Supporting Information

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

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Table of contents

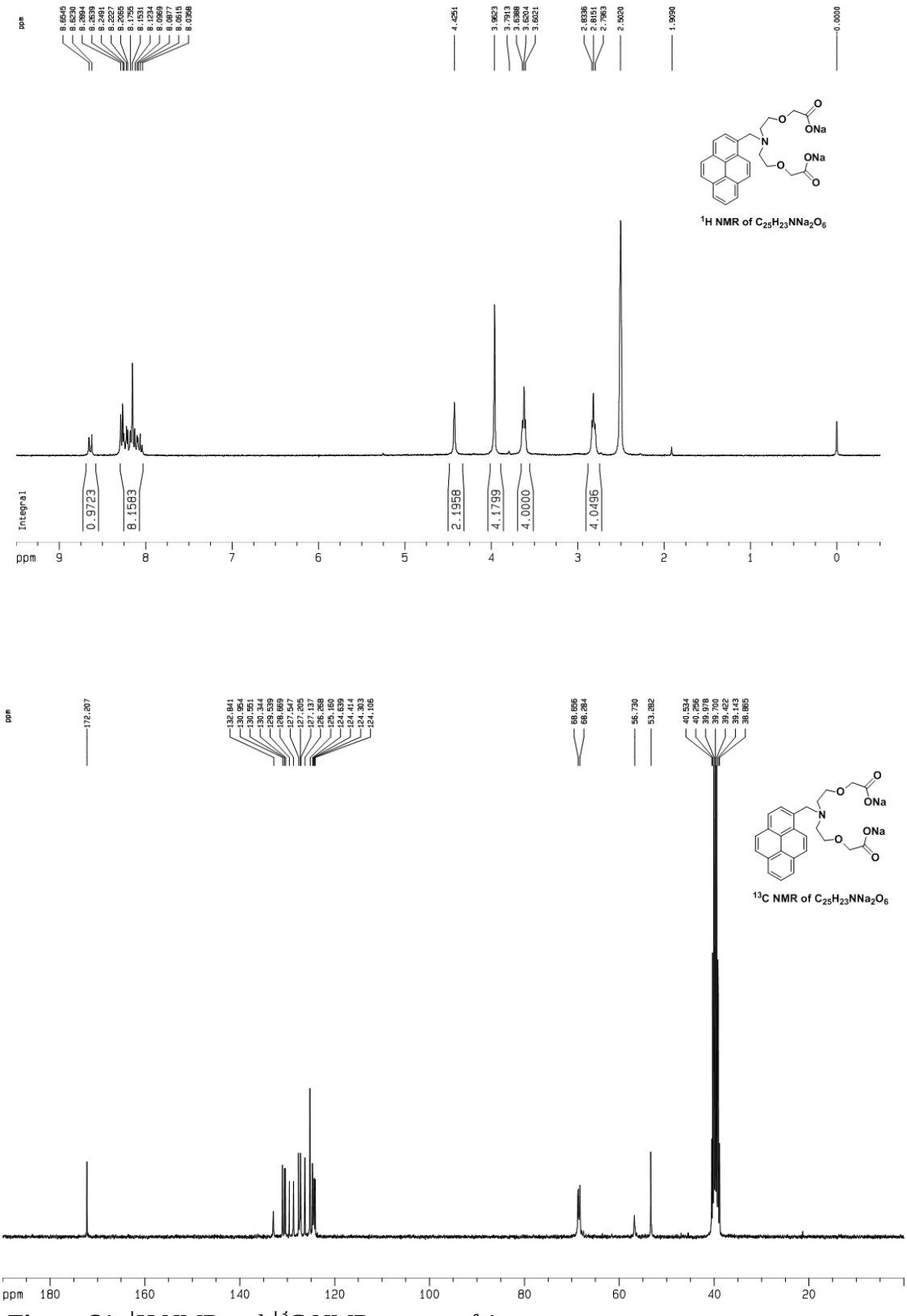

Figure S1. ^{1}H NMR and ^{13}C NMR spectra of **1**

Complete NMR spectral assignments of compound **1**: ^{1}H NMR (300 MHz, DMSO-d6): δ 2.82 (t, J = 5.5 Hz, 4 H, N-C*H*$_2$), 3.62 (t, J = 5.5 Hz, 4 H, O-C*H*$_2$), 3.96 (s, 4H, O-C*H*$_2$CO$_2$), 4.42 (s, 2 H, $C_{16}H_9$C*H*$_2$), 8.04-8.29 (8H, $C_{16}H_9$), δ 8.64 (d, J = 9.4 Hz, 1 H, $C_{16}H_9$) ; ^{13}C NMR (75 MHz, DMSO-d6): δ 172.20(*C*O$_2$Na), 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-*C*H$_2$CO$_2$), 68.28(O*C*H$_2$), 56.73 (N-*C*H$_2$C$_{16}$H$_9$), 53.28(N-*C*H$_2$) .

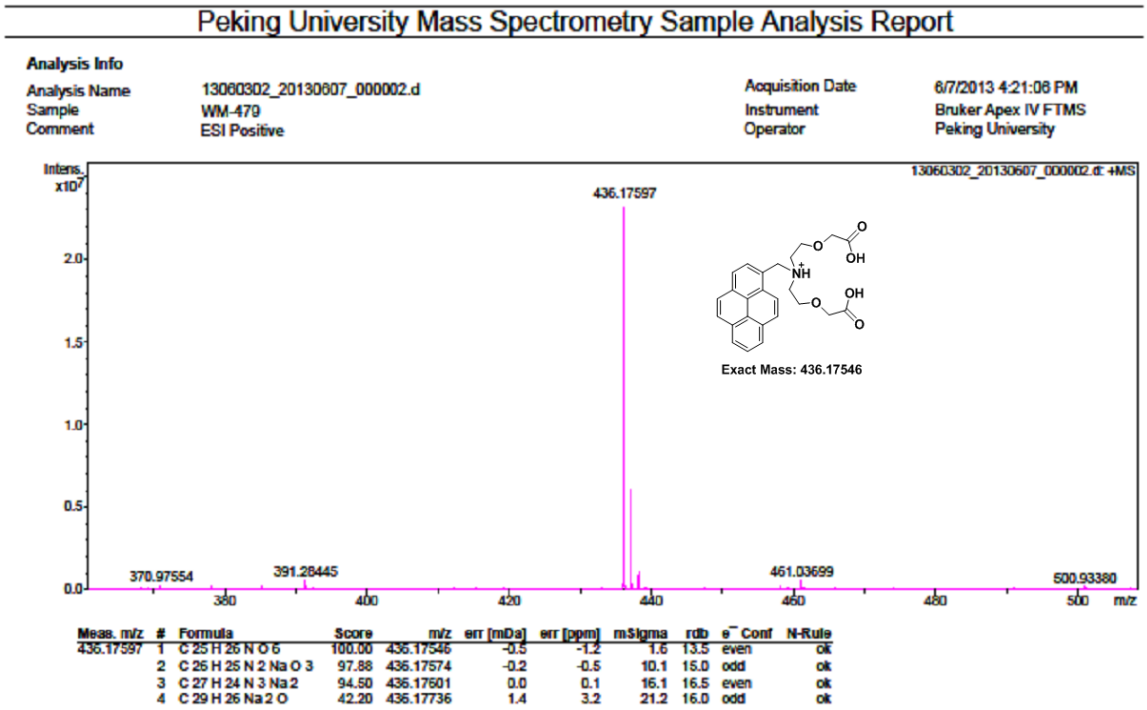

Figure S2. HRMS spectra of **1**

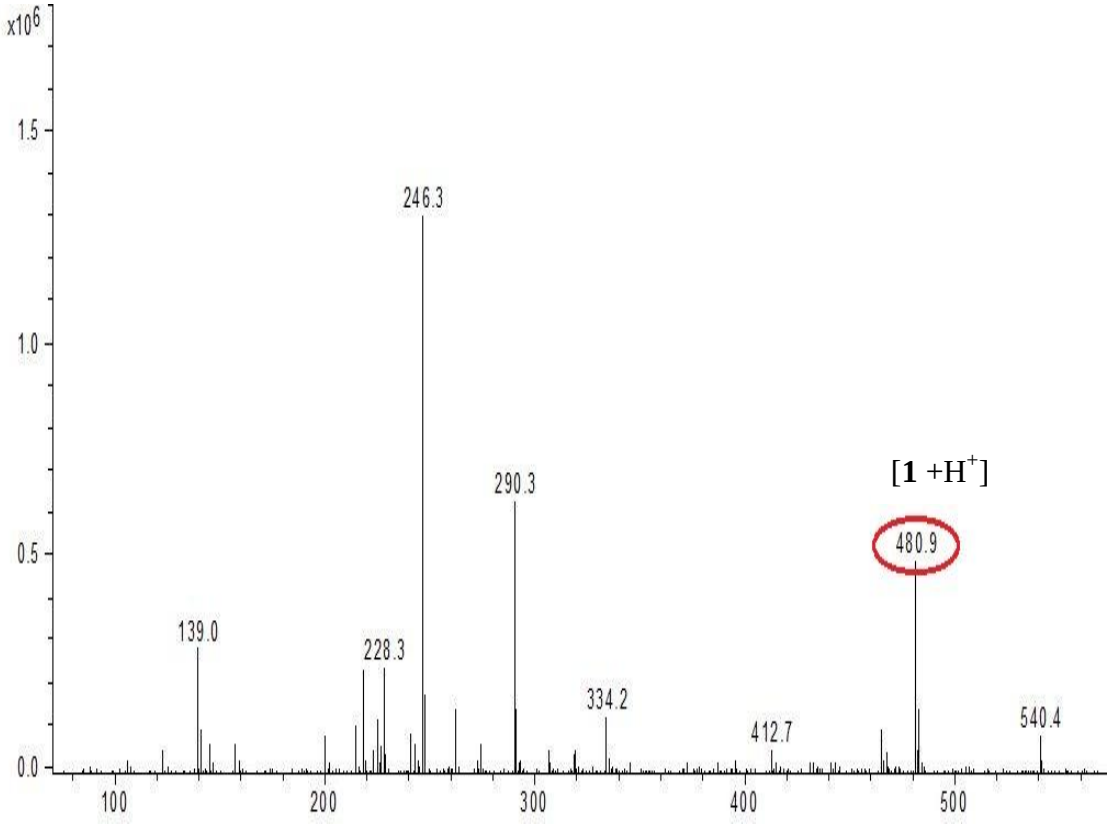

Figure S3. ESI-Mass spectrum of **1**

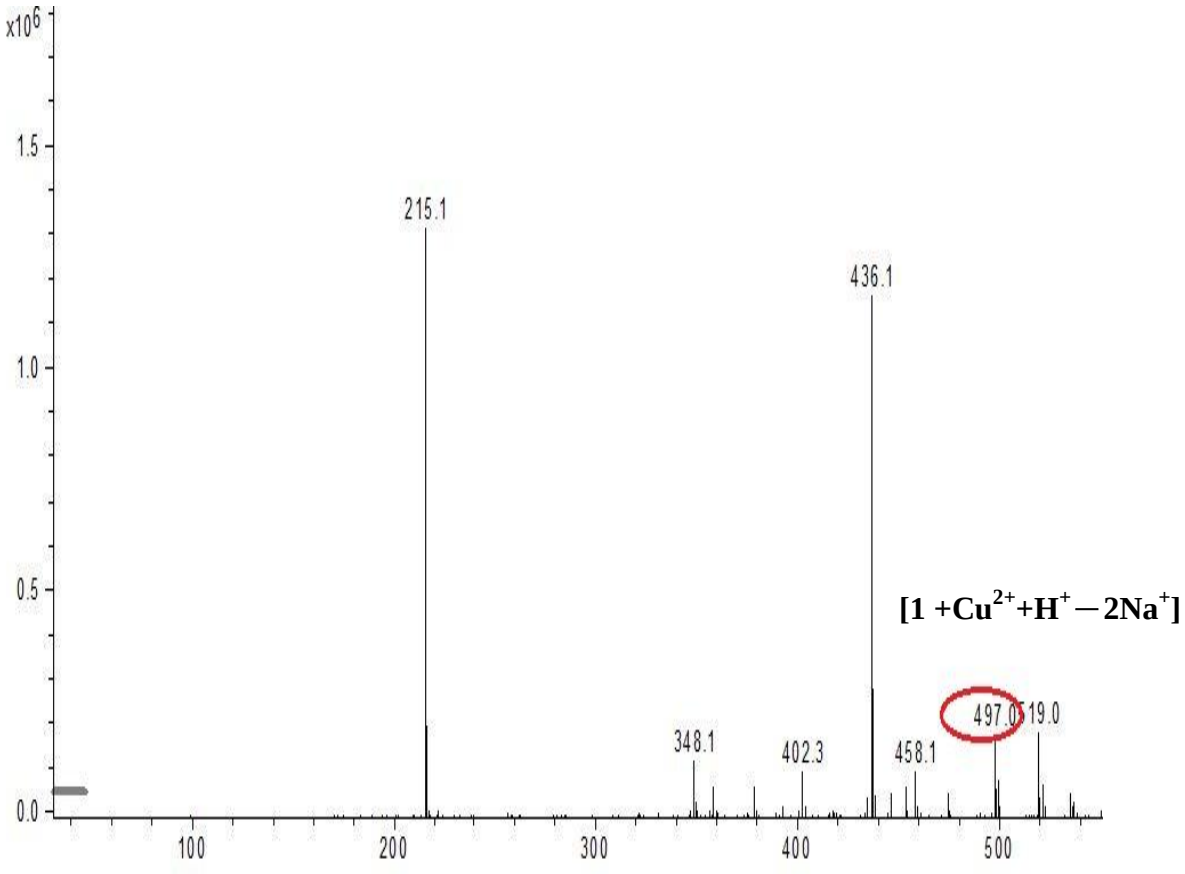

Figure S4. ESI-Mass spectrum of **1•Cu(II)**

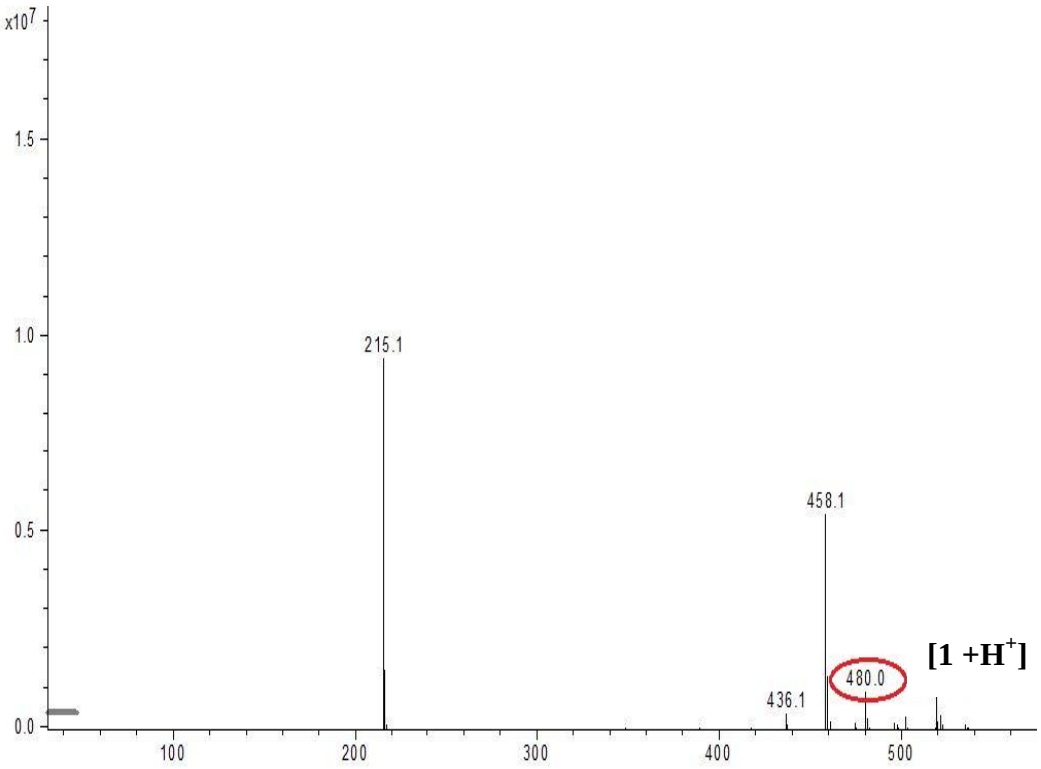

Figure S5. ESI-Mass spectrum of **1•Cu(II) + CN^-**

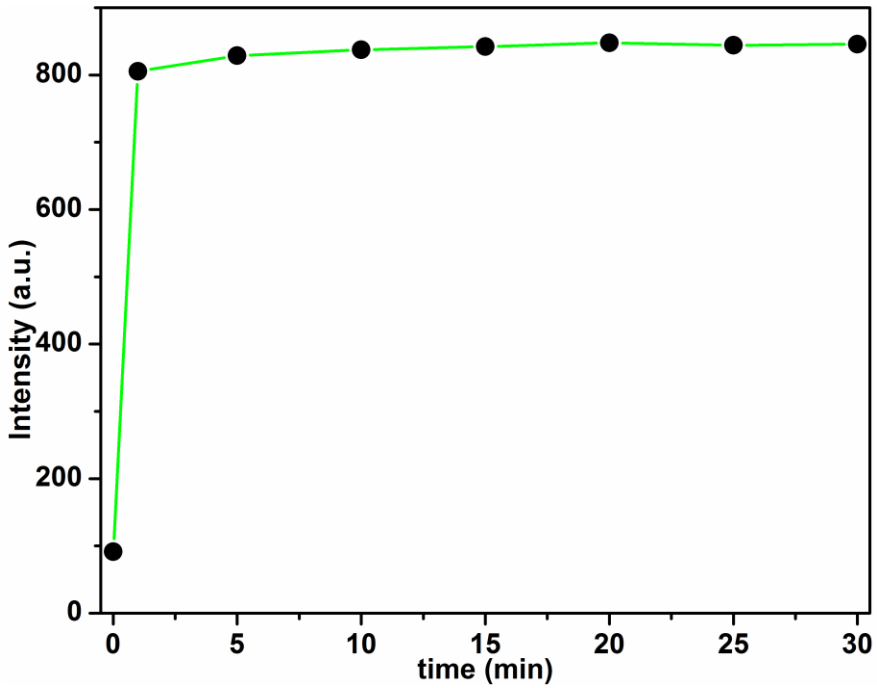

Figure S6. Time-dependent fluorescence spectra of **1** (5 μM) upon addition of cyanide ion (20equiv) in water-MeCN (80:20, v/v) solution. $\lambda_{ex}/\lambda_{em}$ =342 /376nm.

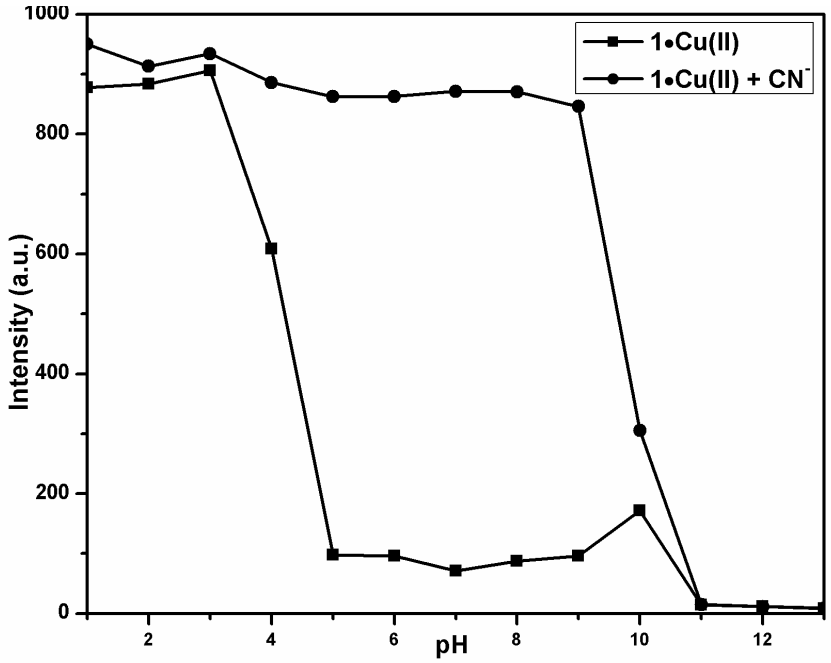

Figure S7. Fluorescence intensity changes of **1**•Cu(II) (5.0×10^{-6} M) in MeCN-H_2O (20:80, v/v) measured with and without CN^- (20.0 equiv.) in different pH value (pH value of the solution was adjusted by $HClO_4$ or NaOH)