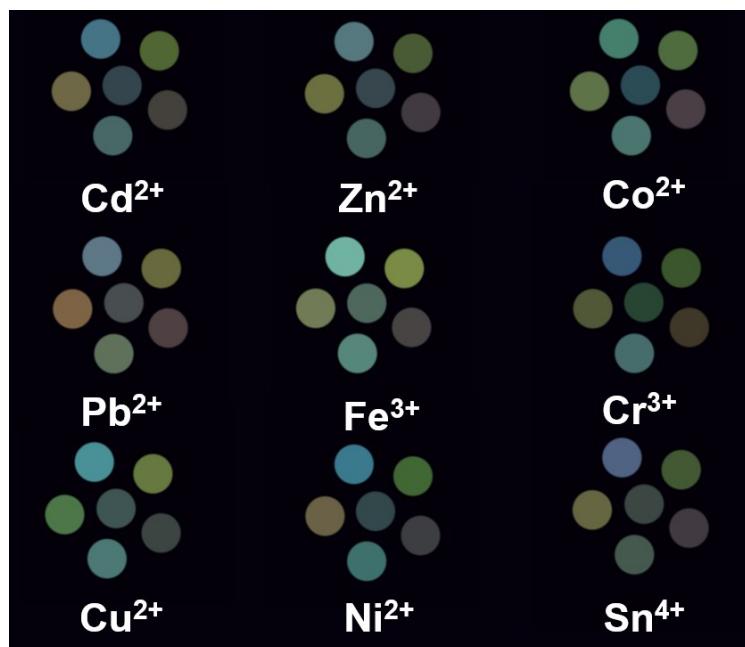


Figure S29. Color-difference patterns of the electronic tongue when exposed to nine metal ions.

Table S3. The identification of unknown metal ions at 1mM using the fluorescent electronic tongue.

| Samples | R1 | G1 | B1 | R2 | G2 | B2 | R3 | G3 | B3 | R4 | G4 | B4 | R5 | G5 | B5 | R6 | G6 | B6 | Identification | Verification |
|---------|-----|------|------|------|------|-----|-----|------|------|-----|------|-----|-----|-----|-----|-----|-----|-----|------------------|------------------|
| 1 | -73 | -100 | -103 | -113 | -105 | -69 | -68 | -116 | -133 | -81 | -105 | -52 | -65 | -68 | -58 | -53 | -68 | -77 | Cd ²⁺ | Cd ²⁺ |
| 2 | -71 | -104 | -101 | -113 | -106 | -69 | -71 | -116 | -135 | -81 | -101 | -50 | -66 | -68 | -62 | -52 | -70 | -79 | Cd ²⁺ | Cd ²⁺ |
| 3 | -74 | -105 | -106 | -110 | -102 | -69 | -68 | -117 | -135 | -81 | -101 | -52 | -71 | -62 | -62 | -54 | -69 | -77 | Cd ²⁺ | Cd ²⁺ |
| 4 | -72 | -104 | -101 | -107 | -102 | -68 | -70 | -115 | -132 | -83 | -105 | -48 | -65 | -63 | -60 | -54 | -67 | -76 | Cd ²⁺ | Cd ²⁺ |
| 5 | -68 | -105 | -103 | -107 | -103 | -73 | -69 | -115 | -134 | -82 | -106 | -49 | -70 | -63 | -60 | -50 | -68 | -75 | Cd ²⁺ | Cd ²⁺ |
| 6 | -69 | -104 | -105 | -111 | -105 | -72 | -70 | -119 | -136 | -82 | -102 | -53 | -68 | -64 | -61 | -51 | -70 | -76 | Cd ²⁺ | Cd ²⁺ |
| 7 | -70 | -102 | -97 | -110 | -107 | -65 | -85 | -120 | -125 | -71 | -89 | -53 | -68 | -57 | -65 | -57 | -72 | -76 | Zn ²⁺ | Zn ²⁺ |
| 8 | -72 | -99 | -100 | -112 | -112 | -62 | -88 | -121 | -129 | -72 | -89 | -51 | -65 | -56 | -62 | -54 | -71 | -77 | Zn ²⁺ | Zn ²⁺ |
| 9 | -71 | -103 | -94 | -106 | -109 | -65 | -84 | -124 | -124 | -71 | -92 | -53 | -66 | -59 | -62 | -54 | -73 | -76 | Zn ²⁺ | Zn ²⁺ |
| 10 | -73 | -104 | -99 | -106 | -113 | -66 | -87 | -123 | -130 | -73 | -93 | -50 | -64 | -59 | -63 | -54 | -67 | -78 | Zn ²⁺ | Zn ²⁺ |
| 11 | -70 | -104 | -94 | -108 | -111 | -65 | -83 | -119 | -124 | -75 | -93 | -52 | -65 | -58 | -66 | -53 | -73 | -78 | Zn ²⁺ | Zn ²⁺ |
| 12 | -75 | -100 | -96 | -108 | -112 | -62 | -85 | -118 | -126 | -74 | -89 | -51 | -67 | -60 | -65 | -55 | -67 | -74 | Zn ²⁺ | Zn ²⁺ |
| 13 | -76 | -117 | -108 | -94 | -118 | -70 | -68 | -129 | -107 | -79 | -109 | -66 | -77 | -65 | -66 | -44 | -77 | -84 | Co ²⁺ | Co ²⁺ |
| 14 | -77 | -119 | -113 | -93 | -114 | -72 | -67 | -129 | -107 | -77 | -111 | -60 | -74 | -63 | -70 | -44 | -76 | -86 | Co ²⁺ | Co ²⁺ |
| 15 | -74 | -118 | -108 | -96 | -118 | -74 | -68 | -125 | -107 | -78 | -106 | -66 | -76 | -60 | -67 | -44 | -77 | -84 | Co ²⁺ | Co ²⁺ |
| 16 | -73 | -116 | -111 | -96 | -116 | -69 | -71 | -127 | -111 | -80 | -108 | -64 | -72 | -63 | -69 | -45 | -78 | -86 | Co ²⁺ | Co ²⁺ |
| 17 | -77 | -114 | -111 | -98 | -113 | -72 | -67 | -129 | -111 | -82 | -105 | -63 | -72 | -60 | -69 | -44 | -75 | -84 | Co ²⁺ | Co ²⁺ |
| 18 | -73 | -118 | -112 | -95 | -113 | -72 | -69 | -128 | -108 | -80 | -111 | -60 | -73 | -65 | -70 | -49 | -75 | -85 | Co ²⁺ | Co ²⁺ |
| 19 | -68 | -88 | -77 | -102 | -105 | -67 | -79 | -102 | -132 | -66 | -88 | -52 | -66 | -57 | -66 | -63 | -69 | -69 | Sn ⁴⁺ | Sn ⁴⁺ |
| 20 | -67 | -91 | -80 | -102 | -105 | -67 | -80 | -97 | -128 | -64 | -94 | -55 | -64 | -59 | -66 | -61 | -72 | -69 | Sn ⁴⁺ | Sn ⁴⁺ |
| 21 | -70 | -87 | -78 | -102 | -99 | -69 | -80 | -99 | -132 | -68 | -93 | -51 | -66 | -61 | -68 | -63 | -71 | -68 | Sn ⁴⁺ | Sn ⁴⁺ |
| 22 | -69 | -93 | -78 | -105 | -100 | -64 | -81 | -97 | -132 | -67 | -88 | -54 | -68 | -60 | -63 | -63 | -69 | -68 | Sn ⁴⁺ | Sn ⁴⁺ |

| Samples | R1 | G1 | B1 | R2 | G2 | B2 | R3 | G3 | B3 | R4 | G4 | B4 | R5 | G5 | B5 | R6 | G6 | B6 | Identification | Verification |
|---------|-----|------|------|------|------|-----|------|------|------|------|------|-----|-----|-----|-----|-----|------|-----|------------------|------------------|
| 23 | -71 | -90 | -81 | -101 | -101 | -68 | -81 | -97 | -132 | -67 | -89 | -51 | -66 | -59 | -65 | -57 | -71 | -67 | Sn ⁴⁺ | Sn ⁴⁺ |
| 24 | -72 | -91 | -80 | -104 | -102 | -66 | -83 | -103 | -127 | -69 | -90 | -55 | -68 | -60 | -66 | -59 | -72 | -69 | Sn ⁴⁺ | Sn ⁴⁺ |
| 25 | -97 | -118 | -93 | -128 | -97 | -67 | -93 | -117 | -134 | -104 | -107 | -61 | -81 | -62 | -64 | -72 | -79 | -78 | Pb ²⁺ | Pb ²⁺ |
| 26 | -93 | -113 | -90 | -125 | -101 | -67 | -93 | -122 | -137 | -106 | -106 | -61 | -78 | -62 | -70 | -74 | -78 | -79 | Pb ²⁺ | Pb ²⁺ |
| 27 | -94 | -117 | -89 | -125 | -102 | -68 | -95 | -121 | -138 | -102 | -104 | -61 | -77 | -66 | -68 | -71 | -77 | -78 | Pb ²⁺ | Pb ²⁺ |
| 28 | -96 | -112 | -93 | -127 | -98 | -73 | -96 | -118 | -134 | -102 | -107 | -62 | -77 | -68 | -65 | -72 | -78 | -80 | Pb ²⁺ | Pb ²⁺ |
| 29 | -94 | -114 | -91 | -125 | -100 | -68 | -96 | -119 | -137 | -106 | -106 | -61 | -79 | -63 | -69 | -70 | -74 | -82 | Pb ²⁺ | Pb ²⁺ |
| 30 | -94 | -112 | -87 | -123 | -102 | -70 | -92 | -122 | -137 | -101 | -106 | -59 | -82 | -63 | -68 | -72 | -74 | -83 | Pb ²⁺ | Pb ²⁺ |
| 31 | -88 | -134 | -120 | -116 | -122 | -85 | -113 | -180 | -165 | -122 | -137 | -71 | -72 | -69 | -72 | -78 | -106 | -96 | Fe ³⁺ | Fe ³⁺ |
| 32 | -87 | -134 | -126 | -114 | -122 | -87 | -114 | -182 | -165 | -123 | -139 | -72 | -74 | -68 | -67 | -76 | -105 | -91 | Fe ³⁺ | Fe ³⁺ |
| 33 | -85 | -137 | -123 | -115 | -126 | -83 | -109 | -178 | -164 | -121 | -142 | -69 | -73 | -70 | -71 | -76 | -104 | -93 | Fe ³⁺ | Fe ³⁺ |
| 34 | -87 | -132 | -120 | -111 | -124 | -85 | -114 | -179 | -161 | -123 | -143 | -68 | -74 | -66 | -66 | -75 | -102 | -93 | Fe ³⁺ | Fe ³⁺ |
| 35 | -88 | -138 | -126 | -117 | -125 | -88 | -113 | -180 | -161 | -117 | -137 | -67 | -72 | -67 | -66 | -80 | -103 | -95 | Fe ³⁺ | Fe ³⁺ |
| 36 | -89 | -132 | -121 | -112 | -122 | -87 | -112 | -178 | -160 | -122 | -137 | -69 | -74 | -68 | -68 | -80 | -102 | -94 | Fe ³⁺ | Fe ³⁺ |
| 37 | -76 | -119 | -118 | -81 | -120 | -71 | -75 | -146 | -149 | -99 | -121 | -64 | -60 | -69 | -63 | -62 | -87 | -84 | Cu ²⁺ | Cu ²⁺ |
| 38 | -77 | -121 | -112 | -77 | -117 | -72 | -75 | -146 | -152 | -101 | -121 | -61 | -62 | -68 | -62 | -65 | -83 | -82 | Cu ²⁺ | Cu ²⁺ |
| 39 | -77 | -120 | -115 | -76 | -117 | -75 | -73 | -143 | -151 | -104 | -122 | -65 | -62 | -67 | -67 | -64 | -87 | -82 | Cu ²⁺ | Cu ²⁺ |
| 40 | -79 | -121 | -116 | -77 | -118 | -75 | -75 | -146 | -150 | -98 | -120 | -62 | -60 | -71 | -67 | -63 | -85 | -84 | Cu ²⁺ | Cu ²⁺ |
| 41 | -76 | -122 | -117 | -79 | -121 | -72 | -72 | -143 | -152 | -100 | -120 | -65 | -62 | -73 | -67 | -61 | -84 | -80 | Cu ²⁺ | Cu ²⁺ |
| 42 | -73 | -120 | -112 | -75 | -120 | -70 | -73 | -144 | -151 | -102 | -123 | -65 | -60 | -67 | -68 | -64 | -83 | -85 | Cu ²⁺ | Cu ²⁺ |
| 43 | -69 | -108 | -106 | -83 | -87 | -56 | -52 | -88 | -122 | -60 | -85 | -46 | -56 | -65 | -54 | -39 | -69 | -52 | Cr ³⁺ | Cr ³⁺ |
| 44 | -70 | -109 | -111 | -83 | -86 | -57 | -53 | -88 | -117 | -58 | -88 | -43 | -57 | -61 | -56 | -39 | -71 | -54 | Cr ³⁺ | Cr ³⁺ |
| 45 | -70 | -111 | -105 | -77 | -90 | -56 | -58 | -87 | -120 | -58 | -84 | -46 | -53 | -60 | -56 | -44 | -66 | -53 | Cr ³⁺ | Cr ³⁺ |
| 46 | -72 | -106 | -108 | -80 | -88 | -58 | -56 | -90 | -117 | -59 | -87 | -47 | -55 | -61 | -57 | -39 | -68 | -49 | Cr ³⁺ | Cr ³⁺ |

| Samples | R1 | G1 | B1 | R2 | G2 | B2 | R3 | G3 | B3 | R4 | G4 | B4 | R5 | G5 | B5 | R6 | G6 | B6 | Identification | Verification |
|---------|-----|------|------|------|------|-----|-----|------|------|-----|------|-----|-----|-----|-----|-----|-----|-----|------------------|------------------|
| 47 | -70 | -112 | -108 | -82 | -91 | -53 | -57 | -93 | -119 | -57 | -86 | -43 | -52 | -65 | -55 | -38 | -69 | -48 | Cr ³⁺ | Cr ³⁺ |
| 48 | -71 | -108 | -110 | -82 | -86 | -57 | -55 | -88 | -120 | -63 | -87 | -41 | -52 | -64 | -53 | -42 | -70 | -52 | Cr ³⁺ | Cr ³⁺ |
| 49 | -63 | -113 | -110 | -107 | -100 | -70 | -58 | -120 | -144 | -64 | -104 | -52 | -60 | -64 | -65 | -51 | -71 | -78 | Ni ²⁺ | Ni ²⁺ |
| 50 | -64 | -114 | -110 | -107 | -98 | -71 | -57 | -121 | -140 | -65 | -104 | -54 | -65 | -64 | -65 | -49 | -75 | -73 | Ni ²⁺ | Ni ²⁺ |
| 51 | -61 | -110 | -106 | -107 | -97 | -67 | -59 | -120 | -143 | -65 | -103 | -52 | -61 | -64 | -65 | -49 | -70 | -74 | Ni ²⁺ | Ni ²⁺ |
| 52 | -63 | -113 | -106 | -109 | -99 | -69 | -59 | -122 | -141 | -67 | -104 | -52 | -59 | -59 | -67 | -47 | -73 | -75 | Ni ²⁺ | Ni ²⁺ |
| 53 | -61 | -114 | -106 | -105 | -98 | -70 | -62 | -123 | -141 | -66 | -102 | -53 | -59 | -61 | -67 | -52 | -70 | -73 | Ni ²⁺ | Ni ²⁺ |
| 54 | -64 | -116 | -110 | -107 | -94 | -70 | -60 | -120 | -144 | -63 | -99 | -56 | -64 | -60 | -64 | -51 | -74 | -77 | Ni ²⁺ | Ni ²⁺ |

Table S4. 18-dimensional vector of 6 sorts of P-SCPNs when soaked in aqueous solutions of metal ions (differences in RGB values).

| Metal Ions | R1 | G1 | B1 | R2 | G2 | B2 | R3 | G3 | B3 | R4 | G4 | B4 | R5 | G5 | B5 | R6 | G6 | B6 |
|------------------|-----|------|------|------|------|-----|-----|------|------|-----|------|-----|-----|-----|-----|-----|-----|-----|
| Cd ²⁺ | -73 | -100 | -103 | -113 | -105 | -69 | -68 | -116 | -133 | -81 | -105 | -52 | -65 | -68 | -58 | -53 | -68 | -77 |
| Cd ²⁺ | -71 | -104 | -101 | -113 | -106 | -69 | -71 | -116 | -135 | -81 | -101 | -50 | -66 | -68 | -62 | -52 | -70 | -79 |
| Cd ²⁺ | -74 | -105 | -106 | -110 | -102 | -69 | -68 | -117 | -135 | -81 | -101 | -52 | -71 | -62 | -62 | -54 | -69 | -77 |
| Cd ²⁺ | -72 | -104 | -101 | -107 | -102 | -68 | -70 | -115 | -132 | -83 | -105 | -48 | -65 | -63 | -60 | -54 | -67 | -76 |
| Cd ²⁺ | -68 | -105 | -103 | -107 | -103 | -73 | -69 | -115 | -134 | -82 | -106 | -49 | -70 | -63 | -60 | -50 | -68 | -75 |
| Cd ²⁺ | -69 | -104 | -105 | -111 | -105 | -72 | -70 | -119 | -136 | -82 | -102 | -53 | -68 | -64 | -61 | -51 | -70 | -76 |
| Ave. | -71 | -104 | -103 | -110 | -104 | -70 | -69 | -116 | -134 | -82 | -103 | -51 | -68 | -65 | -61 | -52 | -69 | -77 |
| Zn ²⁺ | -70 | -102 | -97 | -110 | -107 | -65 | -85 | -120 | -125 | -71 | -89 | -53 | -68 | -57 | -65 | -57 | -72 | -76 |
| Zn ²⁺ | -72 | -99 | -100 | -112 | -112 | -62 | -88 | -121 | -129 | -72 | -89 | -51 | -65 | -56 | -62 | -54 | -71 | -77 |
| Zn ²⁺ | -71 | -103 | -94 | -106 | -109 | -65 | -84 | -124 | -124 | -71 | -92 | -53 | -66 | -59 | -62 | -54 | -73 | -76 |
| Zn ²⁺ | -73 | -104 | -99 | -106 | -113 | -66 | -87 | -123 | -130 | -73 | -93 | -50 | -64 | -59 | -63 | -54 | -67 | -78 |
| Zn ²⁺ | -70 | -104 | -94 | -108 | -111 | -65 | -83 | -119 | -124 | -75 | -93 | -52 | -65 | -58 | -66 | -53 | -73 | -78 |
| Zn ²⁺ | -75 | -100 | -96 | -108 | -112 | -62 | -85 | -118 | -126 | -74 | -89 | -51 | -67 | -60 | -65 | -55 | -67 | -74 |
| Ave. | -72 | -102 | -97 | -108 | -111 | -64 | -85 | -121 | -126 | -73 | -91 | -52 | -66 | -58 | -64 | -55 | -71 | -77 |
| Co ²⁺ | -76 | -117 | -108 | -94 | -118 | -70 | -68 | -129 | -107 | -79 | -109 | -66 | -77 | -65 | -66 | -44 | -77 | -84 |
| Co ²⁺ | -77 | -119 | -113 | -93 | -114 | -72 | -67 | -129 | -107 | -77 | -111 | -60 | -74 | -63 | -70 | -44 | -76 | -86 |
| Co ²⁺ | -74 | -118 | -108 | -96 | -118 | -74 | -68 | -125 | -107 | -78 | -106 | -66 | -76 | -60 | -67 | -44 | -77 | -84 |
| Co ²⁺ | -73 | -116 | -111 | -96 | -116 | -69 | -71 | -127 | -111 | -80 | -108 | -64 | -72 | -63 | -69 | -45 | -78 | -86 |
| Co ²⁺ | -77 | -114 | -111 | -98 | -113 | -72 | -67 | -129 | -111 | -82 | -105 | -63 | -72 | -60 | -69 | -44 | -75 | -84 |
| Co ²⁺ | -73 | -118 | -112 | -95 | -113 | -72 | -69 | -128 | -108 | -80 | -111 | -60 | -73 | -65 | -70 | -49 | -75 | -85 |
| Ave. | -75 | -117 | -111 | -95 | -115 | -72 | -68 | -128 | -109 | -79 | -108 | -63 | -74 | -63 | -69 | -45 | -76 | -85 |
| Sn ⁴⁺ | -68 | -88 | -77 | -102 | -105 | -67 | -79 | -102 | -132 | -66 | -88 | -52 | -66 | -57 | -66 | -63 | -69 | -69 |

| Metal Ions | R1 | G1 | B1 | R2 | G2 | B2 | R3 | G3 | B3 | R4 | G4 | B4 | R5 | G5 | B5 | R6 | G6 | B6 |
|------------------------|-----|------|------|------|------|-----|------|------|------|------|------|-----|-----|-----|-----|-----|------|-----|
| Sn⁴⁺ | -67 | -91 | -80 | -102 | -105 | -67 | -80 | -97 | -128 | -64 | -94 | -55 | -64 | -59 | -66 | -61 | -72 | -69 |
| Sn⁴⁺ | -70 | -87 | -78 | -102 | -99 | -69 | -80 | -99 | -132 | -68 | -93 | -51 | -66 | -61 | -68 | -63 | -71 | -68 |
| Sn⁴⁺ | -69 | -93 | -78 | -105 | -100 | -64 | -81 | -97 | -132 | -67 | -88 | -54 | -68 | -60 | -63 | -63 | -69 | -68 |
| Sn⁴⁺ | -71 | -90 | -81 | -101 | -101 | -68 | -81 | -97 | -132 | -67 | -89 | -51 | -66 | -59 | -65 | -57 | -71 | -67 |
| Sn⁴⁺ | -72 | -91 | -80 | -104 | -102 | -66 | -83 | -103 | -127 | -69 | -90 | -55 | -68 | -60 | -66 | -59 | -72 | -69 |
| Ave. | -70 | -90 | -79 | -103 | -102 | -67 | -81 | -99 | -131 | -67 | -90 | -53 | -66 | -59 | -66 | -61 | -71 | -68 |
| Pb²⁺ | -97 | -118 | -93 | -128 | -97 | -67 | -93 | -117 | -134 | -104 | -107 | -61 | -81 | -62 | -64 | -72 | -79 | -78 |
| Pb²⁺ | -93 | -113 | -90 | -125 | -101 | -67 | -93 | -122 | -137 | -106 | -106 | -61 | -78 | -62 | -70 | -74 | -78 | -79 |
| Pb²⁺ | -94 | -117 | -89 | -125 | -102 | -68 | -95 | -121 | -138 | -102 | -104 | -61 | -77 | -66 | -68 | -71 | -77 | -78 |
| Pb²⁺ | -96 | -112 | -93 | -127 | -98 | -73 | -96 | -118 | -134 | -102 | -107 | -62 | -77 | -68 | -65 | -72 | -78 | -80 |
| Pb²⁺ | -94 | -114 | -91 | -125 | -100 | -68 | -96 | -119 | -137 | -106 | -106 | -61 | -79 | -63 | -69 | -70 | -74 | -82 |
| Pb²⁺ | -94 | -112 | -87 | -123 | -102 | -70 | -92 | -122 | -137 | -101 | -106 | -59 | -82 | -63 | -68 | -72 | -74 | -83 |
| Ave. | -95 | -114 | -91 | -126 | -100 | -69 | -94 | -120 | -136 | -104 | -106 | -61 | -79 | -64 | -67 | -72 | -77 | -80 |
| Fe³⁺ | -88 | -134 | -120 | -116 | -122 | -85 | -113 | -180 | -165 | -122 | -137 | -71 | -72 | -69 | -72 | -78 | -106 | -96 |
| Fe³⁺ | -87 | -134 | -126 | -114 | -122 | -87 | -114 | -182 | -165 | -123 | -139 | -72 | -74 | -68 | -67 | -76 | -105 | -91 |
| Fe³⁺ | -85 | -137 | -123 | -115 | -126 | -83 | -109 | -178 | -164 | -121 | -142 | -69 | -73 | -70 | -71 | -76 | -104 | -93 |
| Fe³⁺ | -87 | -132 | -120 | -111 | -124 | -85 | -114 | -179 | -161 | -123 | -143 | -68 | -74 | -66 | -66 | -75 | -102 | -93 |
| Fe³⁺ | -88 | -138 | -126 | -117 | -125 | -88 | -113 | -180 | -161 | -117 | -137 | -67 | -72 | -67 | -66 | -80 | -103 | -95 |
| Fe³⁺ | -89 | -132 | -121 | -112 | -122 | -87 | -112 | -178 | -160 | -122 | -137 | -69 | -74 | -68 | -68 | -80 | -102 | -94 |
| Ave. | -87 | -135 | -123 | -114 | -124 | -86 | -113 | -180 | -163 | -121 | -139 | -69 | -73 | -68 | -68 | -78 | -104 | -94 |
| Cu²⁺ | -76 | -119 | -118 | -81 | -120 | -71 | -75 | -146 | -149 | -99 | -121 | -64 | -60 | -69 | -63 | -62 | -87 | -84 |
| Cu²⁺ | -77 | -121 | -112 | -77 | -117 | -72 | -75 | -146 | -152 | -101 | -121 | -61 | -62 | -68 | -62 | -65 | -83 | -82 |
| Cu²⁺ | -77 | -120 | -115 | -76 | -117 | -75 | -73 | -143 | -151 | -104 | -122 | -65 | -62 | -67 | -67 | -64 | -87 | -82 |
| Cu²⁺ | -79 | -121 | -116 | -77 | -118 | -75 | -75 | -146 | -150 | -98 | -120 | -62 | -60 | -71 | -67 | -63 | -85 | -84 |

| Metal Ions | R1 | G1 | B1 | R2 | G2 | B2 | R3 | G3 | B3 | R4 | G4 | B4 | R5 | G5 | B5 | R6 | G6 | B6 |
|------------------|-----|------|------|------|------|-----|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|
| Cu ²⁺ | -76 | -122 | -117 | -79 | -121 | -72 | -72 | -143 | -152 | -100 | -120 | -65 | -62 | -73 | -67 | -61 | -84 | -80 |
| Cu ²⁺ | -73 | -120 | -112 | -75 | -120 | -70 | -73 | -144 | -151 | -102 | -123 | -65 | -60 | -67 | -68 | -64 | -83 | -85 |
| Ave. | -76 | -121 | -115 | -78 | -119 | -73 | -74 | -145 | -151 | -101 | -121 | -64 | -61 | -69 | -66 | -63 | -85 | -83 |
| Cr ³⁺ | -69 | -108 | -106 | -83 | -87 | -56 | -52 | -88 | -122 | -60 | -85 | -46 | -56 | -65 | -54 | -39 | -69 | -52 |
| Cr ³⁺ | -70 | -109 | -111 | -83 | -86 | -57 | -53 | -88 | -117 | -58 | -88 | -43 | -57 | -61 | -56 | -39 | -71 | -54 |
| Cr ³⁺ | -70 | -111 | -105 | -77 | -90 | -56 | -58 | -87 | -120 | -58 | -84 | -46 | -53 | -60 | -56 | -44 | -66 | -53 |
| Cr ³⁺ | -72 | -106 | -108 | -80 | -88 | -58 | -56 | -90 | -117 | -59 | -87 | -47 | -55 | -61 | -57 | -39 | -68 | -49 |
| Cr ³⁺ | -70 | -112 | -108 | -82 | -91 | -53 | -57 | -93 | -119 | -57 | -86 | -43 | -52 | -65 | -55 | -38 | -69 | -48 |
| Cr ³⁺ | -71 | -108 | -110 | -82 | -86 | -57 | -55 | -88 | -120 | -63 | -87 | -41 | -52 | -64 | -53 | -42 | -70 | -52 |
| Ave. | -70 | -109 | -108 | -81 | -88 | -56 | -55 | -89 | -119 | -59 | -86 | -44 | -54 | -63 | -55 | -40 | -69 | -51 |
| Ni ²⁺ | -63 | -113 | -110 | -107 | -100 | -70 | -58 | -120 | -144 | -64 | -104 | -52 | -60 | -64 | -65 | -51 | -71 | -78 |
| Ni ²⁺ | -64 | -114 | -110 | -107 | -98 | -71 | -57 | -121 | -140 | -65 | -104 | -54 | -65 | -64 | -65 | -49 | -75 | -73 |
| Ni ²⁺ | -61 | -110 | -106 | -107 | -97 | -67 | -59 | -120 | -143 | -65 | -103 | -52 | -61 | -64 | -65 | -49 | -70 | -74 |
| Ni ²⁺ | -63 | -113 | -106 | -109 | -99 | -69 | -59 | -122 | -141 | -67 | -104 | -52 | -59 | -59 | -67 | -47 | -73 | -75 |
| Ni ²⁺ | -61 | -114 | -106 | -105 | -98 | -70 | -62 | -123 | -141 | -66 | -102 | -53 | -59 | -61 | -67 | -52 | -70 | -73 |
| Ni ²⁺ | -64 | -116 | -110 | -107 | -94 | -70 | -60 | -120 | -144 | -63 | -99 | -56 | -64 | -60 | -64 | -51 | -74 | -77 |
| Ave. | -63 | -113 | -108 | -107 | -98 | -70 | -59 | -121 | -142 | -65 | -103 | -53 | -61 | -62 | -66 | -50 | -72 | -75 |