Supporting Information

A New Fluorescent Probe for Ultrasensitive Detection of Phosgene in Solution and Gas Phase

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Photophysical properties of APQ

Table S1 Photophysical properties of the probe.

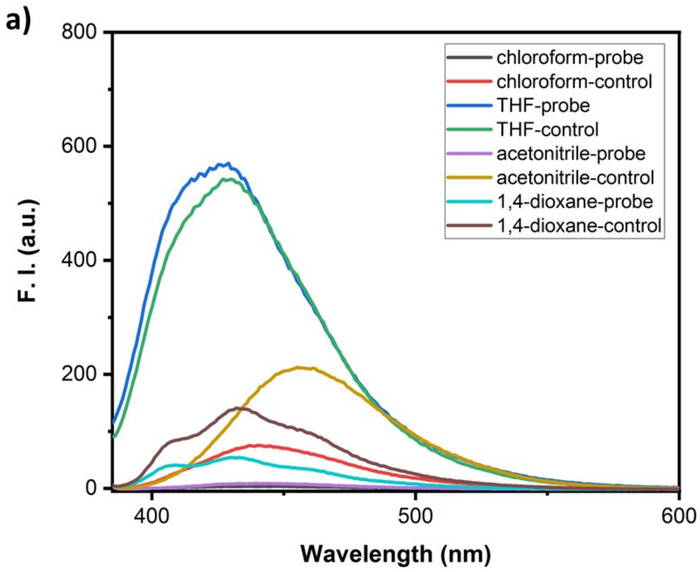
entry	λ_{ab} (nm)	λ_{em} (nm)	Φ^a
APQ	361	447	0.009
APQ+phosgene	357	461	0.192^b

(a) The quantum yield (Φ) of **APQ** and **APQ**-phosgene system were determined according to the literature.[1] (b) Φ was determined in the present of 1.0 equiv. of triphosgene and 2.0 equiv. of TEA.

$$\Phi_{Sample} = \frac{\Phi_{QS} \cdot A_{QS} \cdot F_{Sample} \cdot \lambda_{exQS} \cdot \eta_{Sample}^2}{A_{Sample} \cdot F_{QS} \cdot \lambda_{exSample} \cdot \eta_{QS}^2}$$

Where Φ is quantum yield; A is absorbance at the excitation wavelength; F is integrated area under the corrected emission spectra; λ_{ex} is the excitation wavelength; η is the refractive index of the solution; the Sample and QS refer to the sample and the standard, respectively. We chose quinine sulfate in 0.1N H_2SO_4 as standard, which has the quantum yield of 0.546.[2]

Additional spectroscopic data



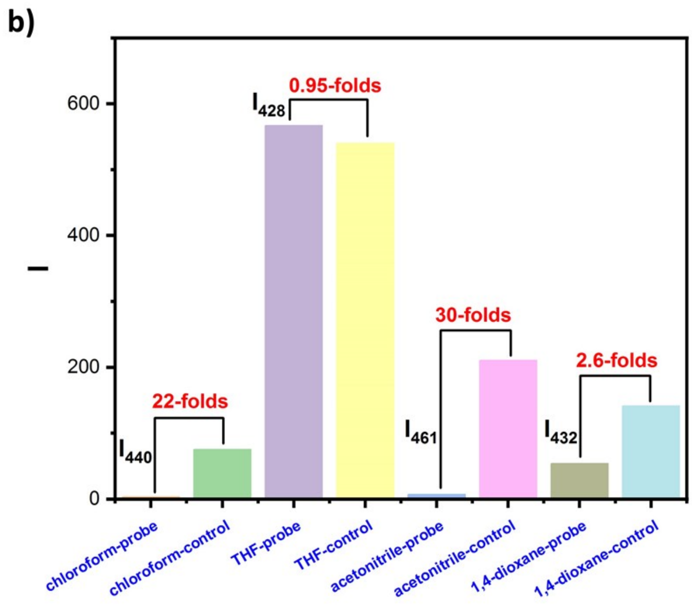


Fig. S1 a) Fluorescence spectra of **APQ** (10.0 μM) in the presence of 1.0 equiv. of triphosgene in chloroform, THF, acetonitrile, and dioxane solution, respectively (containing 1% TEA, λex = 377 nm). b) Fluorescence intensity of a different solution of **APQ** (10.0 μM) before and after addition of 1.0 equiv. of triphosgene (containing 1% TEA).

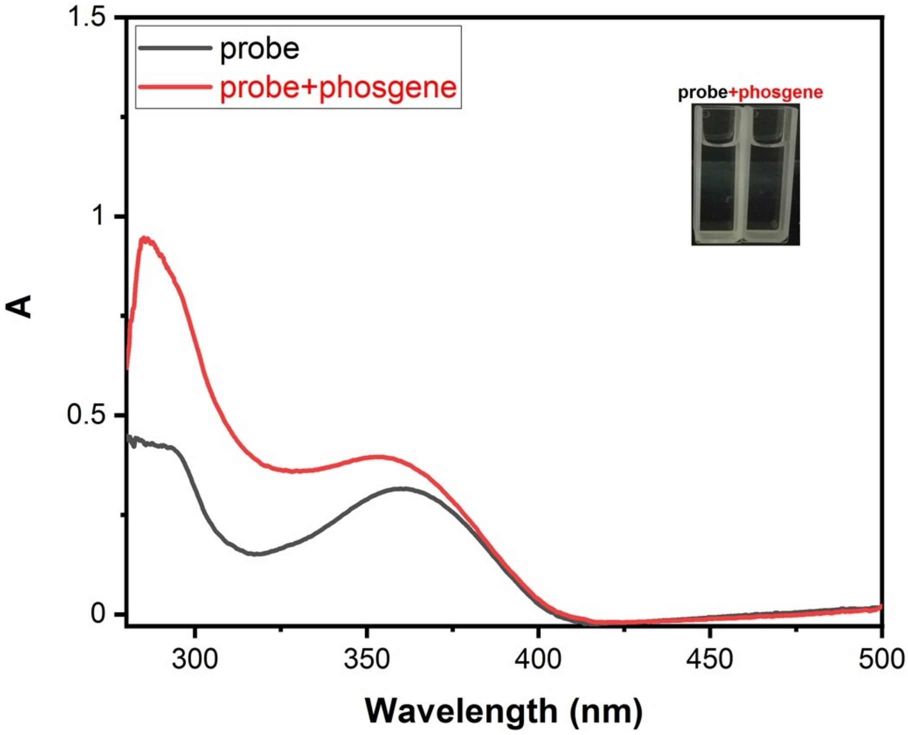


Fig. S2 The UV-vis absorption of **APQ** (20.0 μM) and **APQ** (20.0 μM) in the present of 1.0 equiv. of triphosgene in CH_3CN solution (containing 1% TEA).

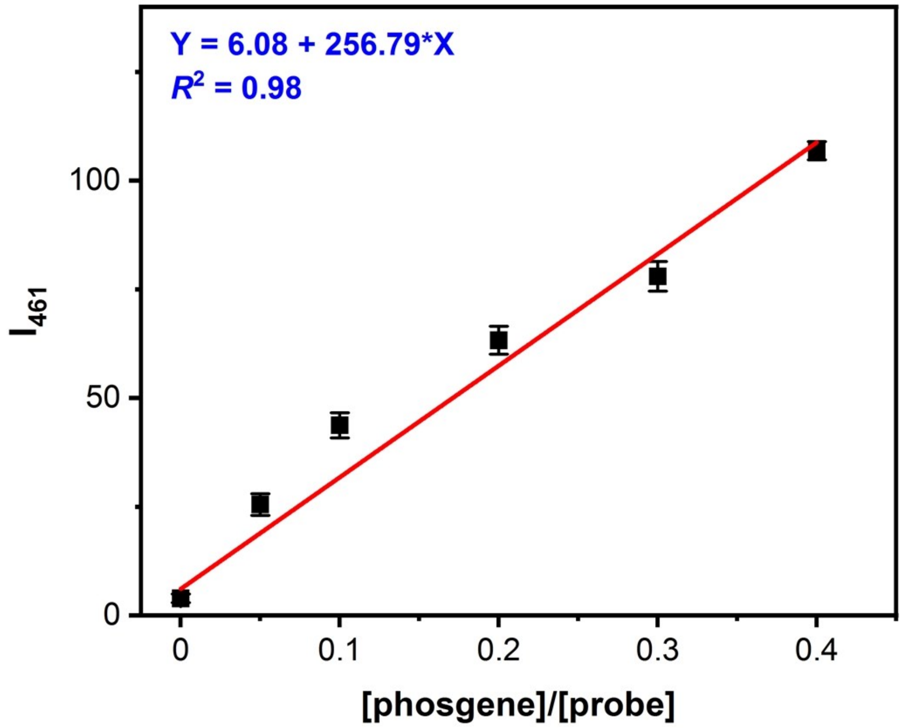


Fig. S3 The changes of the fluorescent intensity of **APQ** (10.0 μM) at at 461 nm (I_{461}) as a function of phosgene concentration (0-4.0 μM) under the same condition as the phosgene titration.

The detection limit (DL) of phosgene using **APQ** was determined from the following equation: [3]

$$DL = 3*\sigma/K$$

Where σ is the standard deviation of the blank solution; K is the slope of the calibration curve.

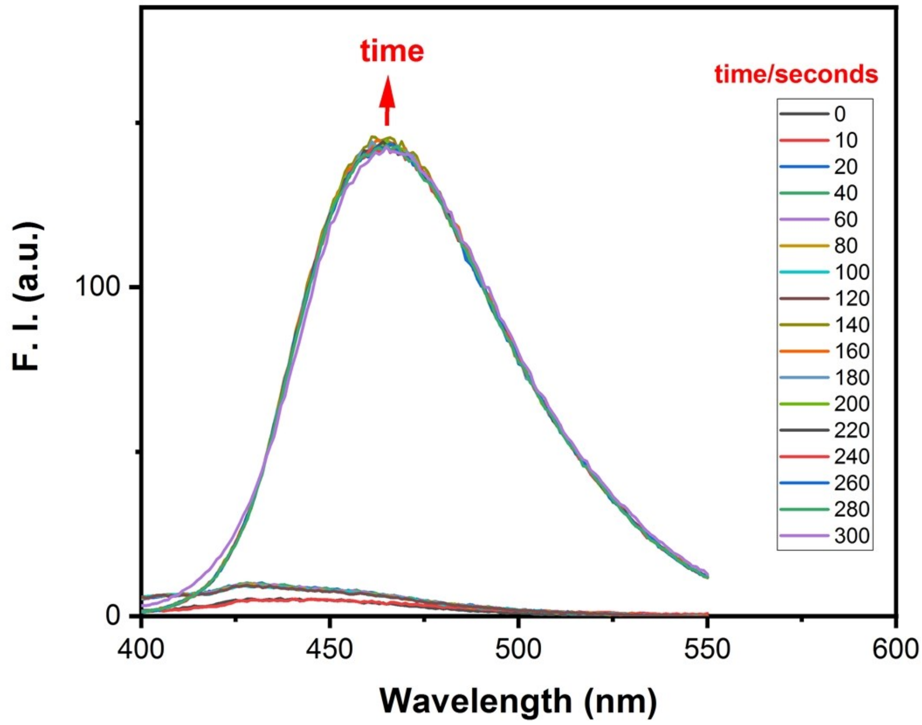


Fig. S4 The fluorescent spectra of **APQ** (10.0 μM) in the present of triphosgene (10.0 μM) in the different reaction time (0-300 s) under the same condition as the phosgene titration.

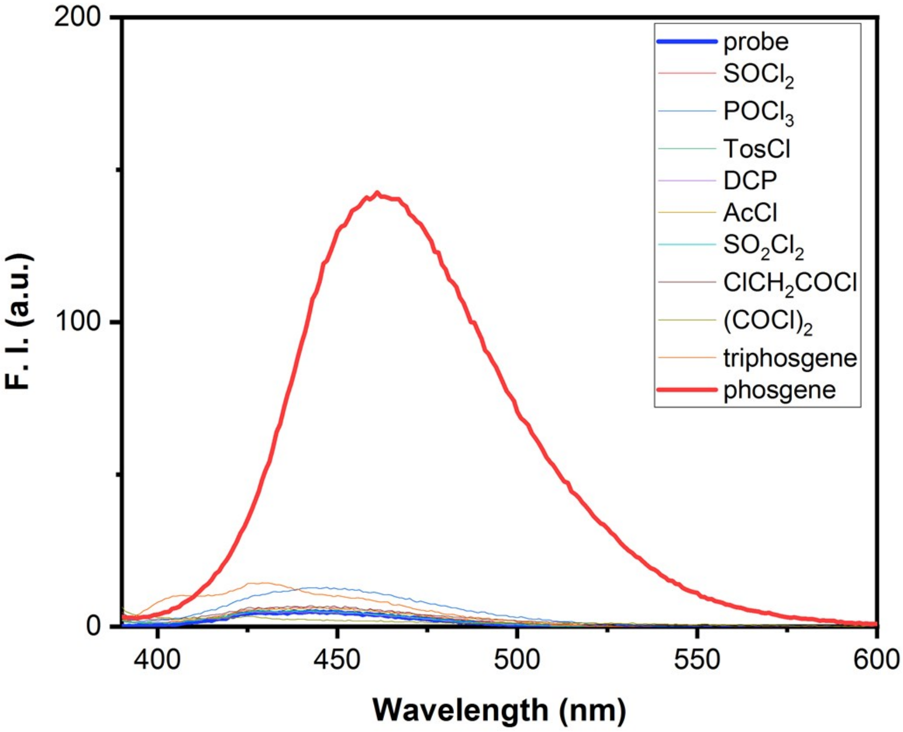


Fig. S5 Fluorescence spectra of a CH_3CN solution of probe **APQ** (10.0 μM) before and after addition of various analytes (including $SOCl_2$, $POCl_3$, TosCl, DCP, AcCl, SO_2Cl_2, $ClCH_2COCl$, $(COCl)_2$, triphosgene, and phosgene (λex = 377 nm).

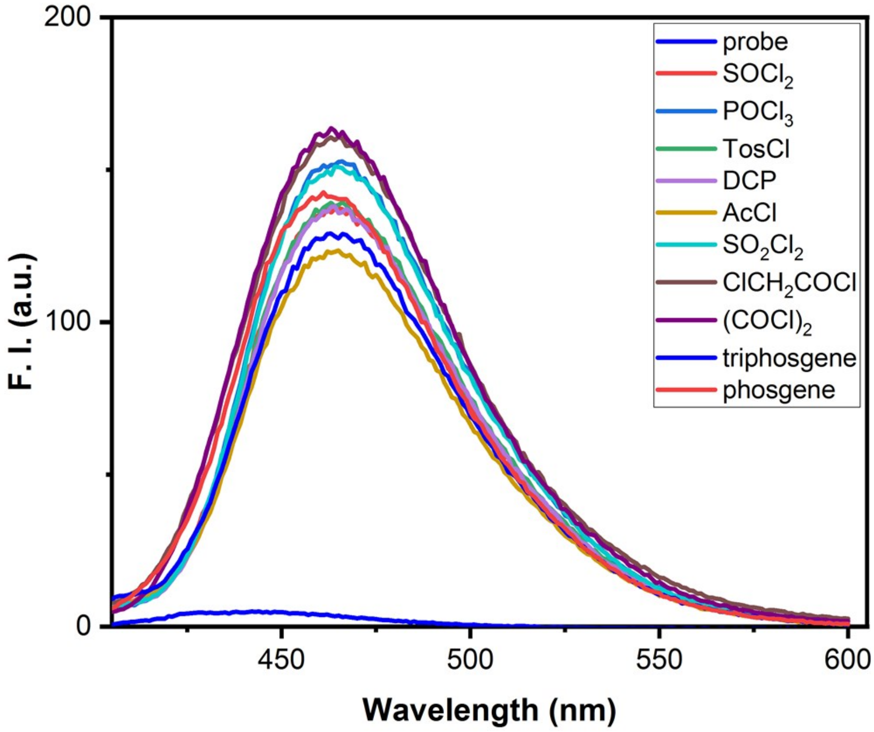


Fig. S6 Fluorescence spectra of a CH_3CN solution of probe **APQ** (10.0 μM) in the presence of 1.0 equiv. of various analytes (including $SOCl_2$, $POCl_3$, TosCl, DCP, AcCl, SO_2Cl_2, $ClCH_2COCl$, $(COCl)_2$, triphosgene, and phosgene, followed by 1.0 equiv. of triphosgene (containing 1% TEA, λex = 377 nm).

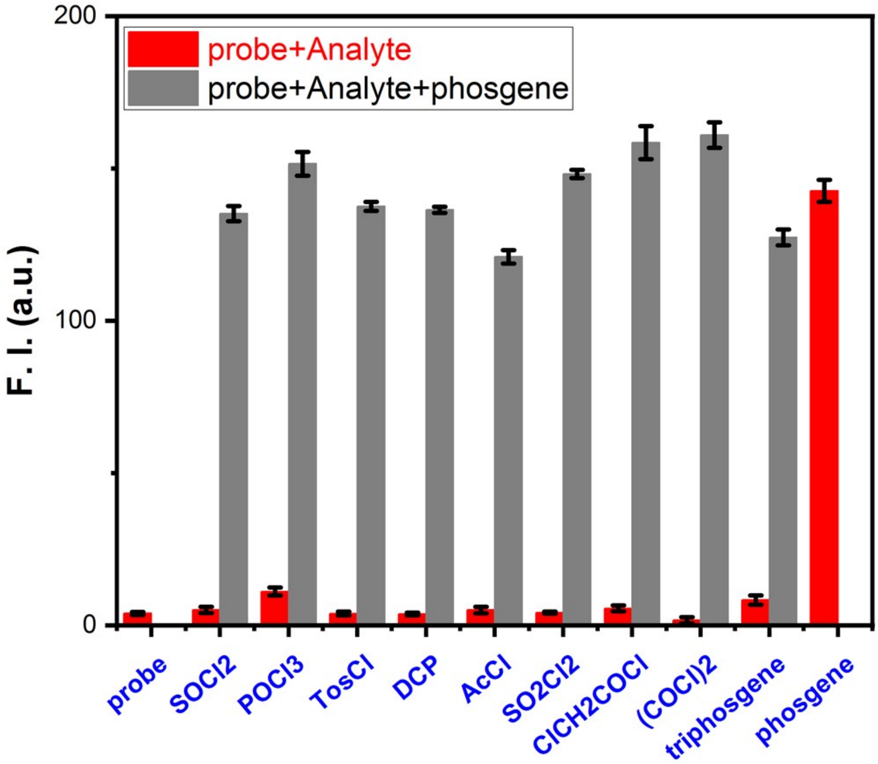


Fig. S7 Fluorescence intensity in 461 nm (I_{461}) of a CH_3CN solution of probe **APQ** (10.0 μM) before and after addition of various analytes (including $SOCl_2$, $POCl_3$, TosCl, DCP, AcCl, SO_2Cl_2, $ClCH_2COCl$, $(COCl)_2$, triphosgene, and phosgene, followed by the addition of 1.0 equiv. of triphosgene (containing 1% TEA, λex = 377 nm).

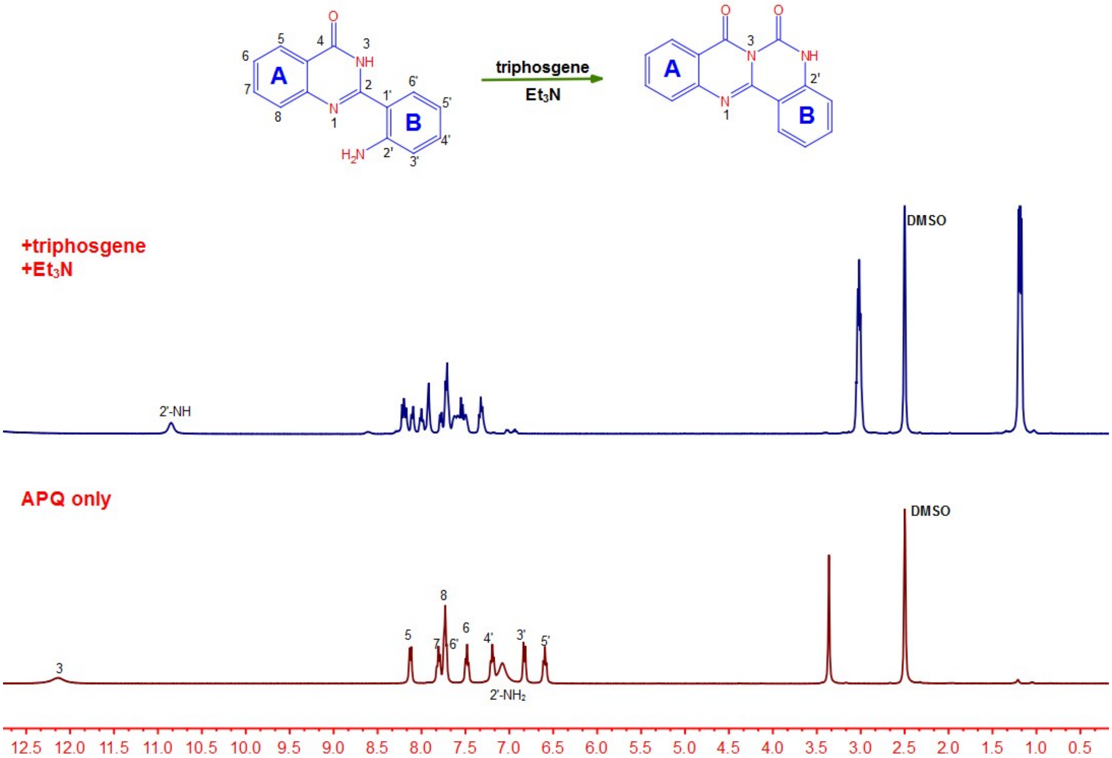


Fig. S8 ^{1}HNMR spectra of **APQ** and **APQ** in the present of phosgene in d_6-DMSO.

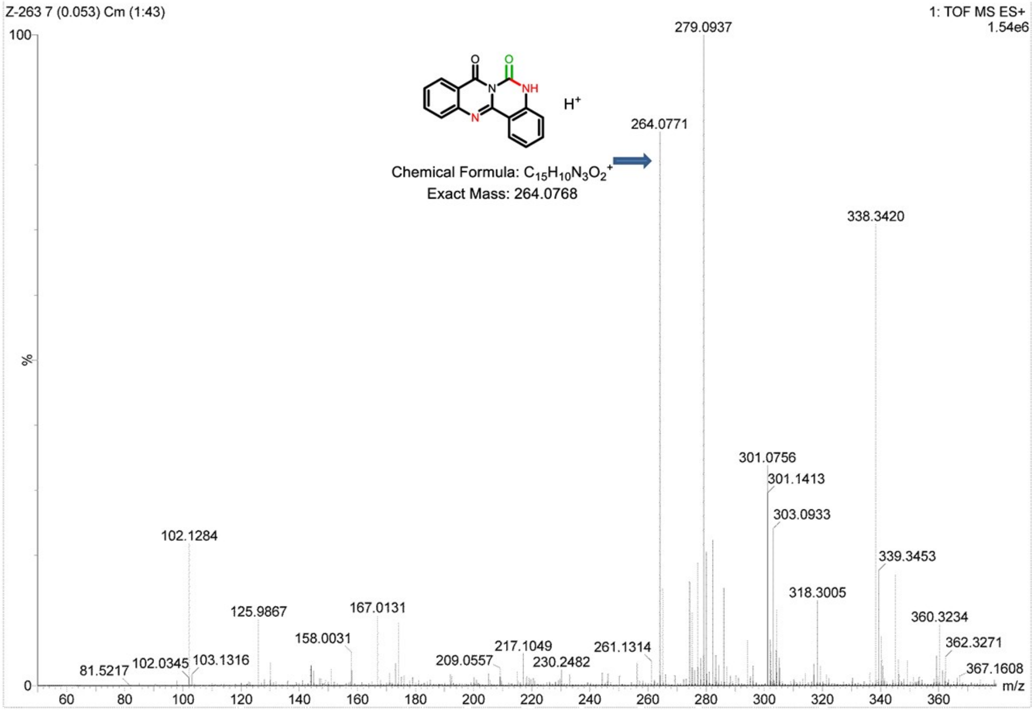


Fig. S9 HR-MS (ESI) spectra of reaction mixture of **APQ** and phosgene.

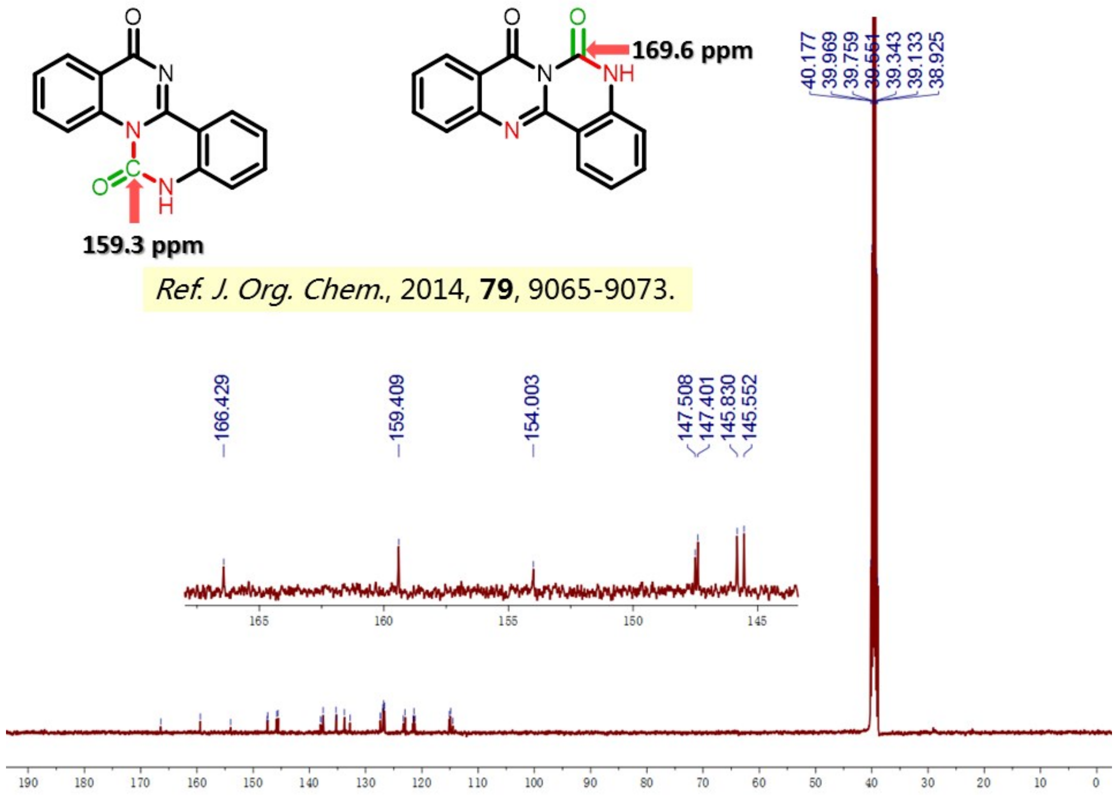


Fig. S10 The [13]C NMR spectrum of the reaction product of **APQ** and phosgene.

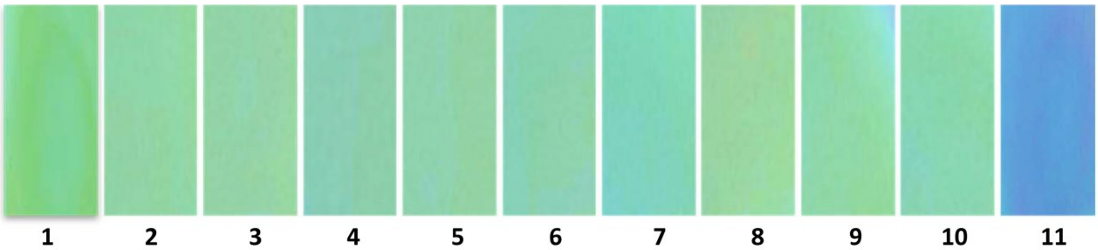
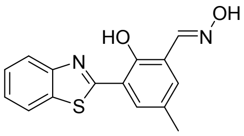
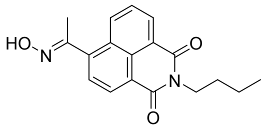
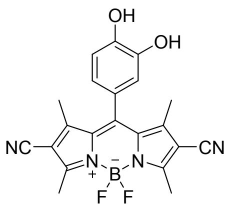
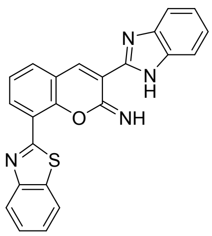
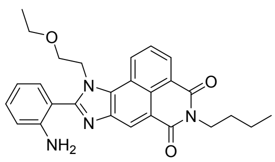
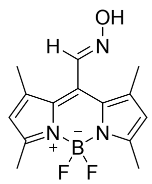
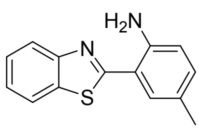
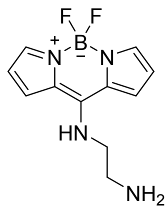
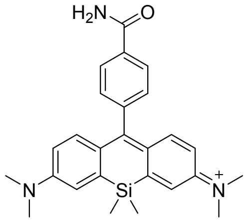
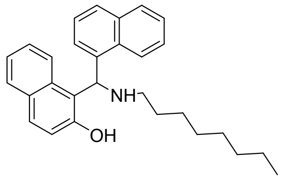
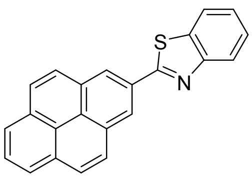
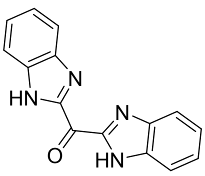
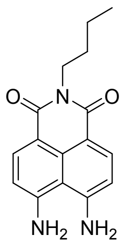
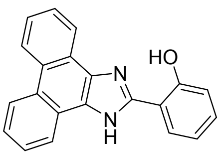
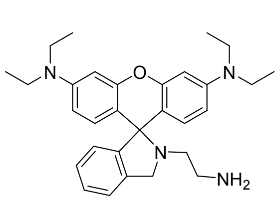
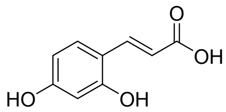
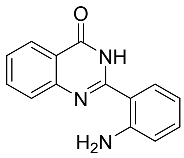


Fig. S11 Photographs of the fluorescence of test strips containing absorbed probe **APQ** exposed for 1 min to vapors containing various analytes, (1) **APQ** only; (2) $SOCl_2$; (3) $POCl_3$; (4) TosCl; (5) DCP; (6) AcCl; (7) SO_2Cl_2; (8) $ClCH_2COCl$; (9) $(COCl)_2$; (10) triphosgene, and (11) phosgene (under a 365 nm hand-held UV lamp).

Table S2 Summary of some reported phosgene fluorescent probes.

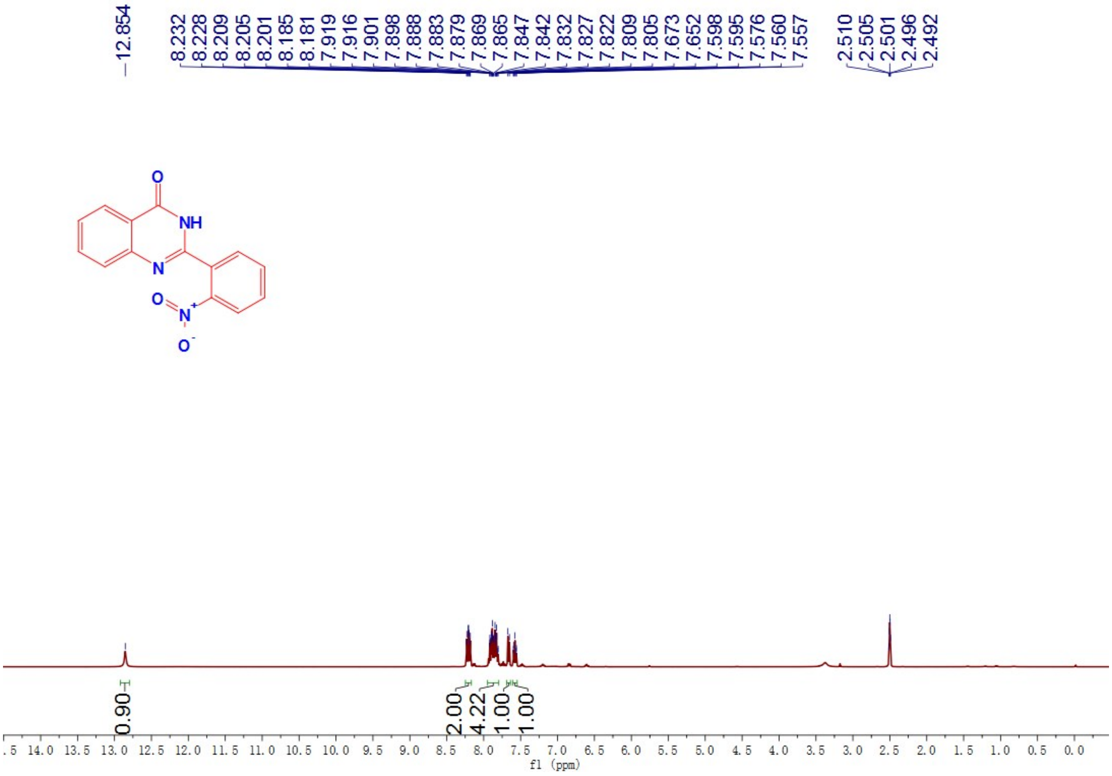
Entry	Structures	Response mode	LOD（in solution）	Response time		References
				In solution	Gaseous	
1		off-on	0.48 nM	20 min	20 min	*Dyes Pigments*, **2019**, 163, 483-488.
2		off-on	6.3 nM	15 in	5 min	*Dyes Pigments*, **2020**, 173, 10784.
3		off-on	124 pM	< 3 S	30 s	*Sens. Actuators. B. Chem.*, **2019**, 283, 458-462.
4		off-on	1.65 nM	3 min	-	*Sens. Actuators. B. Chem.*, **2021**, 326, 128837.
5		ratiometric	526 nM	2.5 s	10 s	*Anal. Chem.*, **2019**, 91, 5690-5697.
6		off-on	0.09 ppb	< 10 s	30 s	*Anal. Chem.*, **2017**, 89, 12837-12842.
7		ratiometric	0.14 ppm	4 min	10 min	*Anal. Chem.*, **2017**, 89, 12596-12601.

8		ratiometric	0.14 ppm	< 1.5 s	< 1 min	*ACS Appl. Mater. Interfaces*, **2017**, 9, 13920-13927.
9		off-on	8.9 nM	< 4 min	5 min	*J. Mater. Chem. C.*, **2018**, 6, 10472-10479.
10		off-on	0.4μM	< 1 min	20 s	*New J. Chem.*, **2019**, 43, 11743-11748.
11		off-on	1.54 nM	< 1.3 min	50 s	*New J. Chem.*, **2019**, 43, 14991-14996.
12		off-on	3.3 nM	< 30 s	10 min	*Anal. Methods,* **2020**, 12, 3123-3129.
13		ratiometric	2.25 μM	10 min	20 min	*J. Chin. Chem. Soc.*, **2020**, 67, 1213-1218.
14		ratiometric	0.14 ppm	< 30 s	< 2 min	*Talanta.*, **2019**, 200, 78-83.

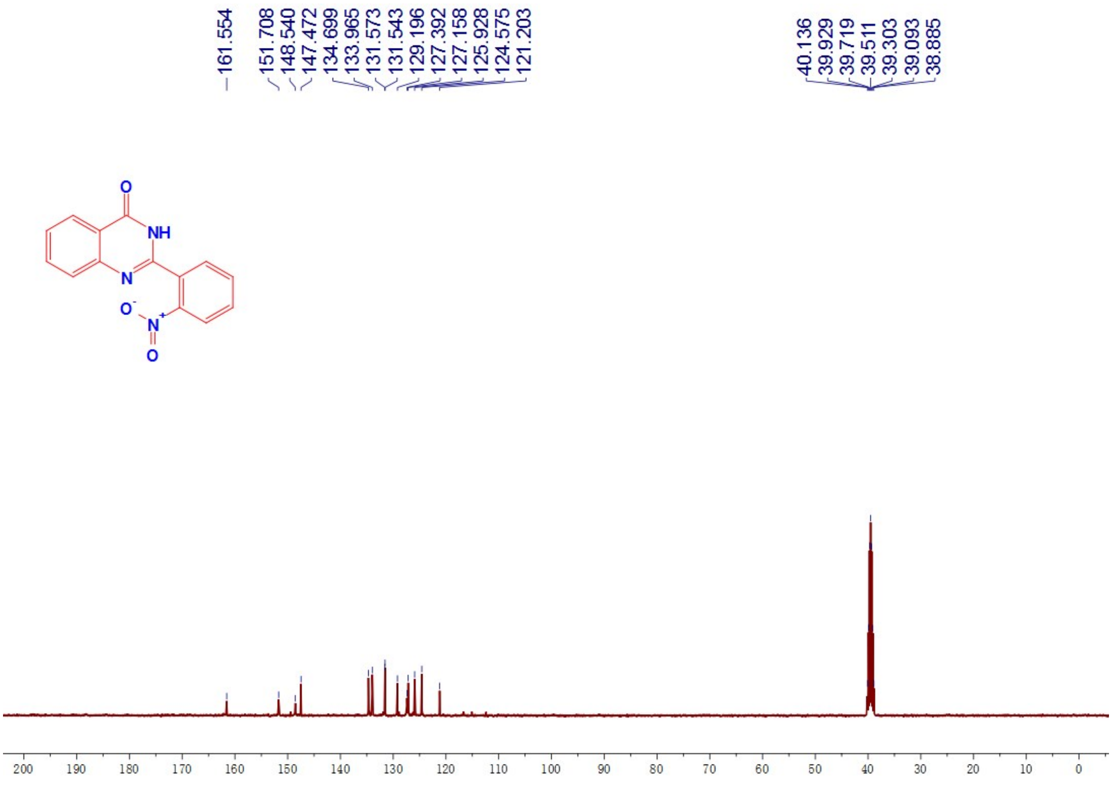
15		off-on	50 μM	-	-	*Chem. Commun.*, **2012**, 48, 1895-1897.
16		off-on	1-18 nM	-	-	*Anal. Chem.*, **2012**, 84, 4594-4597.
17		off-on	0.16 ppm	< 20 s	~ 1 min	This work

The characterization data of APQ

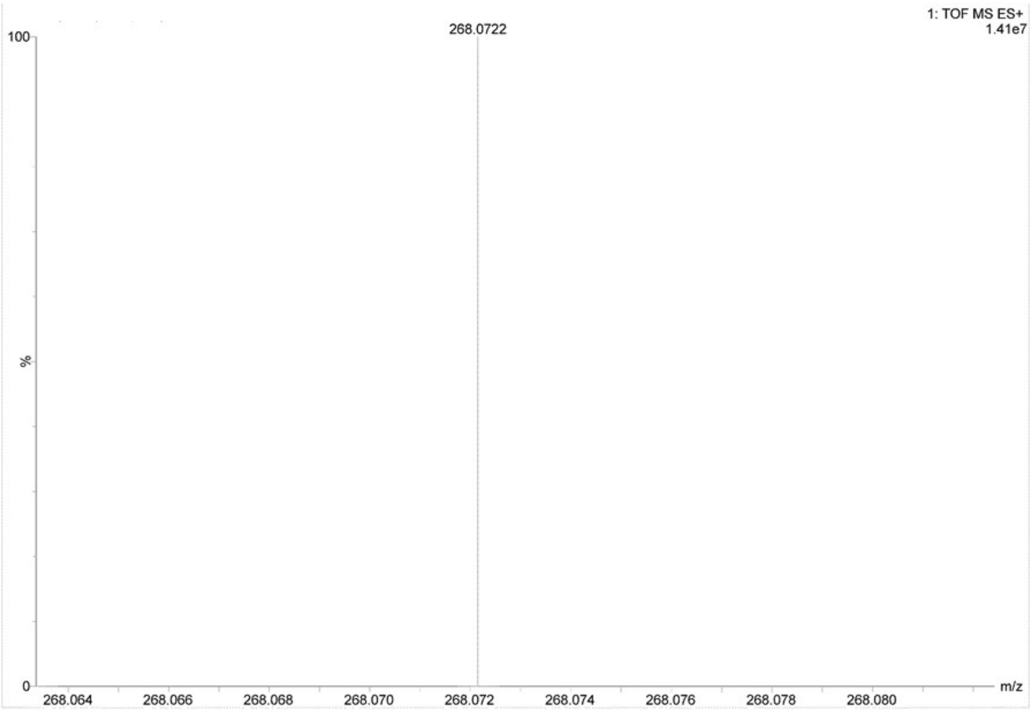
^{1}H NMR of **2-(2-nitrophenyl)quinazolin-4(3H)-one**



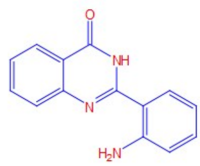
^{13}C NMR of **2-(2-nitrophenyl)quinazolin-4(3H)-one**

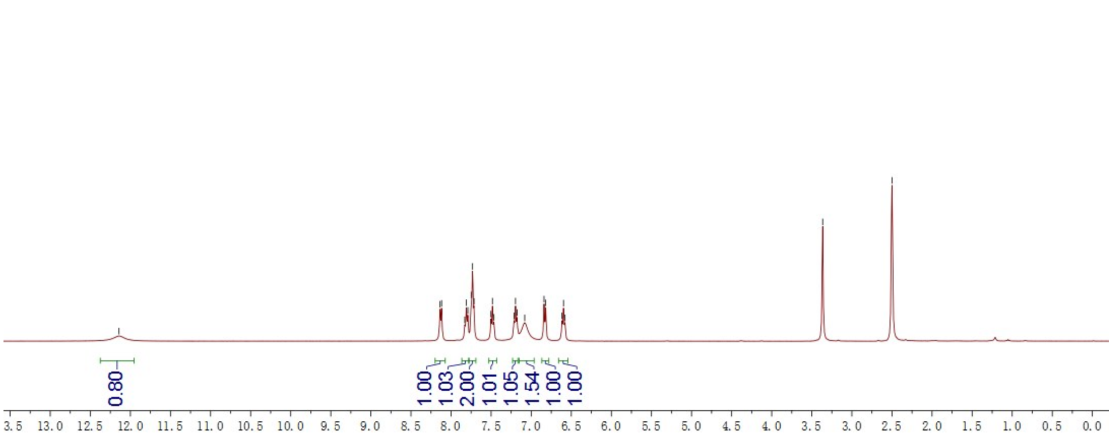


HR-MS of **2-(2-nitrophenyl)quinazolin-4(3H)-one**

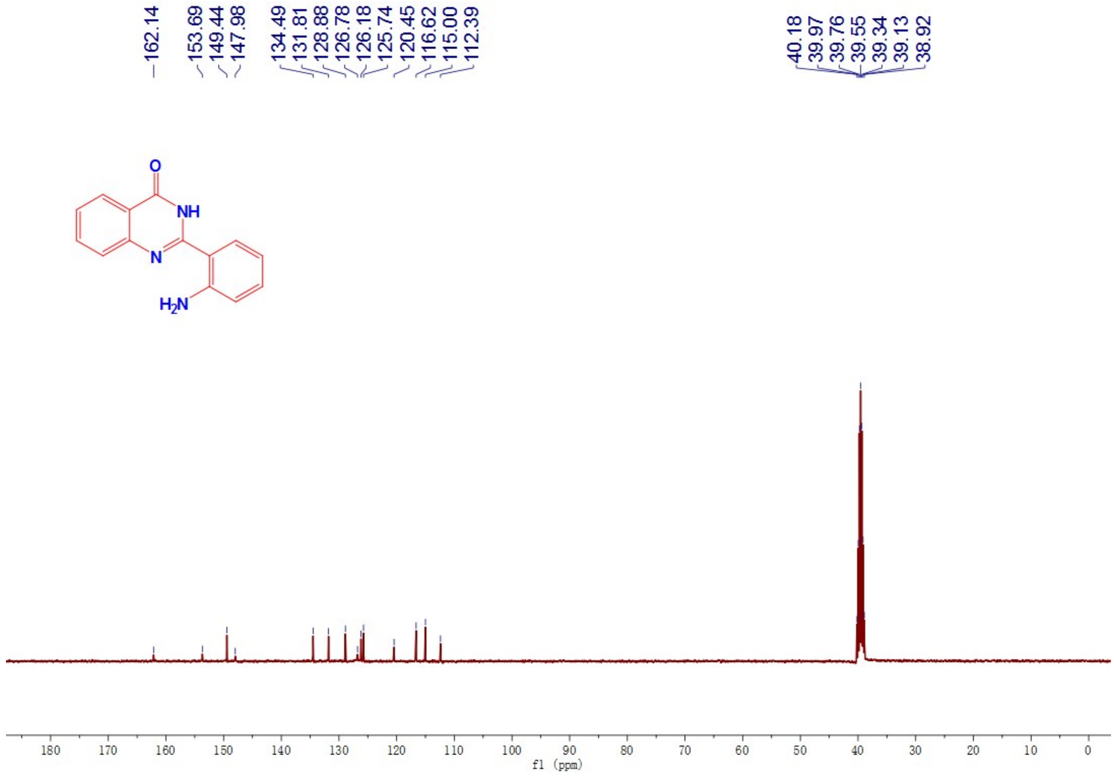


^{1}H NMR of **2-(2-aminophenyl)quinazolin-4(3H)-one (APQ)**

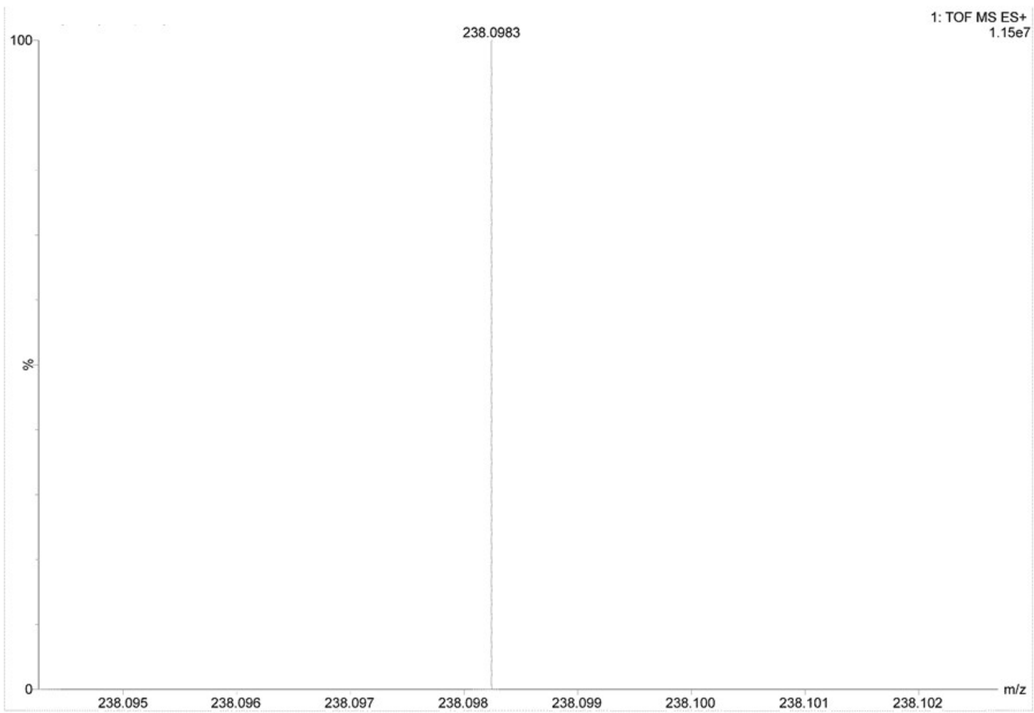




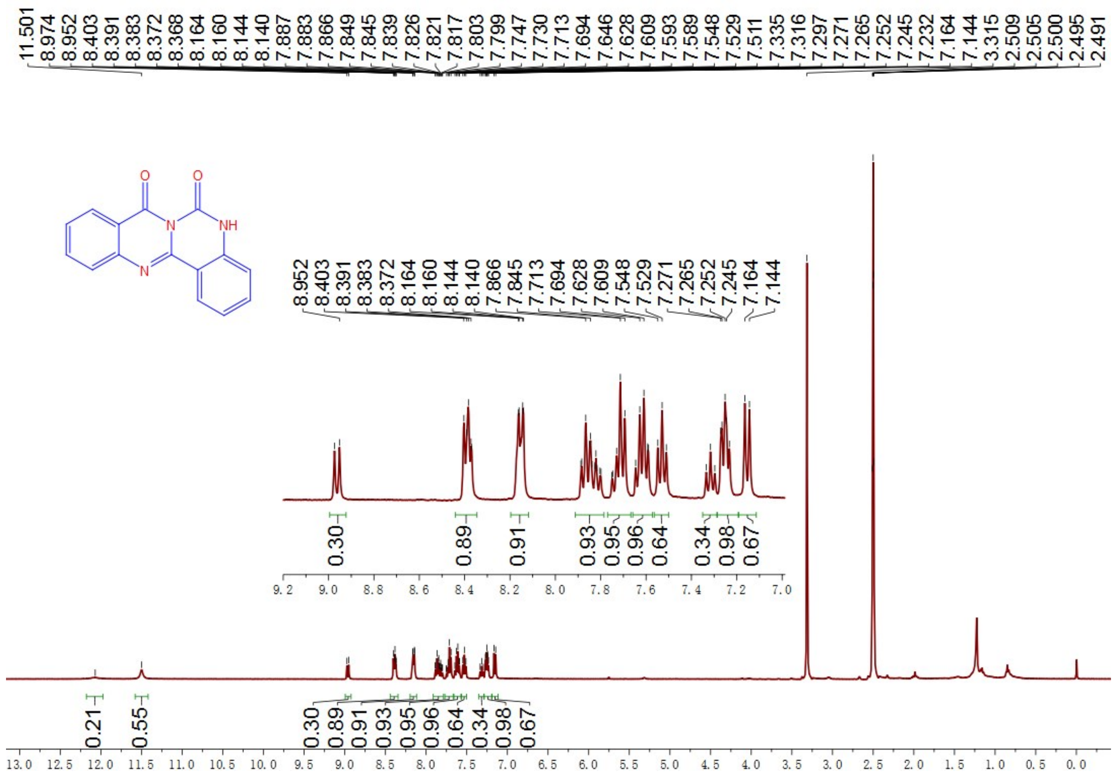
^{13}C NMR of **2-(2-aminophenyl)quinazolin-4(3H)-one (APQ)**



HR-MS of **2-(2-aminophenyl)quinazolin-4(3H)-one (APQ)**



[1]H NMR of **5H-quinazolino[4,3-b]quinazoline-6,8-dione (APQU1)**



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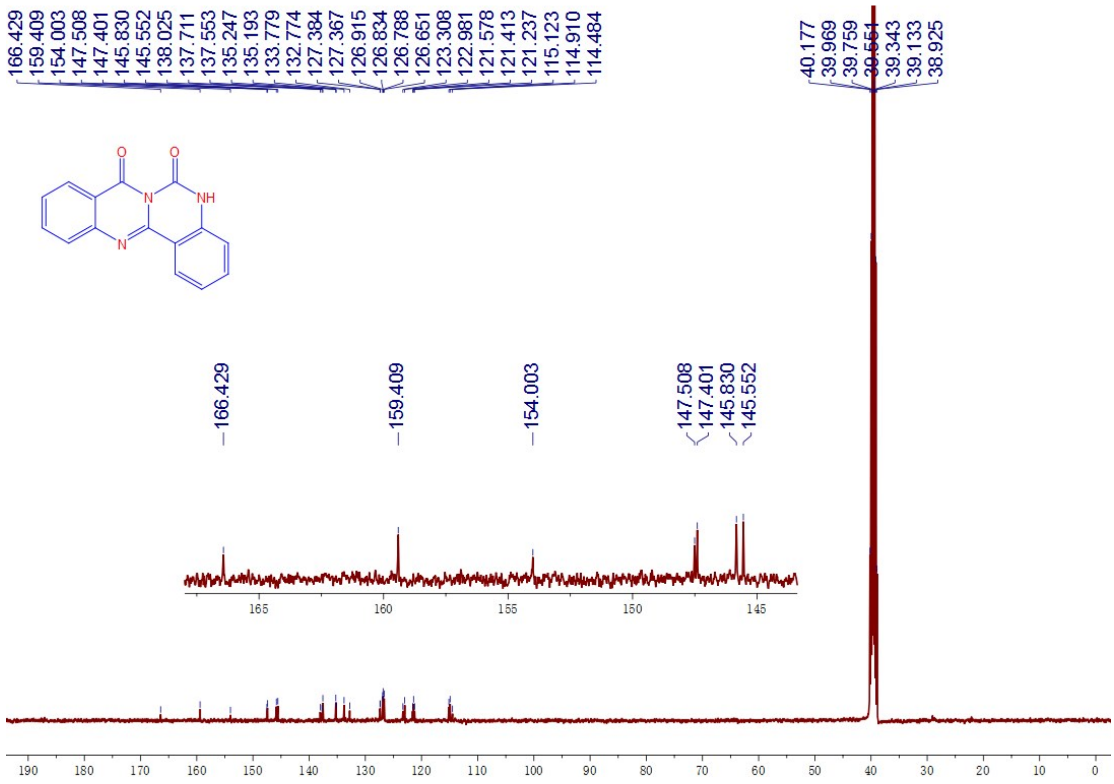
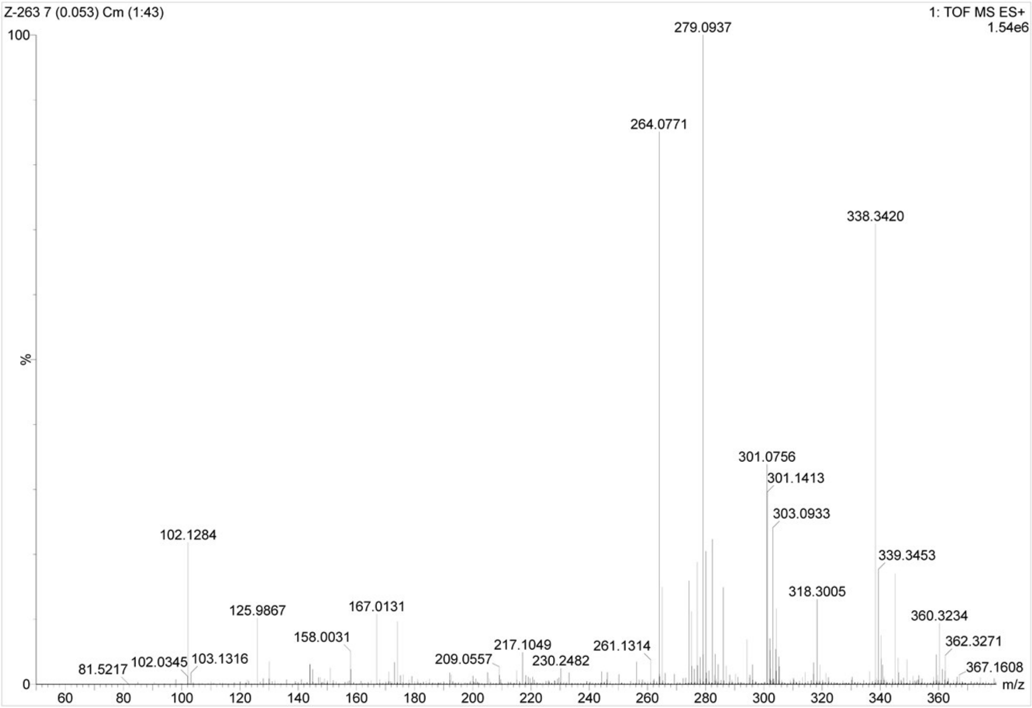


HR-MS of **5H-quinazolino[4,3-b]quinazoline-6,8-dione (APQU1)**



References

1 R. A. Velapoldi, and H. H. Tønnesen, *J. Fluoresc*., 2004, **14**, 465-472.

2 (*a*) D. F. Eaton, *Pure Appl. Chem*., 1988, **60**, 1107-1114; (*b*) D. Magde, R. Wong, and P. G. Seybold, *Photochem. Photobiol*., 2002, **75**, 327-334.

3 (*a*) J. T. Yeh, P. Venkatesan and S. P. Wu, *New J. Chem*., 2014, **38**, 6198-6204. (*b*) A. Roy, D. Kand, T. Saha and P. Talukdar, *Chem. Commun*., 2014, **50**, 5510-5513.