# Instant detection of cyanide in seafood with a tryptophan based fluorescence probe

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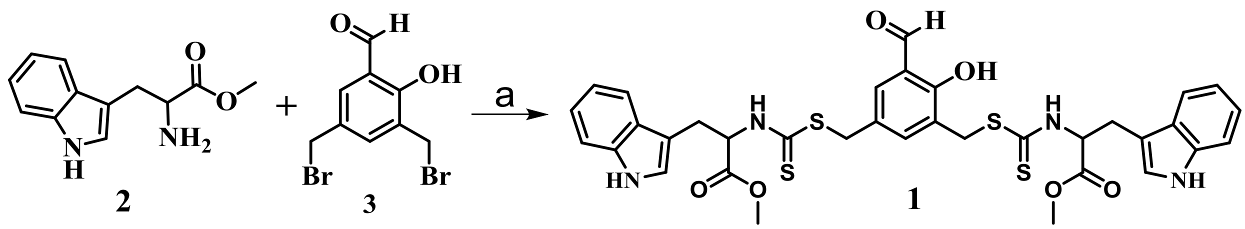
## CONTENTS

1. **Experimental details**

   **Synthesis**



a = Dioxane/$H_2O$, (3:1, v/v), $K_2CO_3$, $CS_2$, 25 °C, **50%**

**Scheme S1**. Synthetic scheme of probe **1**

Compound **2**[1] and compound **3**[2] were prepared following the reported method and compound **1** was synthesized following the reported method of bipodal thiocarbamate synthesis.[3]

**dimethyl 2,2'-(((((5-formyl-4-hydroxy-1,3-phenylene) bis(methylene)) bis(sulfanediyl)) bis(carbonothioyl))bis(azanediyl))bis(3-(1H-indol-3-yl)propanoate) (1)**

Methyl-2-amino-3-(1H-indol-3-yl)propanoate (0.1 g, 0.459 mmol) and $K_2CO_3$ (0.13 g, 0.918 mmol) in dioxane/water (1:4, v/v) was stirred for 5 minutes at 0 °C. Carbon disulfide (1.39 g, 1.10 mL, 18.36 mmol) was added and the mixture was stirred for another 5 minutes. 3,5-*bis*(bromomethyl)-2-hydroxybenzaldehyde (0.07 g, 0.229 mmol) dissolved in dioxane was subsequently added to it dropwise over a period of 10 minutes. The solution was allowed to attain room temperature (25 °C) and stirred for another 60 minutes. The yellowish solution thus obtained was concentrated under reduced pressure and the residue was dissolved in dichloromethane (20 mL). The organic layer was washed with $H_2O$ (20 mL), dried over anhydrous $Na_2SO_4$ and the volatiles were removed under reduced pressure, which on chromatography ($CH_2Cl_2$/$CH_3CN$, 19:1, v/v) yielded compound **1** as a white solid ( 0.17 g, 51%); mp 118-120 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 11.25 (s, 1H, ArOH), 9.59 (s, 1H, ArCHO), 8.22 (s, 1H, ArNH), 8.16 (s, 1H, ArNH), 7.65-7.64 (m, 1H, ArH), 7.52-7.48 (m, 2H, ArH), 7.46-7.40 (m, 2H, ArH), 7.32-7.25 (m, 3H, ArH), 7.17-7.14 (m, 2H, ArH), 7.09-7.01 (m, 2H, ArH), 6.83 (s, 2H, ArH), 5.51-5.48 (m, 2H, $CHCO_2Me$), 4.38-4.31 (m, 4H, $ArCH_2$), 3.67 (s, 3H, $CO_2Me$), 3.66 (s, 3H, $CO_2Me$), 3.58 (d, $J$ = 5.36, 1H, C**H**$_2$CH), 3.55 (d, $J$ = 5.32, 1H, C**H**$_2$CH), 3.37 (d, $J$ = 4.56, 1H, C**H**$_2$CH), 3.33 (d, $J$ = 4.60, 1H, C**H**$_2$CH). $^{13}$C NMR (125 MHz, $CDCl_3$) δ:

197.0, 196.7, 196.2, 171.2, 158.3, 138.1, 135.9, 133.2, 127.9, 127.3, 125.5, 123.1, 123, 122.2, 119.8, 119.7, 118.4, 118.3, 111.4, 111.2, 109.1, 108.9, 66.9, 59.4, 52.6, 38.4, 32.6, 26.5. $\lambda_{abs}$ in $CH_3CN$ (nm, ε): 270 ($1\times10^5$), 340 (5916), 400 (910). FT–IR (KBr, $cm^{-1}$): 3362, 3401, 2958, 2923, 1733, 1649, 1457, 1339, 1213, 772, 744. ESI-MS calculated for $C_{35}H_{34}N_4O_6S_4K^+$ 734.0998, found 734.0997.

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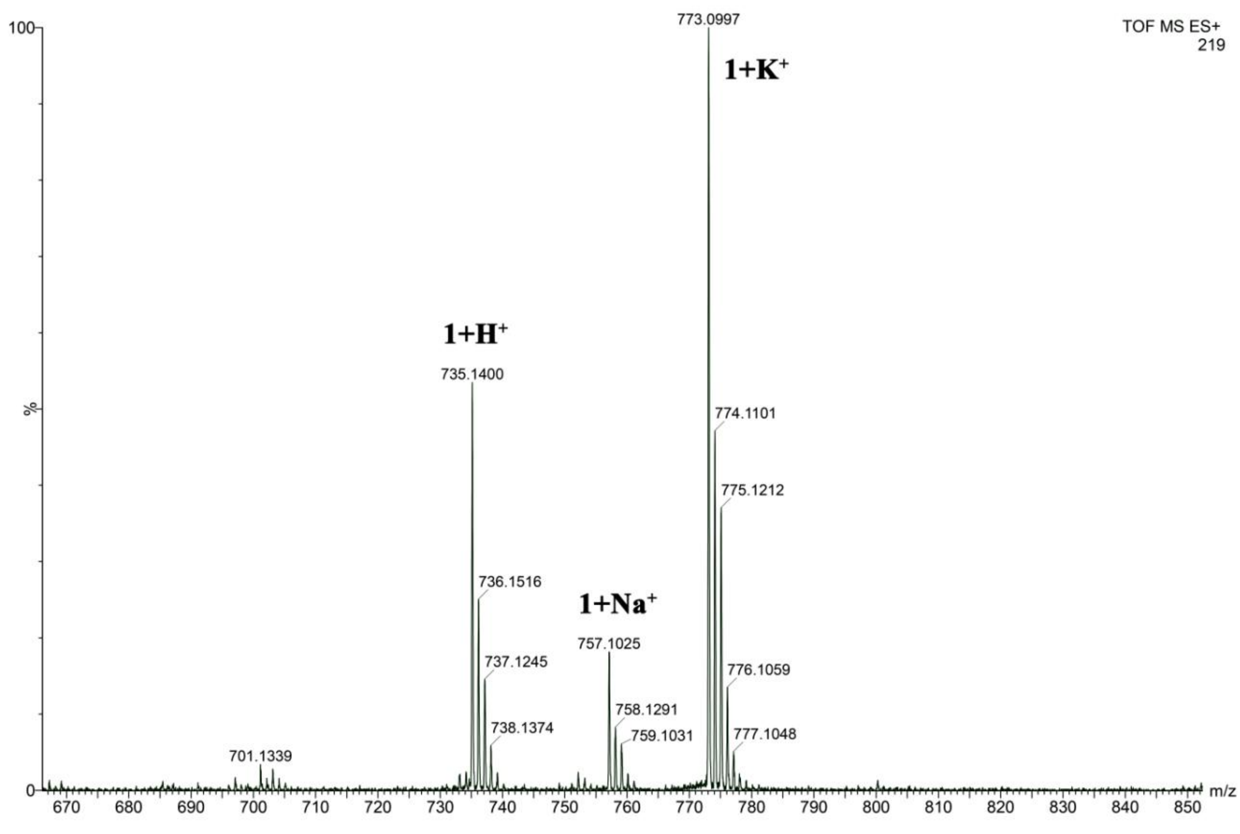


**Figure S1.** ESI mass spectrum of the compound **1**.

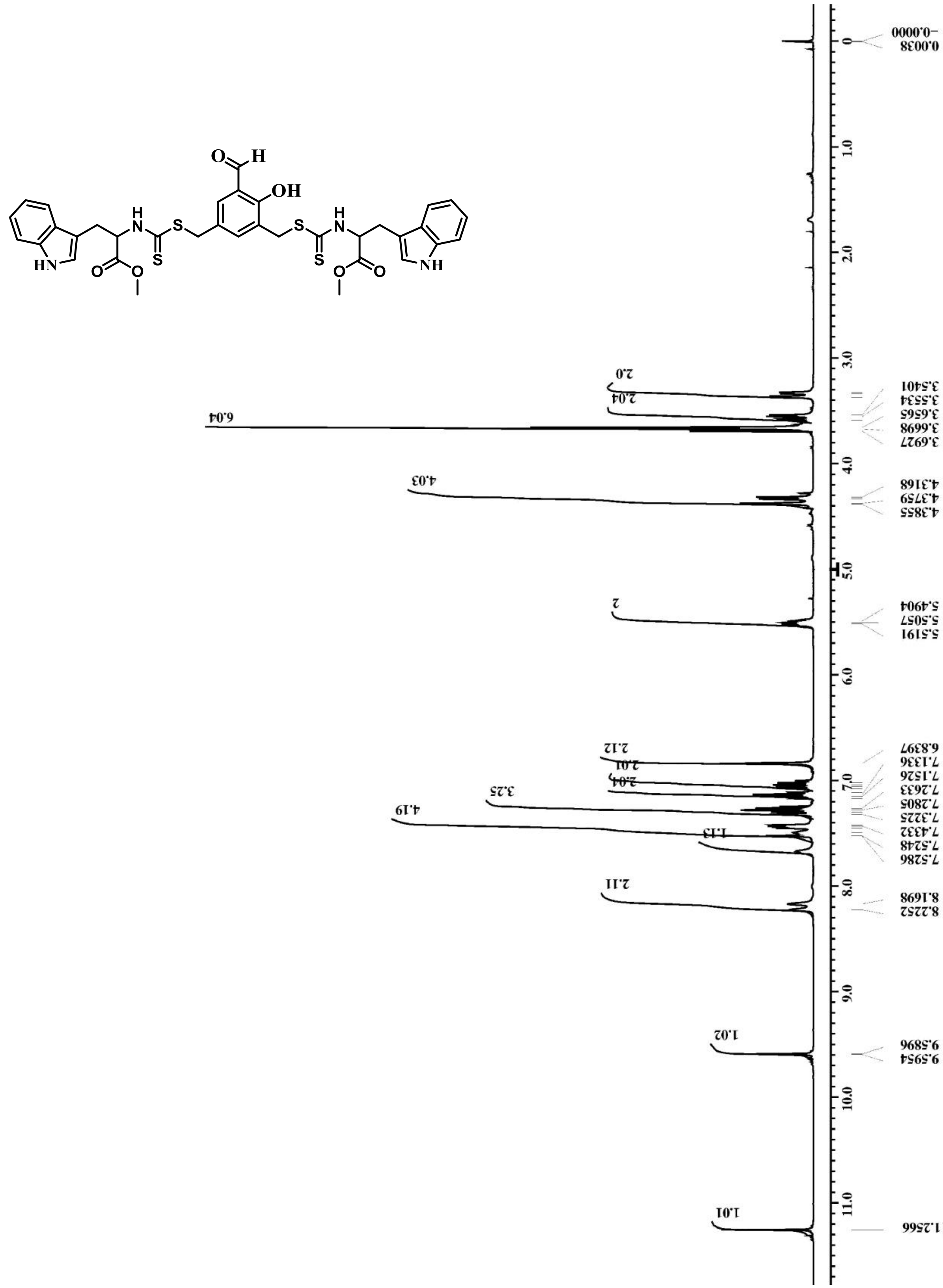

**Figure S2.** $^{1}$H NMR spectrum of chemosensor **1** in $CDCl_3$.

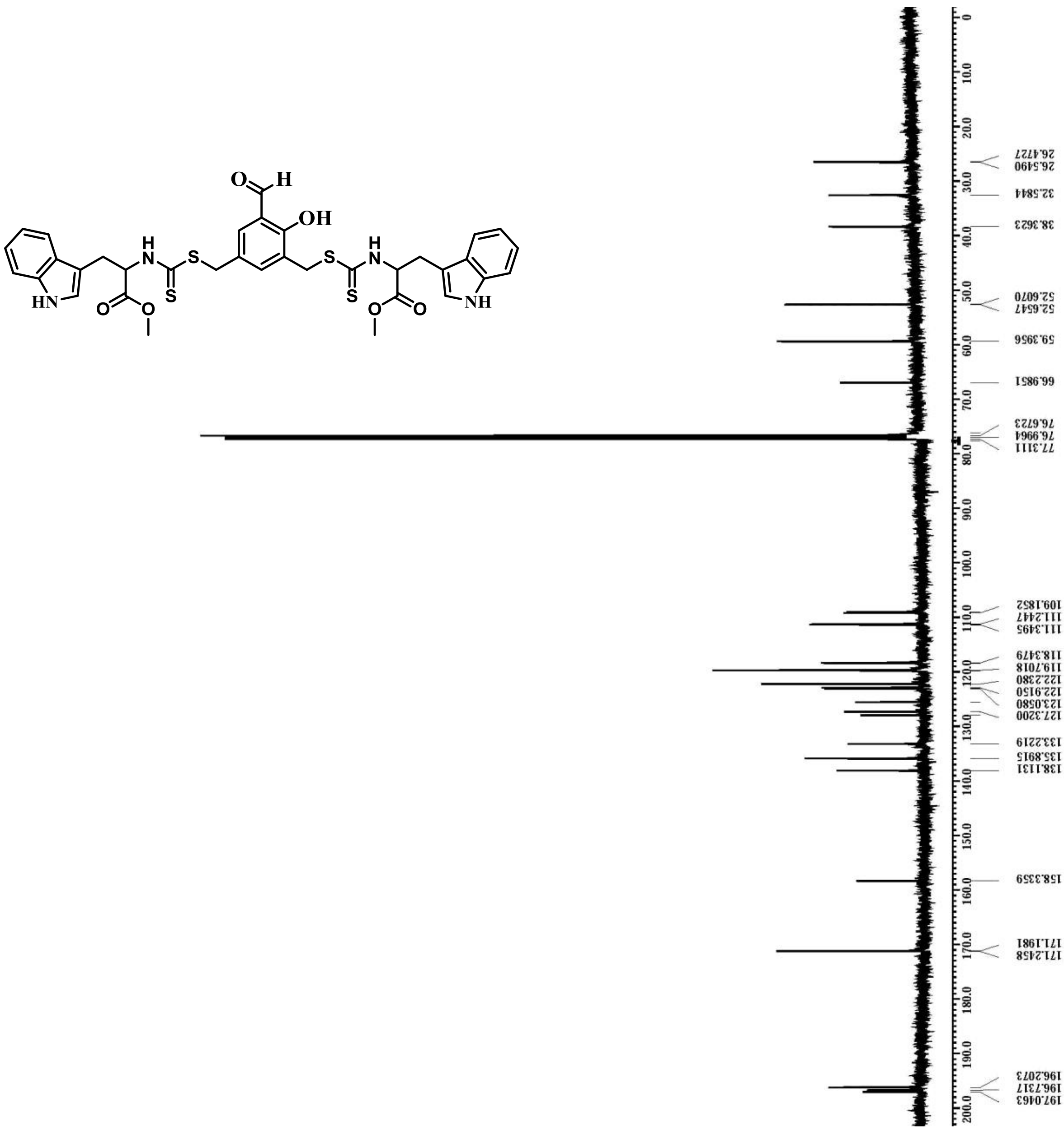


**Figure S3.** $^{13}$C NMR spectrum of chemodosimeter of **1** in $CDCl_3$.

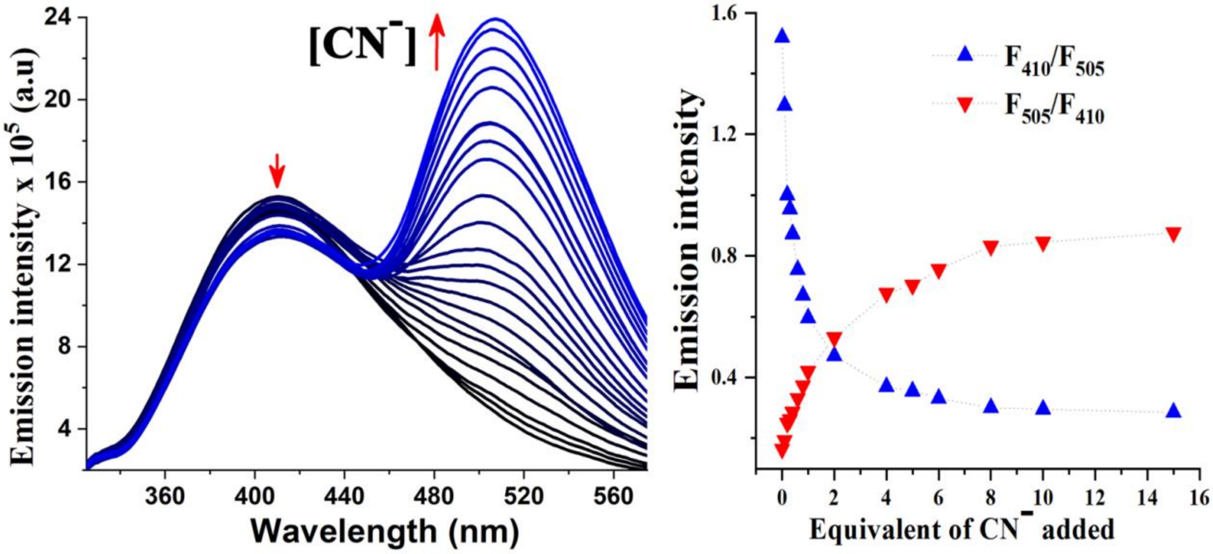


**Figure S4.** (A) Emission spectra of **1** (10 μM) with increasing concentration of CN⁻; (B) Ratiometric behavior of **1** (10 μM) with an increasing concentration of CN¯ (0 to 150 μM) in mixed organic–aqueous media ($CH_3CN/H_2O$, 5:1, v/v).

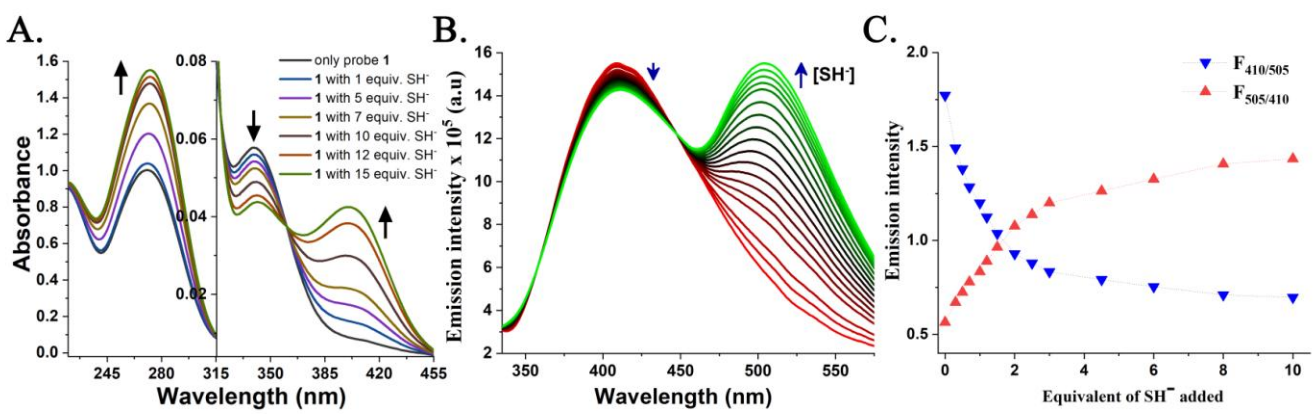


**Figure S5.** (A) UV-vis response of **1** (10 μM) upon addition of SH¯ (150 μM) in mixed media ($CH_3CN/H_2O$, 5:1); (B) Emission spectra of **1** (10 μM) with increasing concentration of SH⁻; (C) Ratiometric behavior of **1** (10 μM) with an increasing concentration of SH¯ (0 to 150 μM) in mixed organic–aqueous media ($CH_3CN/H_2O$, 5:1, v/v).

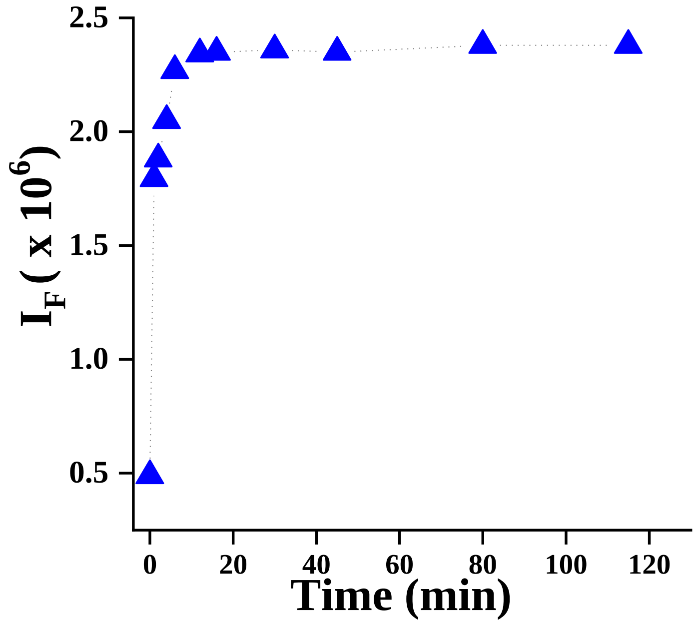


**Figure S6.** Time dependence fluorescence change of chemosensor **1**(10 μM) in presence of $CN^-$ (60 μM) in mixed solvent media.

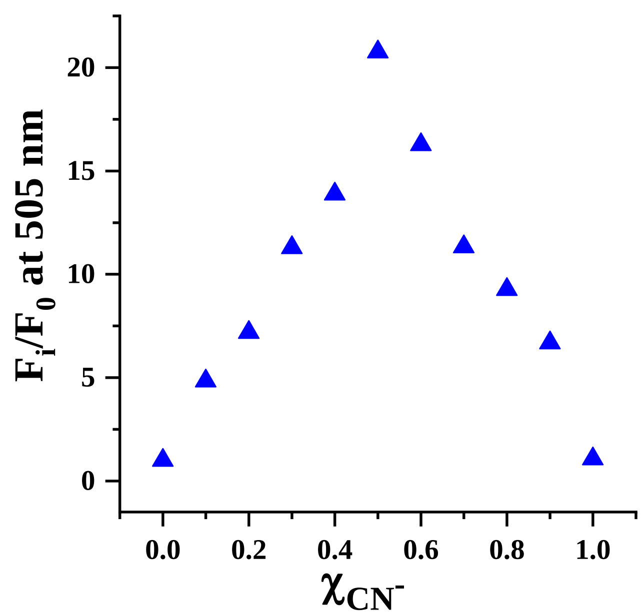


**Figure S7.** Job's plot of **1** with $CN^-$ in mixed organic–aqueous media ($CH_3CN/H_2O$, 5:1, v/v). The total concentration of chemosensor and $CN^-$ kept constant at 8 μM.

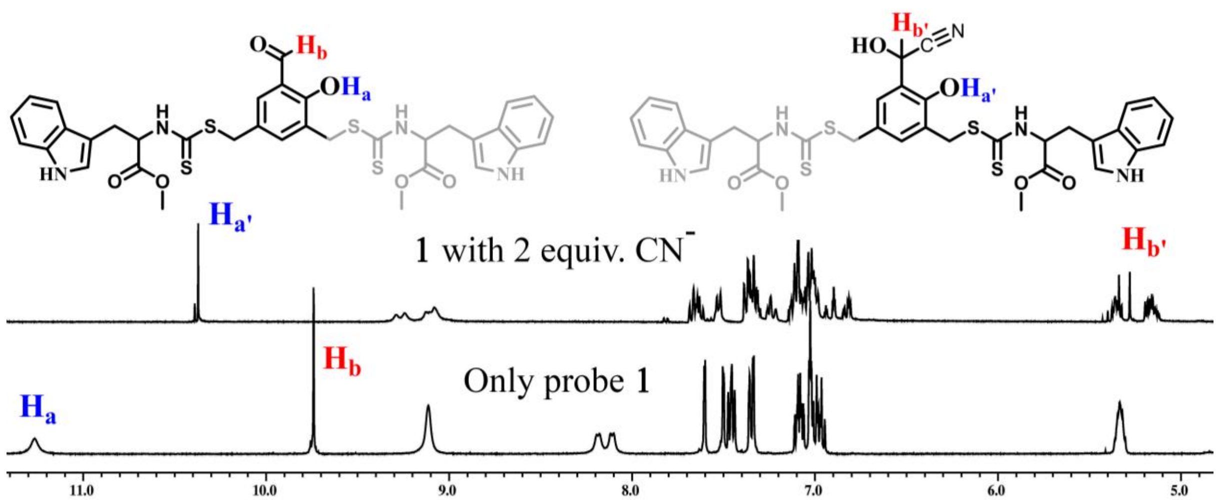


**Figure S8.** $^{1}$H NMR chemical shift of chemodosimeter **1** (10 mM) upon addition of $CN^{-}$ (TBA–CN) in $CD_3CN$.

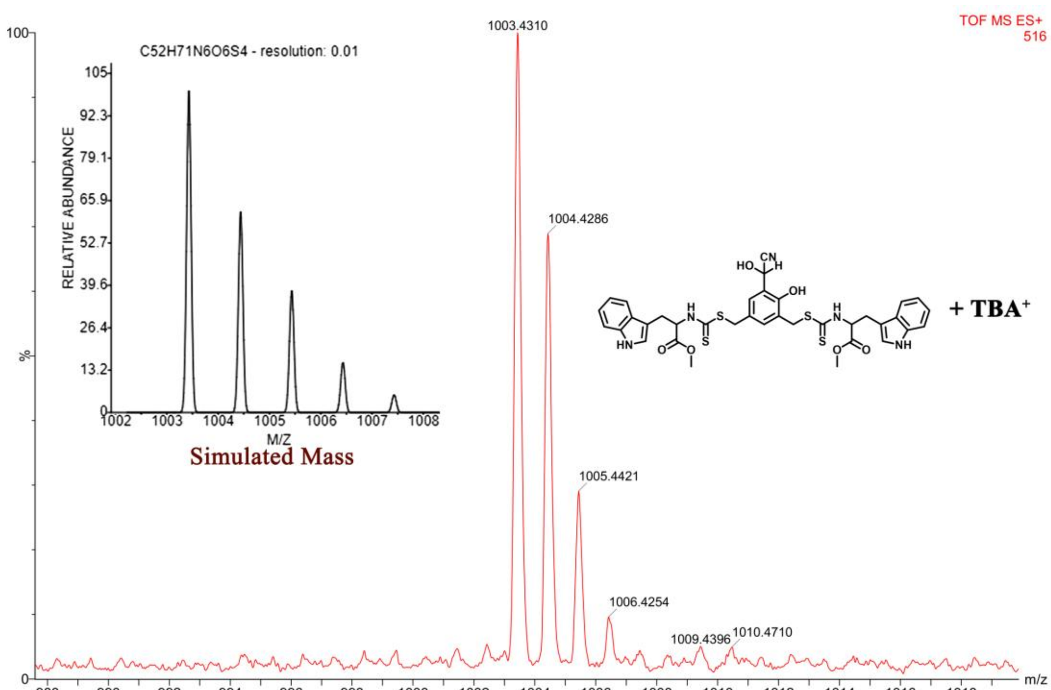


**Figure S9.** ESI-MS isotopic distribution of the $C_{52}H_{71}N_6O_6S_4$ (1-CN + $TBA^{+}$) fragment. The simulated distribution is given in the inset.

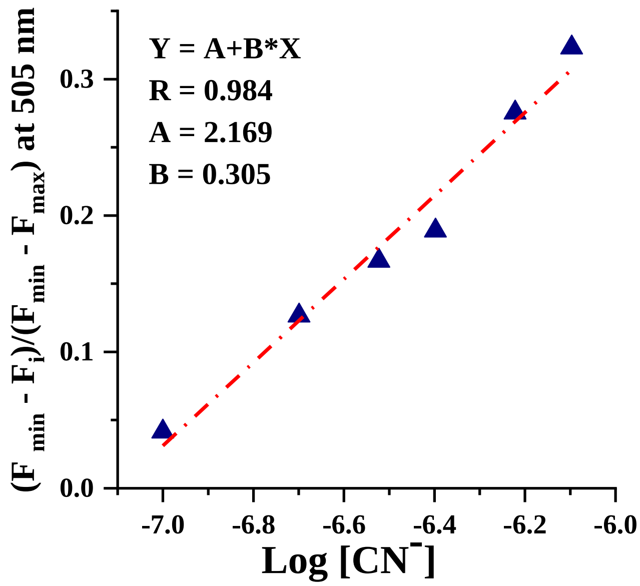


**Figure S10.** Determination of detection limit of chemodosimeter **1** (10 µM) from fluorescence titration in mixed solvent medium ($CH_3CN/H_2O$, 5:1, v/v) at 25 $^{o}$C. The detection limit of chemosensor is 77 nM.

## 2. Determination of cyanide in HeLa S3

Chemosensor **1** was used for the detection of $CN^-$ ion in cells with a fluorescence imaging experiment by using a confocal laser scanning microscope (CLSM). Human epithelial carcinoma cells HeLa S3 were cultured at 37°C in Dulbecco's Modified Eagle's Medium (DMEM), supplemented with 10% fetal bovine serum (FBS), 100 units/mL penicillin,100 µg/mL streptomycin and 5% $CO_2$. Cells ($0.2 \times 10^6$ per mL) were plated on 12 mm sterile cover-slips and were allowed to adhere for 24 h. The cultured cells were first exposed to cyanide ($CN^-$) (40 µM) dissolved in DMEM for 30 min at 37 °C. The cells were washed twice with PBS to remove the retained $CN^-$ ions followed by incubation with dye **1** (10 µM in DMSO) in PBS for 5 min at 25 °C. After incubation, cells were washed twice with PBS to remove residual dye and fixed with 4% paraformaldehyde for 10 minutes. The cells fixed on the cover-slips were washed once and mounted on glass slide and observed under microscope.[4] The slides were observed under Carl Zeiss CLSM-710 (Axio observer microscope version Z.1) microscope using 405 nm excitation argon laser with MBS (main beam splitter) and the observed emission ranged from 515–540 nm. The image acquisition was done under X40 oil immersion lens (NA: 1.3). The frame size of 512 × 512 (8-bit image) was maintained using the software provided (Zen 2010) along with the microscope. The fluorescence imaging obtained by CLSM revealed marked differences in intensity of intracellular fluorescent of $CN^{-}$ strained cells compare to the controls. The fluorescence image of HeLa S3 treated with **1** (Figure 1B, iii) under the same conditions showed weak intercellular fluorescence. In contrast, cells treated with both $CN^{-}$ and dye showed a vivid intercellular fluorescence (Figure 1B, iv). Thus, chemosensor **1** can be used to detect the intracellular $CN^{-}$.

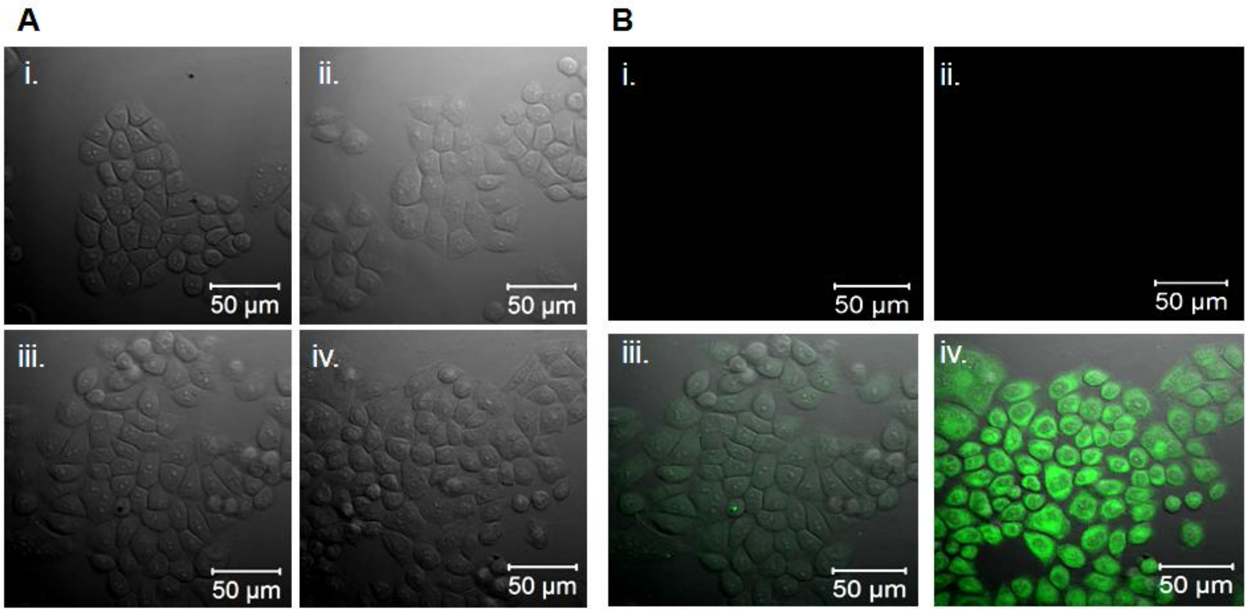


**Figure S11.** Confocal laser scanning microscopic images of HeLa S3: (A) DIC image; (B) corresponding fluorescent images of (i) Only cells; (ii) Cells treated with cyanide salt (40 μM) for 30 min; (iii) Cells treated with dye (10 μM) for 5 min at 37 °C; (iv) Cells treated with cyanide salts (40 μM) for 30 min at 37 °C followed by dye (10 μM) for 5 min at 25 °C. Images are representative of two independent experiments.

### 3. Visual detection of cyanide in shellfish

Chemosensor **1** was used for the detection of cyanide in the adult shellfish. The adult shrimps were treated with aqueous solution of $CN^{-}$ (100 μM) for 1 h at 25 °C followed by washed with PBS to remove any $CN^{-}$ ion adhering to the surface, and were subsequently treated with a solution of dye **1** (100 μM) for 30 min followed by washed with PBS and observed under 366 nm light. The visual images taken with a digital camera (Figure 7) shows striking differences of the samples compared to the controls. The control shellfish incubated with only **1** faintly illuminated, in contrast, the fish exposed to both the dye and $CN^{-}$, a sprightly illuminated yellowish color was observed.

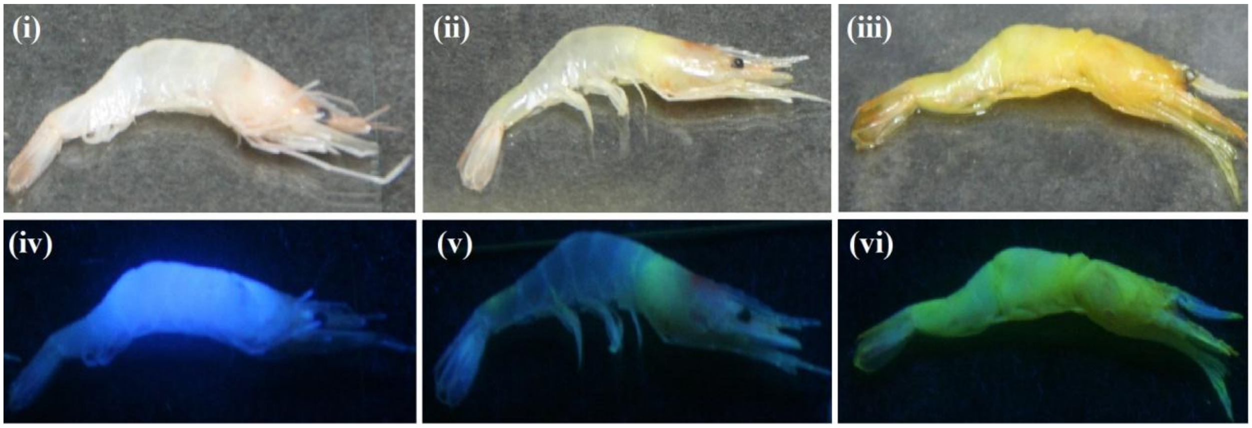


**Figure S12.** Image of fish under visible (panel i, ii, iii) and 366 nm (panel iv, v, vi) light. Fish stained with **1** (100 µM) for 30 min; fish incubated with $CN^{-}$ and subsequently stained with **1** with 0 min (i, iv), 15 min (ii, v,), 30 min (iii, vi) at 25 °C.

## 4. Detection of cyanide in gel samples

Chemosensor **1** was used for the detection of cyanide in the gel samples. Semisolid cyanide containing gel was prepared on addition of alcohol to a saturated solution of calcium acetate and cyanide (10 µM). Cyanide containing gel sample was then exposed with dye **1** (10 µM) and a series of image were taken with a digital camera in different time intervals displayed increased in the bright fluorescence with time. The results demonstrated that dye **1** can be used for the detection of cyanide in the gel samples.

## 5. Detection of cyanide: Paper based strip approach

The positive results of our chemosensor for the detection of $CN^-$ in solution, gel and in cells encouraged us to fabricate a simple paper strip that could detect $CN^-$ ion. Whatmann 1 filter papers of the dimension 5 cm × 0.75 cm was coated with the acetonitrile solution of **1** (100 µM) and was air dried. Careful dipping the dye co ntaining strips to the aqueous solution of $CN^-$ quickly switched the emission color from colorless to deep green under 366 nm UV light.

**Table S1**. Comparison of chemosensor **1** with other probes reported in the literature.

| **S. NO.** | **References** | **Solvent system used for cyanide sensing** | **Detection limit of $CN^-$ ions in solution.** | **Ability to detect cyanide in paper strips and LOD** | **Ability to detect cyanide in fish** | **Ability to detect cyanide in cells** | **Ability to detect cyanide in gel** |
|---|---|---|---|---|---|---|---|
| 1 | *ACS Sens.*, **2016**, *1*, 1265−1271 | HEPES:DMSO (99:1) | 5.77 µM | No | No | Yes (copper complex) | No |
| 2 | *Anal. Chem.*, **2016**, *88*, 6805−6811 | $H_2O$/MeCN (7/3 v/v) | 1 µM | No | No | No | No |
| 3 | *Chem. Commun.*, **2015**, *51*, 8809--8812 | MeCN | 13 µM | No | No | No | No |
| 4 | *Anal. Chem.*, **2015**, *87*, 12396−12403 | $H_2O$/MeCN (1/3 v/v) | 0.23 µM | Yes | No | No | No |
| 5 | *Chem. Asian J.*, **2014**, *9*, 3291 – 3298 | Buffer/$CH_3CN$ (1:3 v/v) | 0.12 µM | Yes | No | No | No |
| 6 | *Anal. Chem.*, **2014**, *86*, 4648−4652 | THF/H2O (8:2) | 2.4 µM | No | No | No | No |
| 7 | *Chem. Commun.*, 2013, **49**, 2912-2914 | $CH_3CN$:$H_2O$ (1:1) | 1.6 mM | No | No | No | No |
| 8 | *Dalton Trans.*, 2013, 42, 4450–4455 | EtOH–$H_2O$ (8 : 2) | 0.026 ppm | No | No | No | No |
| 9 | *Org. Lett.*, 2013, 15, 2386-2389 | DMSO/$H_2O$(99:1) | 0.2 ppm | No | No | No | No |
| 10 | *Dalton Trans.*, 2012, 41, 9607–9610 | $CH_3CN$ | 5 µM | Yes (1 mM) | No | No | No |
| 11 | *Chem. Commun.*, 2011, **47**, 12843–12845 | MeOH/$H_2O$ (1:1) | 0.6 µM | No | No | No | No |
| 12 | *Org. Lett.*, 2011, 13, 3730-3733 | $CH_3CN$ | 0.328 µM | No | No | No | No |
| 13 | *Org. Lett.*, 2011, 13, 5056-5059 | $H_2O$/DMSO (copper complex) | * | No | No | YES (copper complex) | No |
| 14 | *Chem. Eur. J.* 2011, 17, 2057 – 2062 | MeOH/$H_2O$ (4:6) | 50 ppb | No | No | No | No |
| 15 | *Chem. Commun.*, 2013, **49**, 7812--7814 | $H_2O$ | 0.32 µM (AIE) | YES | No | No | No |
| 16 | *Org. Lett.*, 2010, 12, 3406-3409 | $CH_3CN$/$H_2O$ (1:1) | 0.06 ppm | No | No | Yes | No |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 17 | *Chem. Commun., 2009,* 2866–2868 | (0.02 M HEPES)(copper complex) | * | No | No | Yes (copper complex) | No |
| 18 | *Org. Biomol. Chem.*, 2011, **9**, 4954–4958 | DMF/$H_2O$ (9:1) | 0.44 µM | No | No | No | No |
| 19 | *Tetrahedron Letters* 2008, 49, 4102–4105 | $CH_3CN/H_2O$ (9:1) | * | No | No | Yes | No |
| 20 | *Inorg. Chem.*, **2013**, *52* , 4890–4897 | $CH_2Cl_2$ | 6 µM | No | No | No | No |
| 21 | *Org. Biomol. Chem.*, 2008, **6**, 3038–3040 | $CH_3CN/H_2O$(95:5) | 0.51 µM | No | No | No | No |
| 22 | *J. Org. Chem.* **2006**, *71*, 9470-9474 | $CH_3CN$ | 10 µM | No | No | No | No |
| 23 | *Chem. Commun*., 2005, 5260–5262 | $CH_3CN$ | 10 ppm | No | No | No | No |
| 25 | *J. Org. Chem.* **2009**, *74*, 4849–4854 | MeOH/$H_2O$ (10:1) | 3 µM | No | No | No | No |
| **25** | **Present Manuscript** | **$CH_3CN/H_2O$ (5:1)** | **77 nM** | **Yes (0.1 mM)** | **Yes** | **Yes** | **Yes** |

* Not mentioned

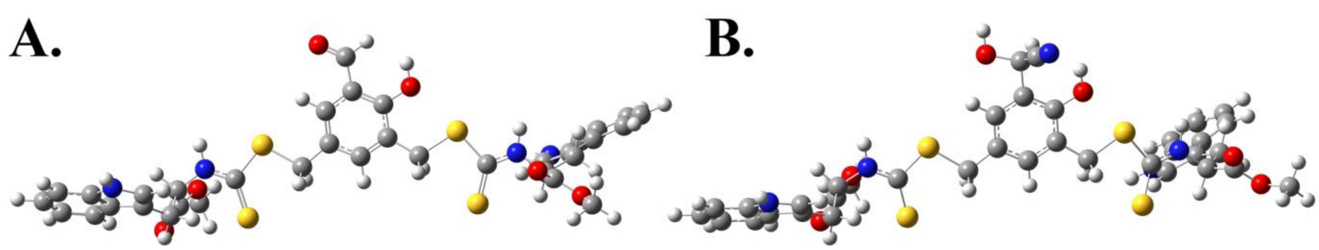


**Figure S13.** (a) The calculated energy minimized structures of (a) the probe **1** and (b) the $CN^-$ bound **1** obtained from the DFT calculation with 6-311G basis.

## 6. DFT computational results:

Cartesian coordinates (X, Y, Z) table and the free energies in atomic unit (a.u.) for the optimized structure of the receptor **1** calculated by DFT methods at the B3LYP/6-311G(d) level.

Receptor **1**  E = -3598.39749949 a.u.

| | | | |
|---|---|---|---|
| C | -1.11252500 | -0.53810100 | 2.35723000 |
| C | -1.10218900 | -0.36459400 | 0.98408900 |
| C | 0.13469200 | -0.46637700 | 0.32088500 |
| C | 1.32982000 | -0.73297700 | 0.98901400 |
| C | 1.29991500 | -0.90679900 | 2.38600200 |
| C | 0.06990100 | -0.80650300 | 3.06435200 |
| C | -2.32523900 | -0.07980900 | 0.13452800 |
| C | 2.56166700 | -0.82281500 | 0.09815400 |
| C | -0.05711600 | -0.97552300 | 4.51745600 |
| O | 2.50208500 | -1.16125900 | 2.99762300 |
| O | -1.12813700 | -0.88183900 | 5.13538300 |
| S | 4.24552300 | -1.09592900 | 0.96004200 |
| C | 5.34156100 | -1.04837600 | -0.53923500 |
| N | 6.62005500 | -1.24147300 | -0.19538100 |
| S | 4.79201400 | -0.74585200 | -2.14169300 |
| S | -3.88057900 | 0.12899700 | 1.20855400 |
| C | -5.14498700 | 0.54108600 | -0.08945200 |
| S | -4.78286100 | 0.69172500 | -1.75482500 |
| C | 7.74287400 | -1.33186000 | -1.14147900 |
| C | 8.99774700 | -0.61306500 | -0.59720100 |
| C | 8.03259700 | -2.81258800 | -1.40432800 |
| O | 9.11035200 | -2.91048200 | -2.24449900 |
| O | 7.38262700 | -3.77172400 | -1.01028200 |
| C | 9.49163600 | -4.28956800 | -2.64252900 |
| C | 8.84132200 | 0.87701700 | -0.44345600 |
| C | -7.58958500 | 0.95395400 | -0.30266900 |
| C | -7.56885100 | 2.32584300 | -0.98350000 |
| C | -7.98750000 | -0.16600700 | -1.31992200 |
| C | -9.08987000 | -1.02981800 | -0.78670300 |
| O | -8.29599000 | 2.60950400 | -1.93714800 |
| O | -6.72948100 | 3.20402100 | -0.37898700 |
| C | -6.69760300 | 4.56535800 | -0.97394200 |
| C | 7.74345900 | 1.66092700 | -0.72658000 |
| N | 8.04702600 | 2.99989300 | -0.47949300 |
| C | 9.35080400 | 3.09900000 | -0.02829500 |
| C | 9.88573200 | 1.77318300 | 0.00970200 |
| C | -10.46331000 | -0.58935900 | -0.65558300 |
| C | -11.20491500 | -1.67306800 | -0.09350200 |
| N | -10.31423800 | -2.71514200 | 0.10517000 |
| C | -9.03967900 | -2.31949300 | -0.31141300 |
| C | 10.11772300 | 4.20771100 | 0.34765700 |
| C | 11.42825600 | 3.98532500 | 0.76022600 |
| C | 11.97177900 | 2.68229100 | 0.80156800 |

| | | | |
|---|---|---|---|
| C | 11.21207500 | 1.57694700 | 0.43175900 |
| C | -11.11207600 | 0.61719500 | -0.97053000 |
| C | -12.47724800 | 0.72277600 | -0.72274000 |
| C | -13.20087200 | -0.35638200 | -0.16728100 |
| C | -12.57846800 | -1.56048500 | 0.15244900 |
| H | -2.02136100 | -0.47725600 | 2.94334500 |
| H | 0.16473200 | -0.33772500 | -0.75667300 |
| H | -2.21469800 | 0.84753500 | -0.43013400 |
| H | -2.52815000 | -0.89739100 | -0.55929900 |
| H | 2.45516200 | -1.65094700 | -0.60452000 |
| H | 2.67741000 | 0.09863800 | -0.47362200 |
| H | 2.44267500 | -1.26076900 | 3.98070000 |
| H | 6.85040900 | -1.42421000 | 0.78351400 |
| H | 7.42332300 | -0.87693400 | -2.08244500 |
| H | 9.28317300 | -1.07263800 | 0.36039100 |
| H | 9.80537900 | -0.83132300 | -1.30310200 |
| H | 10.34528400 | -4.15892900 | -3.30372300 |
| H | 9.76177000 | -4.87391200 | -1.76088900 |
| H | 8.66172800 | -4.77352800 | -3.16098100 |
| H | -8.38945000 | 1.02436300 | 0.44281600 |
| H | -8.33038400 | 0.34040100 | -2.22795400 |
| H | -7.09276600 | -0.73716100 | -1.57756200 |
| H | -5.98975200 | 5.11572500 | -0.35866800 |
| H | -6.36055700 | 4.51090100 | -2.01074500 |
| H | -7.69153200 | 5.01490300 | -0.93469600 |
| H | 6.77275500 | 1.38250900 | -1.10019100 |
| H | 7.40762000 | 3.77337400 | -0.61679000 |
| H | -10.54364100 | -3.62557500 | 0.48502900 |
| H | -8.20222800 | -2.99357300 | -0.23888000 |
| H | 9.70524000 | 5.20915800 | 0.31629300 |
| H | 12.04351000 | 4.82771800 | 1.05480000 |
| H | 12.99672400 | 2.54629200 | 1.12722100 |
| H | 11.63700300 | 0.57975600 | 0.46529500 |
| H | -10.54538500 | 1.44140300 | -1.39157600 |
| H | -12.99855500 | 1.64393100 | -0.95701000 |
| H | -14.26390000 | -0.24485200 | 0.01362700 |
| H | -13.14217700 | -2.38246500 | 0.57752600 |
| N | -6.36183200 | 0.65458200 | 0.45427400 |
| H | -6.46398400 | 0.55741600 | 1.46542100 |
| H | 0.88118400 | -1.17894200 | 5.06315500 |

Receptor **1 with CN**   E = -3691.32577839 a.u.

| | | | |
|---|---|---|---|
| C | -0.96668300 | -2.23369900 | 1.29626500 |
| C | -0.93429100 | -1.38119800 | 0.19233700 |
| C | 0.29945000 | -1.14501600 | -0.42543000 |
| C | 1.48361400 | -1.73913100 | 0.02543000 |
| C | 1.42722700 | -2.60531700 | 1.12798000 |
| C | 0.19918500 | -2.83435700 | 1.75981000 |
| C | -2.15365500 | -0.68662000 | -0.38455300 |

| | | | |
|---|---|---|---|
| C | 2.72919400 | -1.40324500 | -0.77779500 |
| O | 2.61079100 | -3.19661000 | 1.53065800 |
| S | 4.40712200 | -1.71255000 | 0.08488400 |
| C | 5.51936100 | -0.79804000 | -1.08539600 |
| N | 6.78377500 | -0.81787000 | -0.64781000 |
| S | 4.99482200 | -0.05617900 | -2.55164800 |
| S | -3.69097800 | -0.98497000 | 0.69818400 |
| C | -4.91683600 | 0.16592400 | -0.08816600 |
| S | -4.56723500 | 1.17421500 | -1.42930700 |
| C | 7.95039800 | -0.30043700 | -1.37979400 |
| C | 8.85227300 | 0.57009500 | -0.47447300 |
| C | 8.73906700 | -1.48591500 | -1.93625000 |
| O | 9.84404700 | -1.00877400 | -2.59063800 |
| O | 8.45225700 | -2.67228600 | -1.84378200 |
| C | 10.71857200 | -2.03817900 | -3.20797900 |
| C | 8.21646100 | 1.86017100 | -0.02705000 |
| C | -7.28530100 | 0.87396200 | 0.12519500 |
| C | -7.01796300 | 2.38200400 | 0.19340000 |
| C | -7.88849000 | 0.46864500 | -1.26207600 |
| C | -9.26244900 | -0.12460300 | -1.13364600 |
| O | -7.64037800 | 3.22601200 | -0.45344000 |
| O | -6.10197300 | 2.68528200 | 1.14965100 |
| C | -5.81991200 | 4.13329600 | 1.32894700 |
| C | 6.99437200 | 2.38566300 | -0.38549200 |
| N | 6.81139100 | 3.61776800 | 0.24412700 |
| C | 7.91821300 | 3.90435500 | 1.02249400 |
| C | 8.83031900 | 2.81209900 | 0.87702800 |
| C | -10.46345600 | 0.61183300 | -0.79239700 |
| C | -11.53937100 | -0.32895500 | -0.75826200 |
| N | -11.00747200 | -1.56990300 | -1.06576700 |
| C | -9.63506800 | -1.43992900 | -1.29041500 |
| C | 8.21565400 | 5.00186300 | 1.83838500 |
| C | 9.43423600 | 5.00392000 | 2.51085000 |
| C | 10.34604400 | 3.93348400 | 2.37731200 |
| C | 10.05454500 | 2.84032300 | 1.56718800 |
| C | -10.71381900 | 1.96862000 | -0.52148400 |
| C | -12.01519900 | 2.35961900 | -0.22246600 |
| C | -13.06977100 | 1.41964700 | -0.19122400 |
| C | -12.84655900 | 0.07149900 | -0.45784500 |
| H | -1.88116800 | -2.44578000 | 1.83043700 |
| H | 0.34784700 | -0.47961500 | -1.28156200 |
| H | -2.01710700 | 0.39488800 | -0.43008100 |
| H | -2.39594200 | -1.05931800 | -1.38124900 |
| H | 2.75593700 | -1.97345800 | -1.70822500 |
| H | 2.73788800 | -0.34097000 | -1.02412800 |
| H | 2.50348600 | -3.86714800 | 2.25125400 |
| H | 6.99150500 | -1.28357500 | 0.23761800 |
| H | 7.57640800 | 0.28765500 | -2.22130300 |
| H | 9.15222600 | -0.02483300 | 0.40006900 |
| H | 9.76199700 | 0.77052300 | -1.04992200 |
| H | 11.51756700 | -1.47180000 | -3.68102100 |
| H | 11.11108500 | -2.70776400 | -2.44033400 |

| | | | |
|---|---|---|---|
| H | 10.15624200 | -2.61615500 | -3.94366100 |
| H | -8.03505300 | 0.67100600 | 0.89707500 |
| H | -7.93140800 | 1.37420000 | -1.87376000 |
| H | -7.20759900 | -0.23526400 | -1.74504000 |
| H | -5.11859800 | 4.17415300 | 2.15909700 |
| H | -5.37645100 | 4.54093500 | 0.41856300 |
| H | -6.74158300 | 4.67014200 | 1.56023900 |
| H | 6.23401600 | 1.98470800 | -1.03624100 |
| H | 5.99053000 | 4.20244100 | 0.14478800 |
| H | -11.52623400 | -2.43739900 | -1.12819200 |
| H | -9.03465400 | -2.29699600 | -1.54729600 |
| H | 7.51884200 | 5.82476200 | 1.94442200 |
| H | 9.68830300 | 5.84233700 | 3.14917200 |
| H | 11.28625200 | 3.96876600 | 2.91563500 |
| H | 10.76066100 | 2.02318000 | 1.46918700 |
| H | -9.89497900 | 2.67940500 | -0.53973900 |
| H | -12.22889100 | 3.40074300 | -0.00845500 |
| H | -14.07344600 | 1.75475800 | 0.04457500 |
| H | -13.66043600 | -0.64346000 | -0.43287100 |
| N | -6.10200900 | 0.08816000 | 0.51981600 |
| H | -6.21203800 | -0.53009400 | 1.32441100 |
| C | 0.12595900 | -3.74048700 | 2.98632100 |
| H | 0.85051200 | -3.40947800 | 3.74333400 |
| O | -1.24190400 | -3.67093900 | 3.47422200 |
| H | -1.28852700 | -4.18114300 | 4.32689500 |
| C | 0.45196900 | -5.12208500 | 2.60296300 |
| N | 0.67669300 | -6.22514600 | 2.30832800 |

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