

Supporting Information

pH-sensitive multifunctional fluorescent probe based on *N*-annulated perylene for the sensitive and selective detection of hypochlorous acid

Xiao Zhang,^a Yongchao Yan,^a Qing Peng,^b Jian Wang,^a Yandi Hang,^a and Jianli Hua^{*a}

^a *Key Laboratory for Advanced Materials, Institute of Fine Chemicals, College of Chemistry and Molecular Engineering, East China University of Science and Technology, 130 Meilong Road, Shanghai, 200237, China. E-mail: jlhua@ecust.edu.cn; Fax: +86-21-64250940; Tel: +86-21-64250940*

^b *Qingdao Entry Exit Inspection and Quarantine Bureau, 2 Zhongshan Road, Qingdao, 266001, China.*

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1. The absorption responses of PNPM towards HOCl at different pH

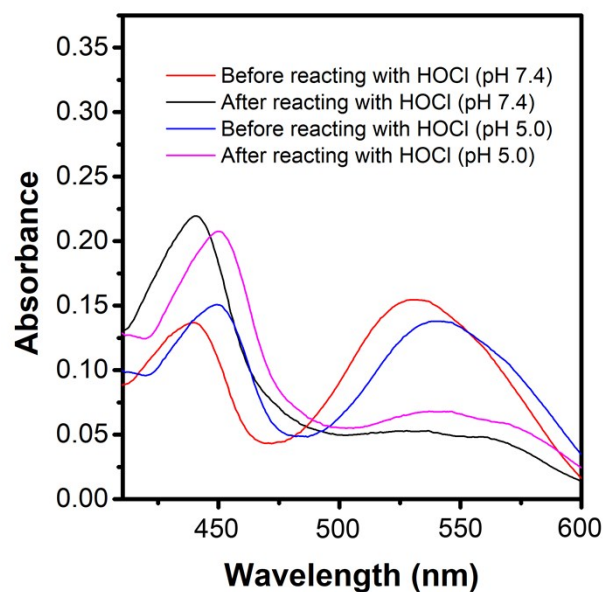


Figure S1. The absorption spectra of PNPM before and after reacting with HOCl under neutral (pH 7.4) or weak acidic (pH 5.0) conditions.

2. The selectivity of probe PNPM (10 μ M) to HOCl at pH 7.4

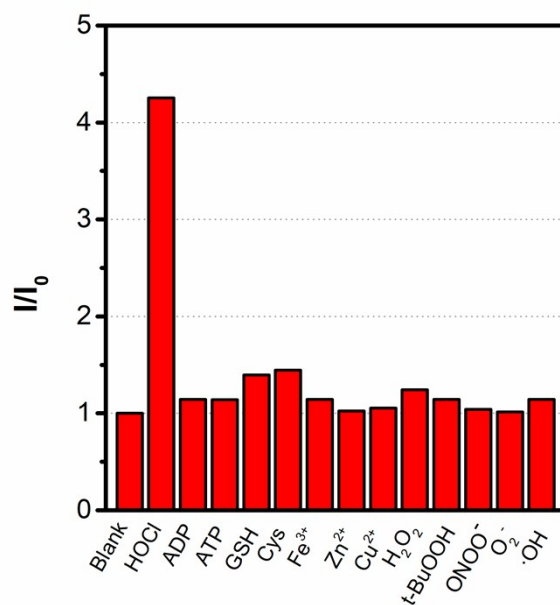


Figure S2. (A) The selectivity of probe **PNPM** (10 μ M) to HOCl at pH 7.4 in the presence of a variety of different biomolecules (ATP, ADP, GSH, Cys, Fe³⁺, Zn²⁺, Cu²⁺, 1 mM) and ROS (H₂O₂, t-BuOOH, ONOO⁻, O₂⁻, •OH).

3. Long-term photostability of probe PNPM

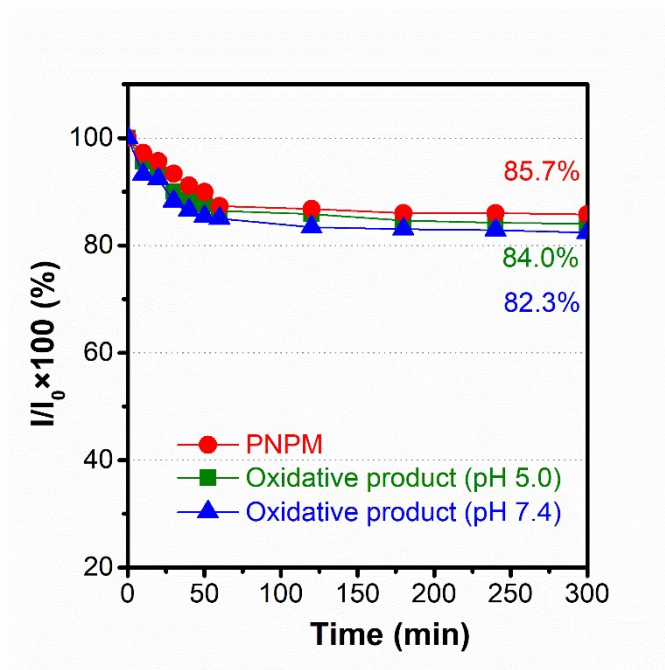


Figure S3. The long-term photostability of PNPM (10 μ M) and its oxidative product at different pH were studied under 200 W/m² light irradiation for 0-300 minutes. I_0 was the initial fluorescent intensity and I was the fluorescent intensity of the sample after the light irradiation at certain time intervals.

4. Detecting HOCl in real water samples

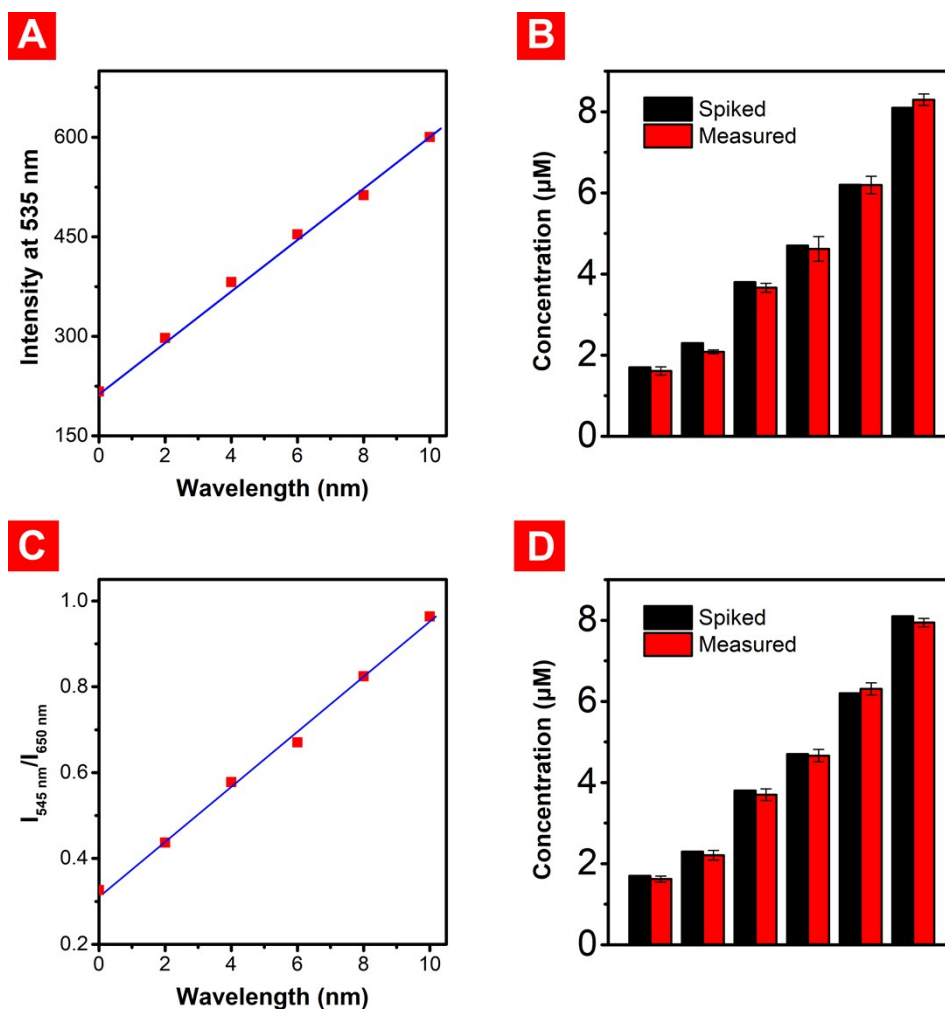


Figure S4. (A) Plotting the fluorescent intensity at 535 nm as a function of low HOCl concentration (0-9 μM) for **PNPM** (10 μM) in the drinking water samples. (B) The spiked (1.7, 2.3, 3.8, 4.7, 6.2 and 8.1 μM) and measured concentrations (1.61, 2.08, 3.66, 4.61, 6.19 and 8.29 μM) of HOCl in in the drinking water samples. (C) Plotting the ratiometric fluorescent changes ($I_{545 \text{ nm}}/I_{650 \text{ nm}}$) at 535 nm as a function of low HOCl concentration (0-10 μM) for **PNPM** (10 μM) in the pool water samples. (B) The spiked (1.7, 2.3, 3.8, 4.7, 6.2 and 8.1 μM) and measured concentrations (1.62, 2.20, 3.70, 4.66, 6.31 and 7.96 μM) of HOCl in in the pool water samples.

5. Characterization of new compounds

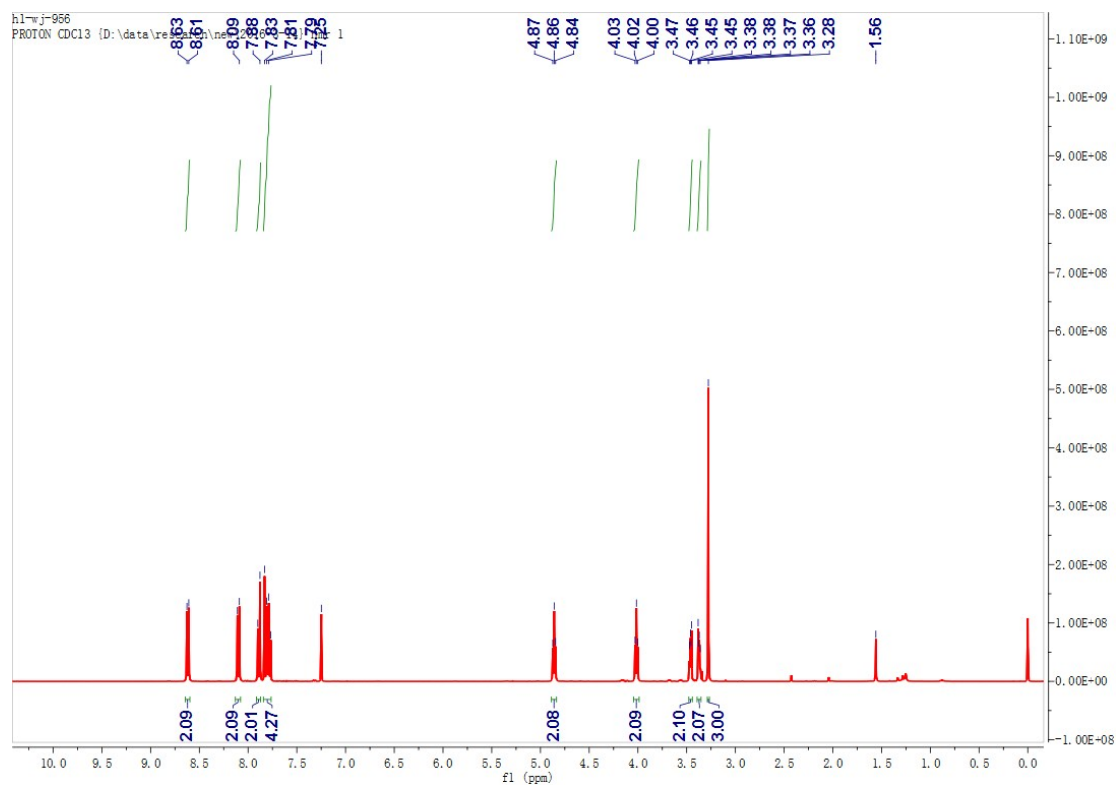


Figure S5. ^1H NMR spectrum of intermediate compound **2** in CDCl_3

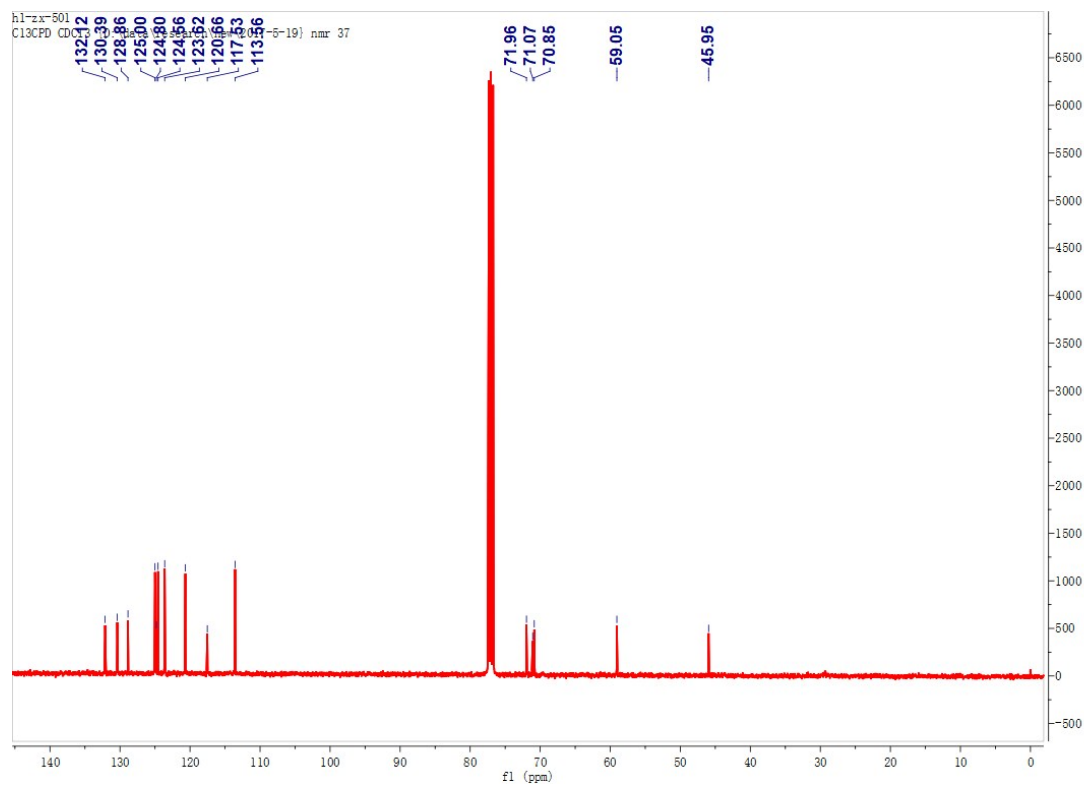


Figure S6. ^{13}C NMR spectrum of intermediate compound **2** in CDCl_3

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-22 N: 0-1 O: 0-2

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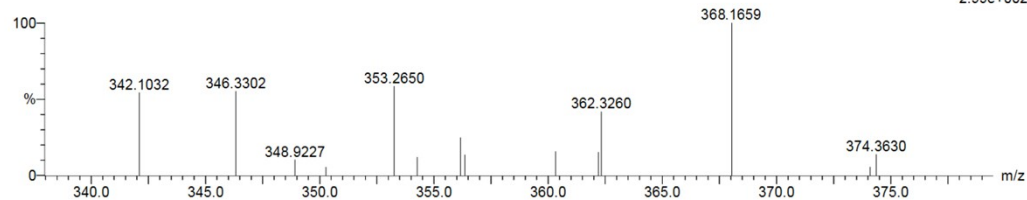
21-Apr-2017

19:05:55

1: TOF MS ES+

2.99e+002

HJL-ZX-553 53 (0.739) Cm (52.54)

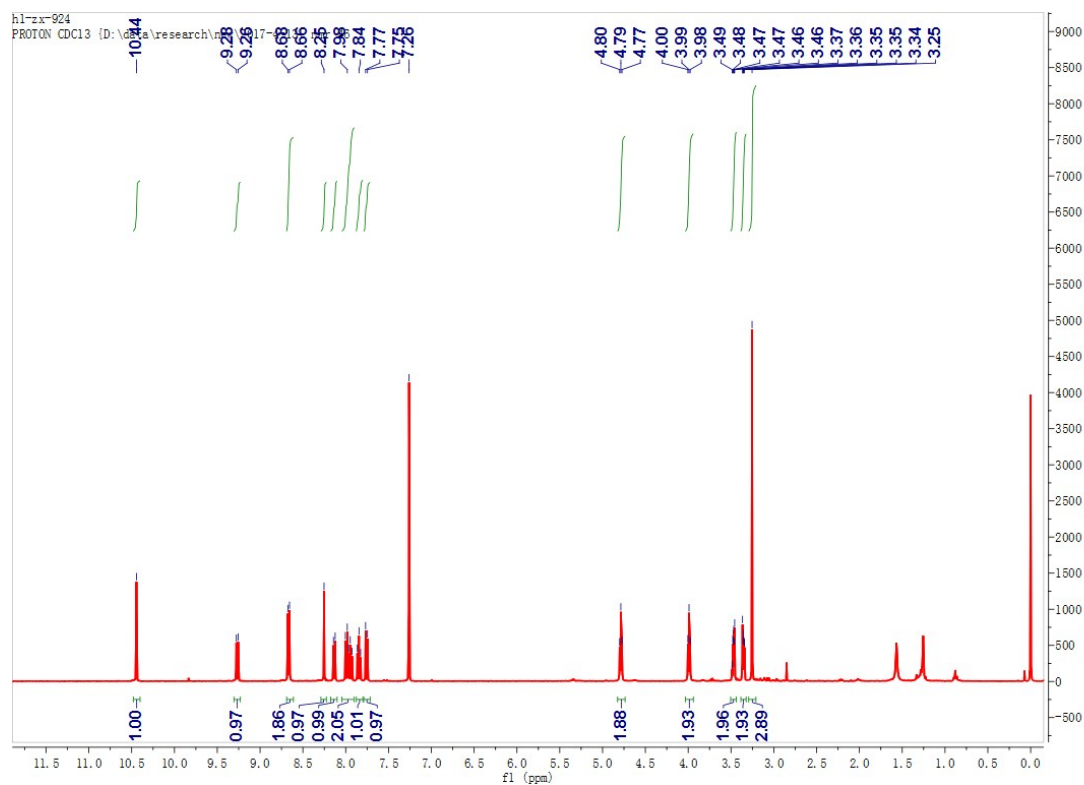


Minimum: 30.0 50.0 -1.5

Maximum: 30.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
368.1659	368.1651	0.1	0.3	10.5	21.2	0.0	C25 H22 N O2

Figure S7. HRMS of intermediate compound 2

Figure S8. ^1H NMR spectrum of intermediate compound 3 in CDCl_3

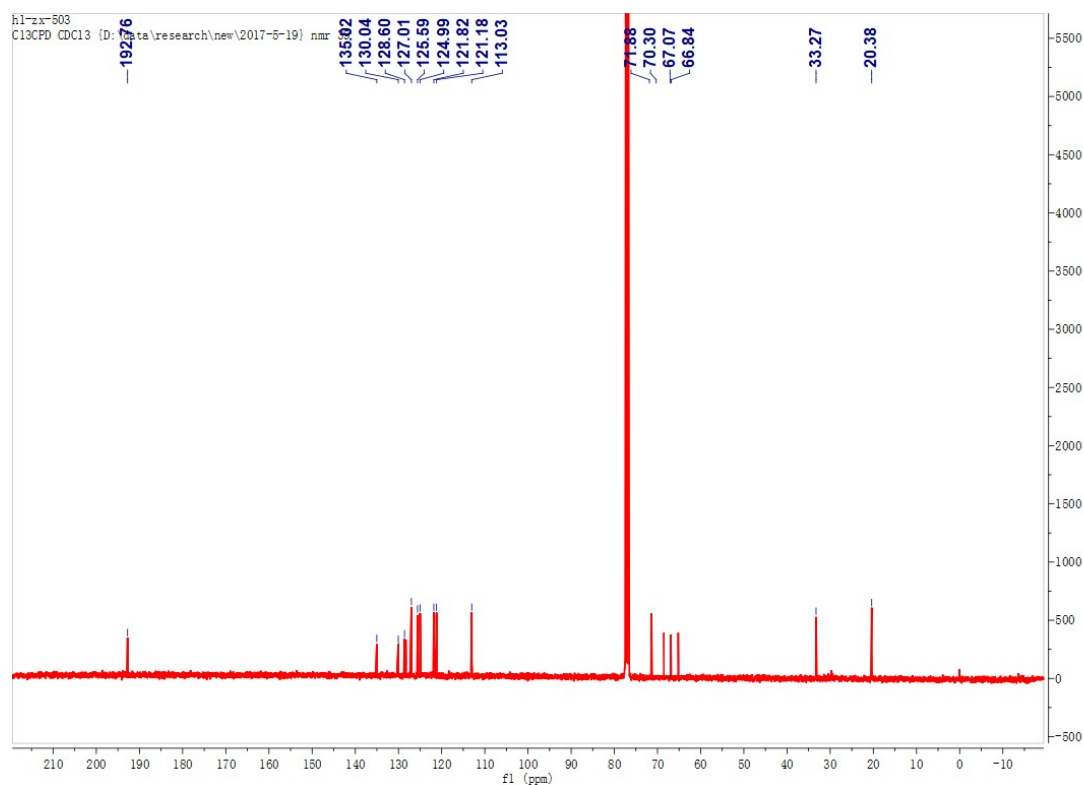


Figure S9. ^{13}C NMR spectrum of intermediate compound **3** in CDCl_3

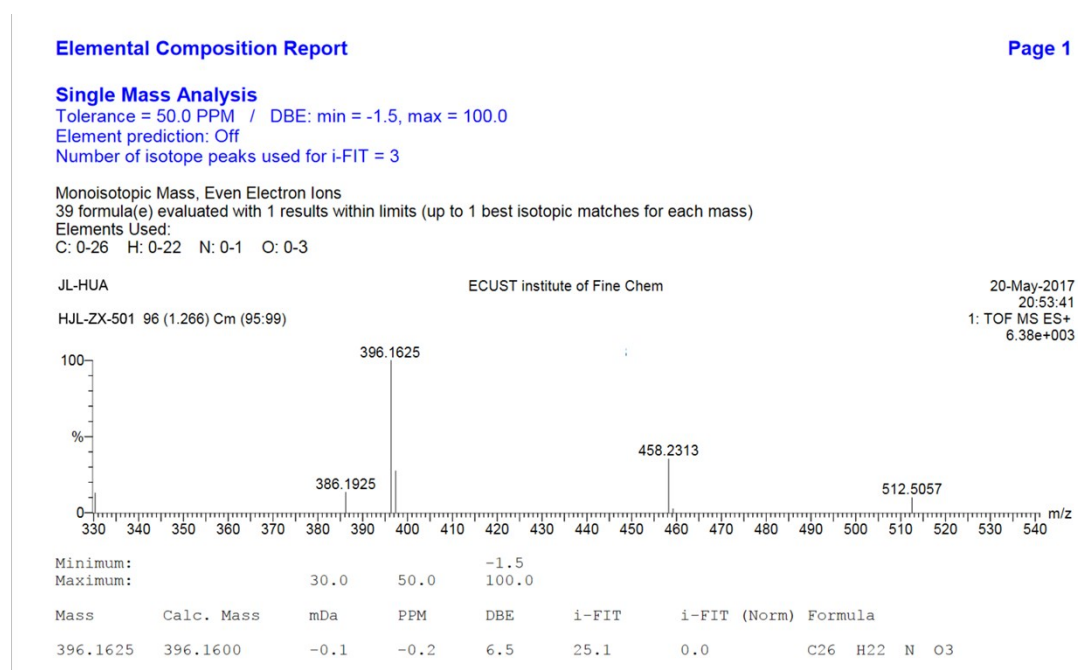


Figure S10. HRMS of intermediate compound **3**

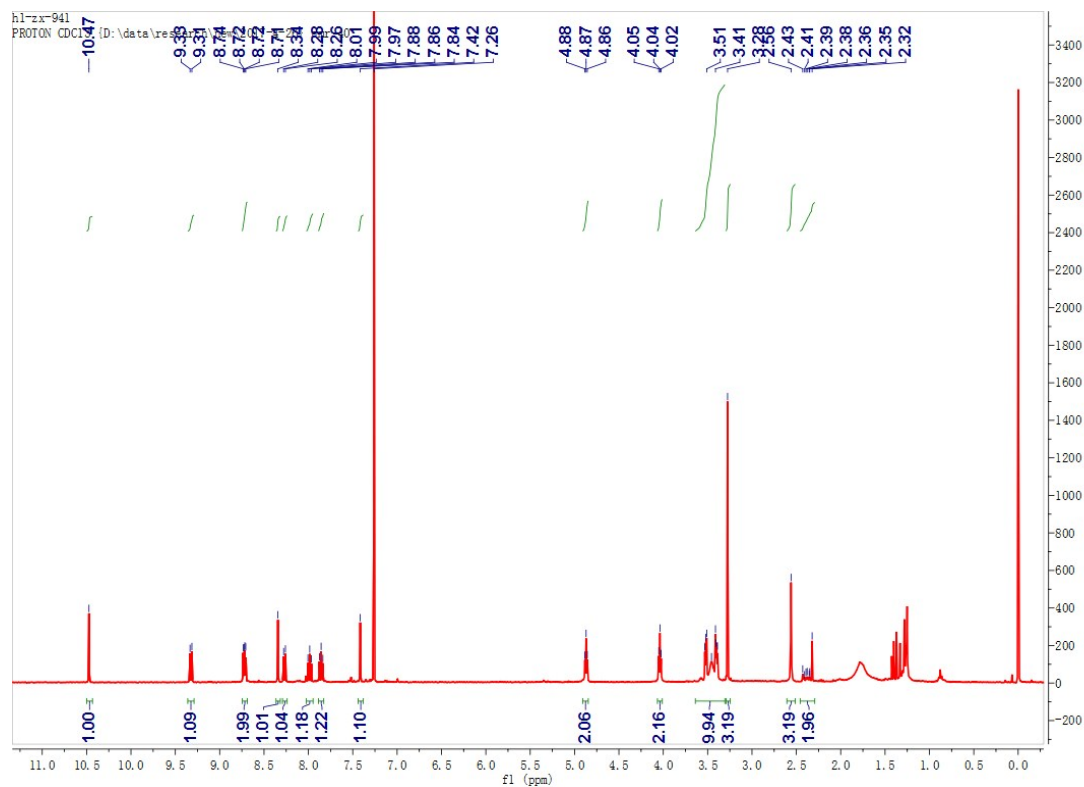


Figure S11. ^1H NMR spectrum of intermediate compound **5**

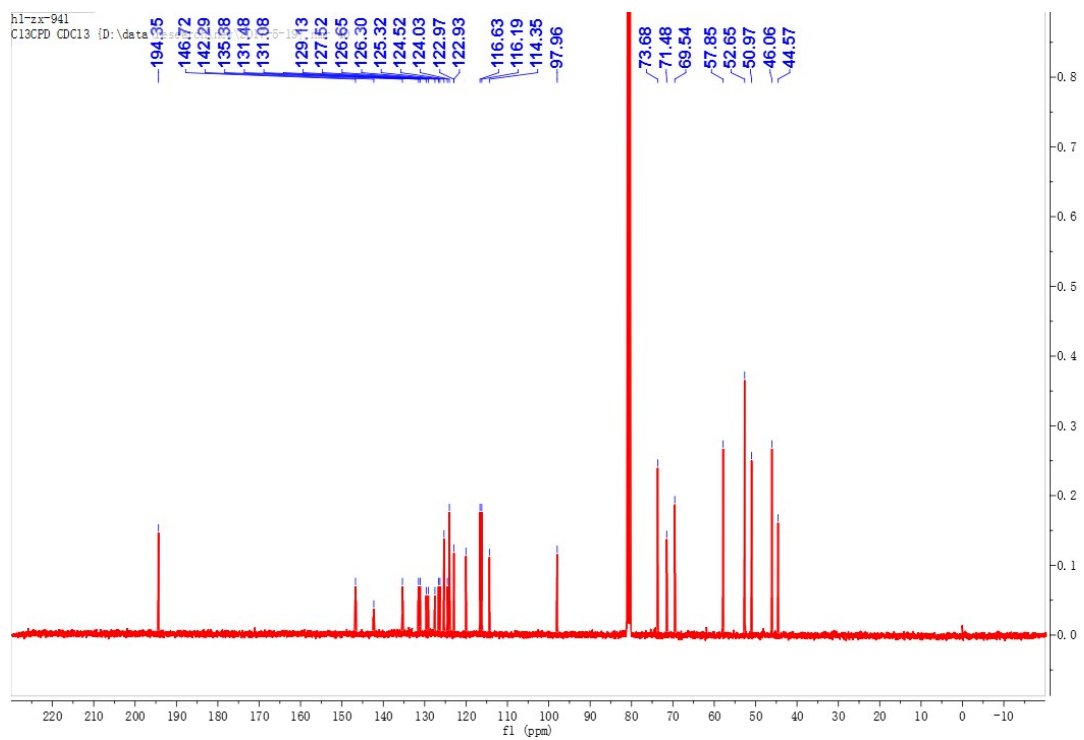


Figure S12. ^{13}C NMR spectrum of intermediate compound **5**

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

40 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-31 H: 0-32 N: 0-3 O: 0-3

JL-HUA

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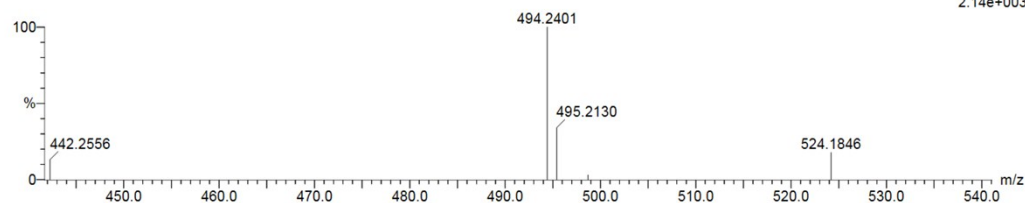
20-May-2017

20:58:48

1: TOF MS ES+

2.14e+003

HJL-ZX-506 49 (0.697) Cm (48:52)



Minimum: -1.5
Maximum: 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
494.2401	494.2444	0.1	0.2	15.5	22.7	0.0	C31 H32 N3 O3

Figure S13. HRMS of intermediate compound 5

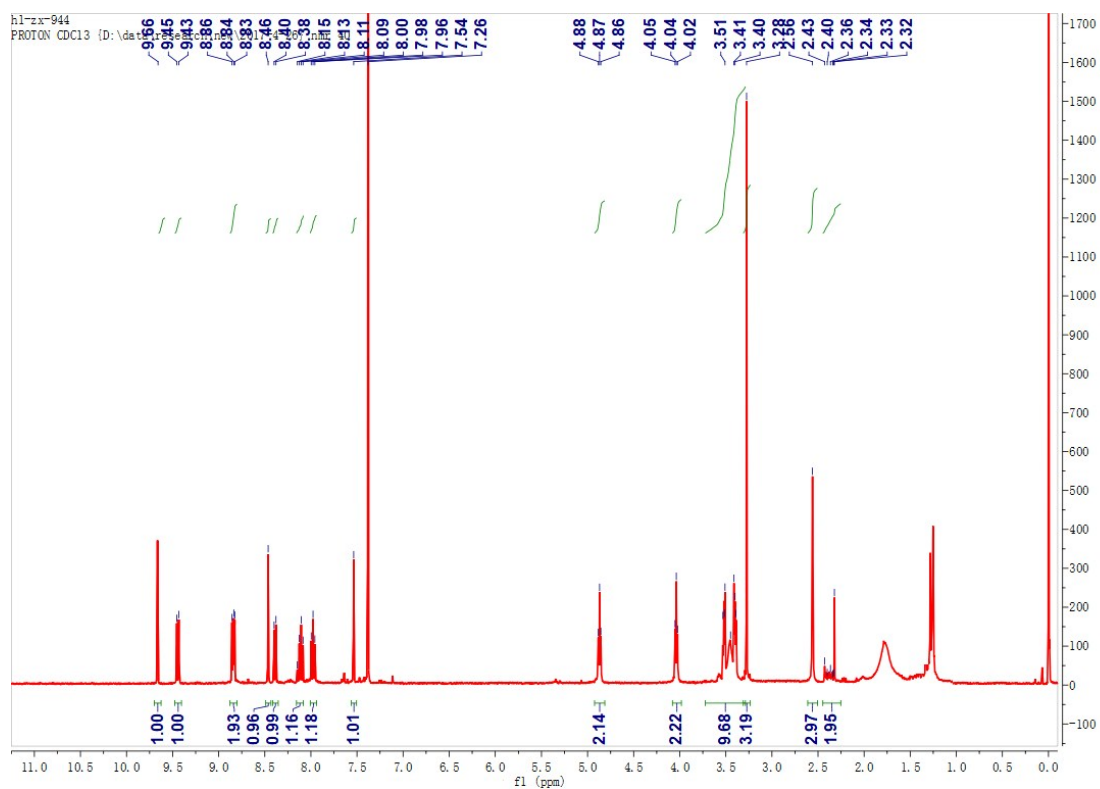


Figure S14. ¹H NMR spectrum of probe PNPM

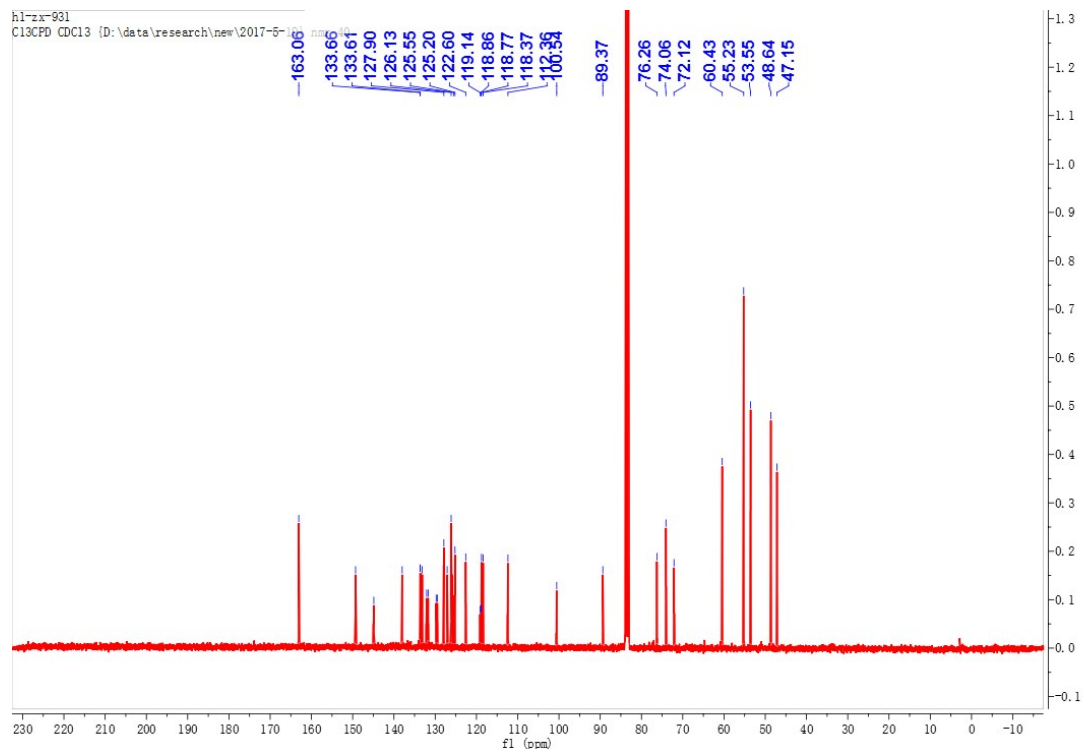


Figure S15. ^{13}C NMR spectrum of probe PNPM

Elemental Composition Report

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Single Mass Analysis

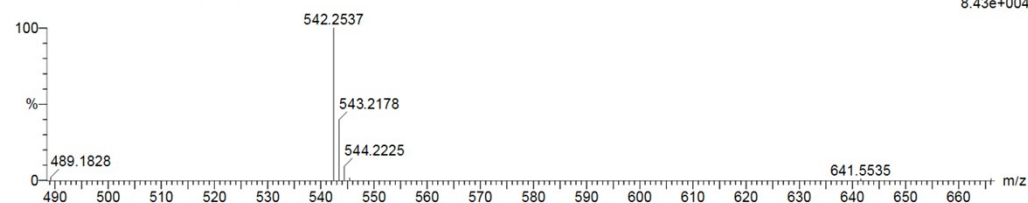
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 23 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
 Elements Used:
 C: 0-34 H: 0-32 N: 0-5 O: 0-3
 JL-Hua

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20-May-2017
 20:34:14
 1: TOF MS ES+
 8.43e+004

HJL-ZX-509 92 (2.093) Cm (90:102)



Minimum: -1.5
 Maximum: 30.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
542.2537	542.2556	0.6	1.0	21.5	14.7	0.0	C ₃₄ H ₃₂ N ₅ O ₃

Figure S16. HRMS of probe PNPM