Supporting information for

Naphthalimide-based fluorescent probe for highly sensitive and selective detection of nerve agent mimic DCP in solution and vapor phase

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1. Determination of detection limit

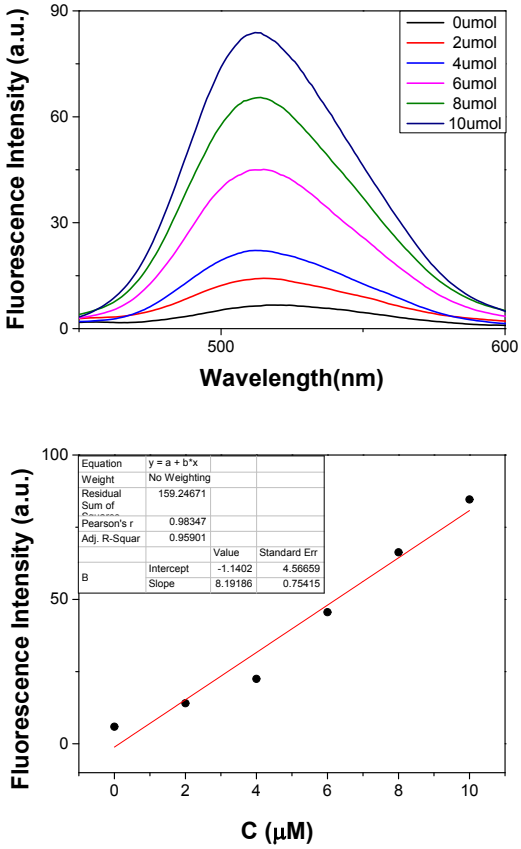


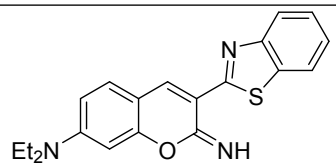
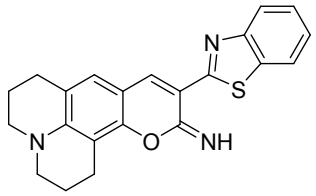
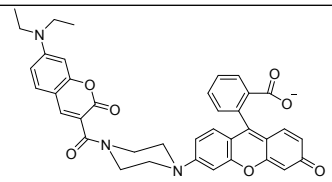
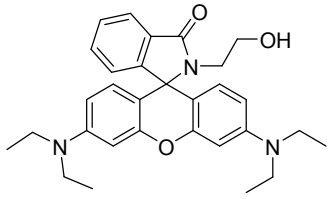
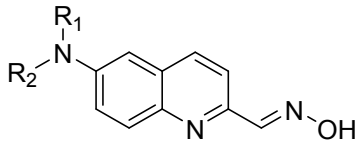
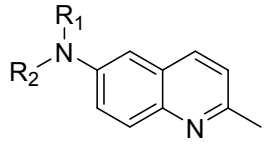
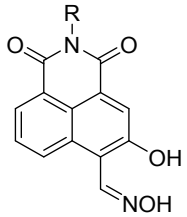
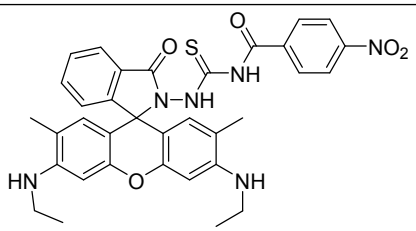
Figure S1. Fluorometric determination of limit of DCP to probe **2** in DMF.

LOD = 3 Sb / m (Sb is the ratio signal and noise, m is the slope of the linearity)

Slope = 8.19186 Standard Deviation = 0.015169 K=3

LOD = K × Standard Deviation / Slope = 3 × 0.015169 / 8.19186 = 0.0055 μM=5.5nm

2. The LOD of reported fluorescent probe for DCP

Probe	LOD	References
	0.065 μM	J. Hazard. Mater., 2018, 342, 10–19
	0.21 μM	J. Hazard. Mater., 2018, 342, 10–19
	0.17 ppm	Chem.Commun., 2013, 49, 10474–10476
	25 ppm	Chem.Commun.,2011, 47, 11468–11470
	21 nM	J. Mater. Chem. C, 2017, 5, 7337--7343
	8 nm	ACS Sens. 2017, 2, 834−841
	21.9 nM	Chem. Eur.J. 2017, 23,7785 –7790
	0.142 μmol	Sensor. Actuators B Chem. 235 (2016) 447–456

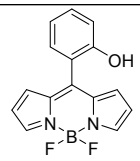
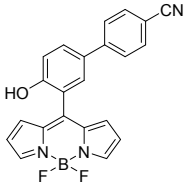
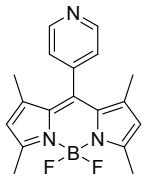
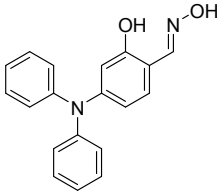
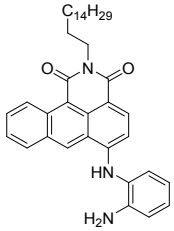
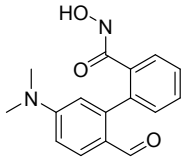
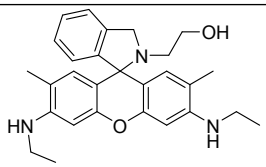
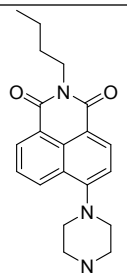
	0.71μg/L	Anal. Chem. 2016, 88, 9259−9263
	1.87 ppb	Sensor. Actuators B Chem. 255 (2018) 176–182
	3.36 μmol	Sensor. Actuators B Chem. 238 (2017) 145–149
	140 nM	Dyes and Pigments 170 (2019) 107585
	88nm	Anal. Chem. 2019, 91, 12070−12076
	10.4nm	Anal. Chem. 2019, 91, 10979−10983
	9.6nm	Dyes and Pigments 171 (2019) 107712
	5.5 nM	This work

Table S1. The LOD of reported fluorescent probe for DCP

3. HCl effect

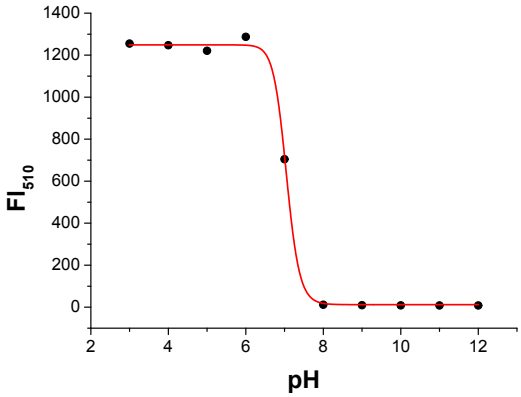


Figure S2. The fluorescence intensity of probe **2** (10.0 μM) at 510 nm in the presence and absence of DCP in DMF: H_2O 1:1 v/v (10.0 μM) under different pH (3.0-12.0)

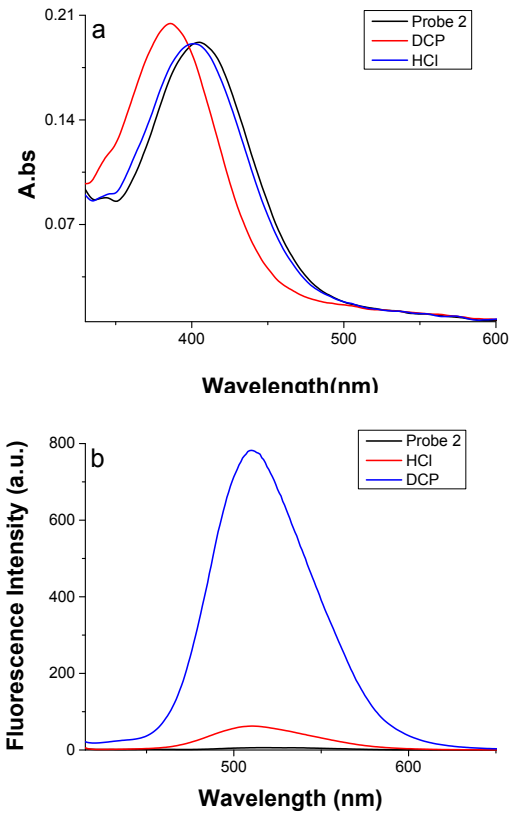


Figure S3. (a) Absorption and (b) emission spectra of probe **2** (10 μM) in the presence of DCP (50.0 μM) or HCl (50.0 μM) in DMF.

4. Kinetic study

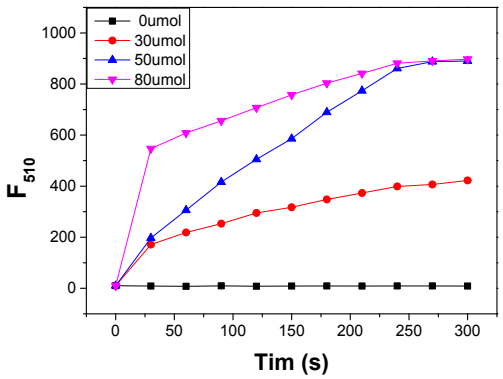


Fig. S4. Kinetic profile of the reaction between probe **2** and DCP in DMF

5. Fluorescence images of above solutions

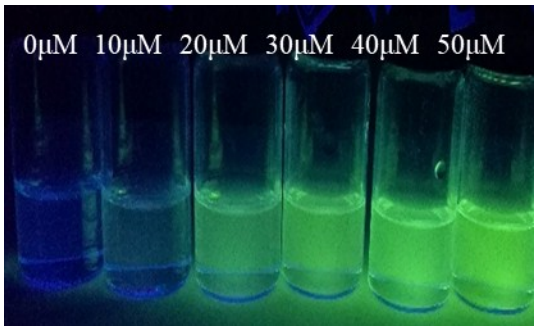


Fig. S5. Photographs of probe **2** in DMF with different amounts of DCP after a 5 min incubation under UV light (365 nm).

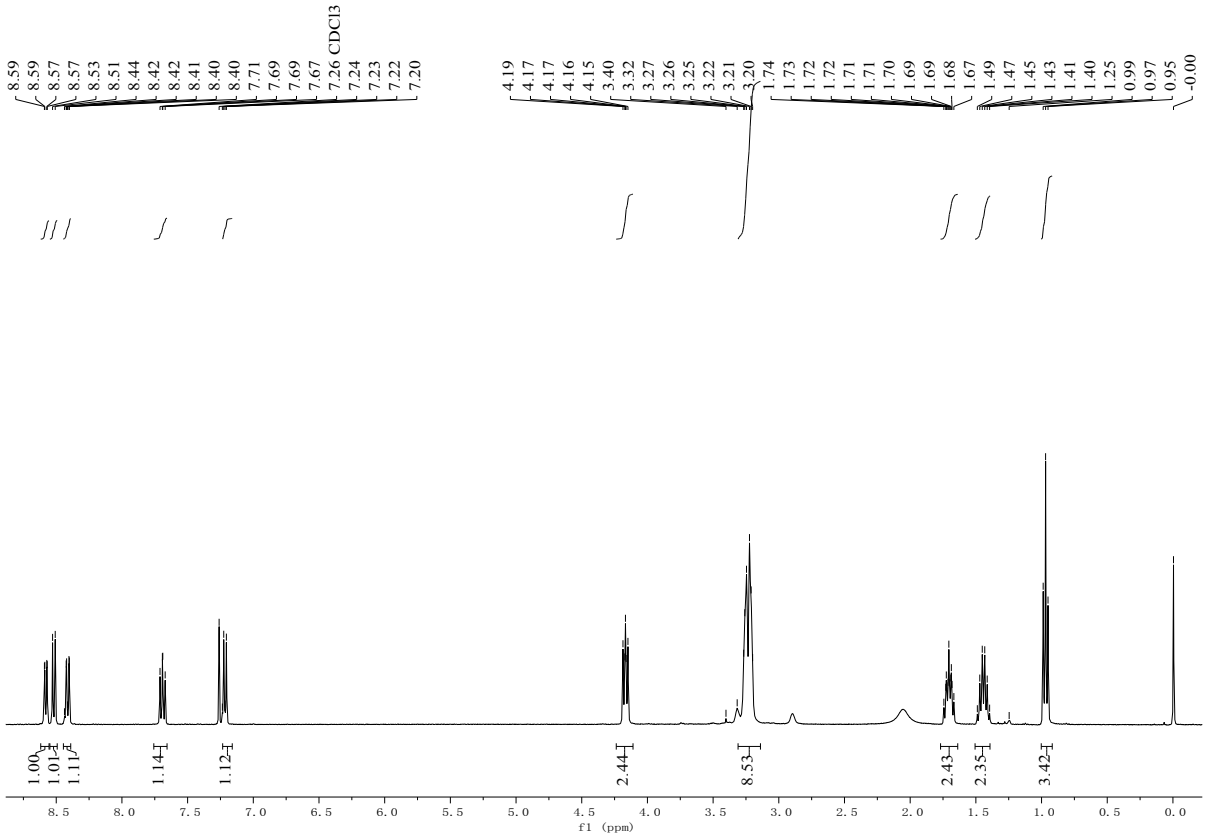
6. Quantum yield

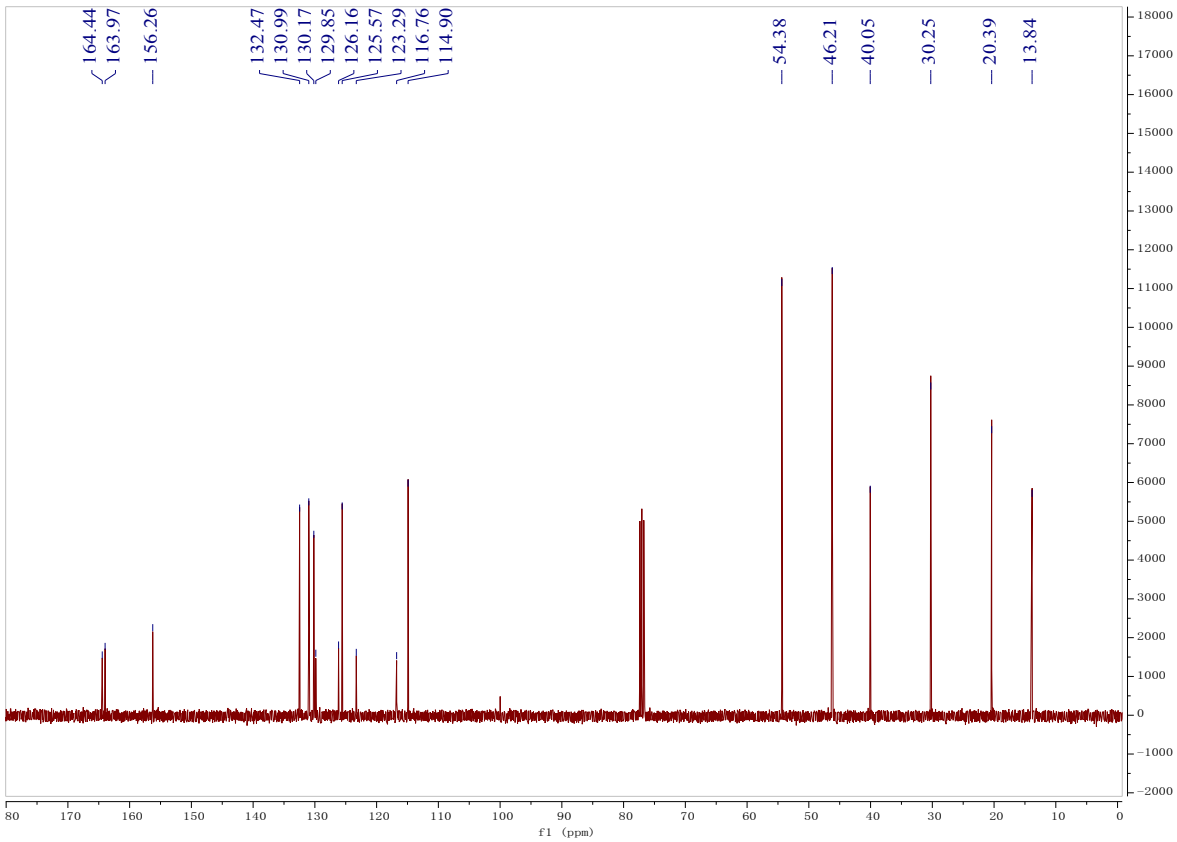
$$\Phi_I = \frac{\Phi_B I_I A_B \lambda_{exB} \eta_I}{I_B A_I \lambda_{exI} \eta_B}$$

Where φ is quantum yield; I is integrated area under the corrected emission spectra; A is absorbance at the excitation wavelength; λex is the excitation wavelength; η is the refractive index of the solution; the subscripts 1 and B refer to the unknown and the standard, respectively. Fluorescence quantum yields were determined in solution, using Rhodamine B (Acid) in alcohol as a standard (ΦF = 0.49). ΦF=0.005 for probe **2** and ΦF=0.48 for probe **2**@DCP.

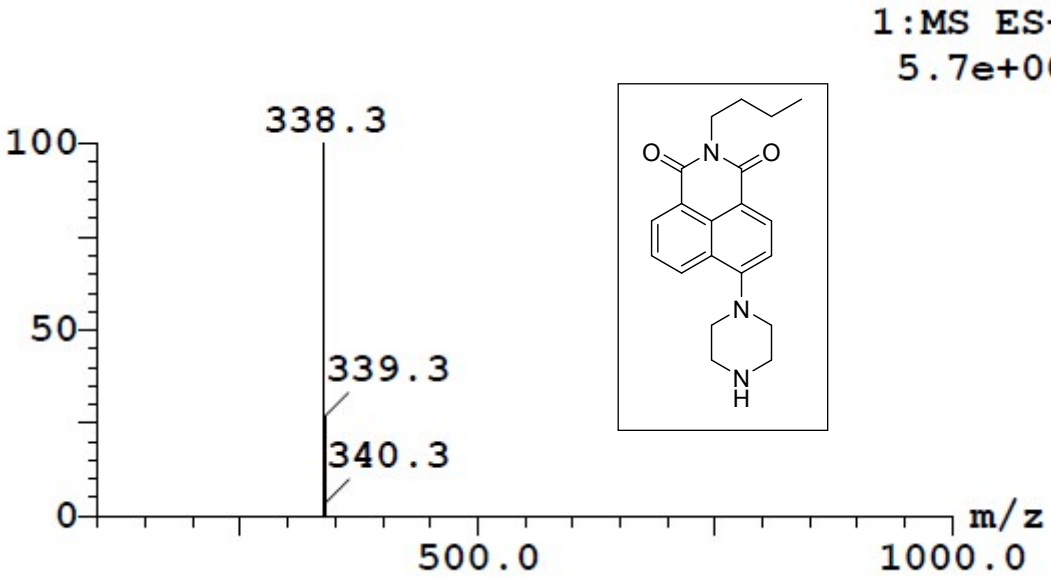
7. Characterization

NMR spectra of probe 2

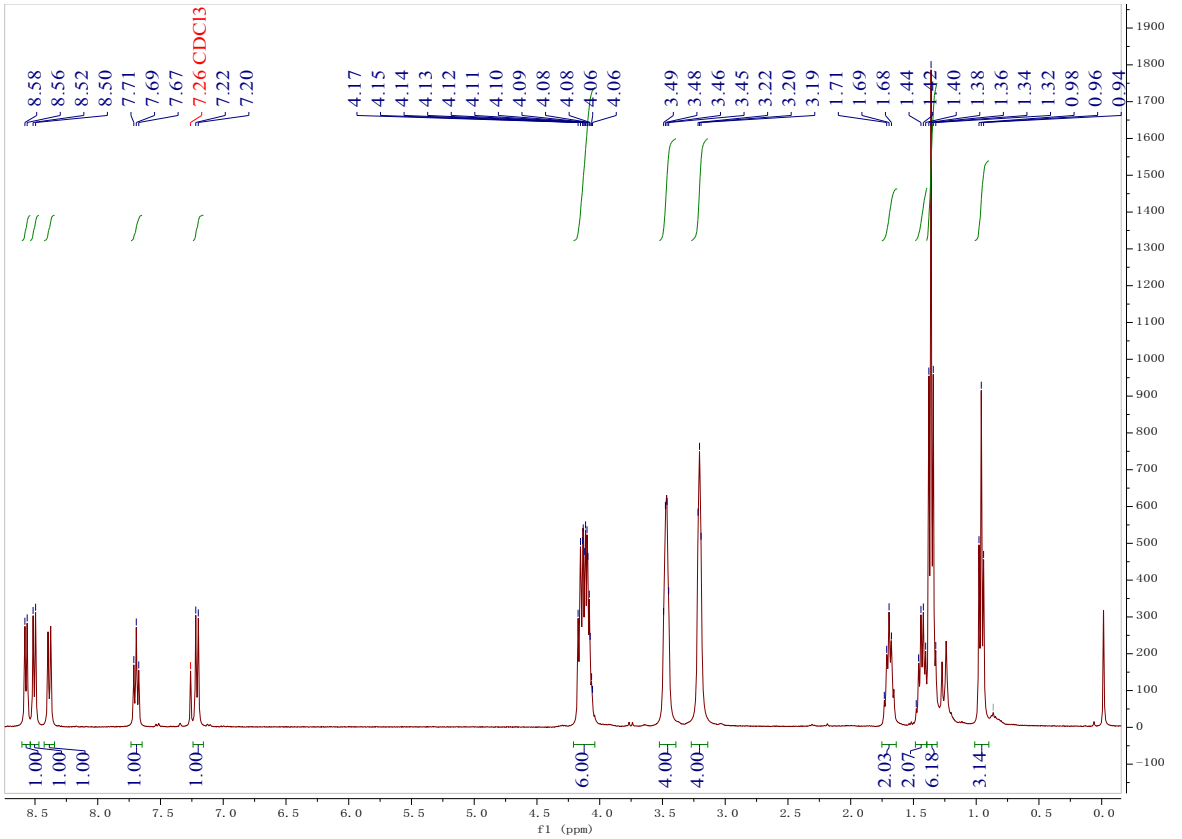


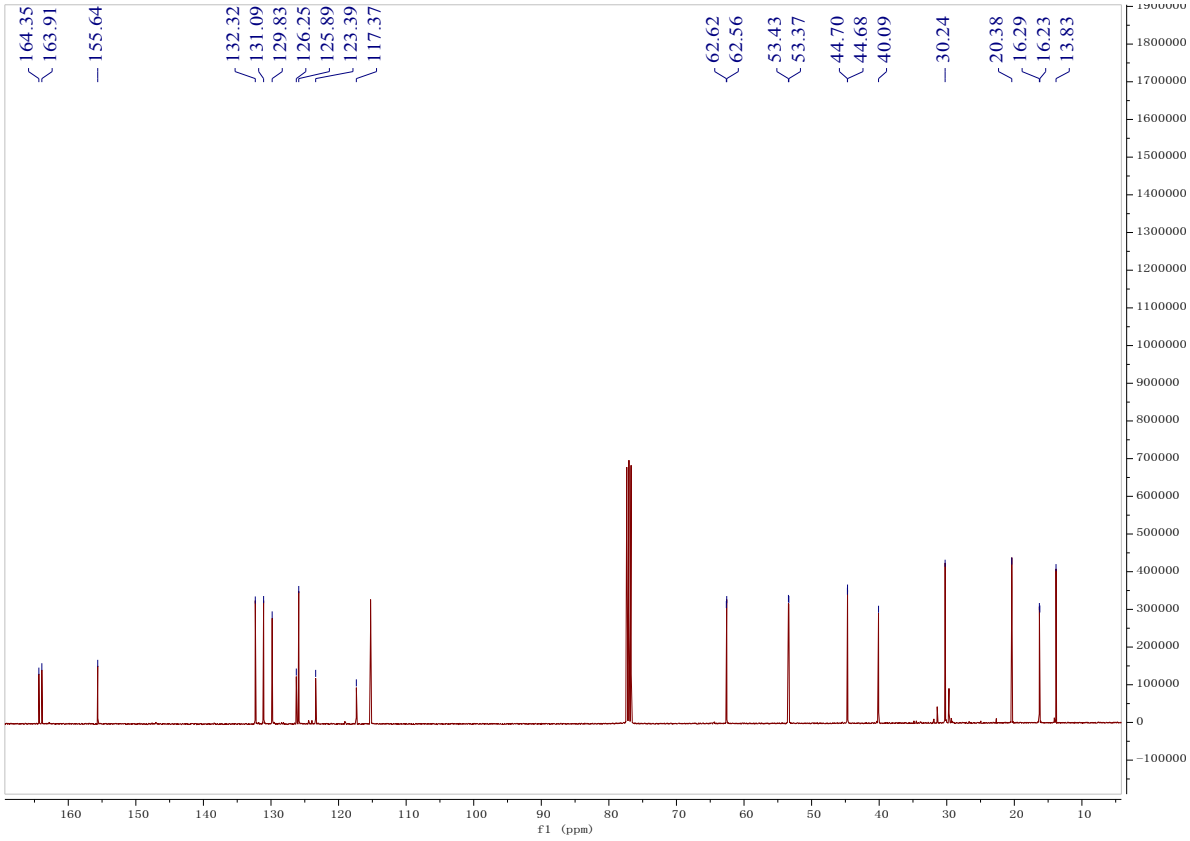


MS spectrum of probe 2

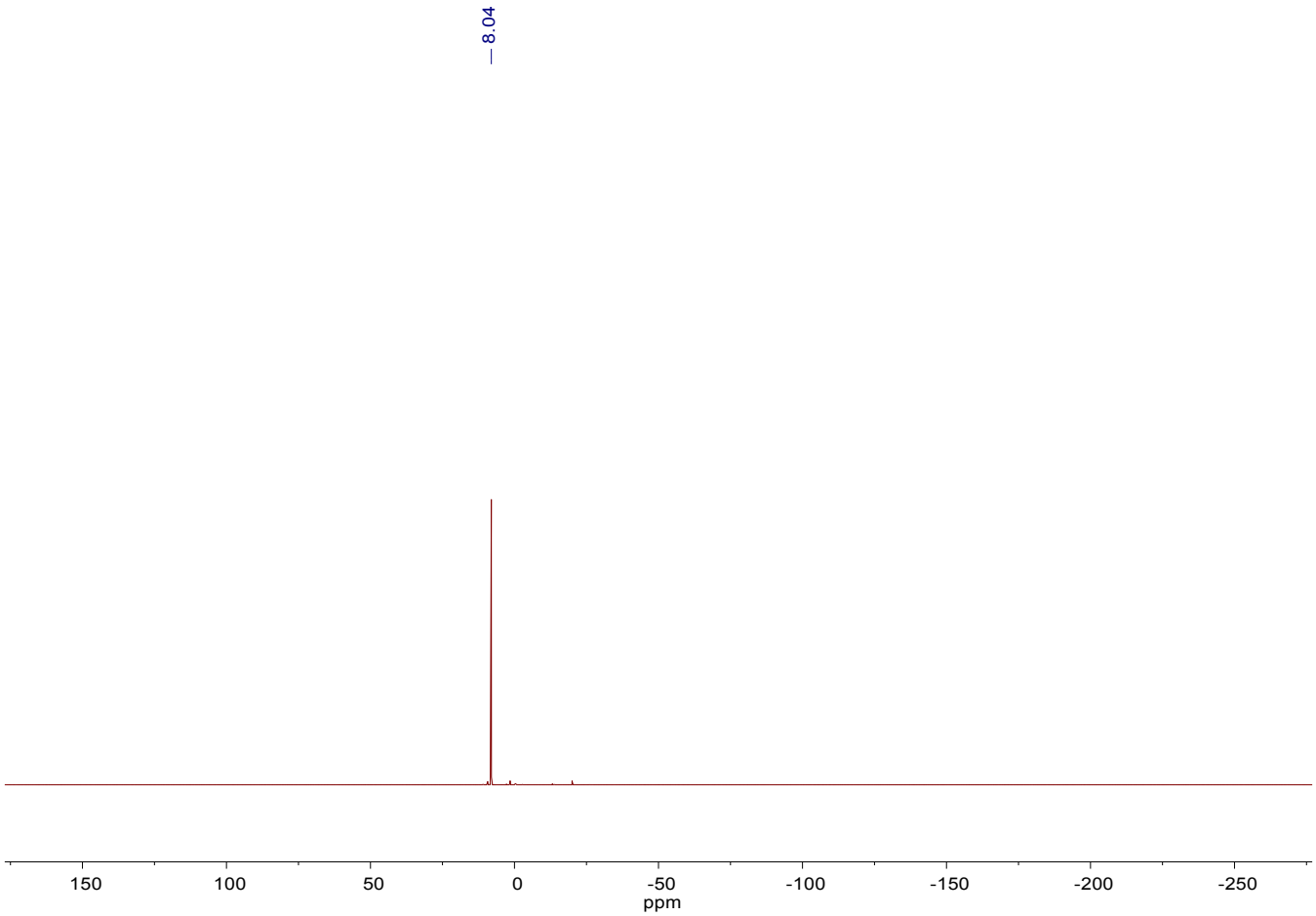


NMR spectra of compound 3

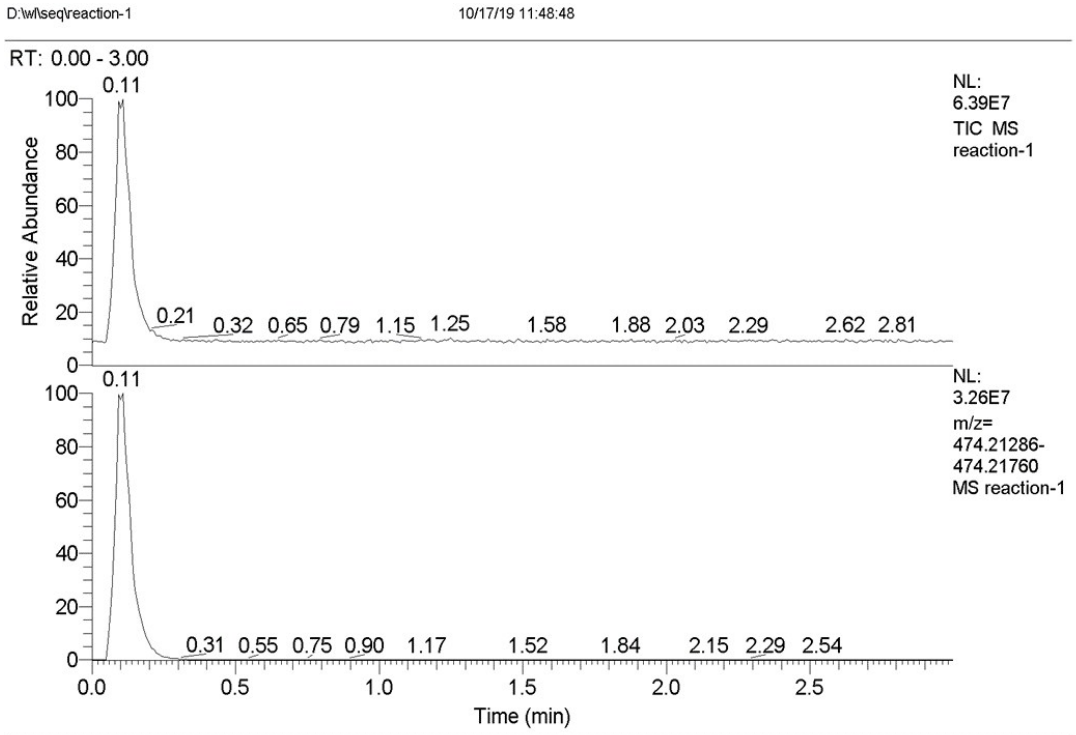

8.58
8.56
8.52
8.50
7.71
7.69
7.67
7.26 CDCl3
7.22
7.20
4.17
4.15
4.14
4.13
4.12
4.11
4.10
4.09
4.08
4.08
4.06
4.06
3.49
3.48
3.46
3.45
3.22
3.20
3.19
1.71
1.69
1.68
1.44
1.42
1.40
1.38
1.36
1.34
1.32
0.98
0.96
0.94
1.00
1.00
1.00
1.00
1.00
6.00
4.00
4.00
2.03
2.07
6.18
3.14
f1 (ppm)

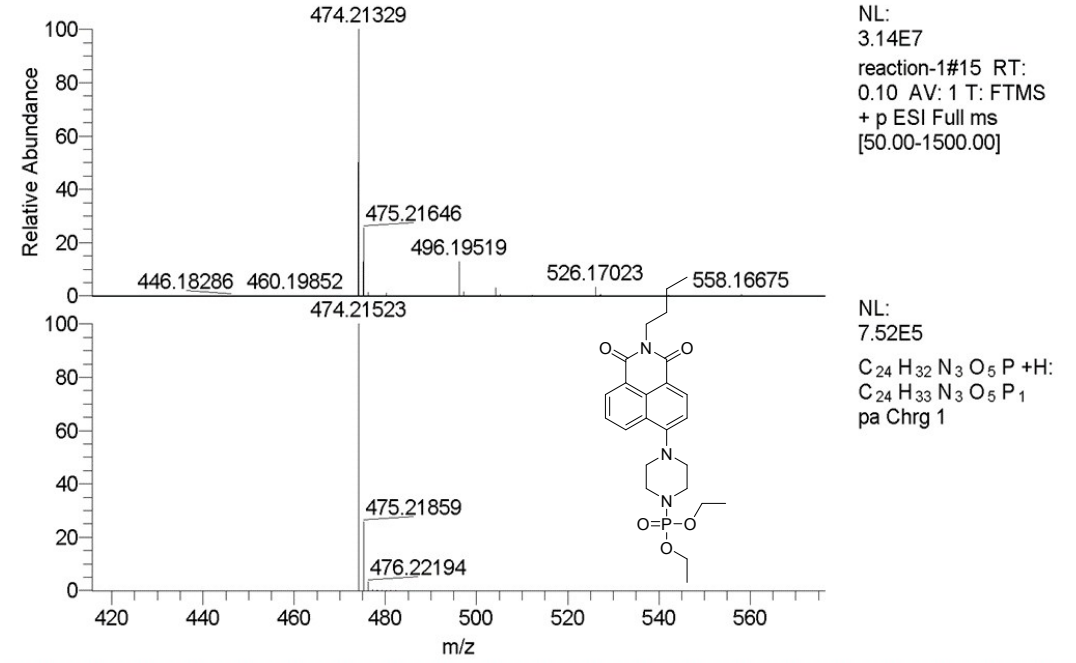

164.35
163.91
155.64
132.32
131.09
129.83
126.25
125.89
123.39
117.37
62.62
62.56
53.43
53.37
44.70
44.68
40.09
30.24
20.38
16.29
16.23
13.83
f1 (ppm)

^{31}P NMR spectra of compound 3



HR-MS spectrum of compound 3





IR spectrum of compound 3