

Supporting Information

Highly sensitive turn-off fluorescent detection of cyanide in aqueous medium using dicyanovinyl substituted phenanthridine fluorophore

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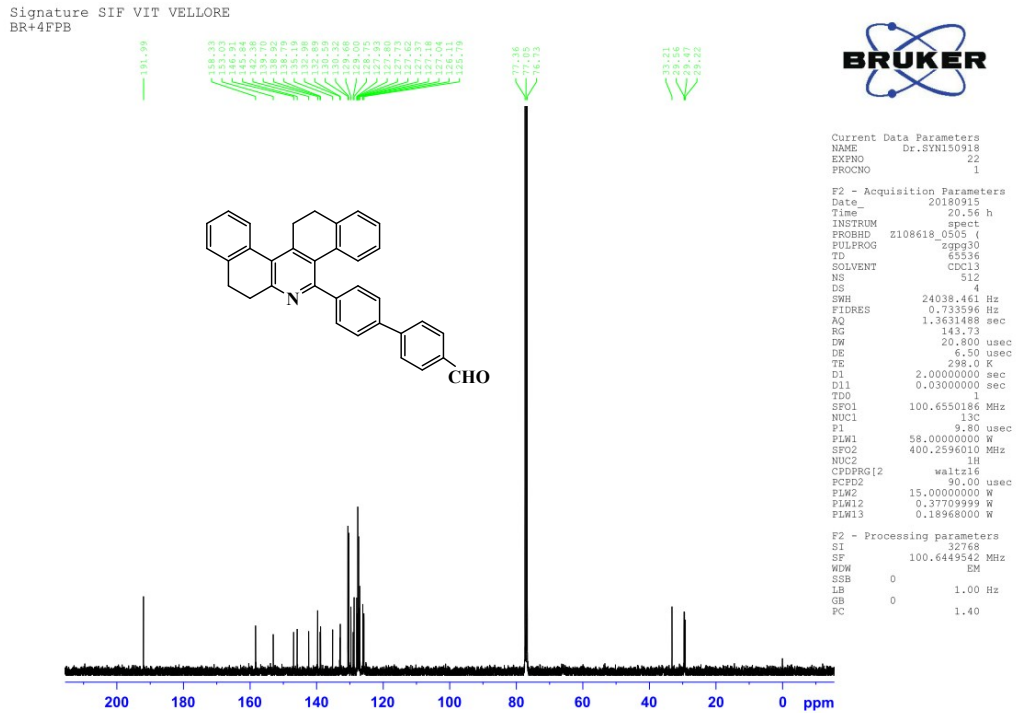
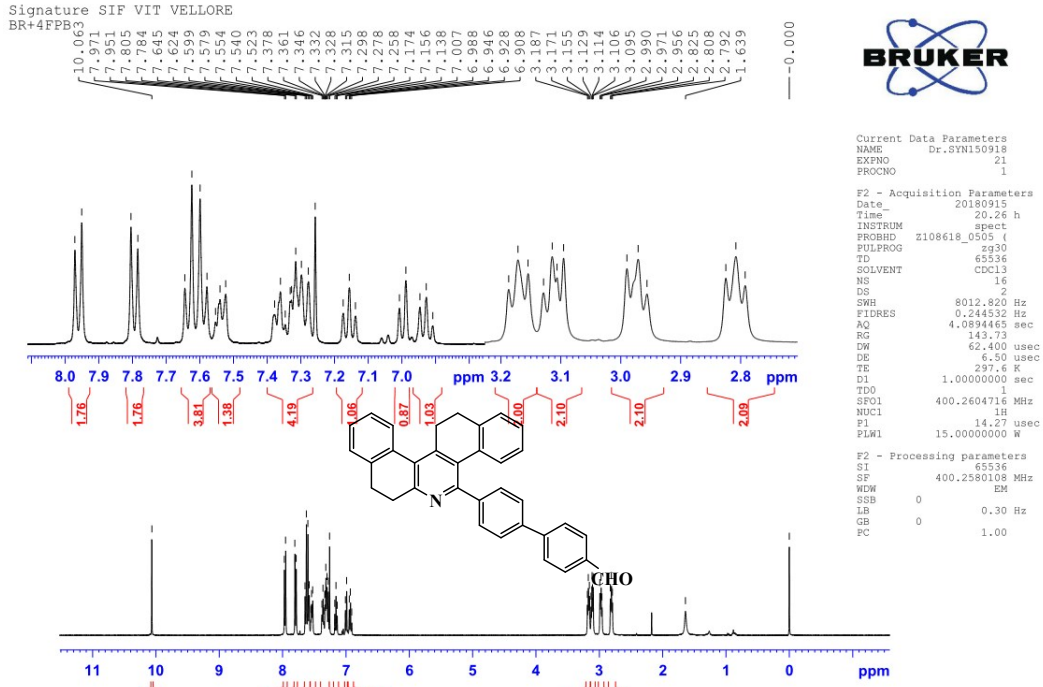
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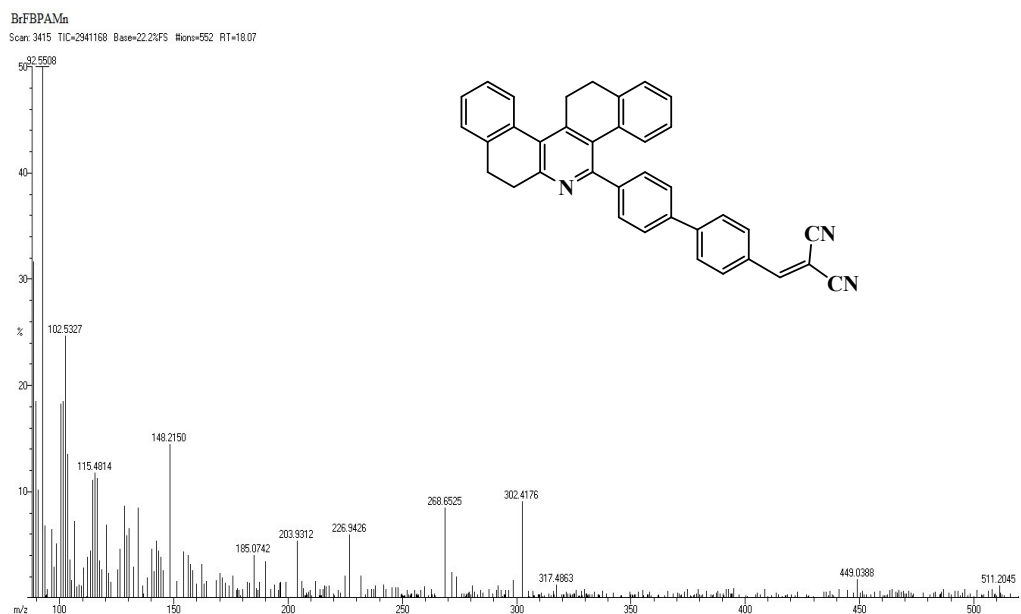
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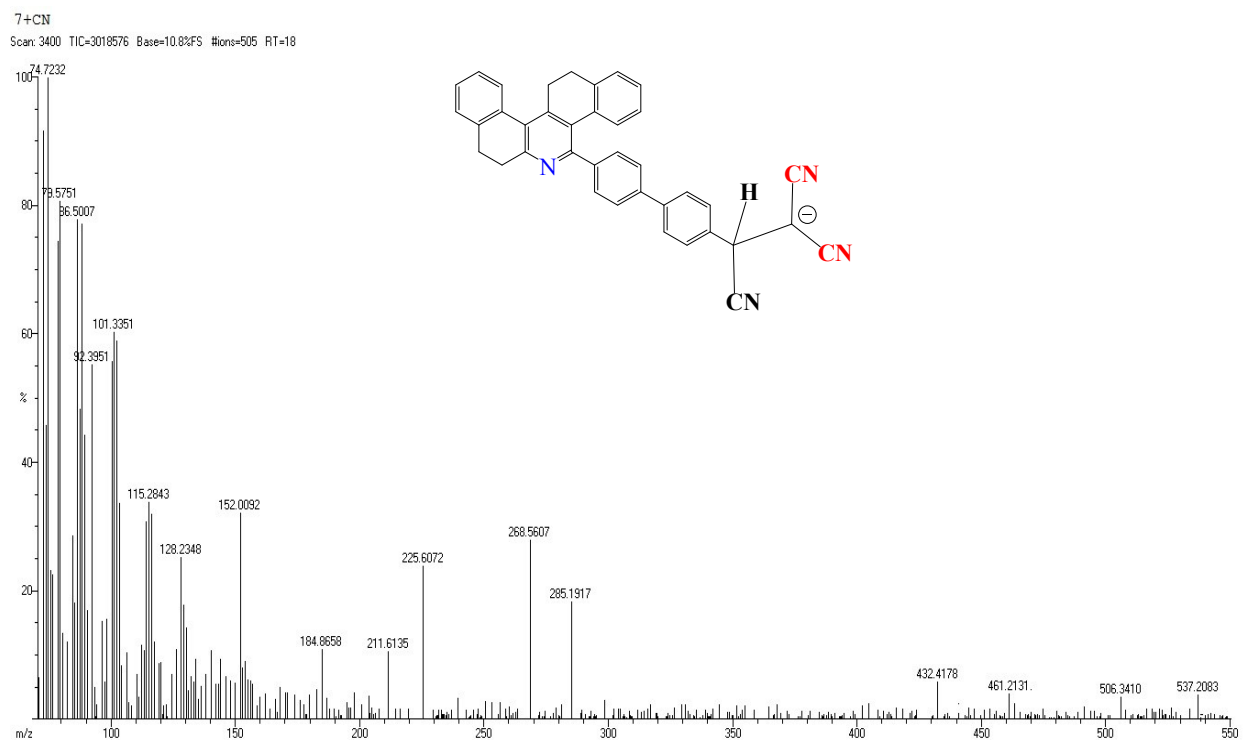
SI Figure S2 ¹H and ¹³C NMR spectra of compound 5



SI Figure S6 HRMS spectra of compound: 7



SI Figure S7 HRMS spectra of compound: 7+CN. Exact mass (M) calculated 537.2085, mass obtained in m/z 537.2083



SI Table S1 The comparisons of Fluorescence “off” cyanide detection sensor LOD of 7 in the previous and present works

| Name of the receptor | Solvent/supported systems | Method used | Detection limit | Application | References |
|--|-----------------------------------|----------------------|---------------------|---|---|
| Calorimetric sensing of cyanide based on dipyrin adducts | Dichloromethane | Calorimetric sensing | 3.6, 4.2 and 7.1 μM | - | Org. Biomol. Chem., 2012 , 10, 4201 |
| Carbazole based hemicyanine | Acetonitrile | Ratiometric sensing | 0.54 μM | TLC Plate | Dalton Trans., 2013 , 42, 10682 |
| Cyanide detection in aqueous solution using carbazole | ACN:H ₂ O (9:1) | Fluorescence “off” | 0.126 μM | Test paper Strips | RSC. Adv., 2014 , 4, 22902 |
| Solvatochromic AIE luminogens as supersensitive and highly efficient CN ⁻ detection | Aqueous solution | Fluorescence “off” | 0.2 μM | Test paper Strips | Chem. Sci., 2014 , 5, 2710 |
| Cyanide detection based on triphenylimidazole derivatives | Acetonitrile | Fluorescence “off” | 0.1 μM | - | Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 2014 , 124, 97-101 |
| A new coumarin based fluorogenic cyanide sensing | ACN:H ₂ O (1:1) | Fluorescence “on” | 0.14 μM | CN ⁻ detection visualized on TLC Plate and CN ⁻ determination in water samples. | RSC. Adv., 2015 , 5, 96905 |
| Cyanide in aqueous media using novel AIEE fluorophores | DMSO | Fluorescence “off” | 0.29 μM | - | RSC. Adv., 2015 , 5, 12191 |
| 7-azaindole based ratiometric fluorescent sensor | THF:H ₂ O (9:1) | Ratiometric sensing | 2.1 μM | Test paper Strips | Dyes and Pigments, 2015 , 123, 1-7 |
| Detection of cyanide based on a novel dicyanovinyl phenylacetylene | ACN:HEPES buffered solution (9:1) | Fluorescence “on” | 0.68 μM | CN ⁻ determination in water samples | New. J. Chem., 2017 , 41, 4058 |
| Selective recognition of cyanide based on the FRET mechanism | Dimethylformamide | Fluorescence “on” | 63 nM | Color changes in Silica gel plates | J.Org. Chem. 2017 , 82, 6259-6267 |
| Detection of cyanide based on a dicyanovinyl pyrazoles | ACN:H ₂ O 1% | Fluorescence “off” | 6.8 μM | Test paper Strips | J.Org. Chem. 2017 , 82, 13376-13385 |
| Carbazole based cyanide detection | DMSO | Fluorescence “off” | 67.4 nM | Test paper Strips | Dyes and Pigments, 2019 , 164, 165-173 |
| Pheanthridine based cyanide detection | Acetonitrile-water (1%) | Fluorescence “off” | 39.3 nM | CN ⁻ detection visualized on Test paper Strips, Logic gate and CN ⁻ determination in water samples. | Present work |

Table S2 UV-Vis spectra characteristic of **7** and **7+CN⁻** by experimental and theoretical

| Compound | Experimental | | Theoretical | | | |
|-----------------|-----------------------------|------------|--------------------|----------------------------|-----------------------|-------------------------------|
| | λ_{abs} (nm) | ϵ | Wavelength | Oscillator strength | State Involved | Key Transitions |
| 7 | 368 | 0.51 | 365.63 | 0.4252 | S3 \rightarrow S0 | HOMO-1 \rightarrow LUMO 89% |
| 7+CN | 320 | 0.27 | 332.91 | 0.5462 | S10 \rightarrow S0 | HOMO-2 \rightarrow LUMO 98% |