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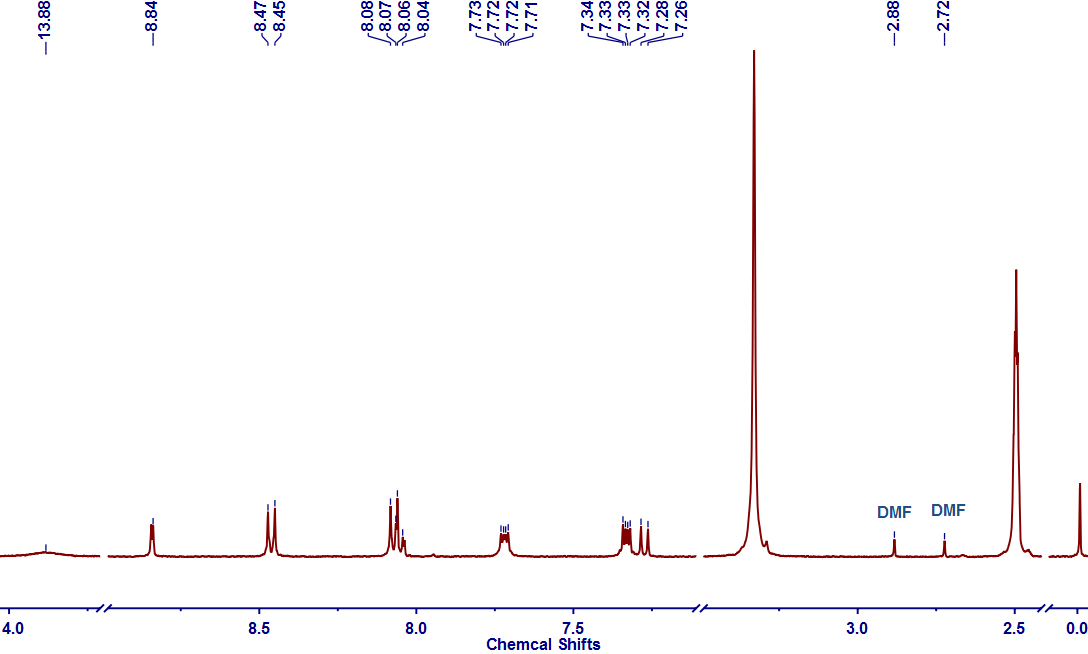


Figure **S1**. 1H NMR spectrum of **S1** in DMSO-d6.

In Figure **S1**, the signals of 2.72 and 2.88 ppm colud be assigned to the solvent impurities of dimethylformamide (DMF). In our experiments, the dimethyl sulfoxide (DMSO) was used as the polar solvent. DMF is also a polar solvent, which is always used for the investigation of sensing behavior [1], and there isn’t much difference among λmax of sensor in DMSO or DMF solvent. That is, the negative effects generated from the traces of DMF can be ignored.

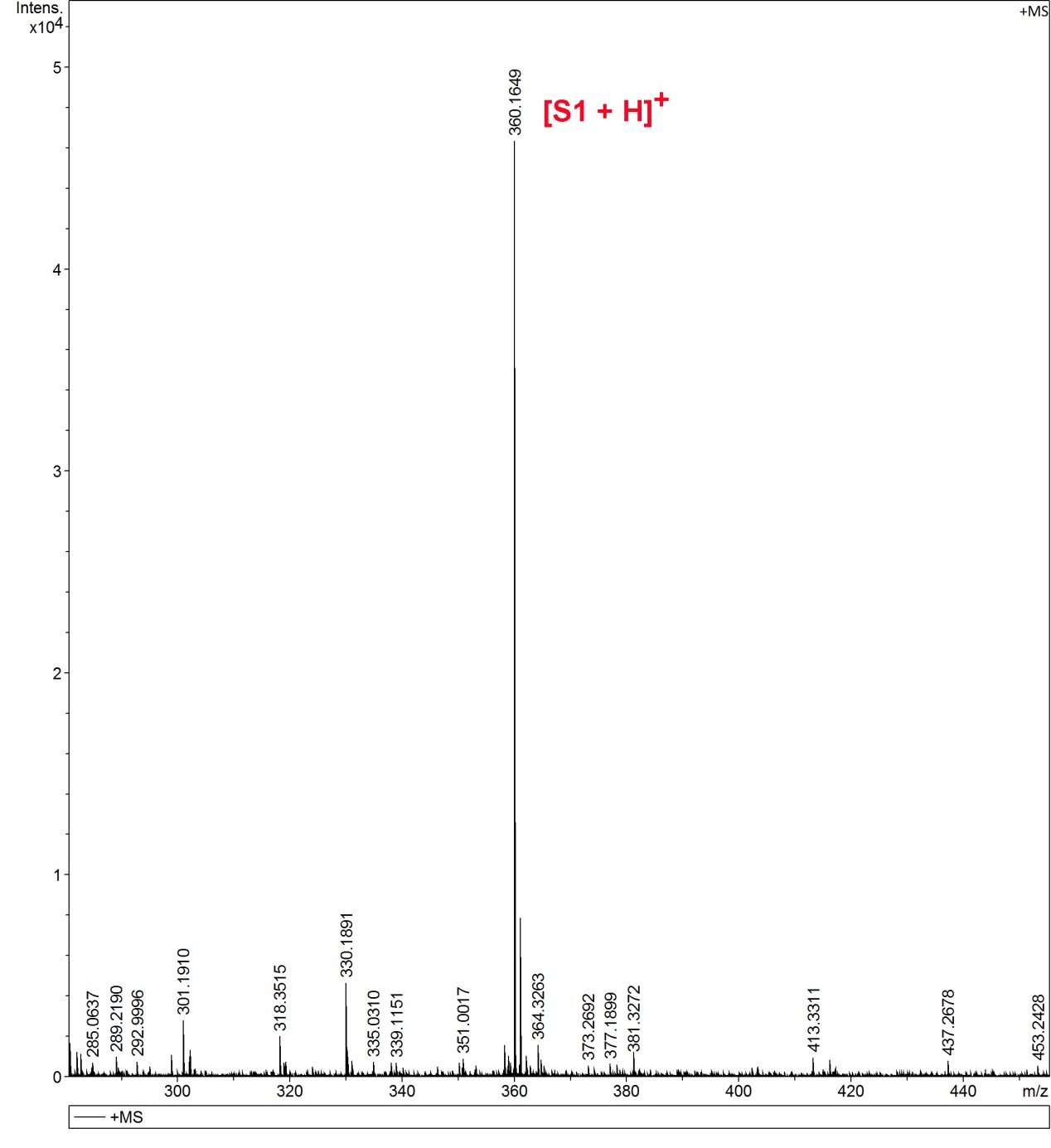
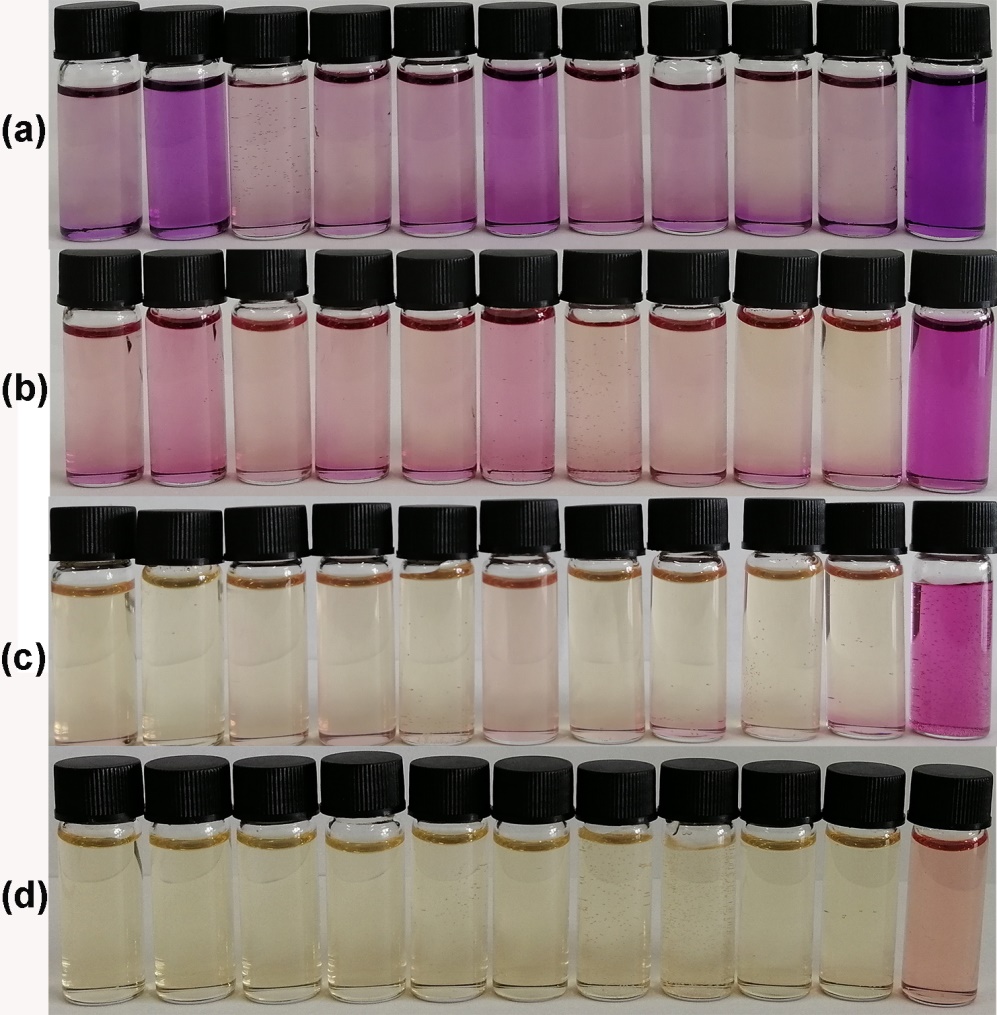
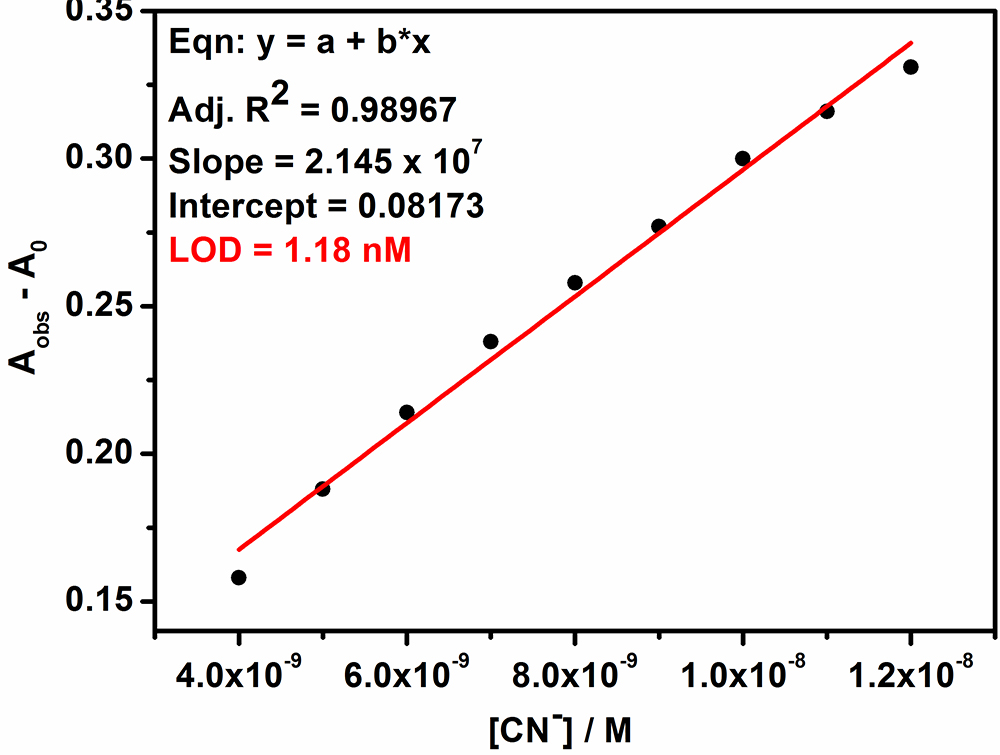


Figure **S2**. ESI-MS spectrum of **S1,** calc. for C19H14N5O3 , 360.1097, found: 360.1649.



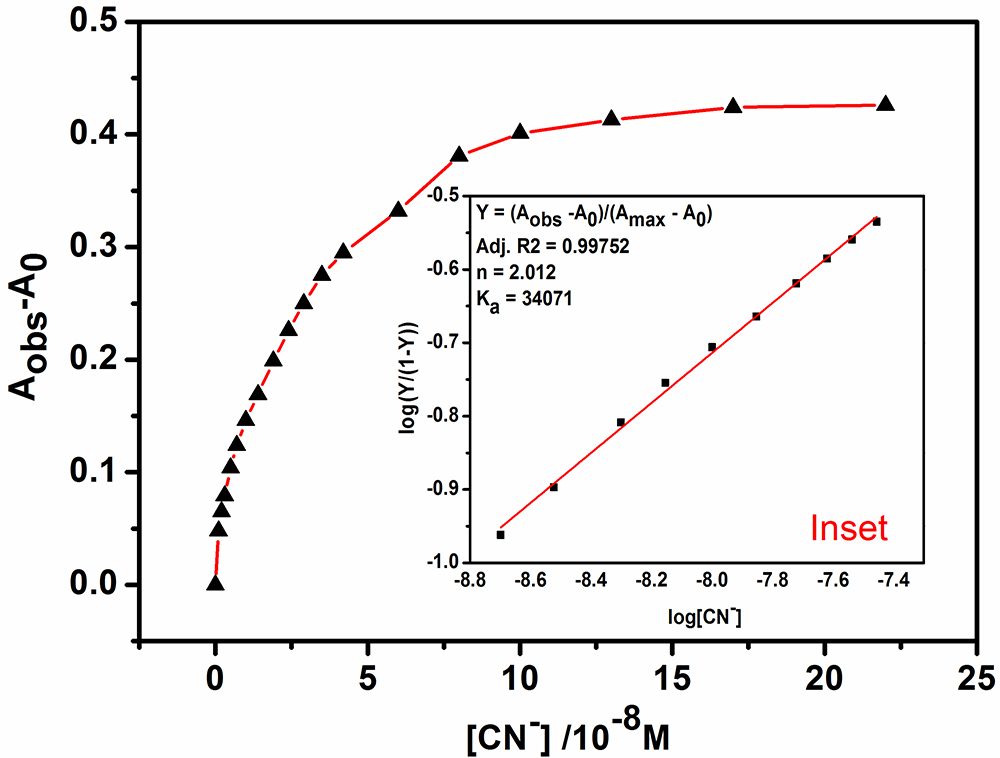
**Figure S3**. Visual color changes of **S1** (20 *μ*M) in (a) HEPES–DMSO (1:9, *V*/*V*, pH = 7.0); (b) HEPES–DMSO (2:8, *V*/*V*, pH = 7.0); (c) HEPES–DMSO (3:7, *V*/*V*, pH = 7.0); (d) HEPES–DMSO (1:1, *V*/*V*, pH = 7.0) (v/v) after addition of 10 equiv. corresponding anions (F−, Cl−, Br−, I−, AcO−, H2PO4−, ClO4−, HSO4−, SCN− and CN−, respectively).



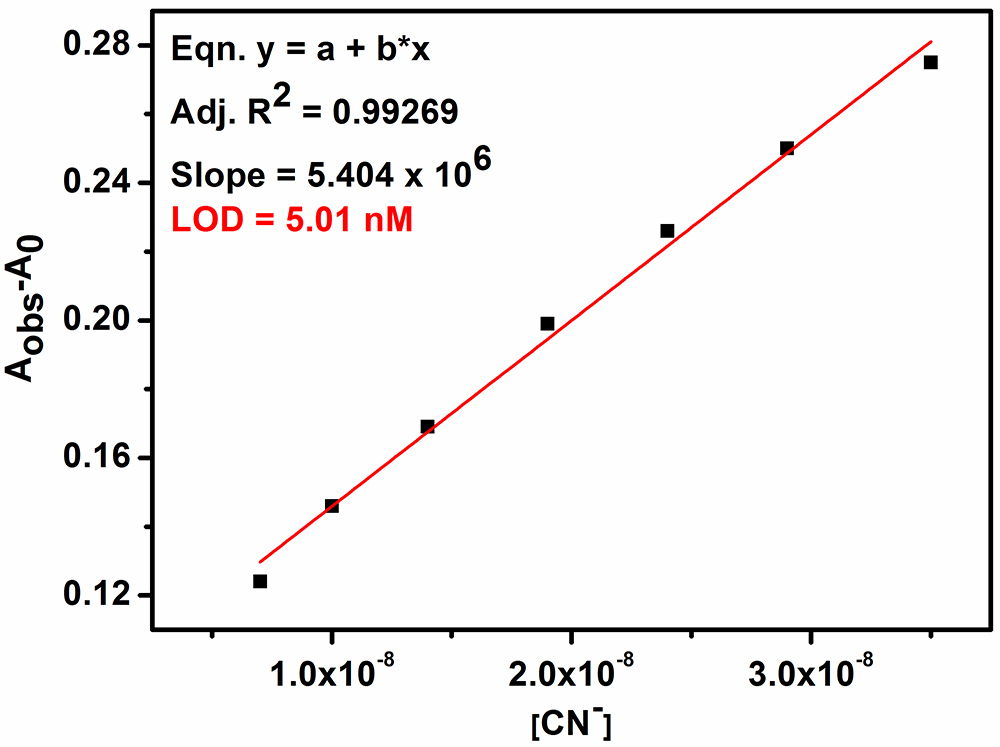
**Figure S4**. Linear plot of **S1** (20 *μ*M) against CN− ( 0 – 1.2 × 10-8 M) in HEPES–DMSO (1:9, *V*/*V*, pH = 7.0) for calculating detection limit of CN−.

**SD = =** 0.008412

LOD = 3 × SD **/** Slope = 3× 0.008412/(2.145 × 107)= 1.18 × 10-9 M



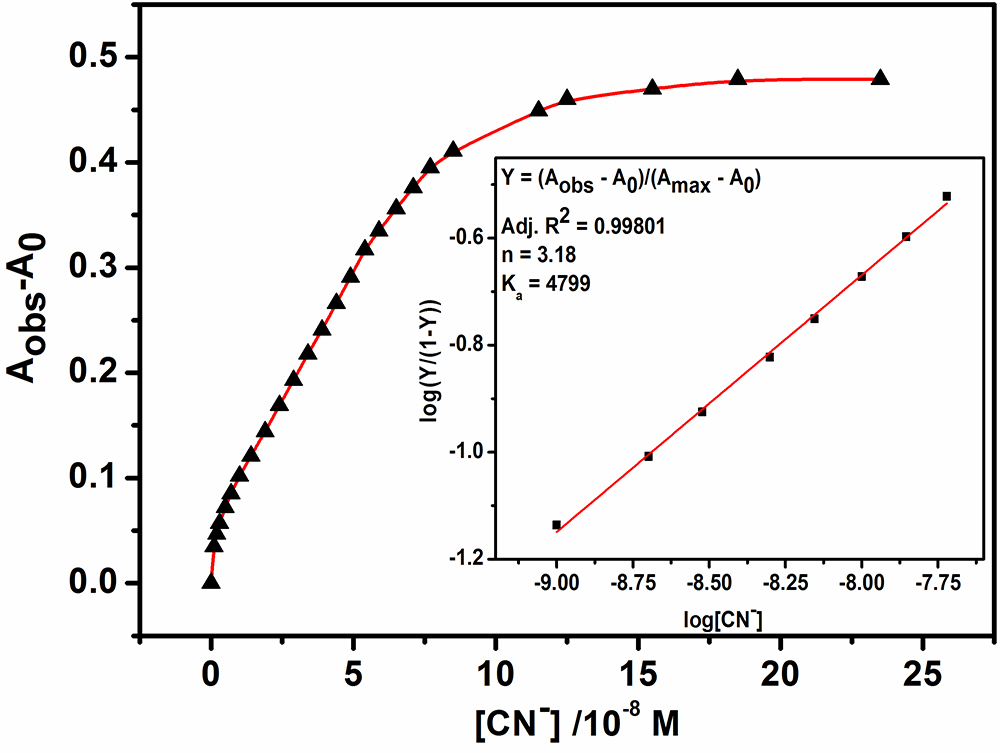
**Figure S5**. The resulting titration curve of **S1** with CN− in HEPES–DMSO (2:8, *V*/*V*, pH = 7.0) (Inset: the result of the Hill plot analysis)



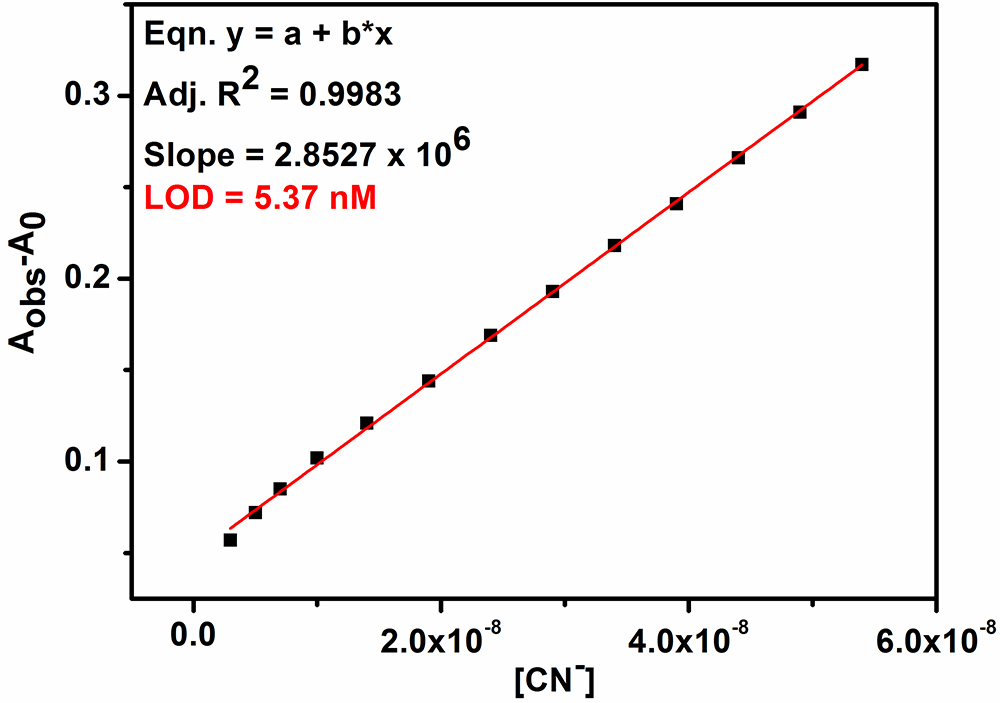
**Figure S6**. Linear plot of **S1** (20 *μ*M) against CN− ( 0 – 3.5 × 10-8 M) in HEPES–DMSO (2:8, *V*/*V*, pH = 7.0) for calculating detection limit of CN−.

**SD = =** 0.009018

LOD = 3 × SD **/** Slope = 3× 0.009018/(5.404 × 106)= 5.01 × 10-9 M



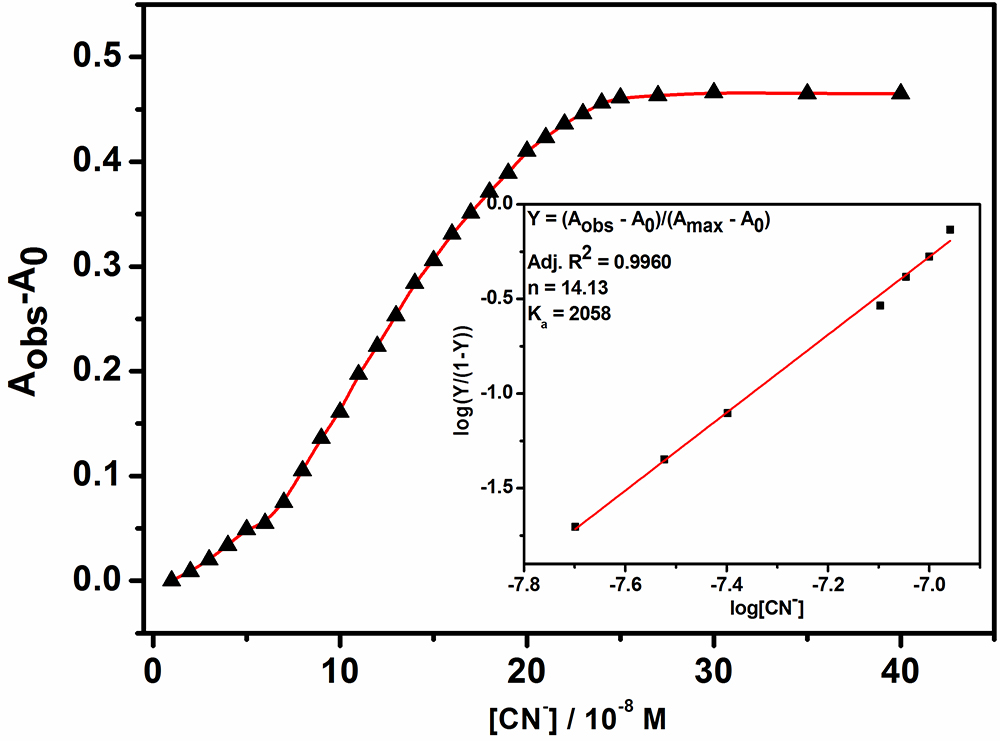
**Figure S7**. The resulting titration curve of **S1** with CN− in HEPES–DMSO (3:7, *V*/*V*, pH = 7.0) (Inset: the result of the Hill plot analysis)



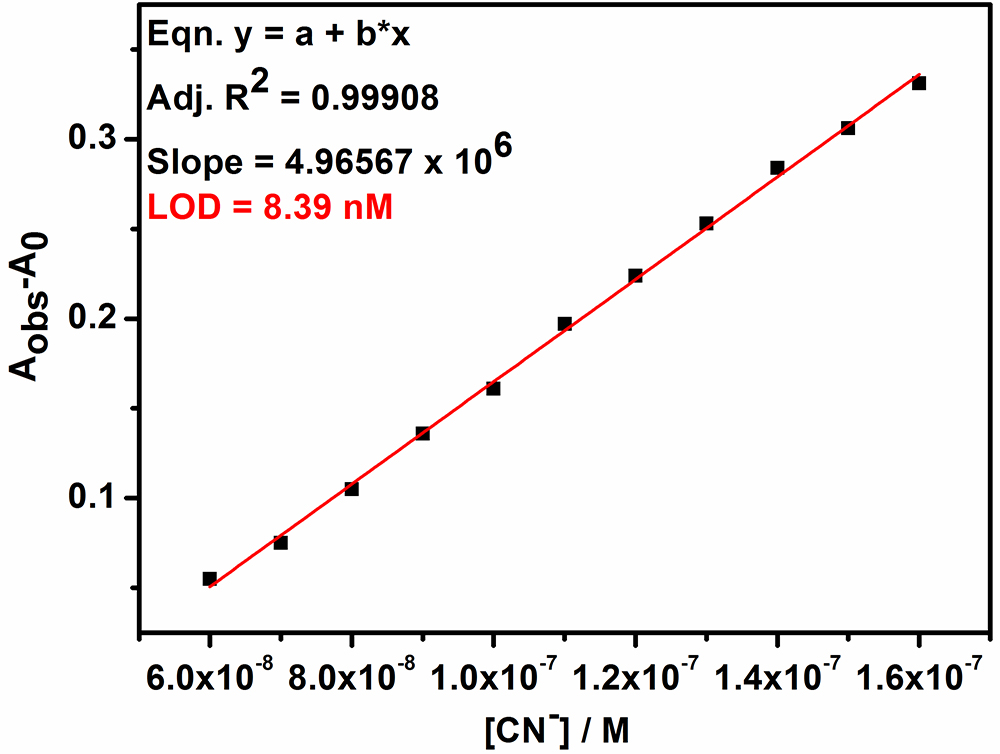
**Figure S8**. Linear plot of **S1** (20 *μ*M) against CN− ( 0 – 5.4 × 10-8 M) in HEPES–DMSO (3:7, *V*/*V*, pH = 7.0) for calculating detection limit of CN−.

**SD = =** 0.005106

LOD = 3 × SD **/** Slope = 3× 0.005106/ (2.8527 × 106 ) = 5.37 × 10-9 M



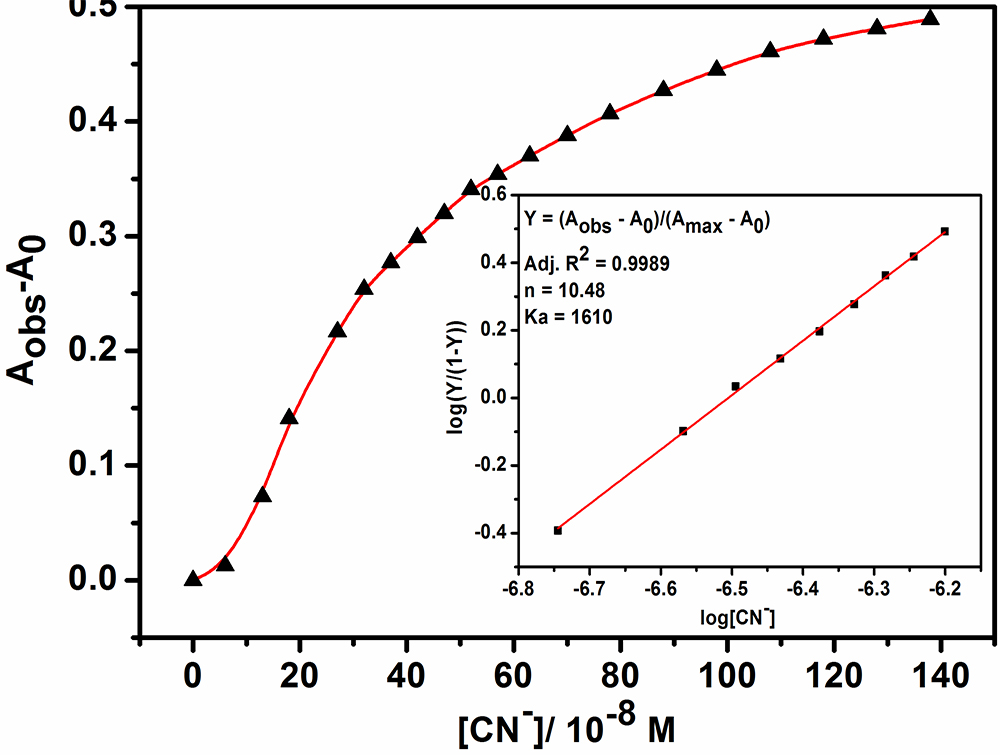
**Figure S9**. The resulting titration curve of **S1** with CN− in HEPES–DMSO (4:6, *V*/*V*, pH = 7.0) (Inset: the result of the Hill plot analysis).



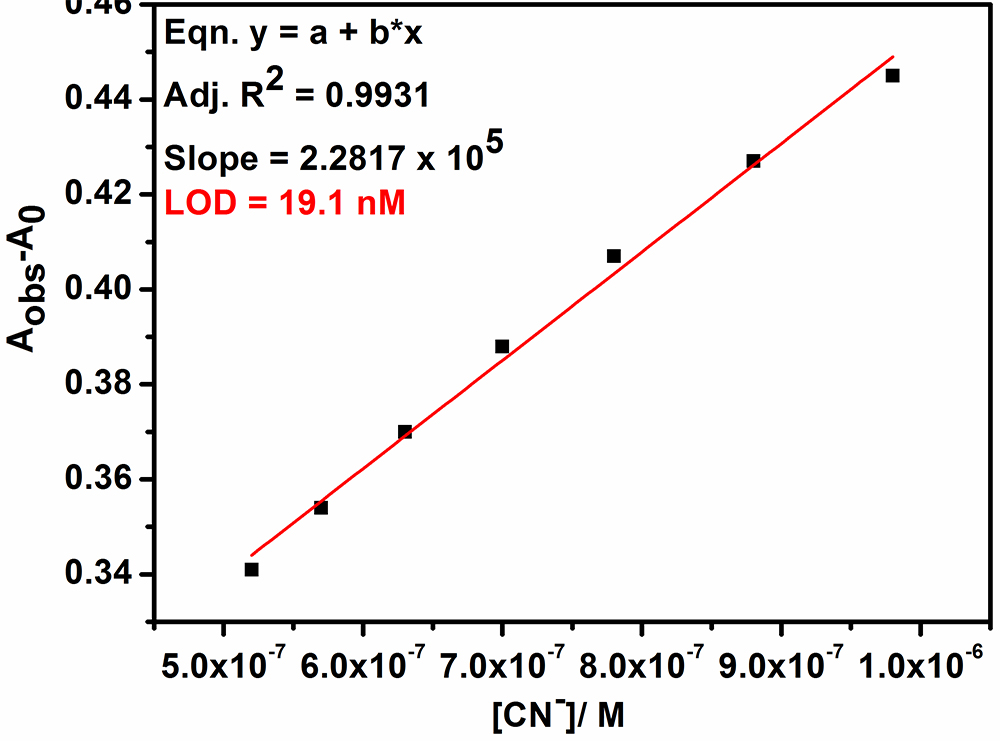
**Figure S10**. Linear plot of **S1** (20 *μ*M) against CN− ( 0 – 5.4 × 10-8 M) in HEPES–DMSO (4:6, *V*/*V*, pH = 7.0) for calculating detection limit of CN−.

**SD = =** 0.013895

LOD = 3 × SD **/** Slope = 3× 0.013895/(4.96567 × 106)= 8.39 × 10-9 M



**Figure S11**. The resulting titration curve of **S1** with CN− in HEPES–DMSO (1:1, *V*/*V*, pH = 7.0) (Inset: the result of the Hill plot analysis).



**Figure S12**. Linear plot of **S1** (20 *μ*M) against CN− ( 0 – 5.4 × 10-8 M) in HEPES–DMSO (1:1, *V*/*V*, pH = 7.0) for calculating detection limit of CN−.

**SD = =** 0.00145

LOD = 3 × SD **/** Slope = 3× 0.00145/(2.2817 × 105)= 19.1 × 10-9 M

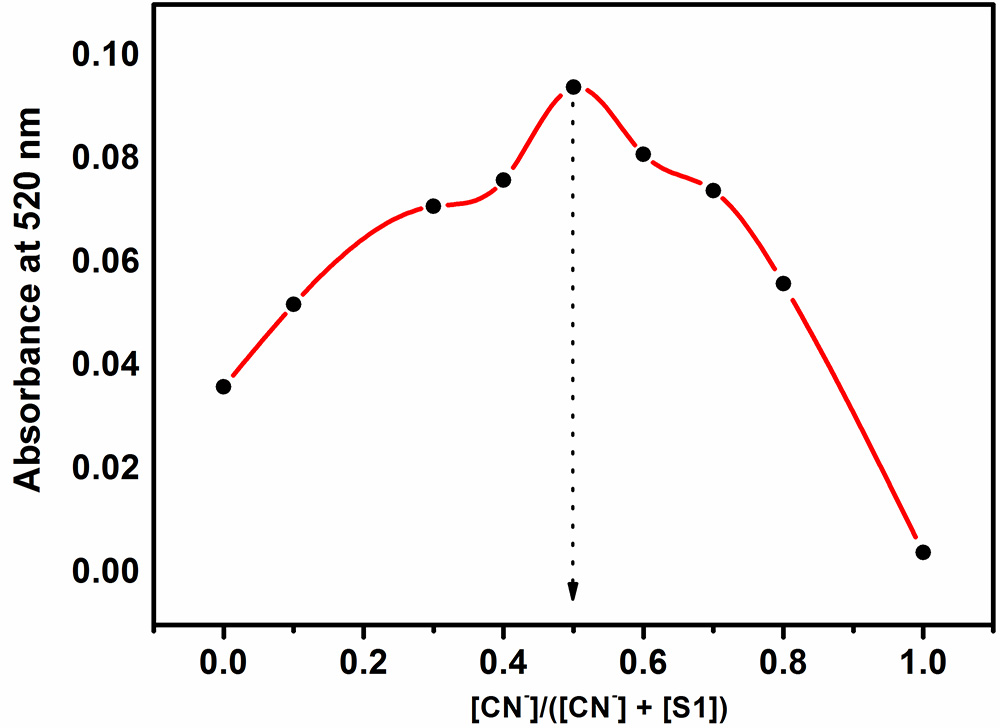


Figure **S13**. Jobs’ plot of **S1** with CN- ([S**1 + CN**−] = 20 *μ*M) in HEPES–DMSO (4:6, *V*/*V*, pH = 7.0) shows 1:1 stoichiometry.

C:\Users\yj\Desktop\WANGJUN160831_2NEG.tif

Figure **S14**. ESI-MS spectrum of **S1** afterthe addtion of excess of CN− (m/z: calcd for C19H12N5O3 : 358.0940 [**S1** - H+]-; found: 358.1638).

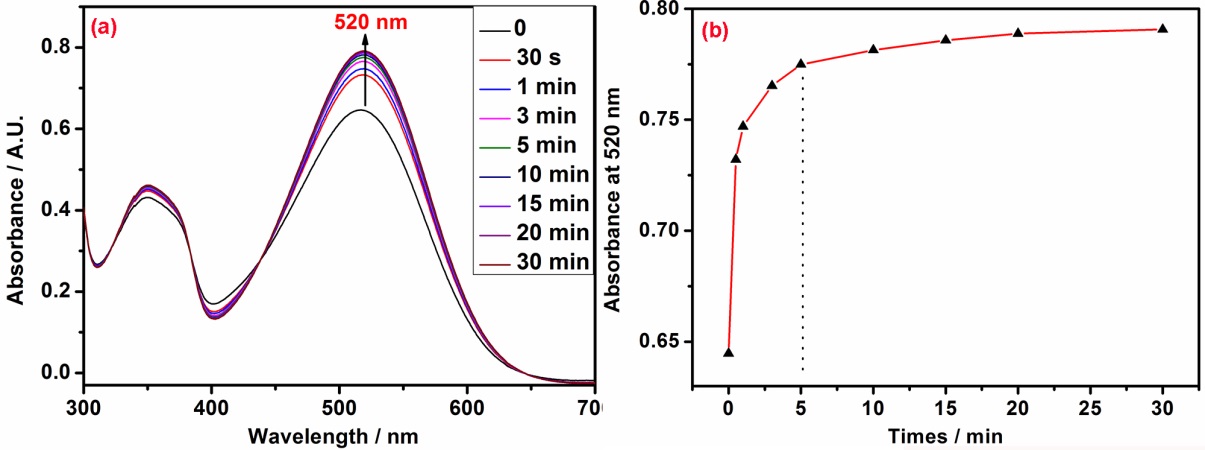
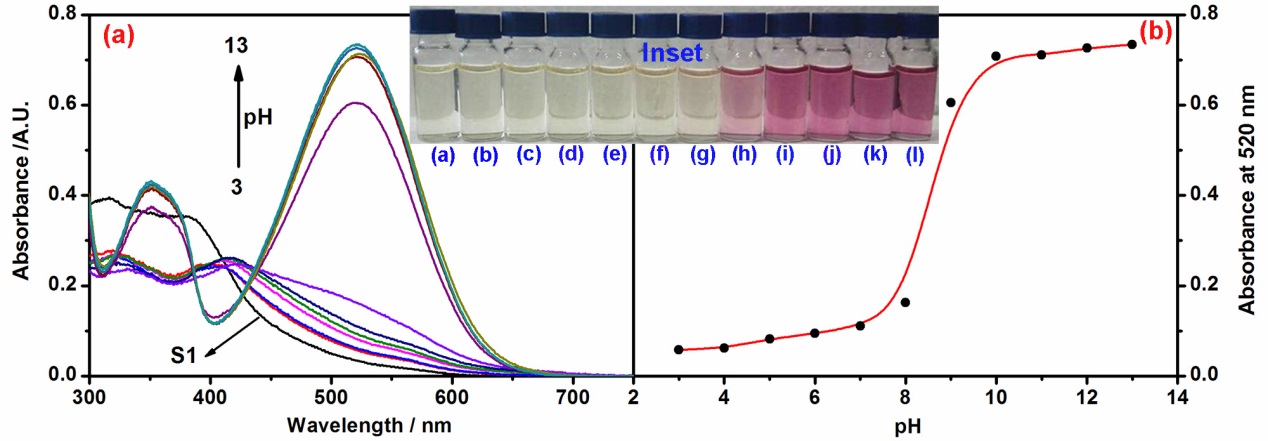
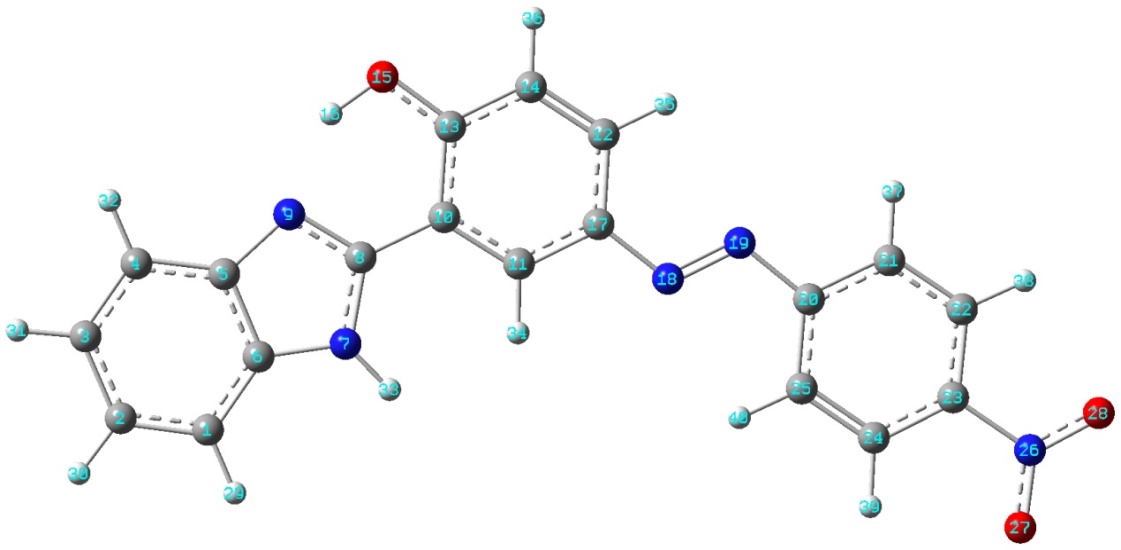


Figure **S15**. Effect of time (from 0 to 30 minutes) on the UV-vis spectra (a) and on the absorbance at 520 nm (b) for **S1** (20 *μ*M) in HEPES–DMSO (4:6, *V*/*V*, pH = 7.0) (*V/V*) solution after addtion of 10 equiv. CN−.



**Figure S16**. (a) Effect of pH (from 3 to13) on the UV-vis spectra for **S1** (20 *μ*M) in 40% H2O-60% DMSO (*V/V*) solution, pH values were controlled by the HEPES solution; (b) the change curve of **S1** with different pH values (Inset: color change of **S1** atdifferent pH values, (a) **S1** only, from (b) to (l) pH value is 3 to 13, respectively).



**Figure S17**. Labels of C, H, O, N atoms in optimized structure of **S1**.

Table **S1** representative interatomic distance

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| SN | O15-H16 | C13-O15 | C8-C10 | C8-N9 | C8-N7 | C8-N9 | N7-H33 | H16-N9 |
| S1 | 0.9980 | 1.3296 | 1.4561 | 1.3234 | 1.3744 | 1.4240 | 1.0063 | 1.7020 |

Table **S2** Correlative calculation results of different species

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| SN | *E* | *H* | *G* | *S* | HOMO | LUMO | ΔEa | ΔEa |
| units | a.u. | a.u. | a.u. | cal/(mol‧K) | eV | eV | kJ/mol | eV |
| CN− | -92.8616 | -92.8583 | -92.8806 | 47.019 |  |  |  |  |
| HCN | -93.4356 | -93.4321 | -93.4549 | 48.043 |  |  |  |  |
| **S1** | -1231.19 | -1231.17 | -1231.24 | 156.91 | -6.24 | -3.15 | 297.99 | **3.09** |
| **S1**-H | -1230.67 | -1230.65 | -1230.72 | 156.94 | -2.37 | -0.12 | 217.01 | **2.25** |

a: ΔE = Δ(LUMO-HOMO)

***Reference***

[1] [Balamurugan](https://pubs.rsc.org/en/results?searchtext=Author%3AGopal%20Balamurugan), G.; [Velmathi](https://pubs.rsc.org/en/results?searchtext=Author%3ASivan%20Velmathi), S. *Anal. Methods* **2016**, *8*, 1705-1710.