

Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

A highly selective pyrene based “off-on” fluorescent chemosensor for cyanide

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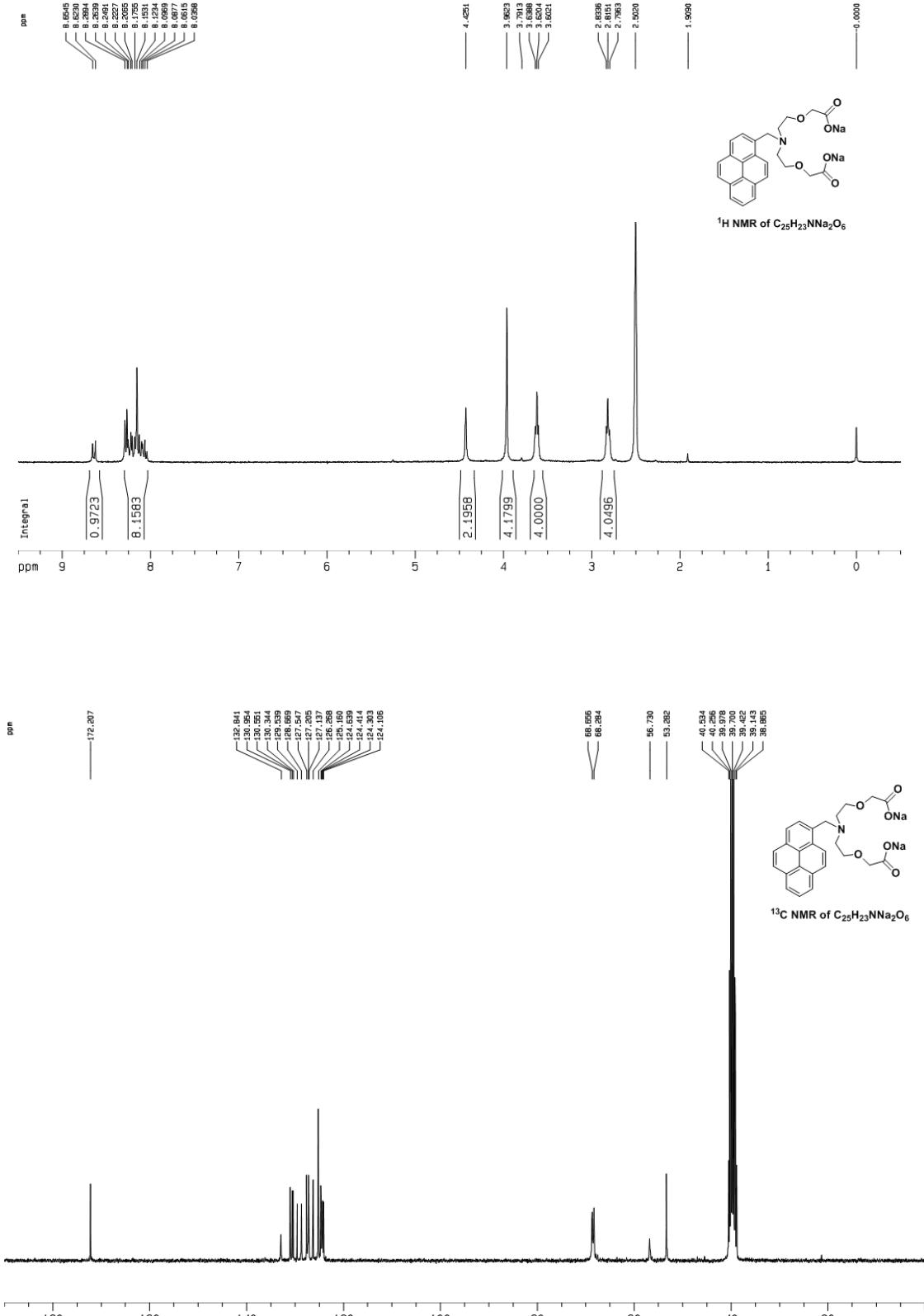


Figure S1. ¹H NMR and ¹³C NMR spectra of **1**

Complete NMR spectral assignments of compound **1**: ¹H NMR (300 MHz, DMSO-d6): δ 2.82 (t, $J = 5.5$ Hz, 4 H, N-CH₂), 3.62 (t, $J = 5.5$ Hz, 4 H, O-CH₂), 3.96 (s, 4H, O-CH₂CO₂), 4.42 (s, 2 H, C₁₆H₉CH₂), 8.04-8.29 (8H, C₁₆H₉), δ 8.64 (d, $J = 9.4$ Hz, 1 H, C₁₆H₉) ; ¹³C NMR (75 MHz, DMSO-d6): δ 172.20(CO₂Na), 132.84, 130.95, 130.55, 130.34, 129.53, 128.66, 127.54, 127.20, 127.13, 126.26, 125.16, 124.63, 124.41, 124.30, 124.10 (aromatic carbons), 68.65(O-CH₂CO₂), 68.28(OCH₂), 56.73 (N-CH₂C₁₆H₉), 53.28(N-CH₂) .

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name: 13060302_20130607_000002.d
Sample: WM-479
Comment: ESI Positive

Acquisition Date: 6/7/2013 4:21:08 PM
Instrument Operator: Bruker Apex IV FTMS
Peking University

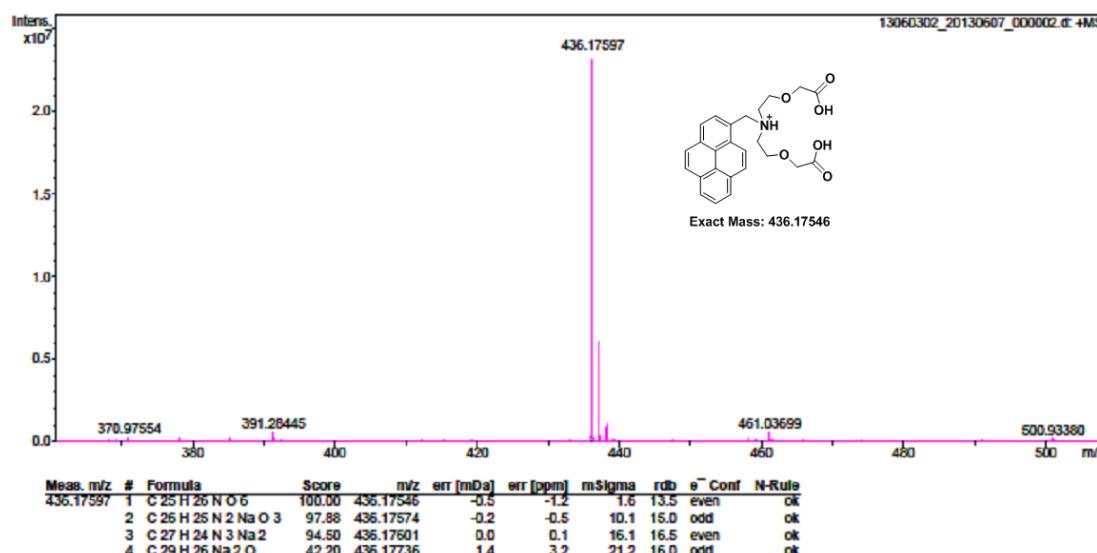


Figure S2. HRMS spectra of 1

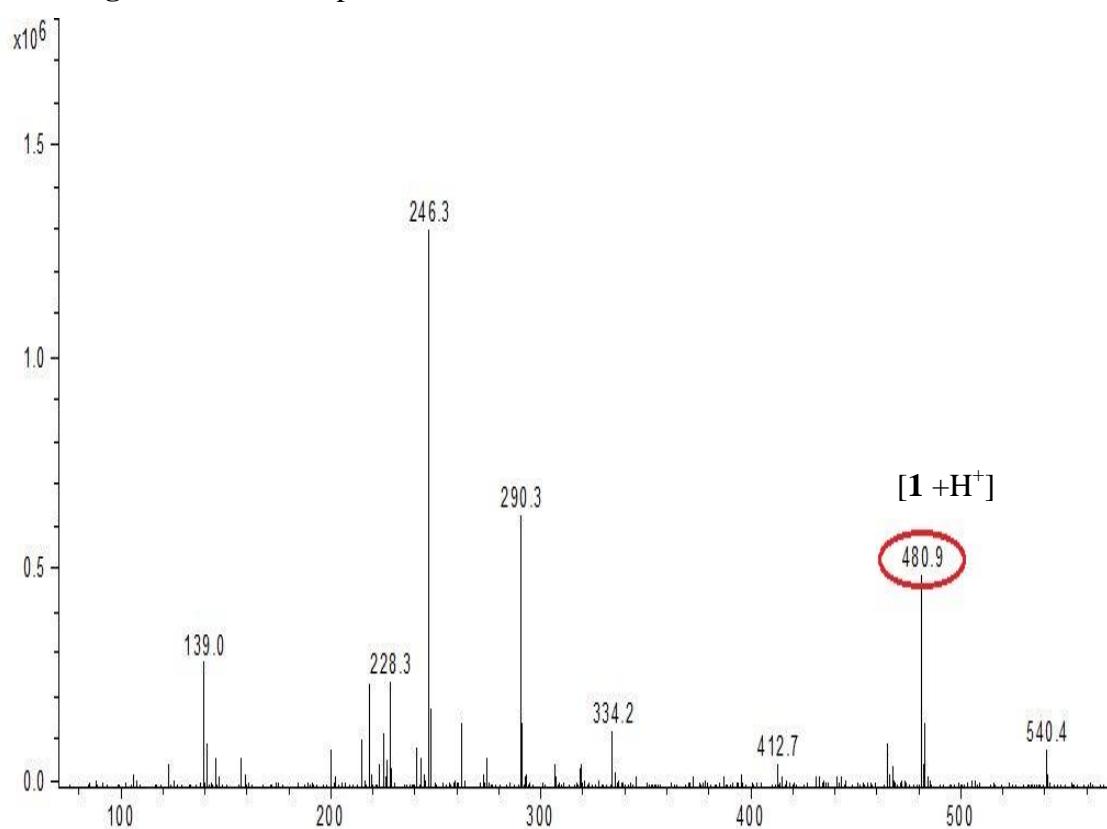


Figure S3. ESI-Mass spectrum of 1

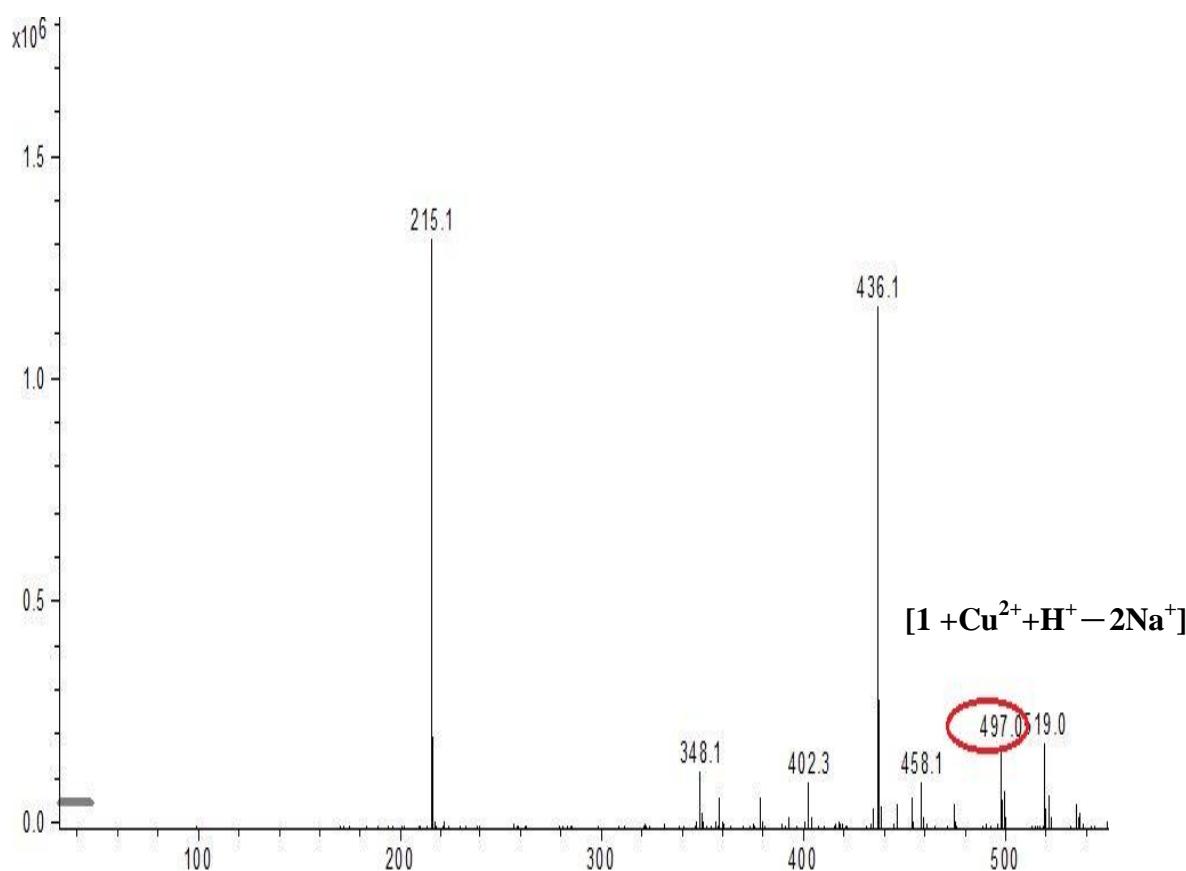


Figure S4. ESI-Mass spectrum of **1•Cu(II)**

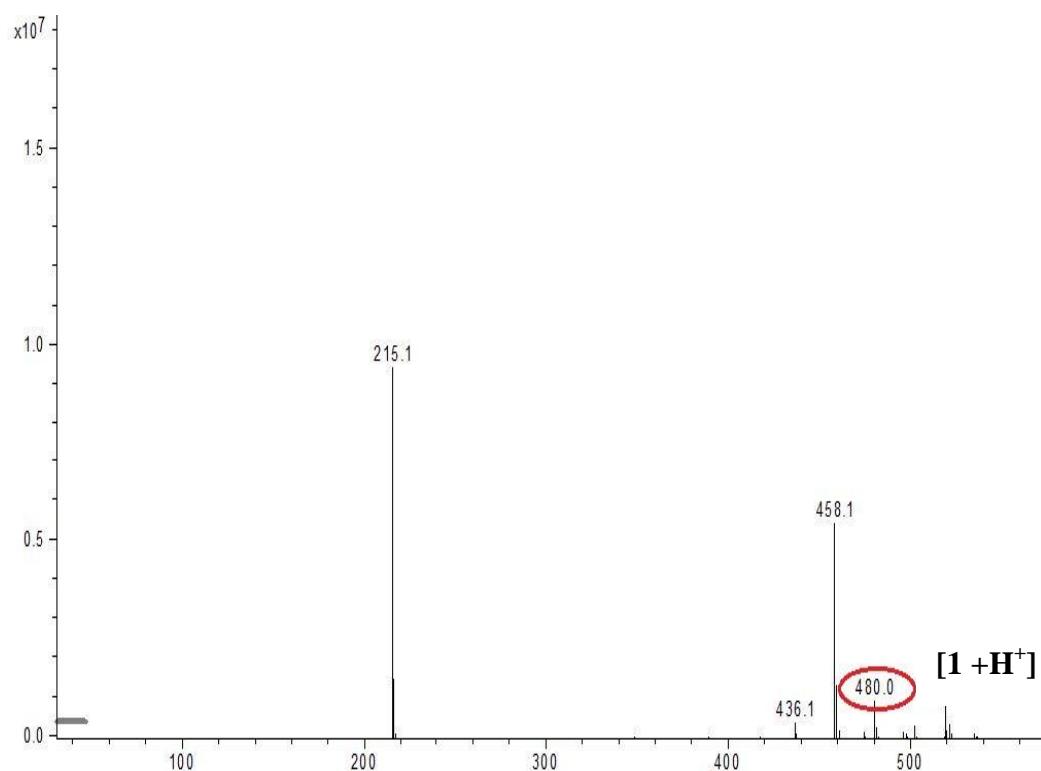


Figure S5. ESI-Mass spectrum of **1•Cu(II) + CN⁻**

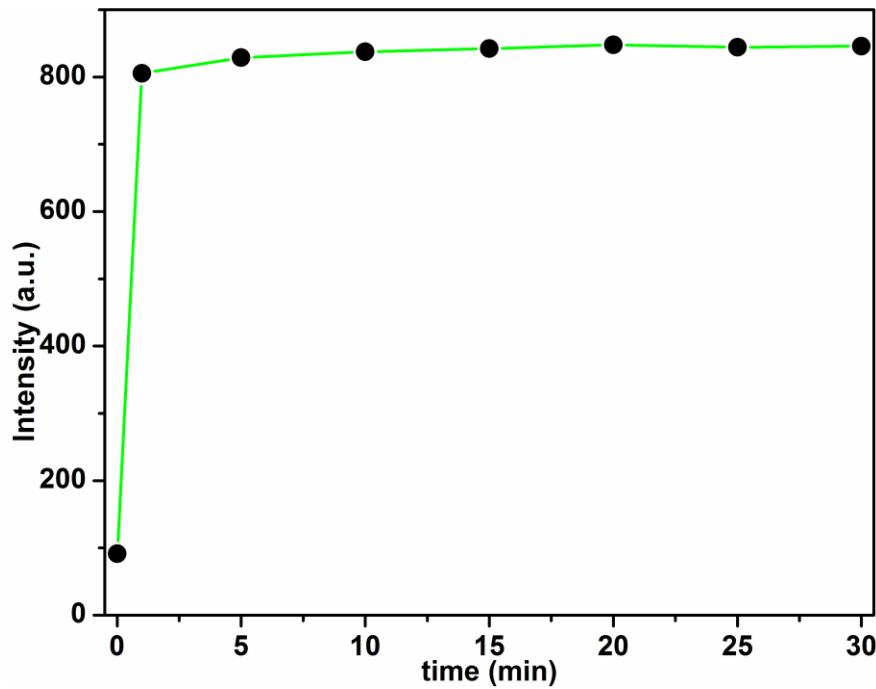


Figure S6. Time-dependent fluorescence spectra of **1** (5 μ M) upon addition of cyanide ion (20 equiv) in water-MeCN (80:20, v/v) solution. $\lambda_{\text{ex}}/\lambda_{\text{em}} = 342 / 376 \text{ nm}$.

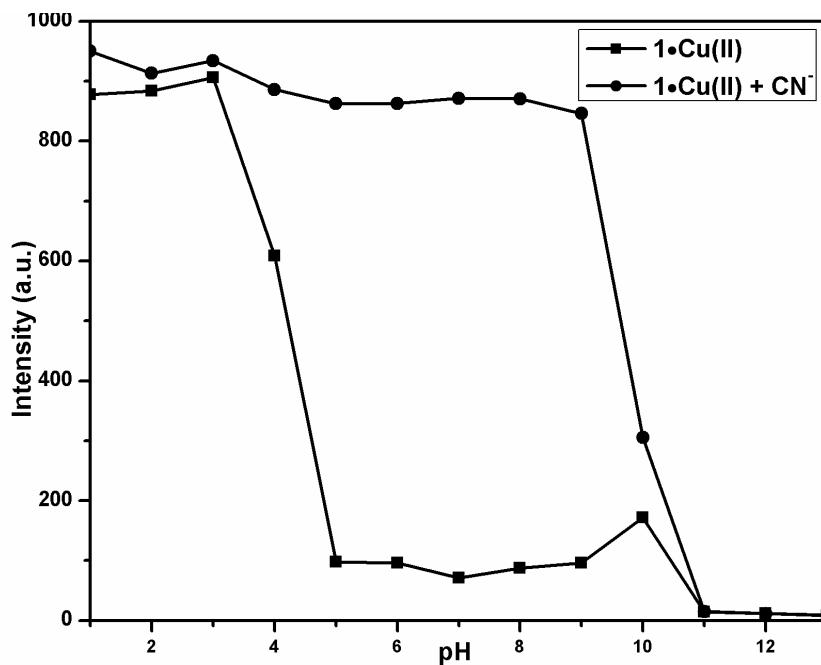


Figure S7. Fluorescence intensity changes of **1**•Cu(II) ($5.0 \times 10^{-6} \text{ M}$) in MeCN-H₂O (20:80, v/v) measured with and without CN⁻ (20.0 equiv.) in different pH value (pH value of the solution was adjusted by HClO₄ or NaOH)