

Supporting Information

1-*m*-Nitrobenzoyl semicarbazide: reversible colorimetric cascade indicators for fluoride and moisture†

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Table of contents

<i>1. Supporting information Scheme S1</i>	<i>S3</i>
<i>2. Supporting information Figure S1</i>	<i>S3</i>
<i>3. Hydrogen bonding parameters: Table S1</i>	<i>S3</i>
<i>4. Supporting information Figure S2</i>	<i>S4</i>
<i>5. Supporting information Figure S3</i>	<i>S5</i>
<i>6. Supporting information Figure S4</i>	<i>S6</i>
<i>7. Supporting information Figure S5</i>	<i>S7</i>
<i>8. Supporting information Figure S6</i>	<i>S8</i>
<i>9. Supporting information Figure S7</i>	<i>S8</i>
<i>10. Supporting information Figure S8</i>	<i>S9</i>
<i>11. Supporting information Figure S9</i>	<i>S10</i>
<i>12. Supporting information Figure S10</i>	<i>S10</i>
<i>13. Supporting information Figure S11</i>	<i>S11</i>
<i>14. Supporting information Figure S12</i>	<i>S11</i>
<i>15. Supporting information Figure S13</i>	<i>S12</i>
<i>15. Supporting information Scheme S2</i>	<i>S12</i>
<i>16. Supporting information Scheme S3</i>	<i>S12</i>
<i>16. Supporting information Figure S14</i>	<i>S13</i>
<i>17. Supporting information Figure S15</i>	<i>S13</i>
<i>18. Supporting information Figure S16</i>	<i>S13</i>
<i>19. Supporting information Figure S17</i>	<i>S14</i>
<i>20 Supporting information Figure S18</i>	<i>S14</i>
<i>21 Supporting information Figure S19</i>	<i>S15</i>
<i>21 Supporting information Figure S20</i>	<i>S15</i>
<i>20. Supporting information Figure S21</i>	<i>S16</i>
<i>21. Supporting information Figure S22</i>	<i>S16</i>

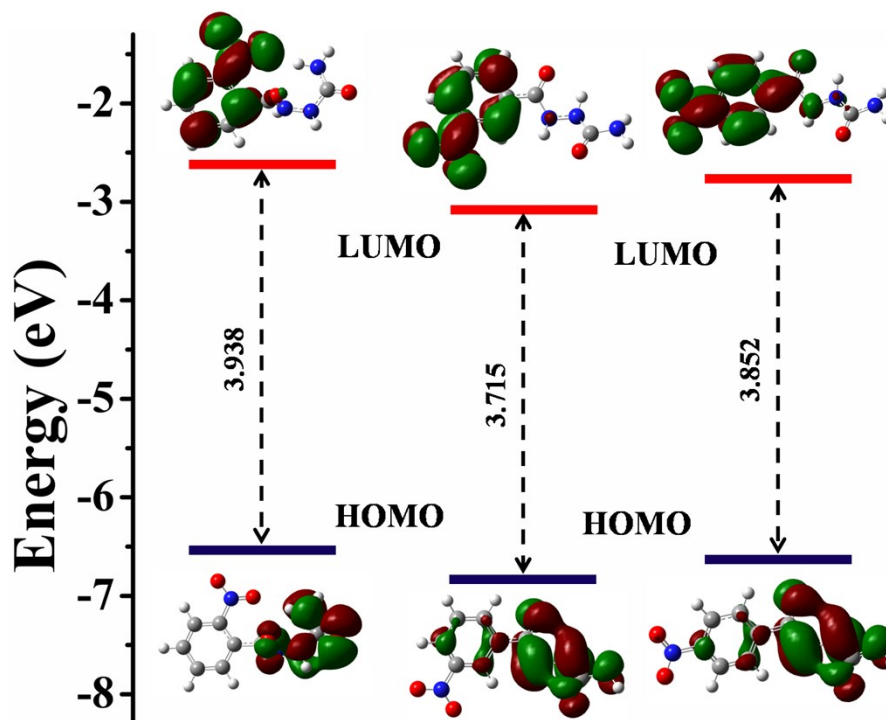
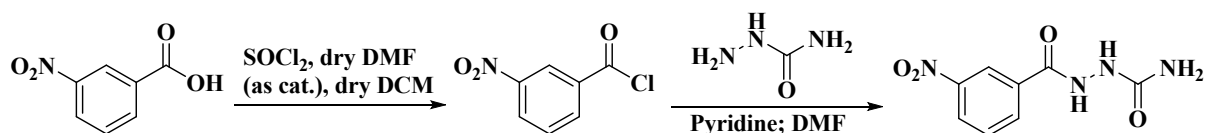


Figure S1: The molecular orbital diagram of the 1-*o*-nitrobenzoyl semicarbazide **2** (HOMO - 6.562; LUMO -2.624), 1-*m*-nitrobenzoyl semicarbazide **1** (HOMO -6.809, LUMO -3.094) and 1-*p*-nitrobenzoyl semicarbazide **3** (HOMO -6.635; LUMO -2.783).



Scheme S1: Schematic representation for the formation of compound **1**.

Table S1:

Hydrogen bonding parameters for compound **1**:

D–H···A	D···H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
N2 --- H2 O4 ^a	0.8800	2.2100	2.8532(18)	129.00
N3 --- H3 O4 ^b	0.8800	2.0200	2.7884(17)	146.00
N4 --- H4A ... O3 ^c	0.8800	2.1400	2.9931(19)	163.00
N4 --- H4B ... O4 ^b	0.8800	2.5100	3.0897(17)	124.00
N4 --- H4B ... O3 ^d	0.8800	2.4300	3.0508(19)	128.00
N4 --- H4B ... N3 ^d	0.8800	2.5500	3.2833(19)	141.00

Symmetry: a = 1-x,1-y,1-z; b = x,1+y,z; c = -x,1-y,1-z; d = -x,2-y,1-z

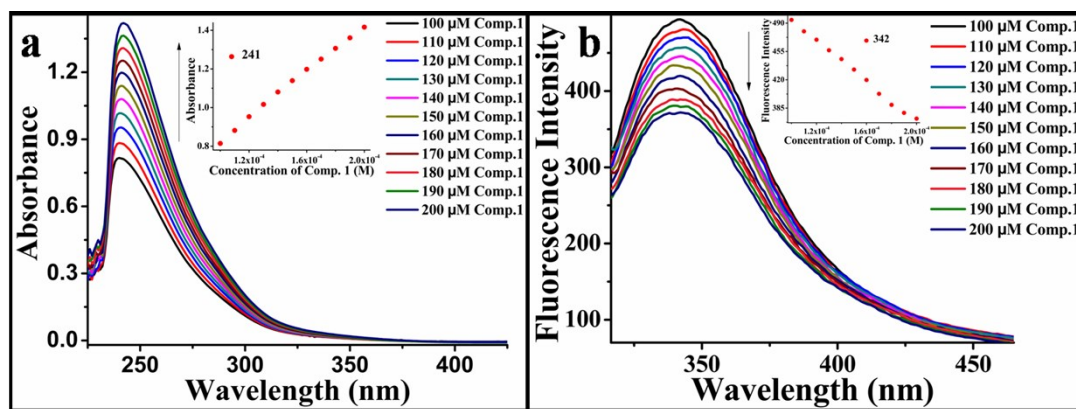


Figure S2: Concentration-dependent UV-Vis (a) and fluorescence spectra (excitation at 254 nm) (b) (inset graph indicate the linear increment and decrement with conc. respectively).

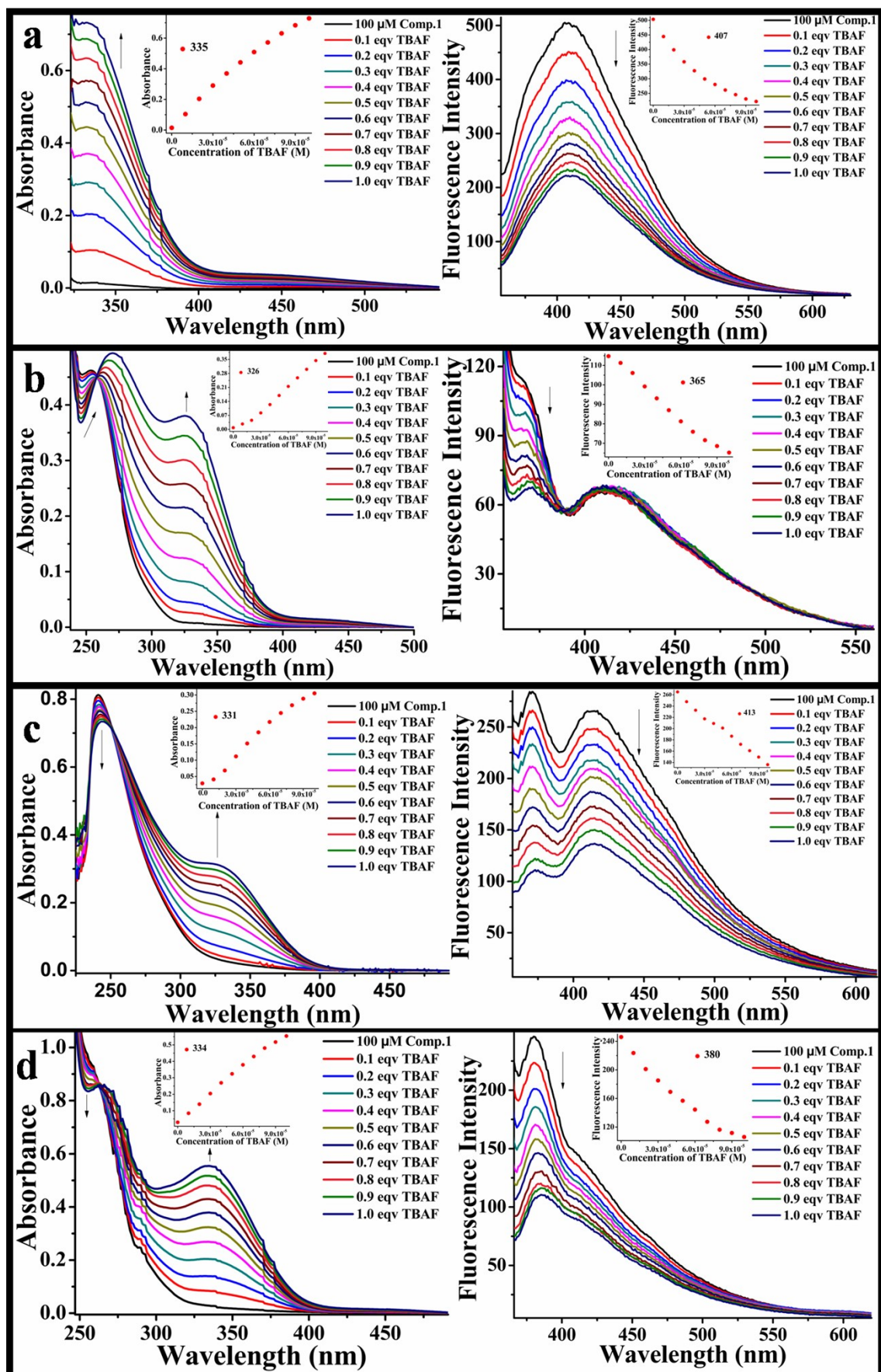


Figure S3: Absorption and emission spectra (excitation at 330 nm) of compound 1 with the gradual addition of fluoride ion in different solvents, (a) Acetone; (b) ACN; (c) DMSO; (d) THF (inset graph indicate the linear increment and decrement with TBAF conc. respectively).

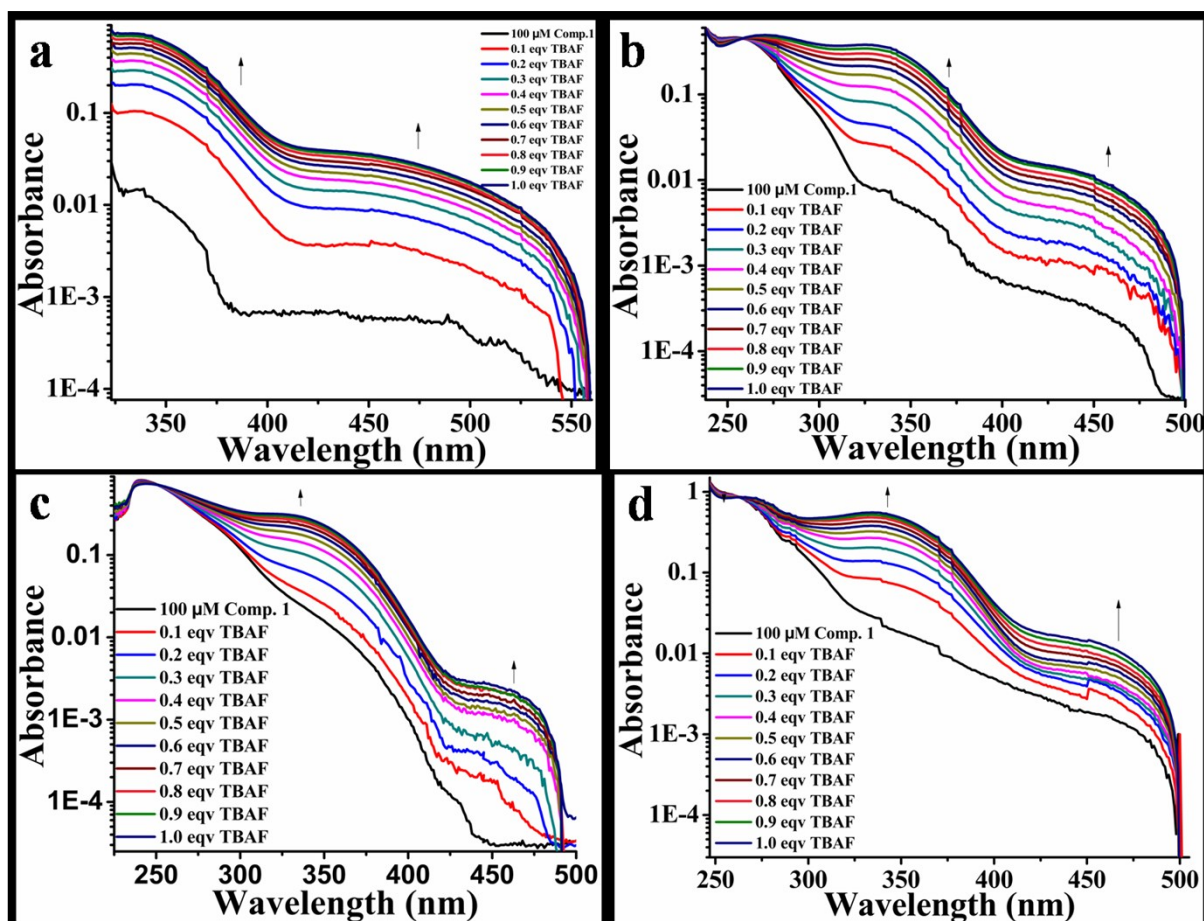


Figure S4: Absorption spectra of compound 1 with the gradual addition of fluoride ion in different solvents, (a) Acetone; (b) ACN; (c) DMSO; (d) THF (Every graph as represented in logarithmic scale for better understanding of the band at around 466 nm).

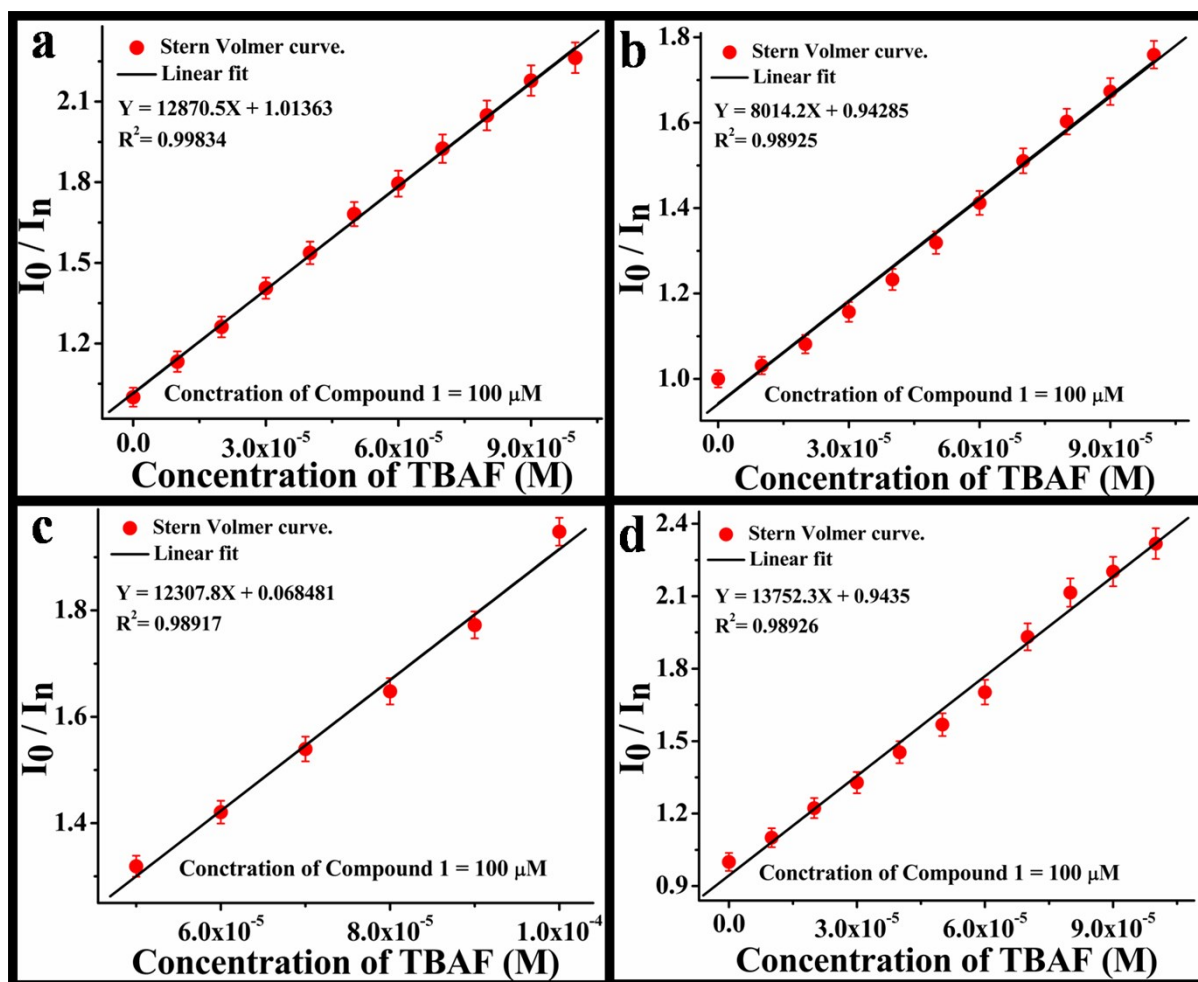


Figure S5: Stern-Volmer plot for fluoride ion binding in different solvents, (a) Acetone; (b) ACN; (c) DMSO; (d) THF.

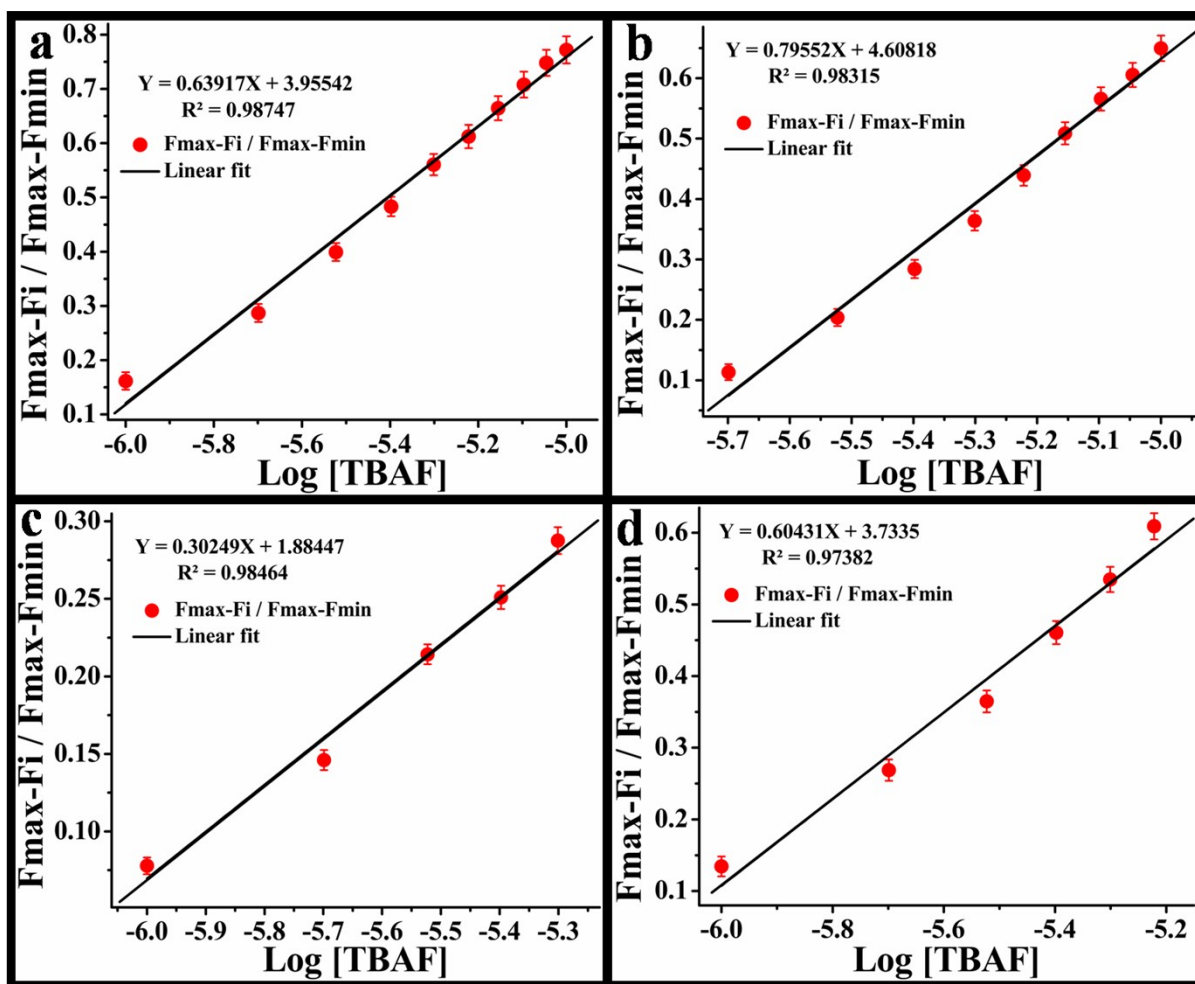


Figure S6: Detection limit calculation for fluoride ion in different solvents, (a) Acetone; (b) ACN; (c) DMSO; (d) THF.

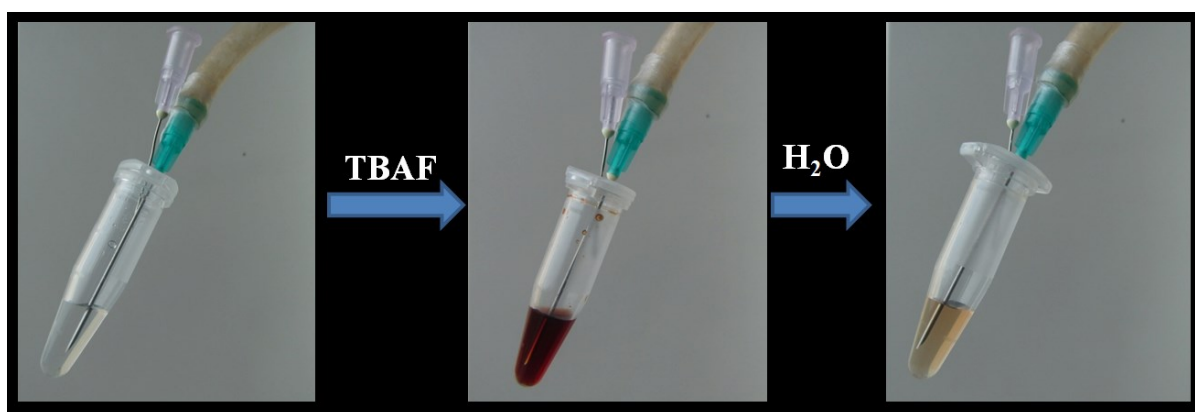


Figure S7: Reversible colour changes of compound **1** in DMSO with the addition of TBAF and by the introduction of a trace amount of water in the solvents.

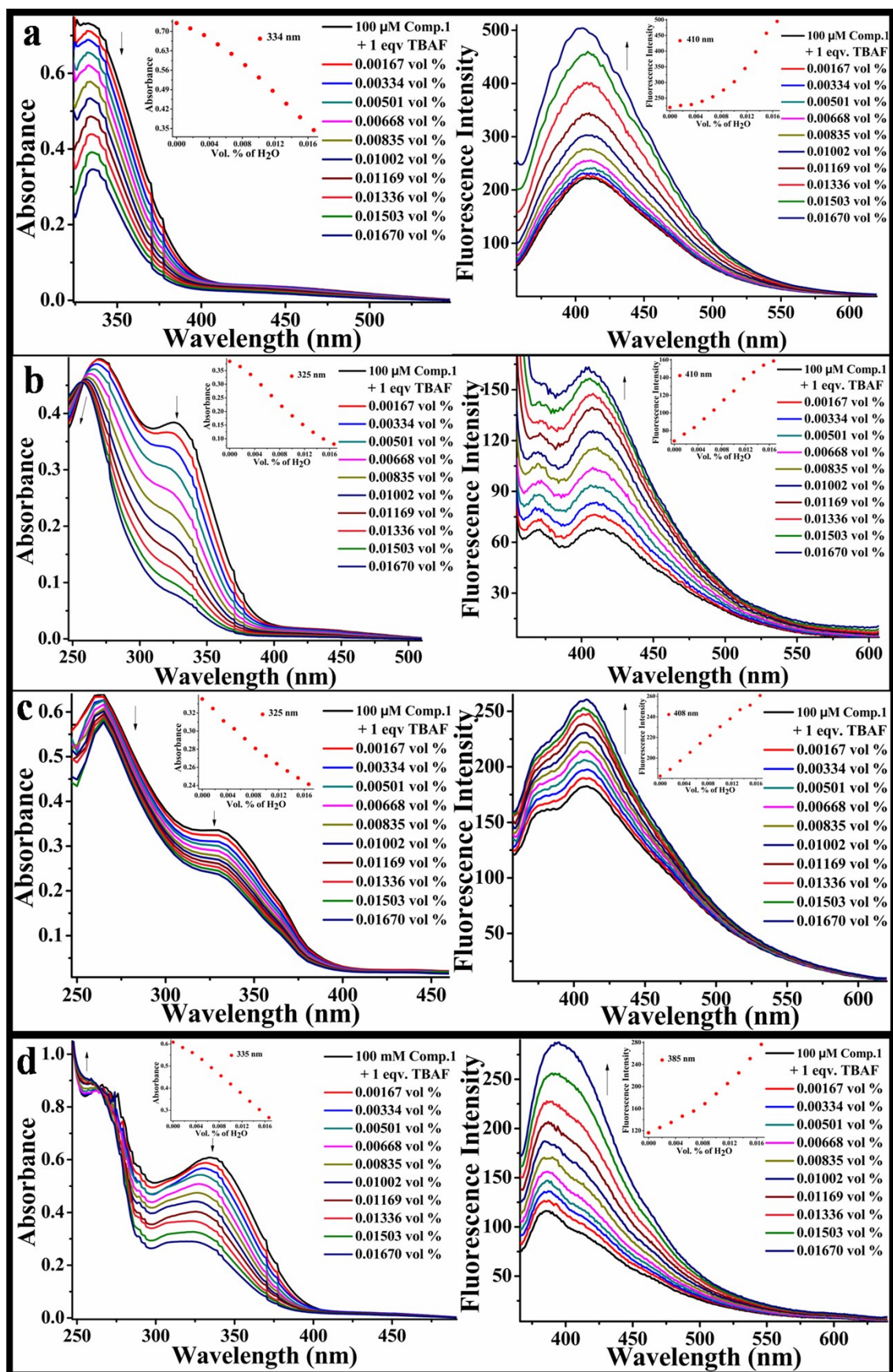


Figure S8: Absorption and emission spectra(excitation at 330 nm) of 1.F with the gradual addition of water in different solvents, (a) Acetone; (b) ACN; (c) DMSO; (d) THF (inset graph indicate the linear decrement and increment with different wt% of water respectively).

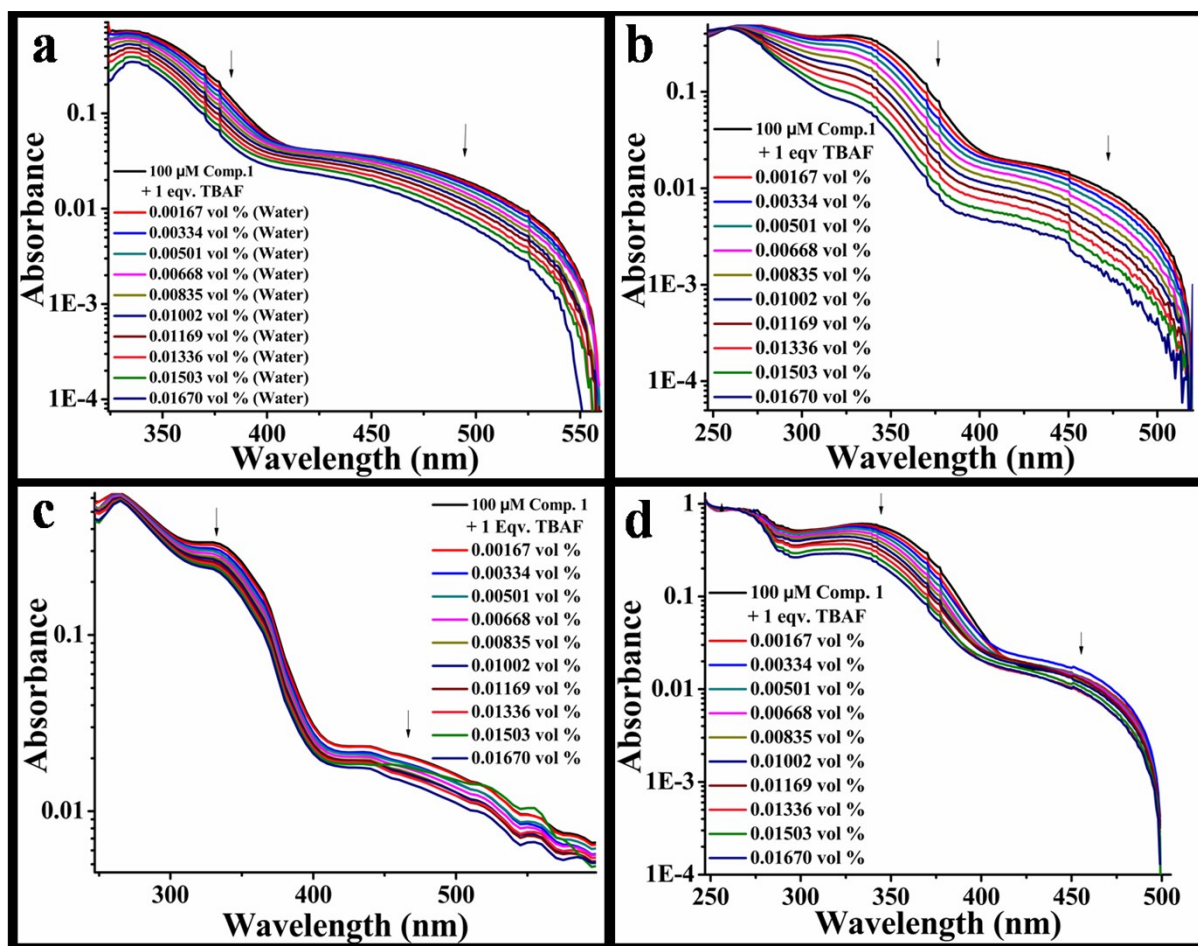


Figure S9: Absorption spectra of compound **1.F** with the gradual addition of water in different solvents, (a) Acetone; (b) ACN; (c) DMSO; (d) THF (Every graph as represented in logarithmic scale for better understanding of the band at around 464 nm).

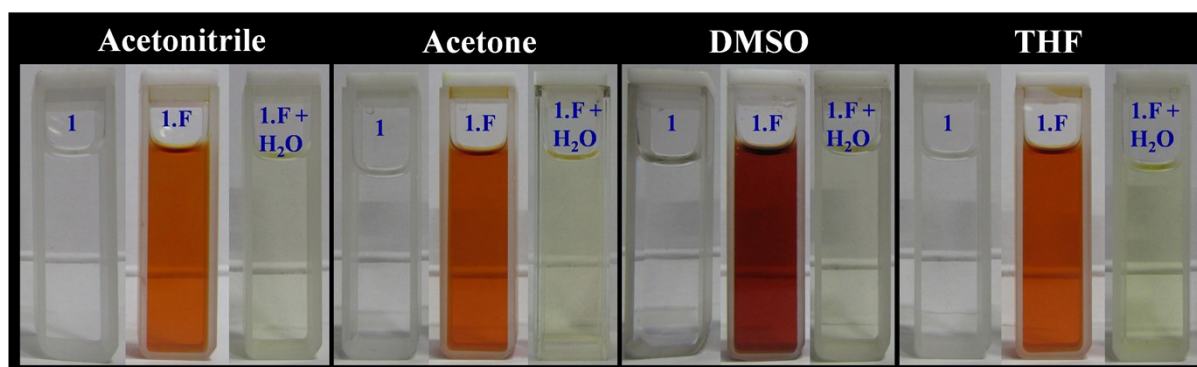


Figure S10: Reversible color changes of compound **1** in acetone, ACN, DMSO, and THF with the addition of TBAF and by the introduction of a trace amount of water in the solvents.

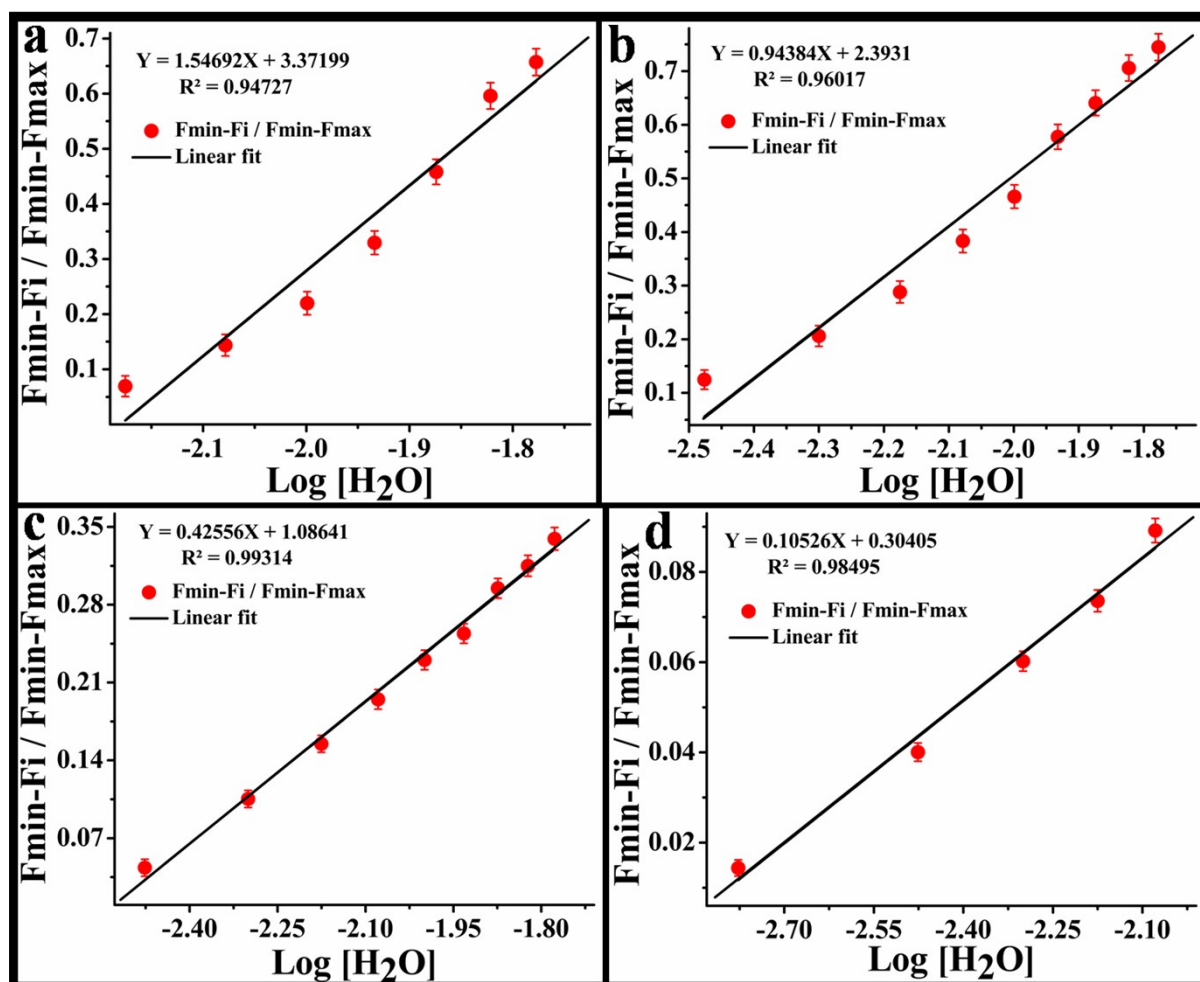


Figure S11: Detection limit calculation for moisture in different solvents, (a) Acetone; (b) ACN; (c) DMSO; (d) THF.

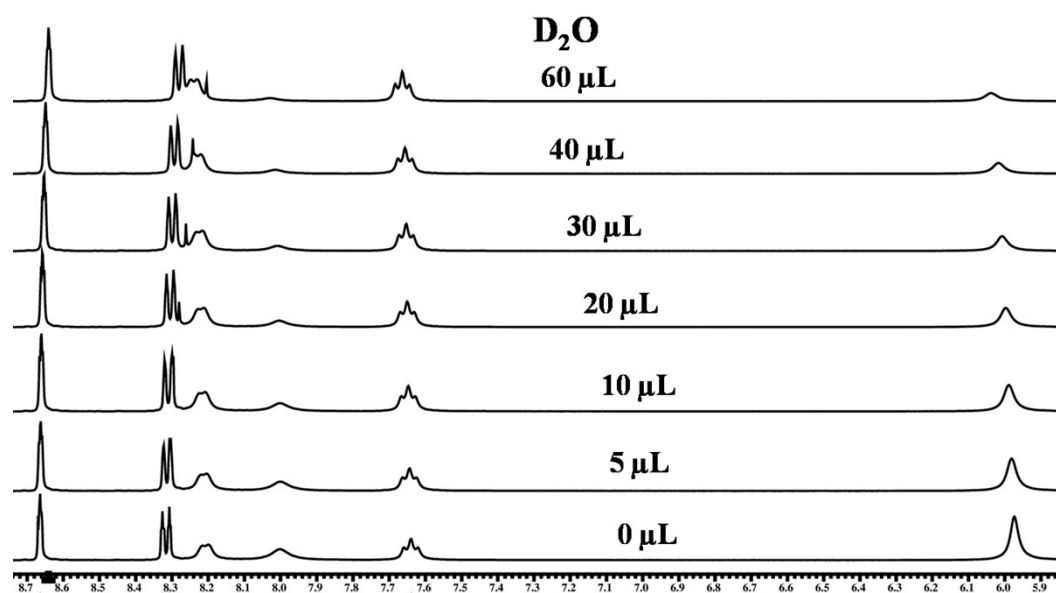


Figure S12: NMR titration with the gradual addition of D₂O in **1.F** using DMSO-d₆ as a solvent.

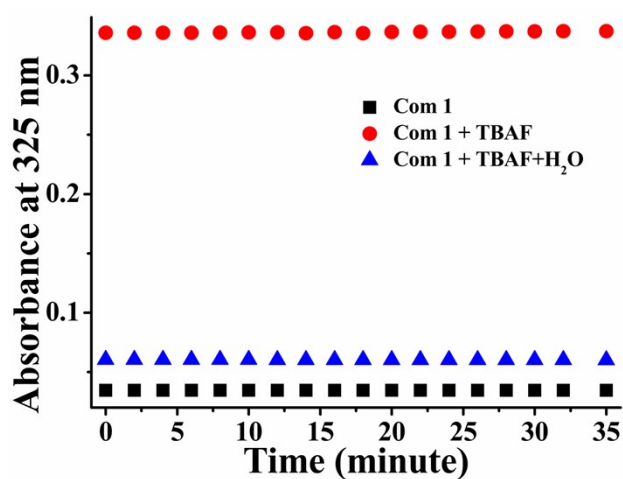
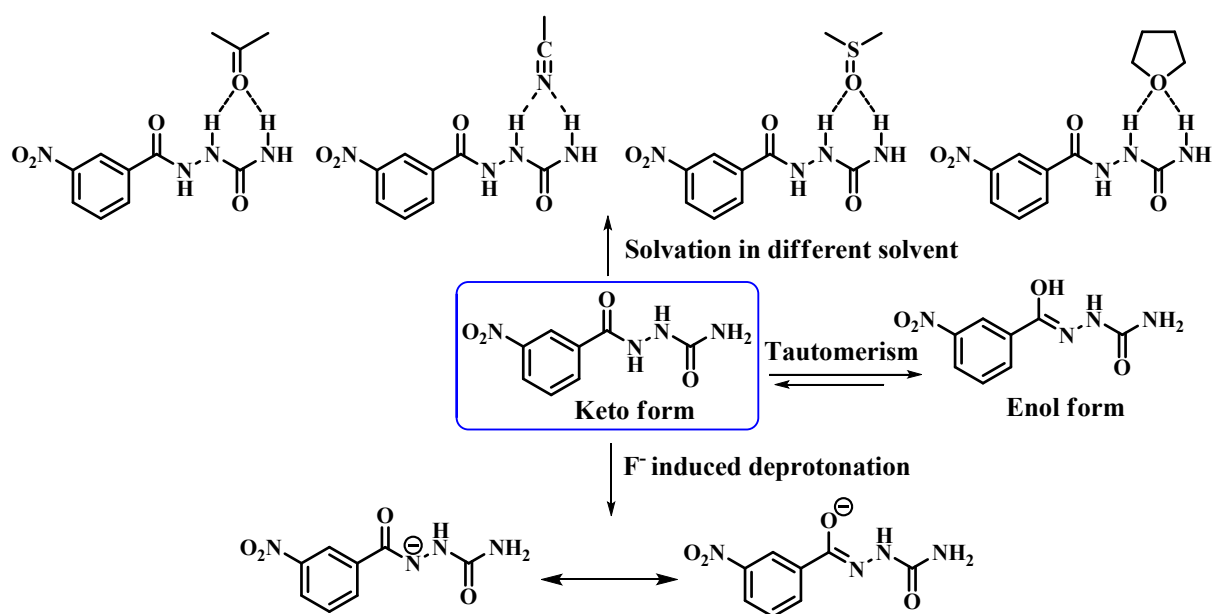
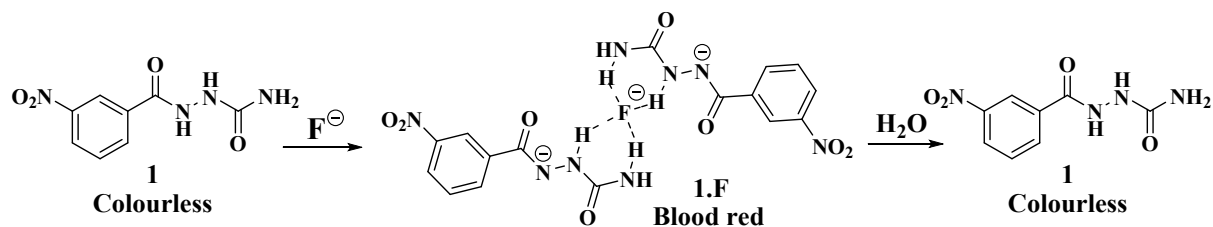


Figure S13. Time-dependent absorbance change of **1.F** with 0.016 vol. % of water.



Scheme S2: Possible structures of compound **1** from solvation in different solvent and the interaction with the fluoride ion.



Scheme S3: Proposed mechanism for the detection of fluoride and moisture.

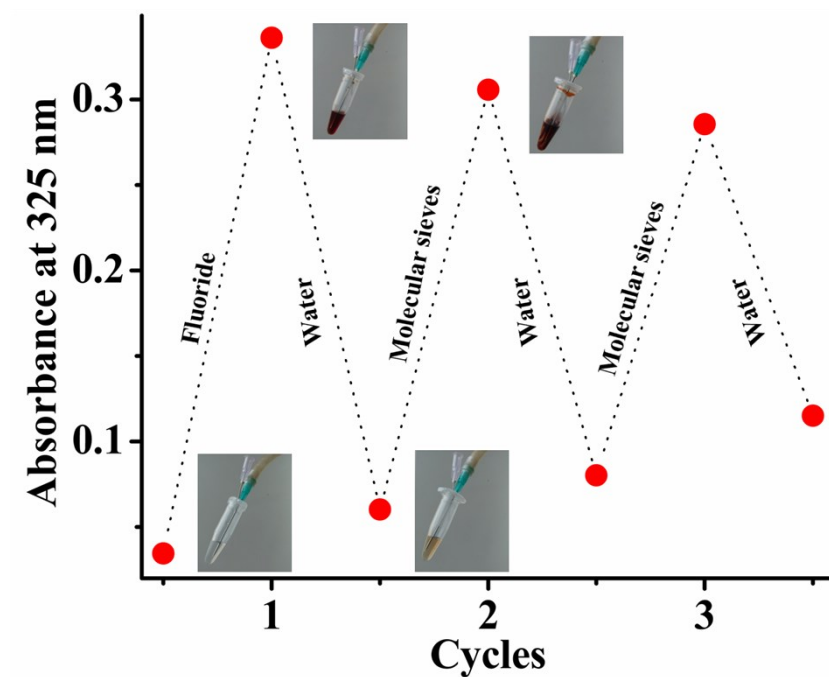


Figure S14. Change in absorbance of **1.F** upon the alternate addition of water and molecular sieves.

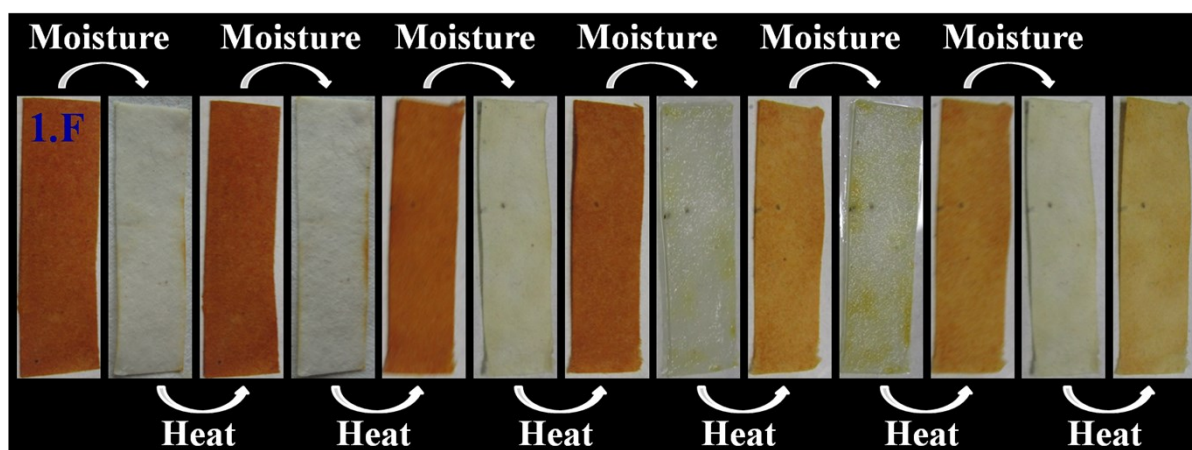


Figure S15: Reversibility of mobile test paper strip in the presence of moisture and heat, respectively.

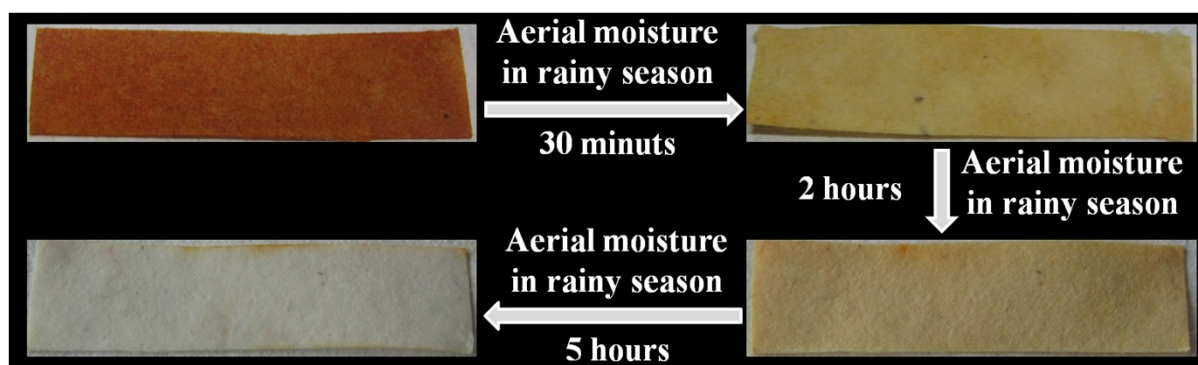


Figure S16: Aerial moisture detection by reversible mobile test paper strip.

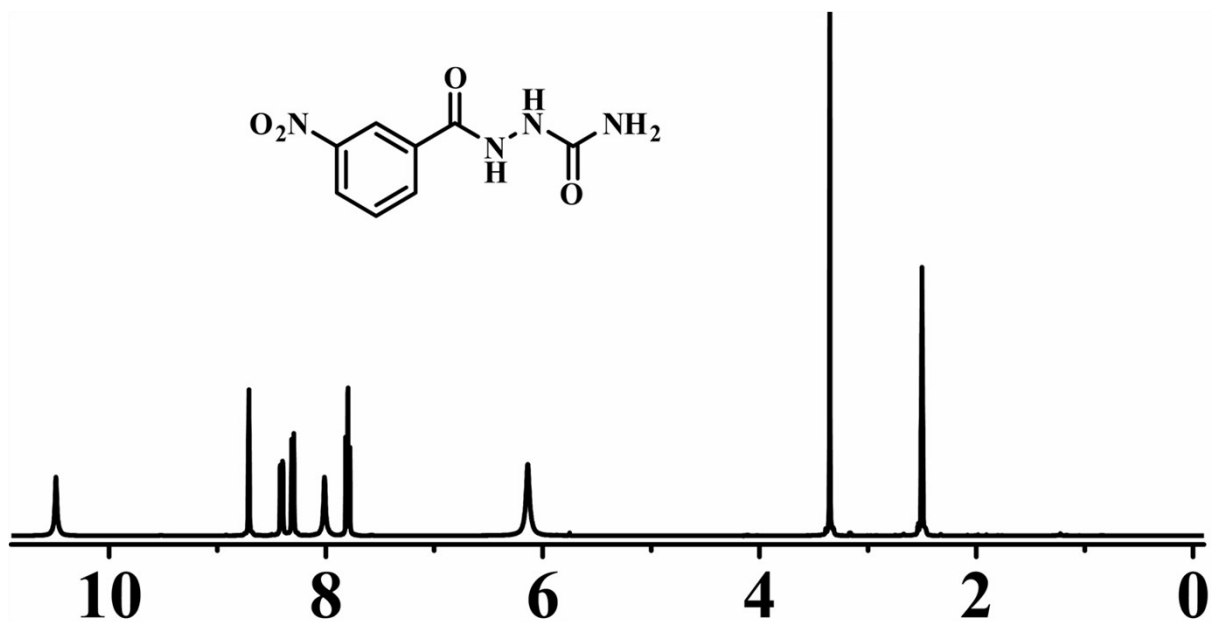


Figure S17: ¹H NMR (400 MHz, DMSO-*d*₆, δ in ppm, 298K) spectra of compound 1.



Figure S18: ¹³C NMR (100 MHz, DMSO-*d*₆, δ in ppm, 298K) spectra of compound 1.

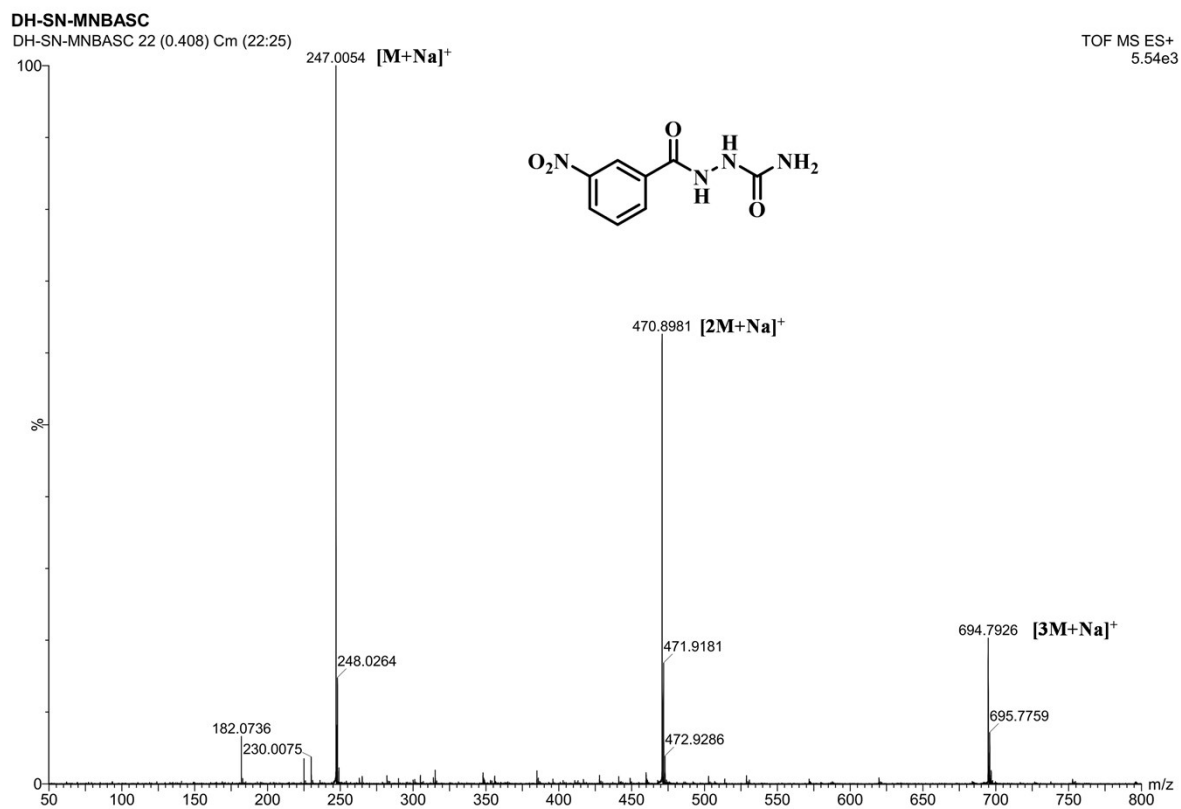


Figure S19: Mass spectrum of compound 1.

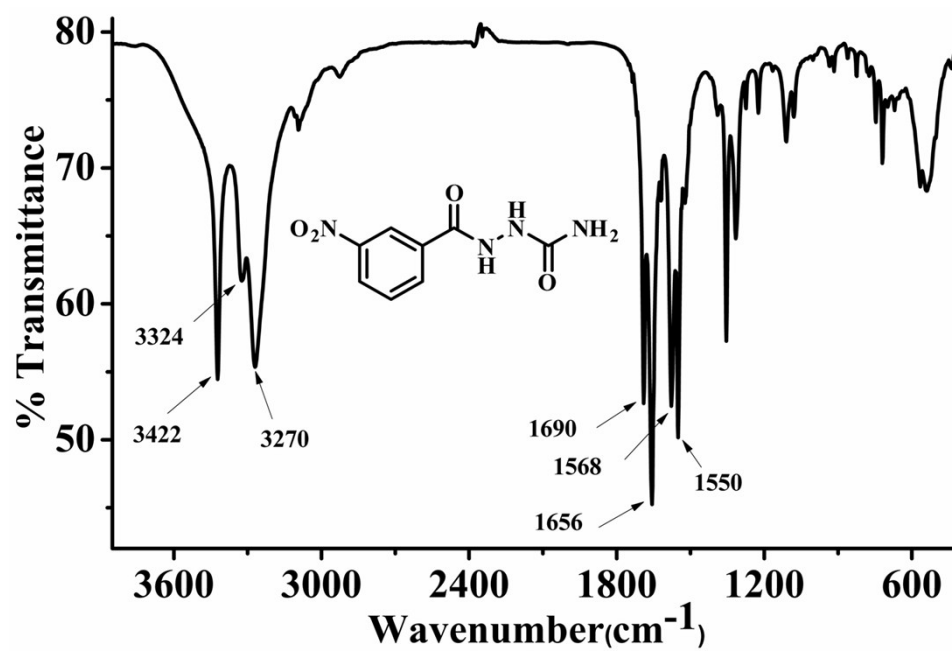


Figure S20: IR spectra of compound 1.

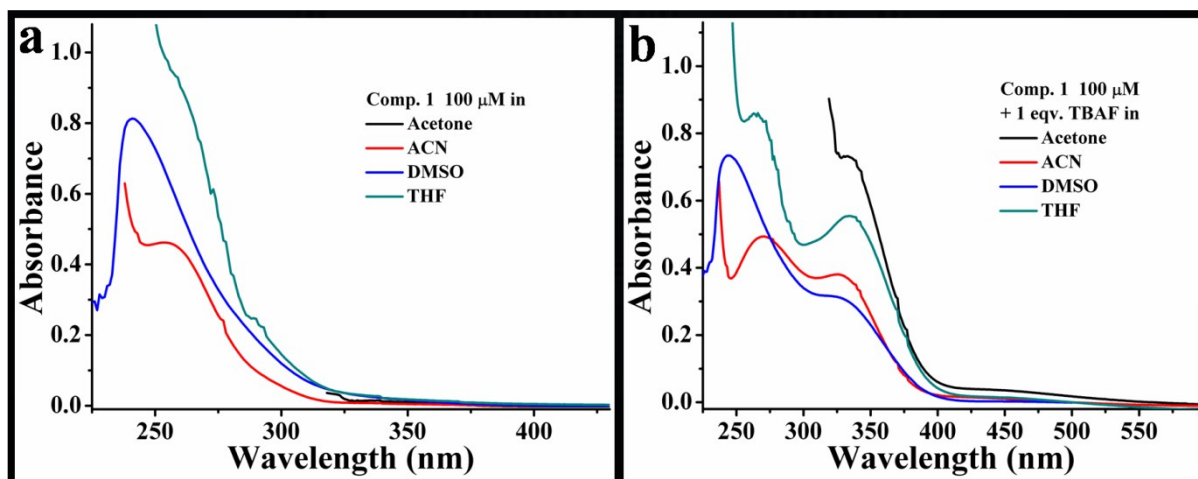


Figure S21: Effect of addition of fluoride ion on compound 1.

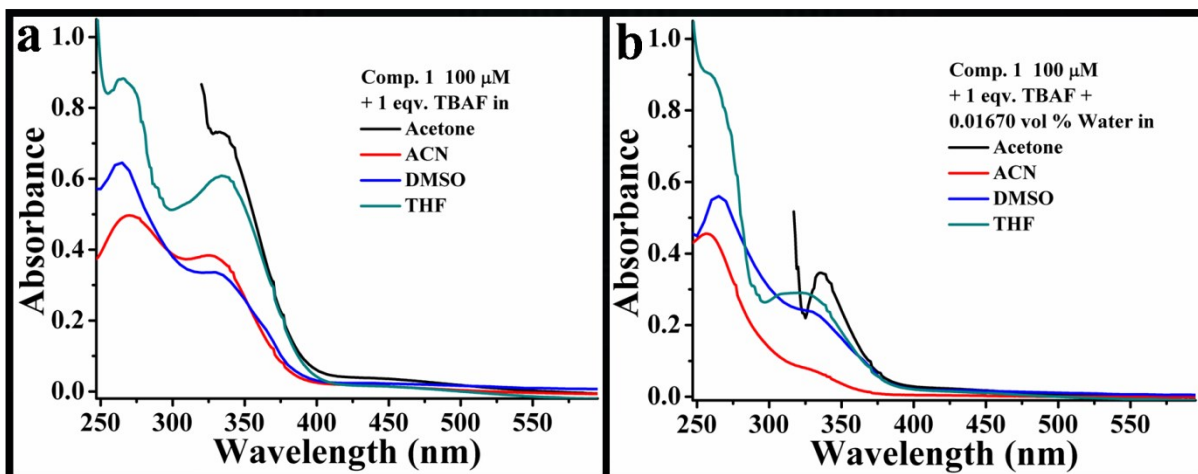


Figure S22: Effect of water on 1-*m*-nitrobenzoyl semicarbazide-fluoride complex.

Chemical Structure of TBAF:

