Electronic Supplementary Information (ESI) for

Selective and visual detection of a nerve agent mimic by phosphorylation and protonation of quinolin oximes

Yuan-Chao Cai, Chen Li and Qin-Hua Song*

Department of Chemistry, University of Science and Technology of China, Hefei 230026, China

E-mail address: qhsong@ustc.edu.cn (Q.-H. Song)

Contents

II. UV/Vis absorption and fluorescence spectra of three sensors

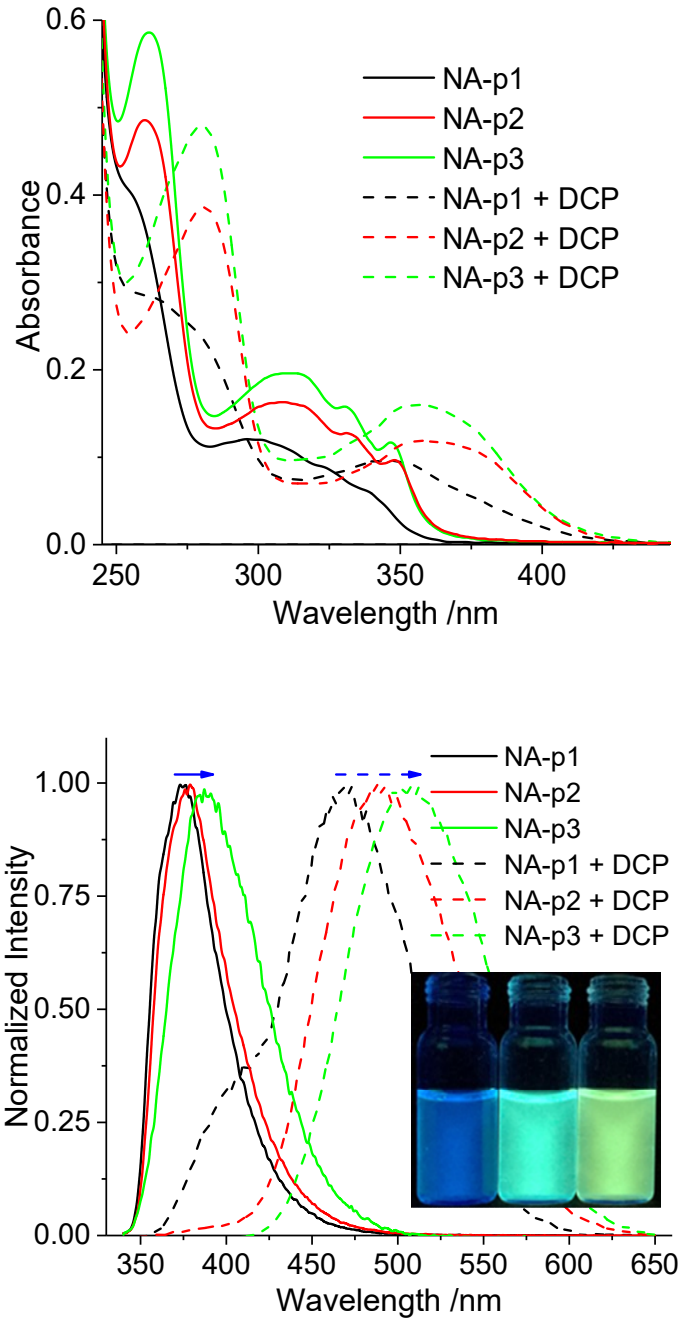


Fig. S1 Absorbance (left) and normalized fluorescent (right) spectra of three probes (10 μM) in CH_3CN containing 1% DMSO before and after addition of the solution of DCP (5 equiv.) in CH_3CN (λ_{ex}=330 nm).

II. Spectral response of the sensors to different amounts of DCP

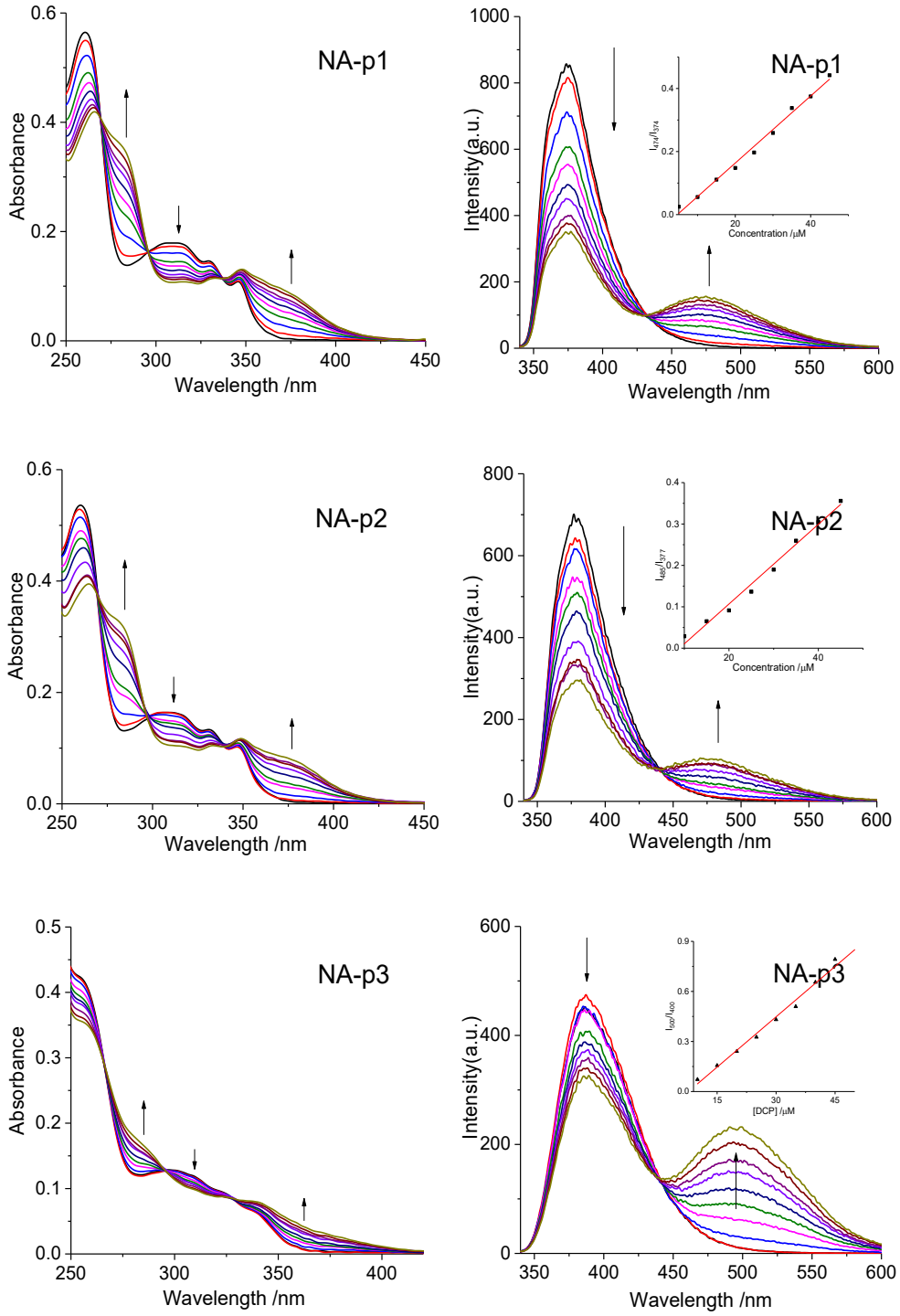


Fig. S2 Absorbance (left) and fluorescence (middle) spectra of sensors (10 μM) upon gradual addition of a solution of DCP (0–4.5 equiv.) in CH_3CN containing 1% DMSO (λ_{ex}=330 nm). Right: Linear correlation between florescent ratio of F_{500}/F_{400} and the concentration of DCP solutions.

III. HRMS evidence of the sensing mechanism of NA-p3

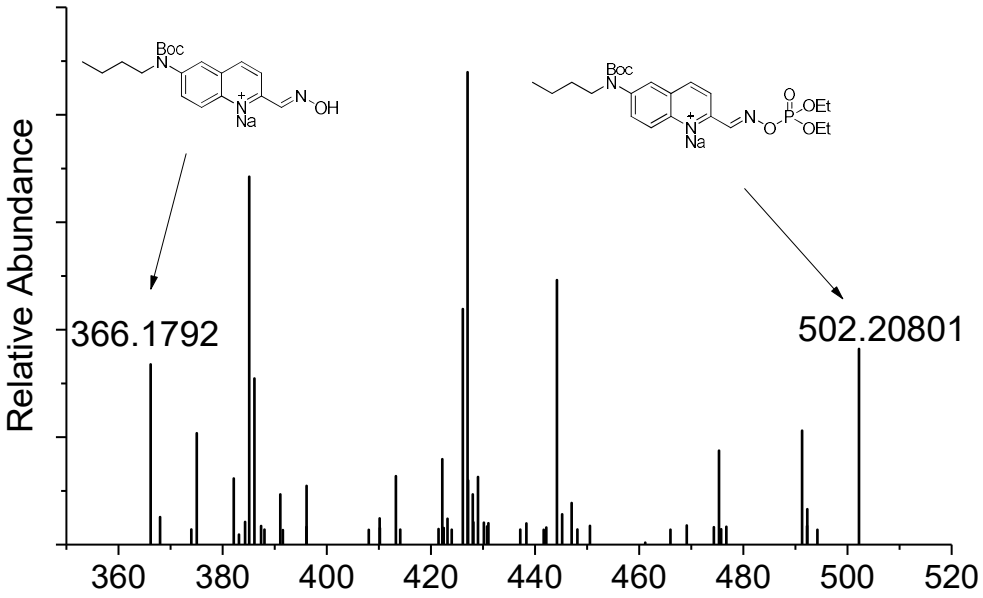


Fig. S3 HRMS of the reaction mixture of NA-p3 with DCP in CH_3CN

IV. Measurements of pKa values

The measurements of pK_a were performed through recording UV/Vis absorption spectra of a sensor in aqueous solutions at different pH, which were DMSO/buffer (1:99 v/v) solvent mixtures, and four buffers over a pH range of 2.2-13.0, including 0.1 M critric acid-0.1 M Na_2HPO_4 buffer for pH 2.2-8, 0.1 M KCl-0.1 M H_3BO_3-0.1 M NaOH buffer for pH 8-10, 0.1 M $NaHCO_3$-0.1 M NaOH buffer for pH 10-11 and 0.1 M KCl-0.1 M NaOH buffer for pH 12-13.

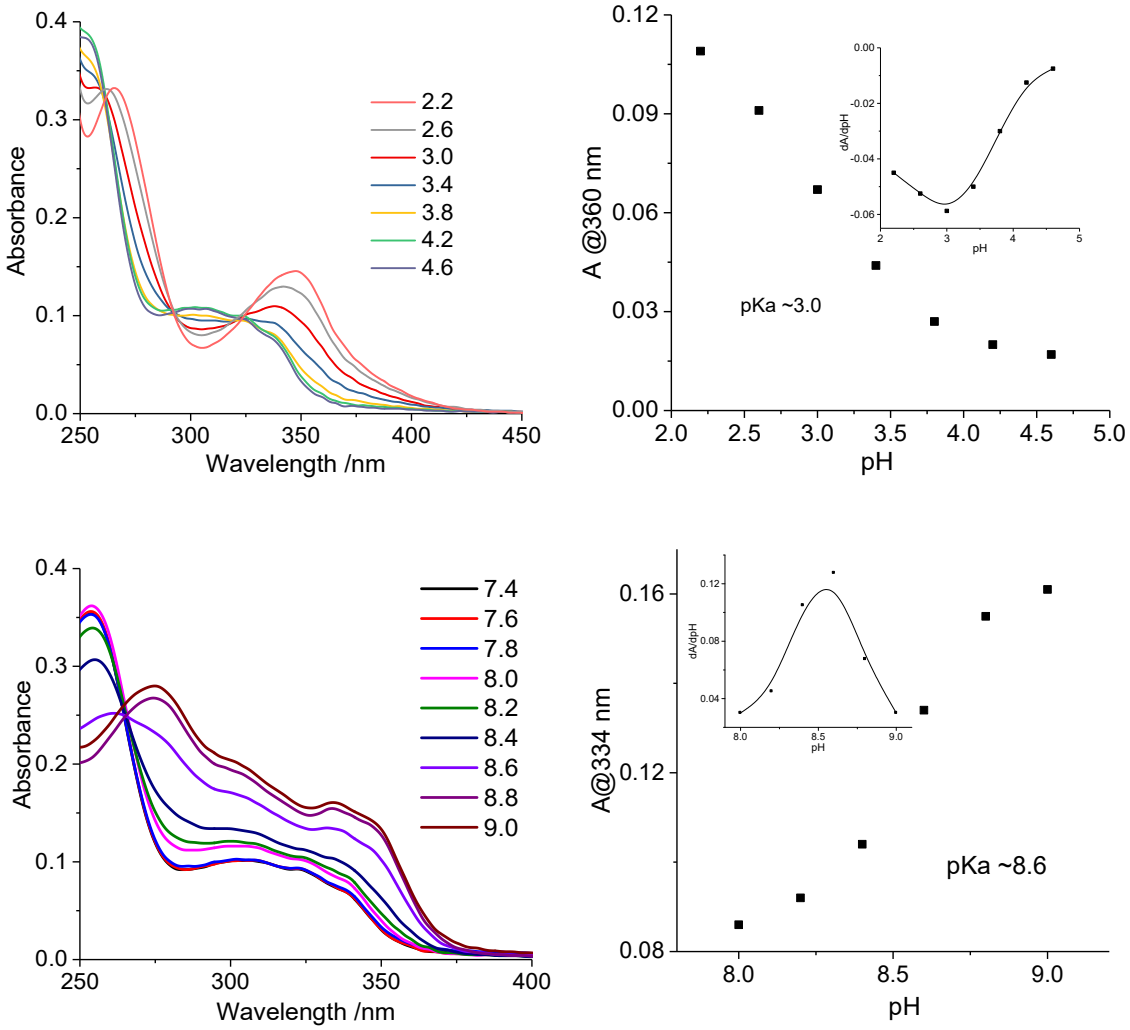


Fig. S4 UV/Vis absorption spectra (left) in various pH solutions and plots of absorbance (right) of NA-p3 at certain wavelength *vs*. pH value.

V. Effects of water on the sensing performance of NA-p3

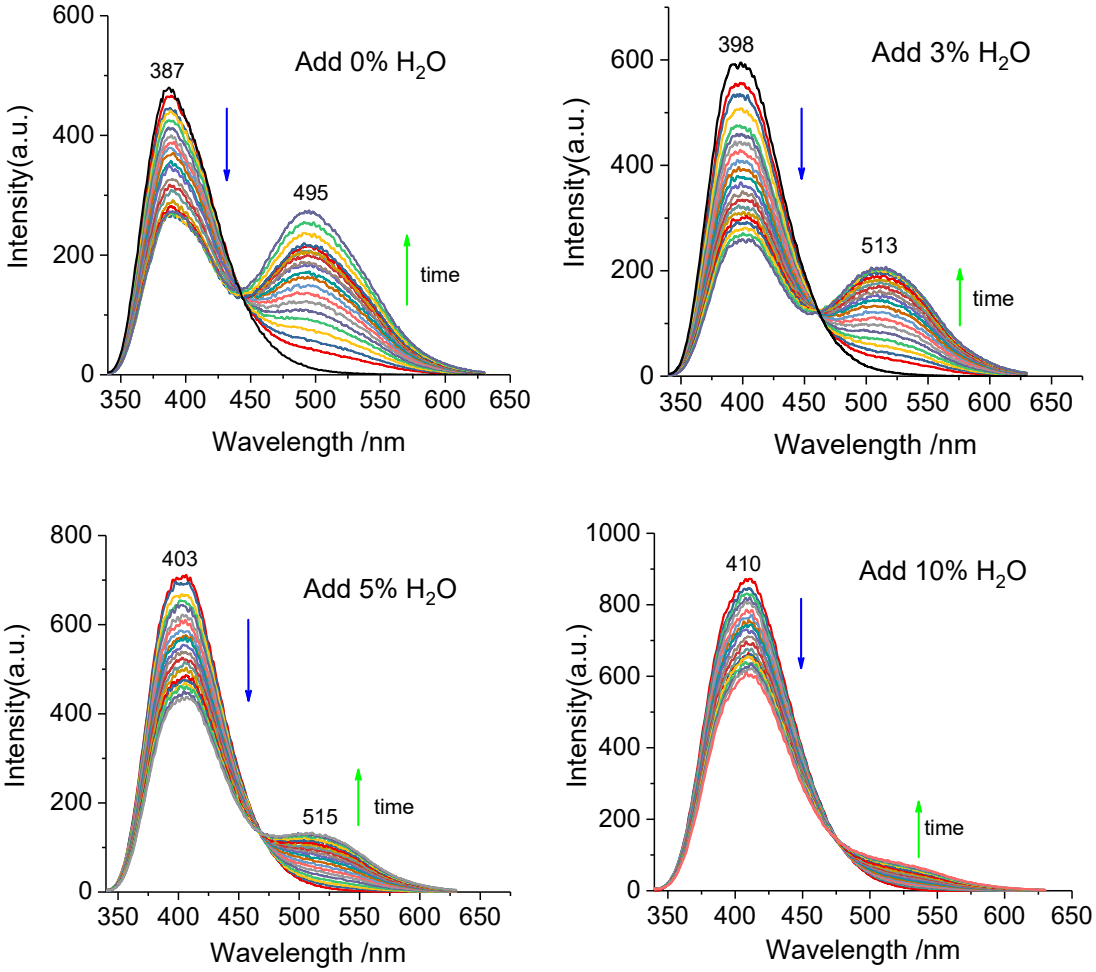


Fig. S5 Time-dependent fluorescence spectra of 10 μM NA-p3 after the addition of 5 equiv. DCP in acetonitrile solutions upon adding different amounts of water (0-10%), recorded once every minute for 20 min, excitation at 330 nm.

VI. Experiments for the selectivity of the sensors

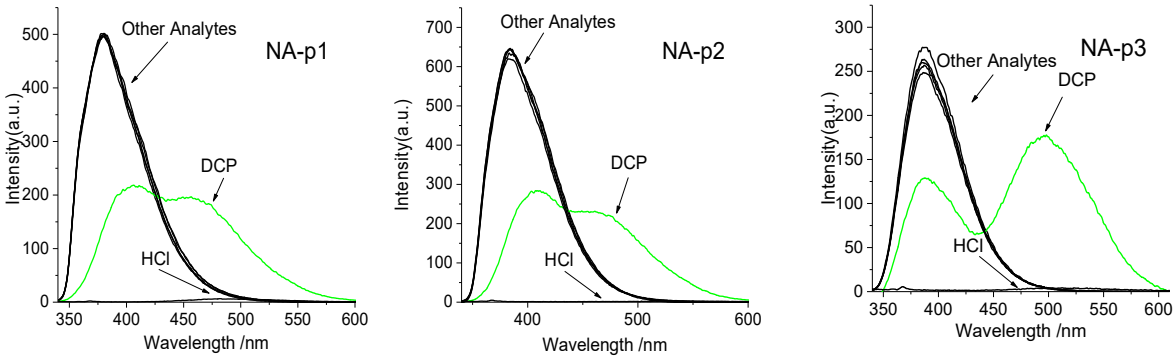


Fig. S6a Fluorescence intensity of the probe (10 μM) upon addition of 4.5 equiv. of DCP or 100 equiv. of other analytes (DCNP, HAc, HCl, DMMP and TEP).

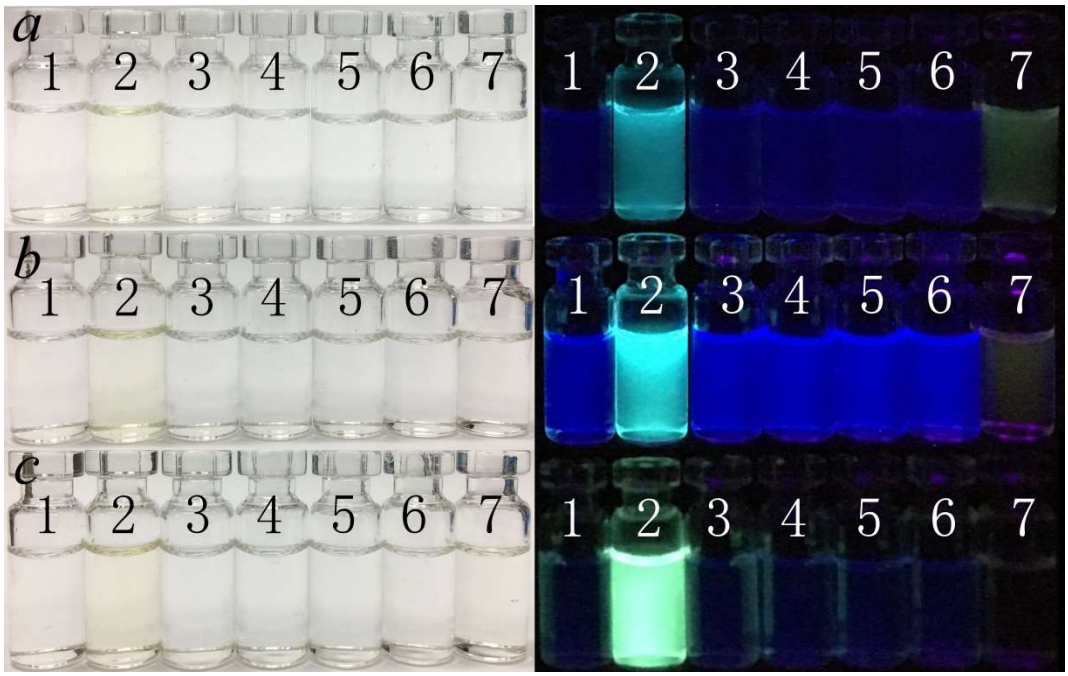
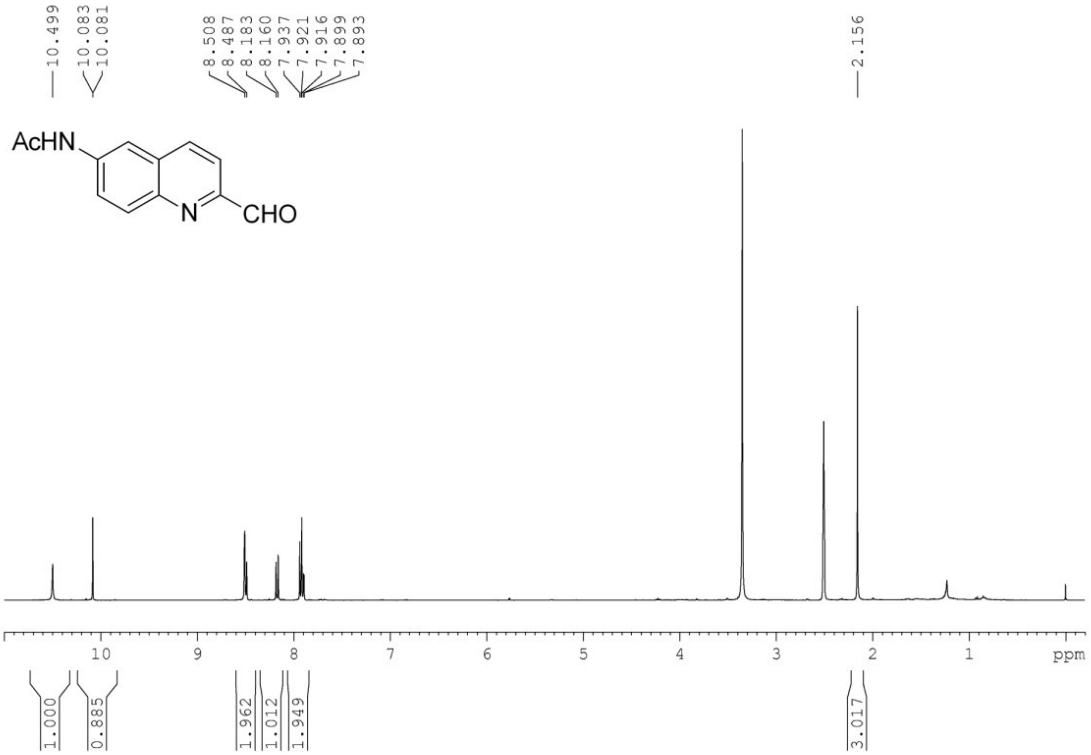
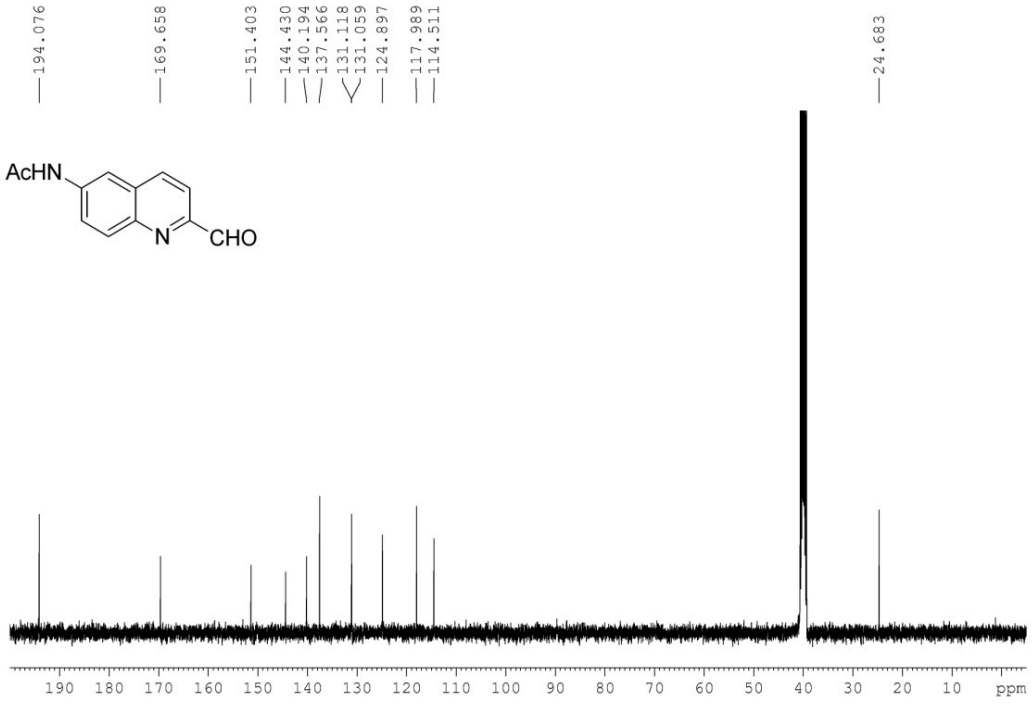


Fig. S6b Chromatic (left) and fluorescent (right) response of 20 μM NA-p1 (a), NA-p2 (b) and NA-p3 (c) before (1) and after addition of 2: DCP (45 μM), 3: DCNP (1 mM), 4: HAc (1 mM), 5: DMMP (1 mM), 6: TEP (1 mM) or 7: HCl (1 mM).

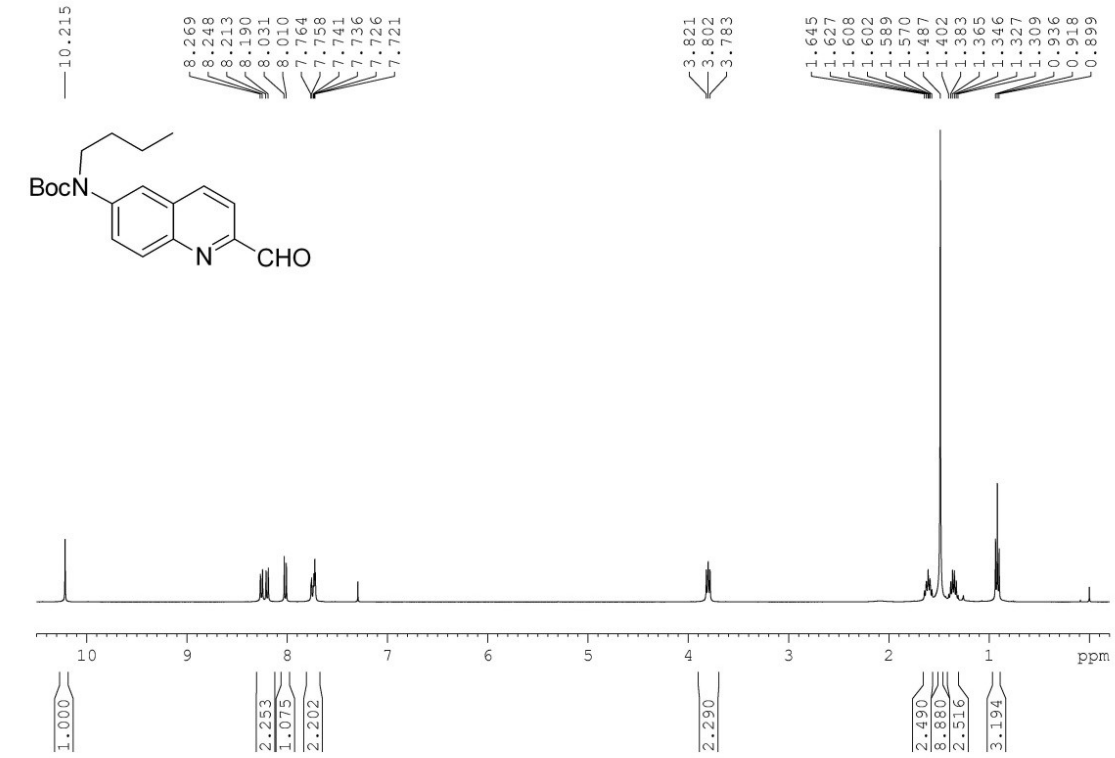
VII. Copies of NMR spectra of relevant compounds

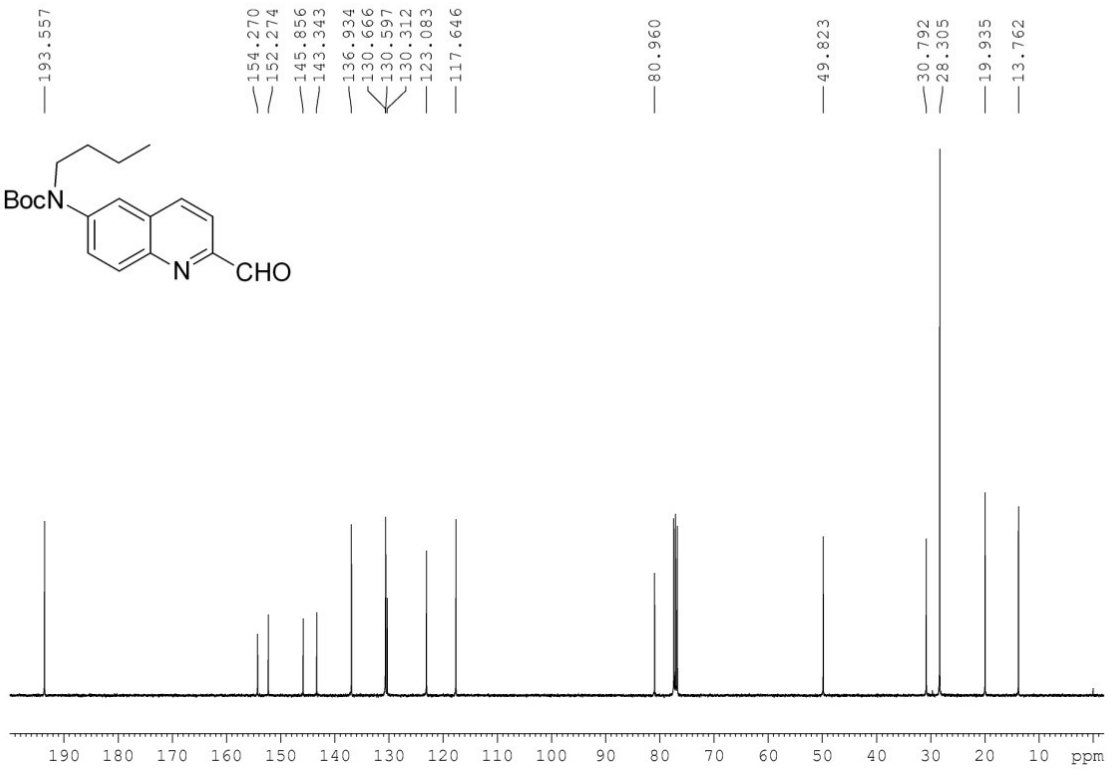
Copies of NMR spectra of compound **2a**



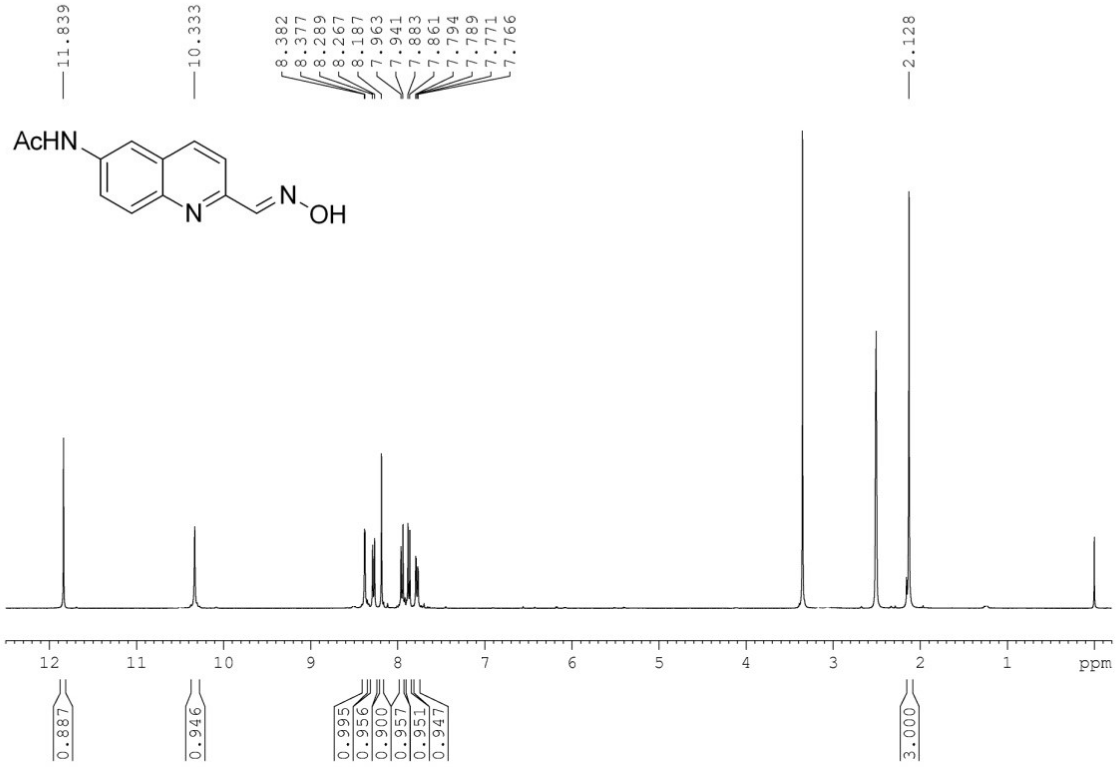


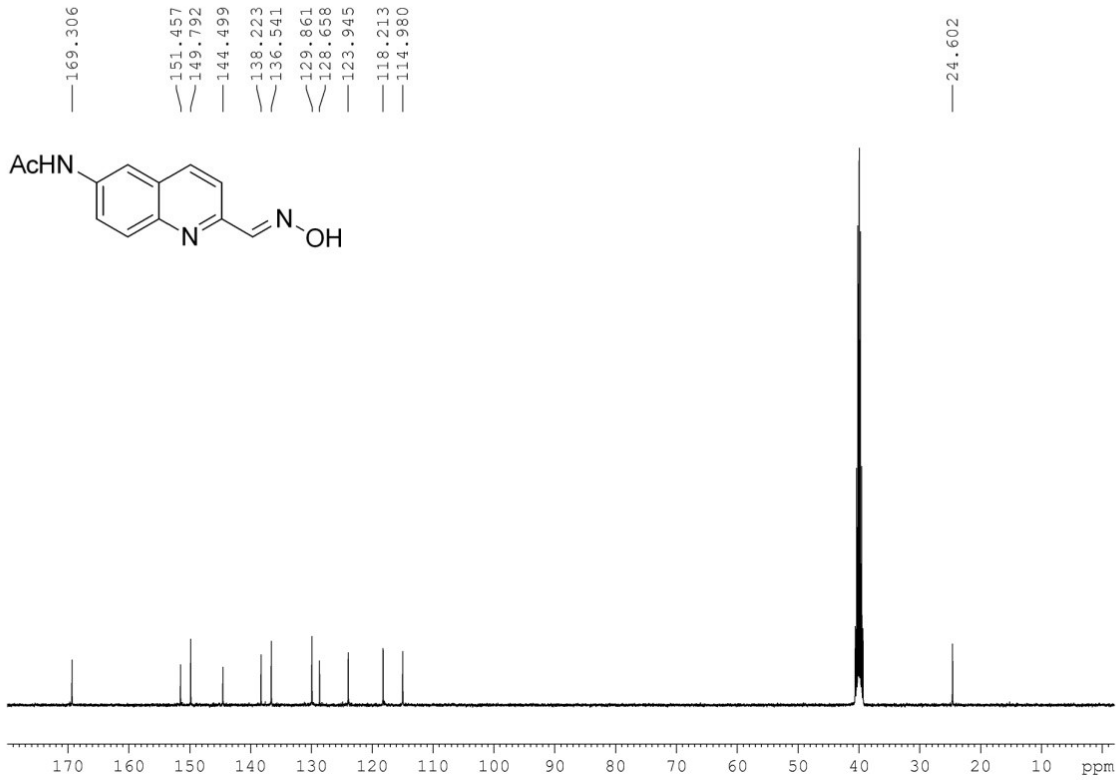
Copies of NMR spectra of compound **2c**



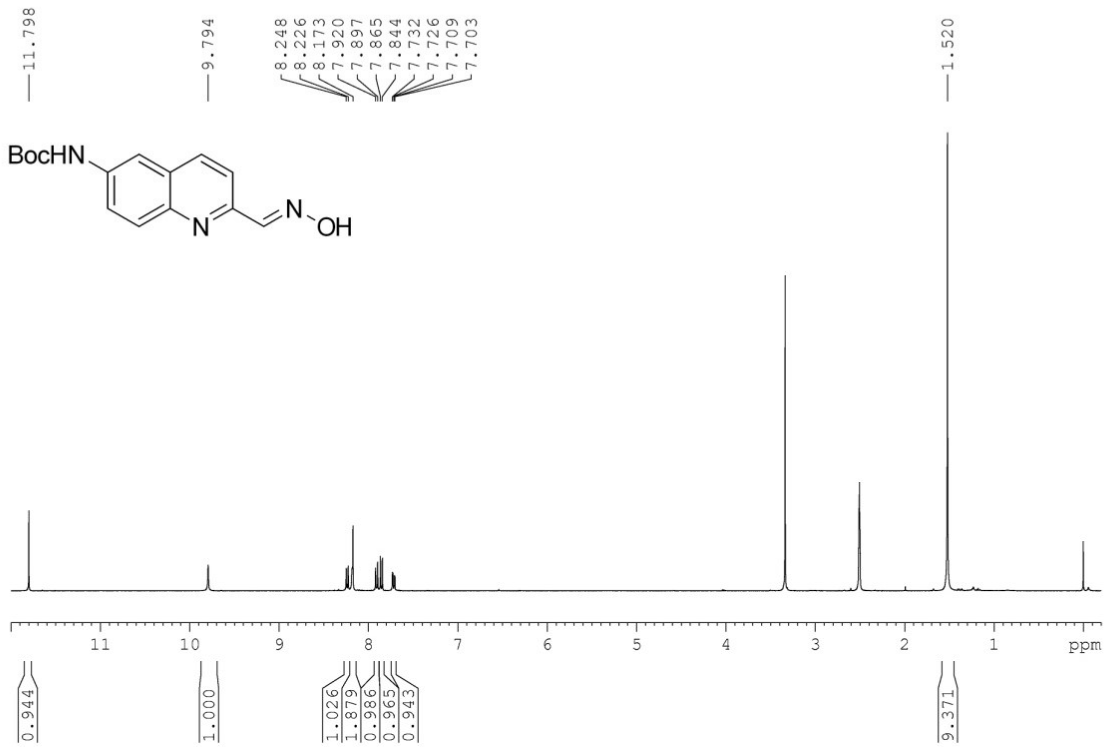


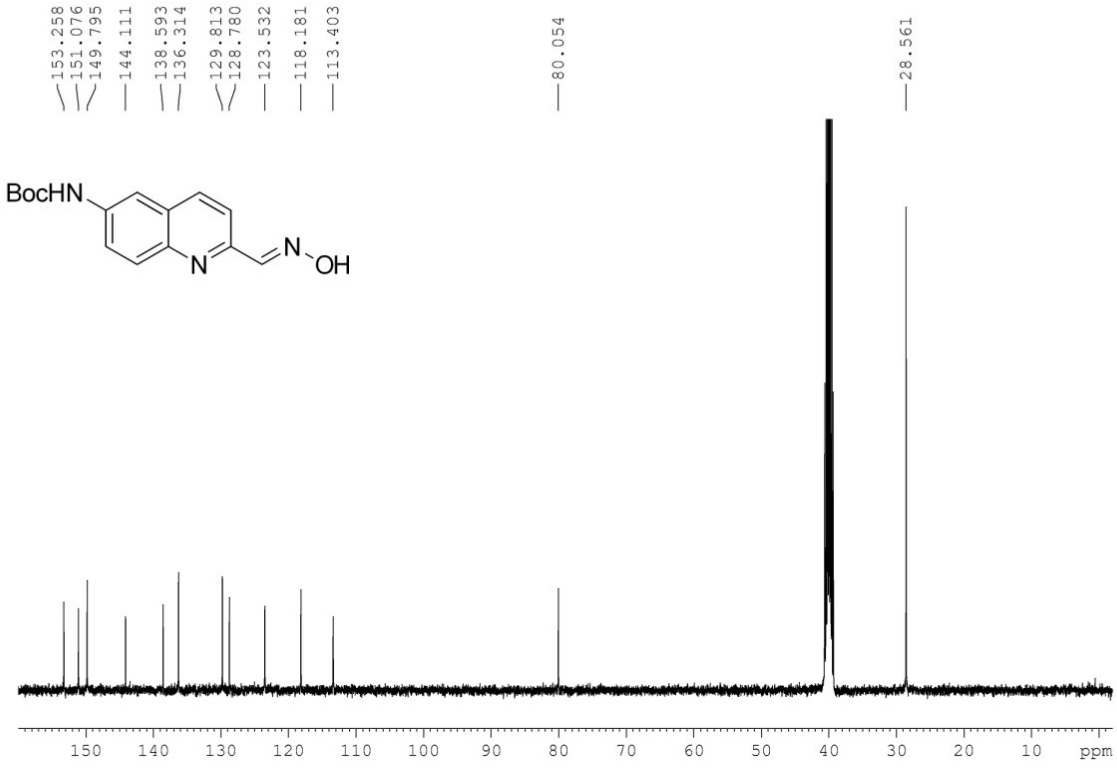
Copies of NMR spectra of NA-p1





Copies of NMR spectra of NA-p2





Copies of NMR spectra of NA-p3