# Design, Synthesis and Performance Test of a Hydrogen Peroxide Fluorescent Probe Based on Selenamorpholine and Pyrimidine

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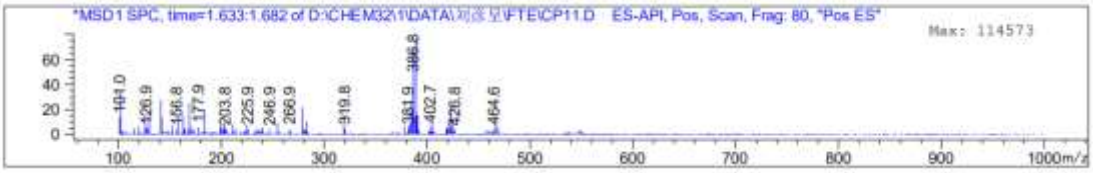


**Fig. S1** MS spectrum of **Pyrimidine-Se** reaction with $H_2O_2$

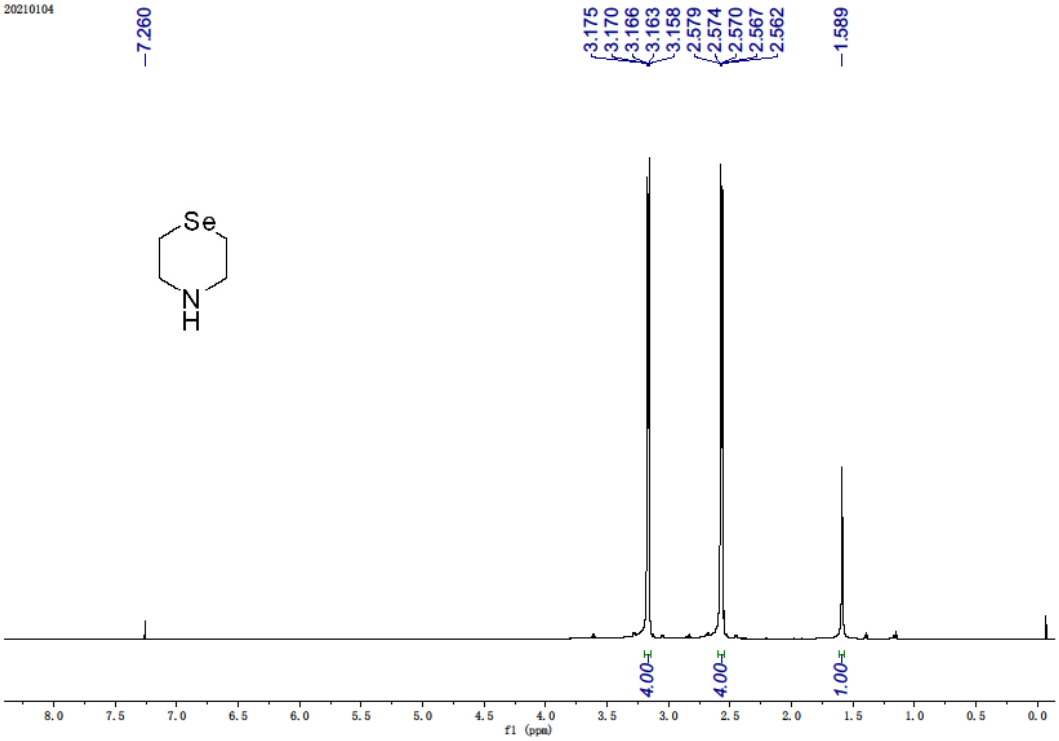


**Fig. S2** $^1$H NMR spectrum ($CDCl_3$, 600 MHz) of **Selenamorpholine**

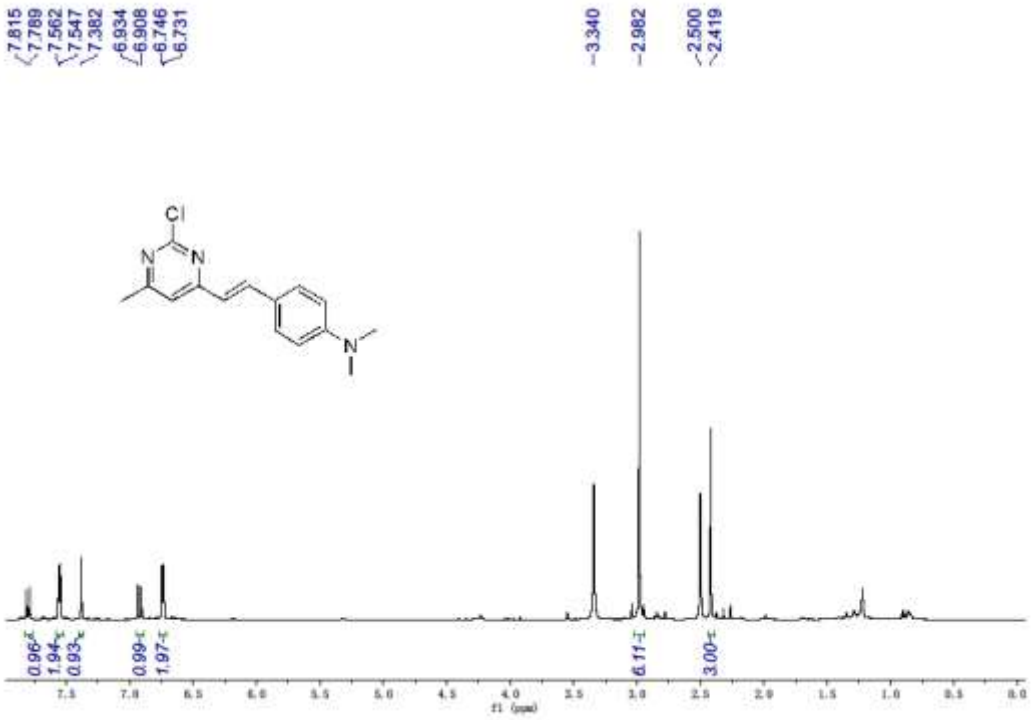


**Fig. S3** $^{1}$H NMR spectrum ($CDCl_3$, 600 MHz) of compond **1**

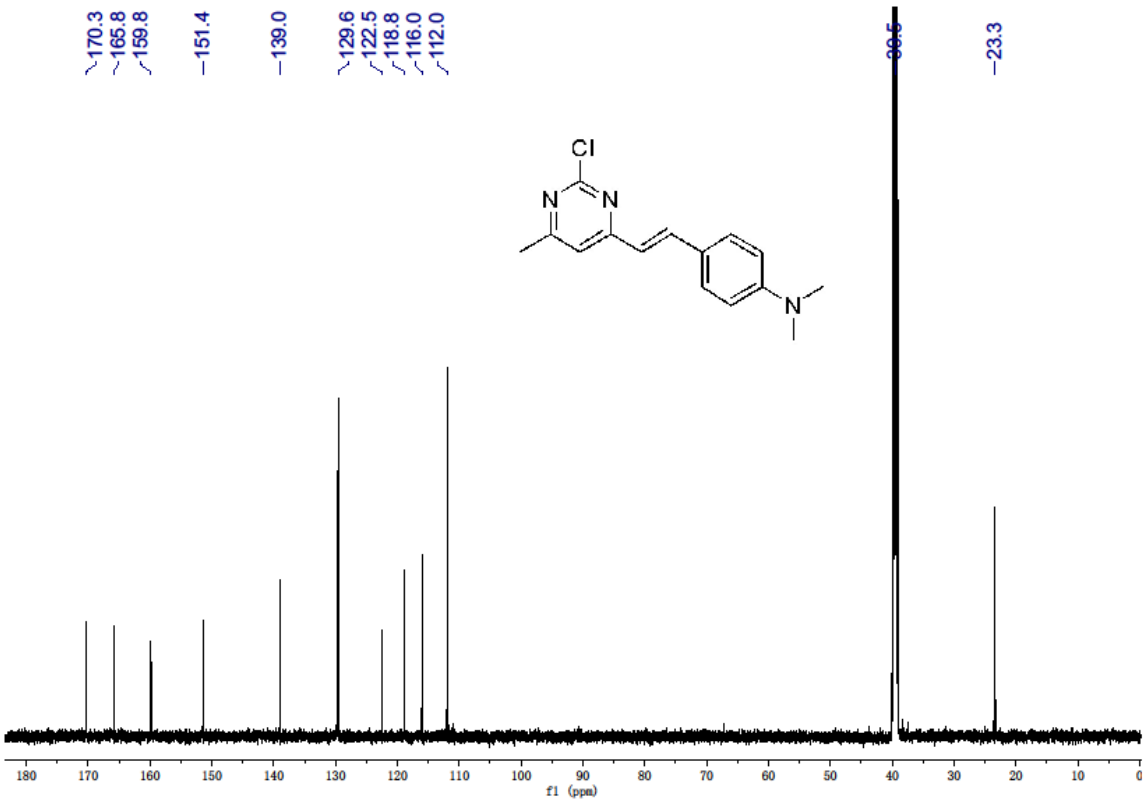


**Fig. S4** $^{13}$C NMR spectrum ($CDCl_3$, 151 MHz) of Compound **1**

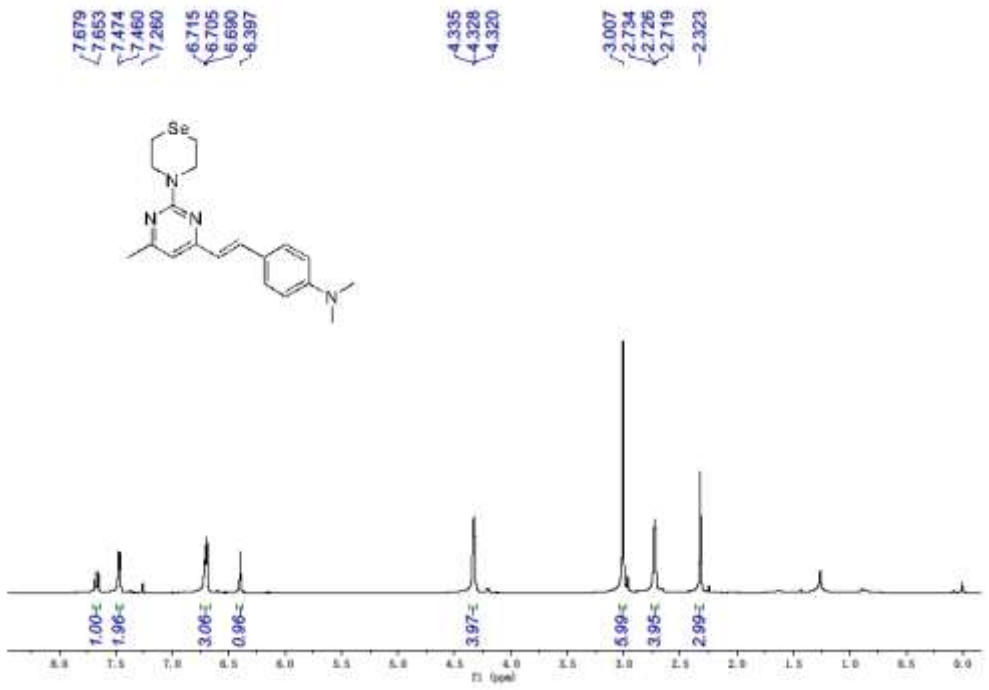


**Fig. S5** $^{1}$H NMR spectrum ($CDCl_3$, 600 MHz) of **Pyrimidine-Se**

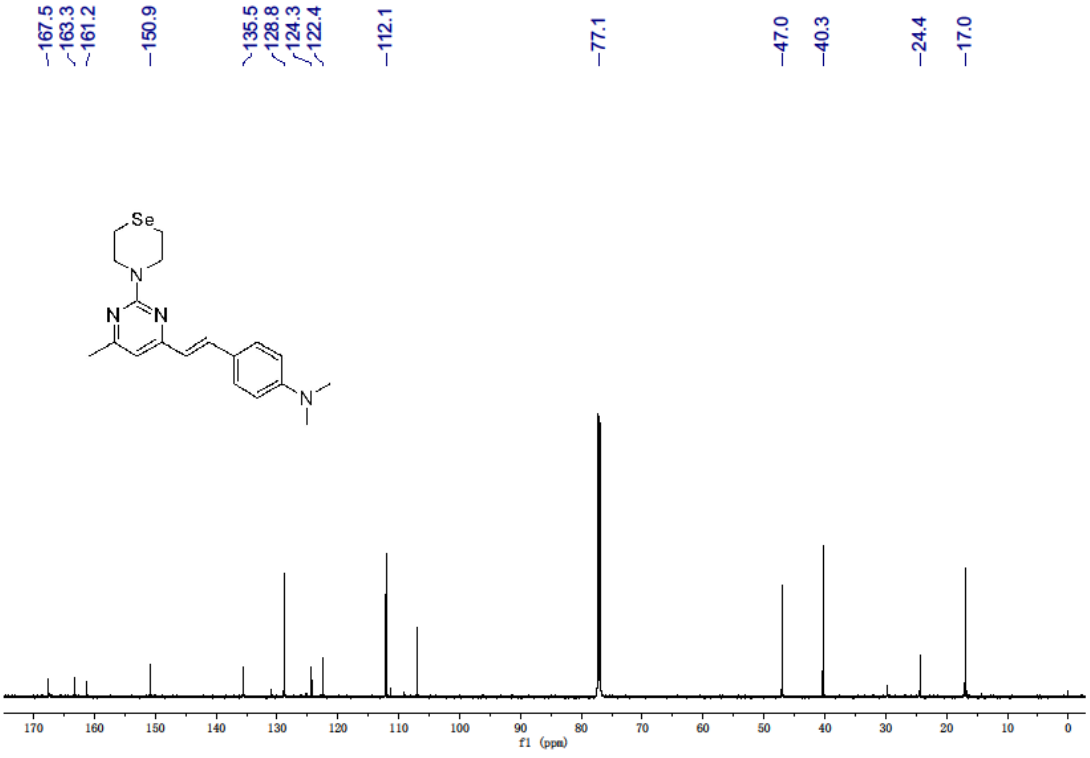


**Fig. S6** $^{13}$C NMR spectrum ($CDCl_3$, 151 MHz) of **Pyrimidine-Se**

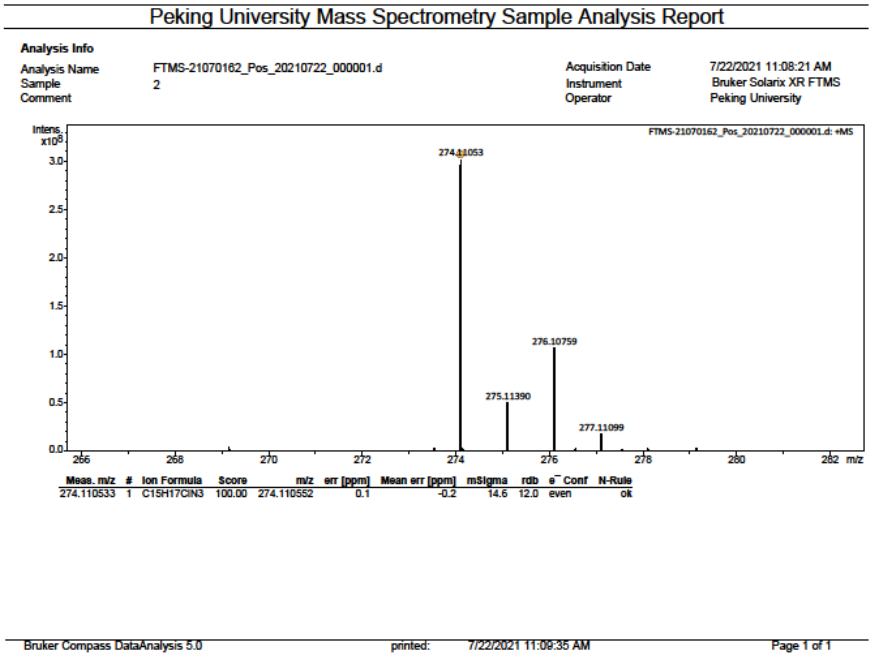


**Fig. S7** HR-ESI-MS spectrum of Compound **1**

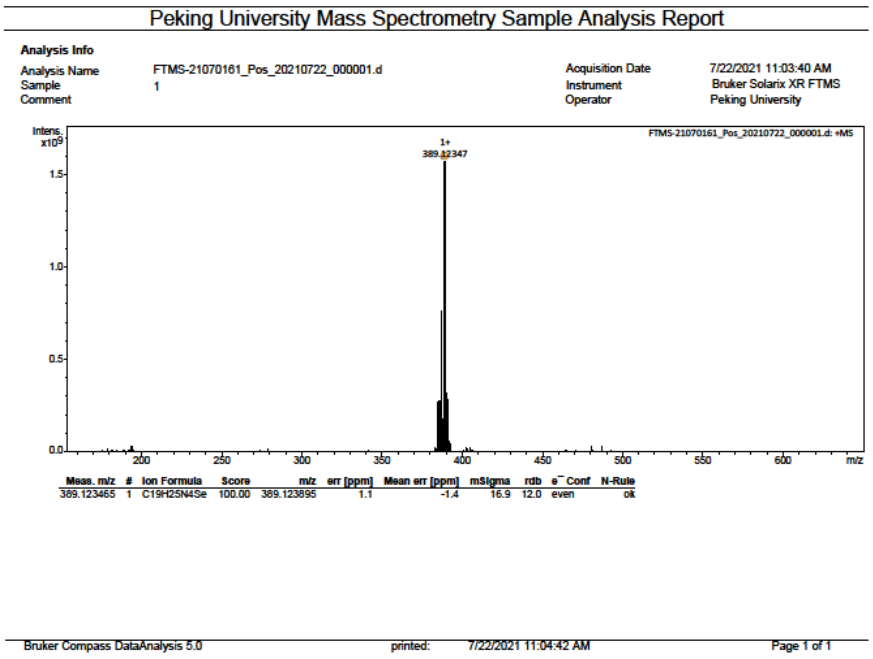


**Fig. S8** HR-ESI-MS spectrum of **Pyrimidine-Se**

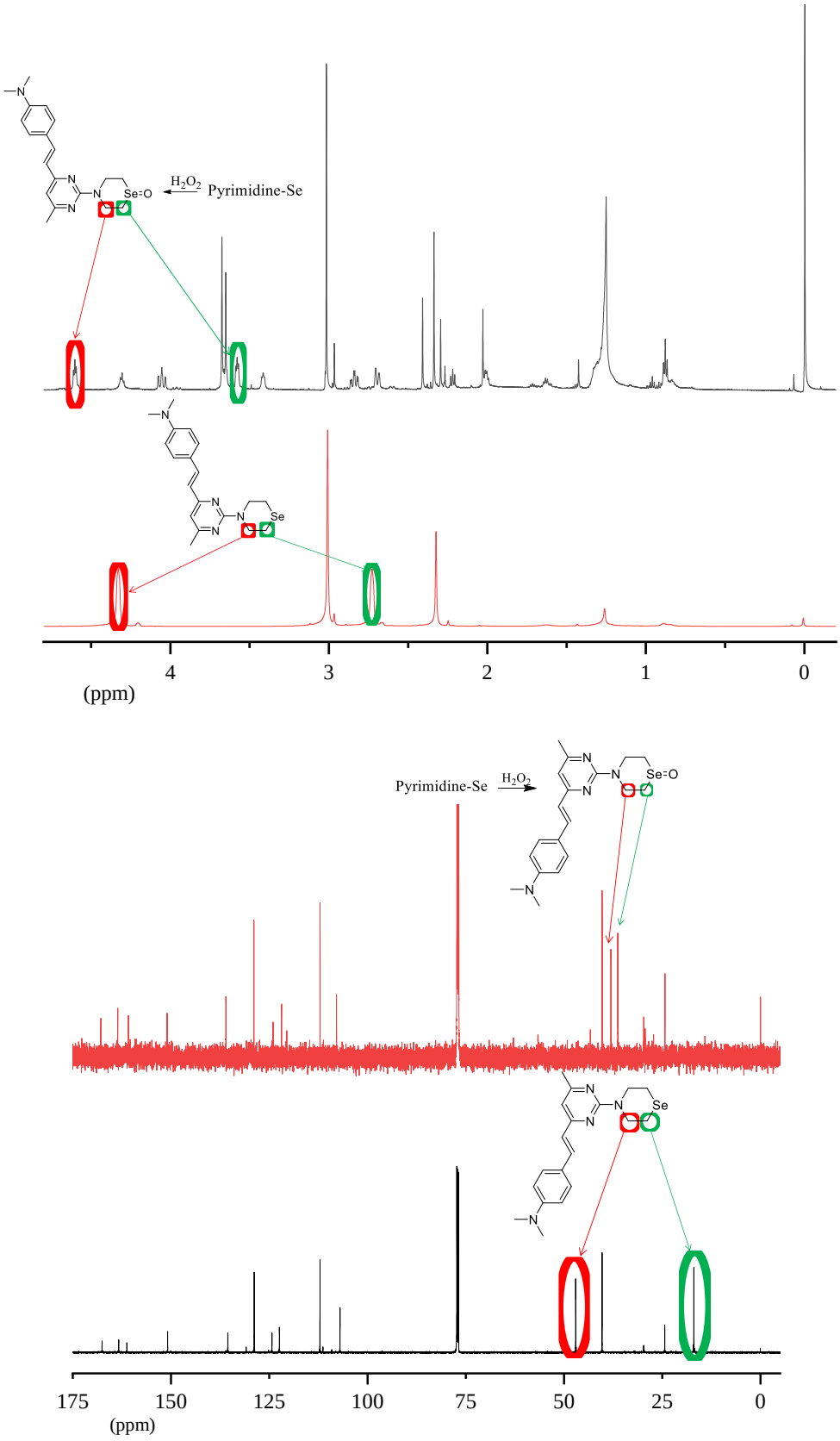


**Fig. S9** $^{1}$H NMR and $^{13}$C NMR titration spectra of sensor **Pyrimidine-Se** upon addition of 1 equiv. $H_2O_2$

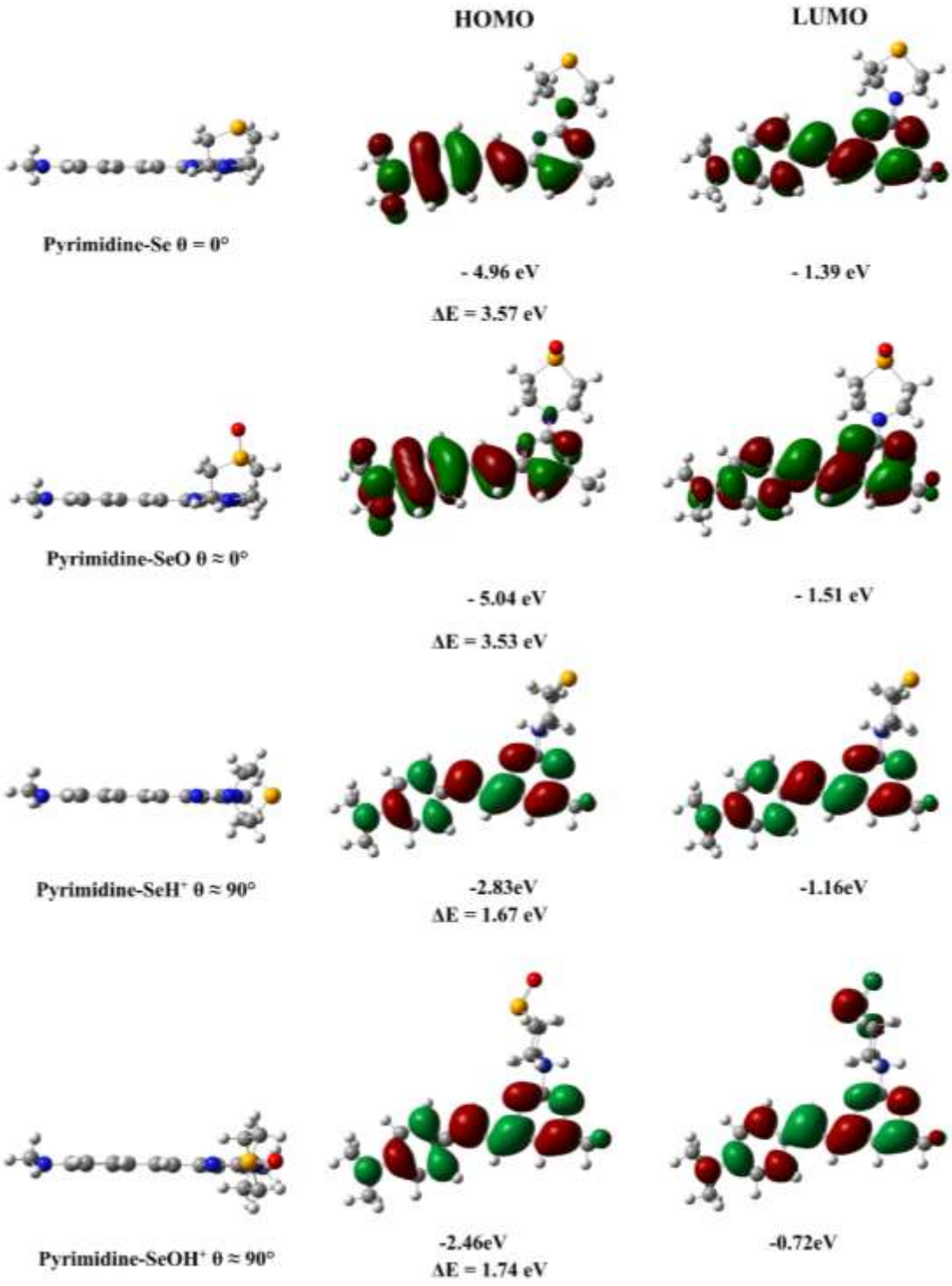


**Fig. S10** DFT calculated molecular orbitals and molecular electrostatic potential diagrams of **Pyrimidine-Se**, **Pyrimidine-SeO**, **Pyrimidine-SeH$^+$** and **Pyrimidine-SeOH$^+$**

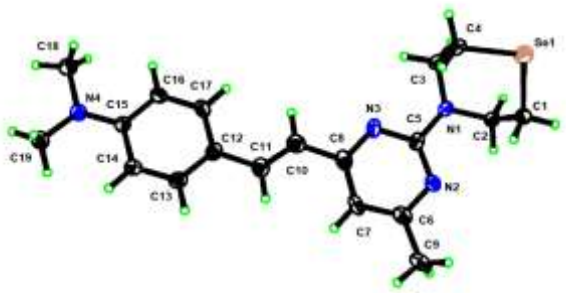


**Fig.S11** Crystal 1 Crystal structure of **Pyrimidine-Se**

**Table 1** Crystal data and structure refinement for **Pyrimidine-Se**

| Compond | **Pyrimidine-Se** |
|---|---|
| Empirical formula | $C_{19}H_{24}N_4Se$ |
| Formula weight | 387.38 |
| Temperature/K | 170.0 |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 8.4463(5) |
| b/Å | 7.5471(5) |
| c/Å | 28.3974(18) |
| α/° | 90 |
| β/° | 90.409(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 1810.1(2) |
| Z | 4 |
| ρcalcg/cm$^3$ | 1.421 |
| μ/mm$^{-1}$ | 2.082 |
| F(000) | 800.0 |
| Crystal size/mm$^3$ | 0.11 × 0.04 × 0.02 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.822 to 52.772 |
| Index ranges | ? ≤ h ≤ ?, ? ≤ k ≤ ?, ? ≤ l ≤ ? |
| Reflections collected | 3638 |
| Independent reflections | 3638 [Rint = ?, Rsigma = 0.0877] |
| Data/restraints/parameters | 3638/7/220 |
| Goodness-of-fit on F$^2$ | 1.057 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0612, $wR_2$ = 0.1062 |
| Final R indexes [all data] | $R_1$ = 0.1076, $wR_2$ = 0.1199 |
| Largest diff. peak/hole/eÅ$^{-3}$ | 0.68/-0.55 |

**Table 2** Excitation wavelength and emission wavelength of sensor **Pyrimidine -Se**

| Solvent | $\lambda_{ex}$ | $\lambda_{em}$ |
|---|---|---|
| DMSO | 382 nm | 496 nm |
| DMF | 383 nm | 492 nm |
| MeOH | 380 nm | 506 nm |
| EtOH | 378 nm | 498 nm |
| MeCN | 379 nm | 489 nm |
| PBS Buffer | 390 nm | 469 nm |