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Supporting Information

Tuning of H-bonding ability of imidazole N-H towards colorimetric sensing of fluoride and cyanide ions as their sodium salt in aqueous medium

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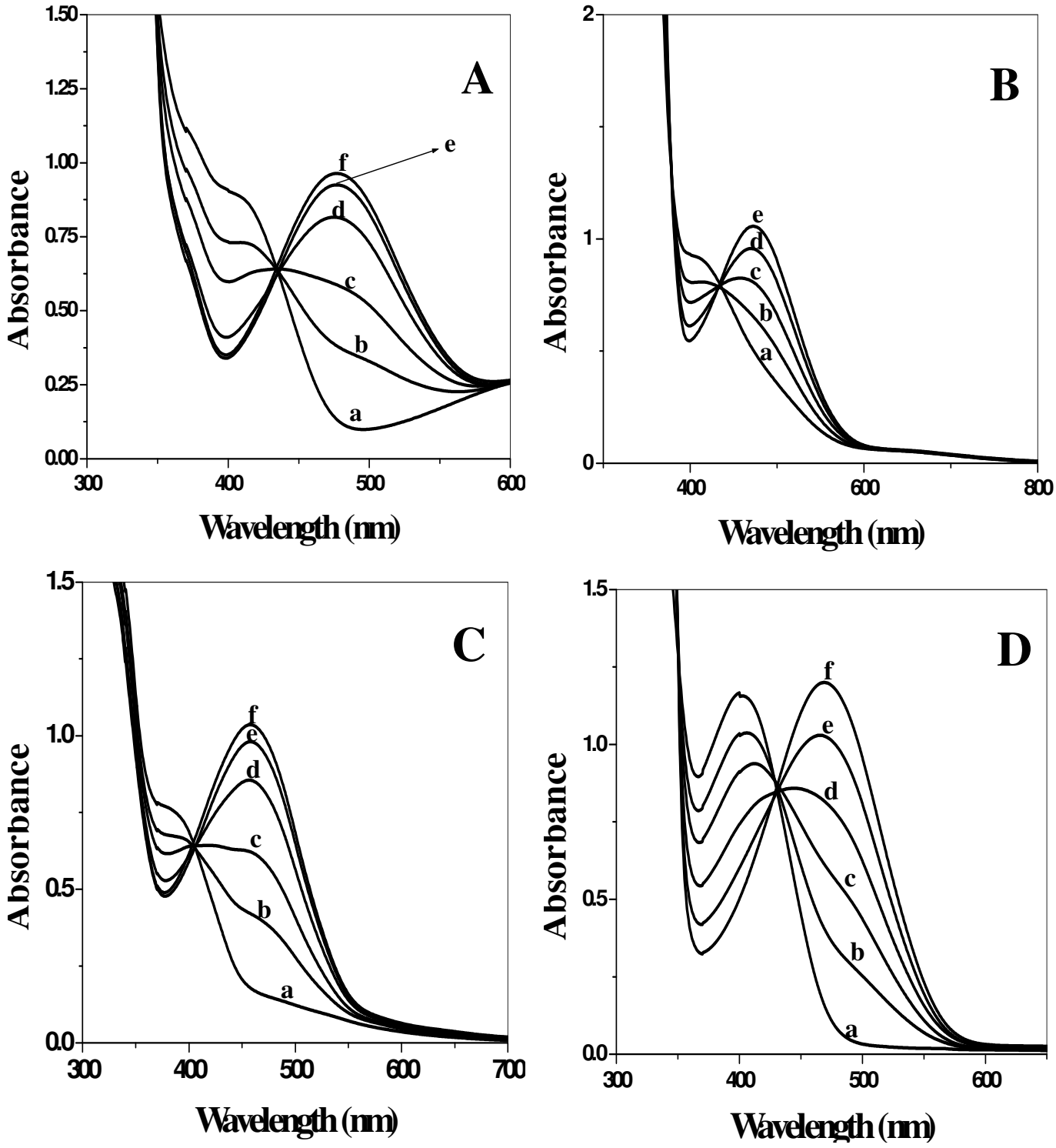


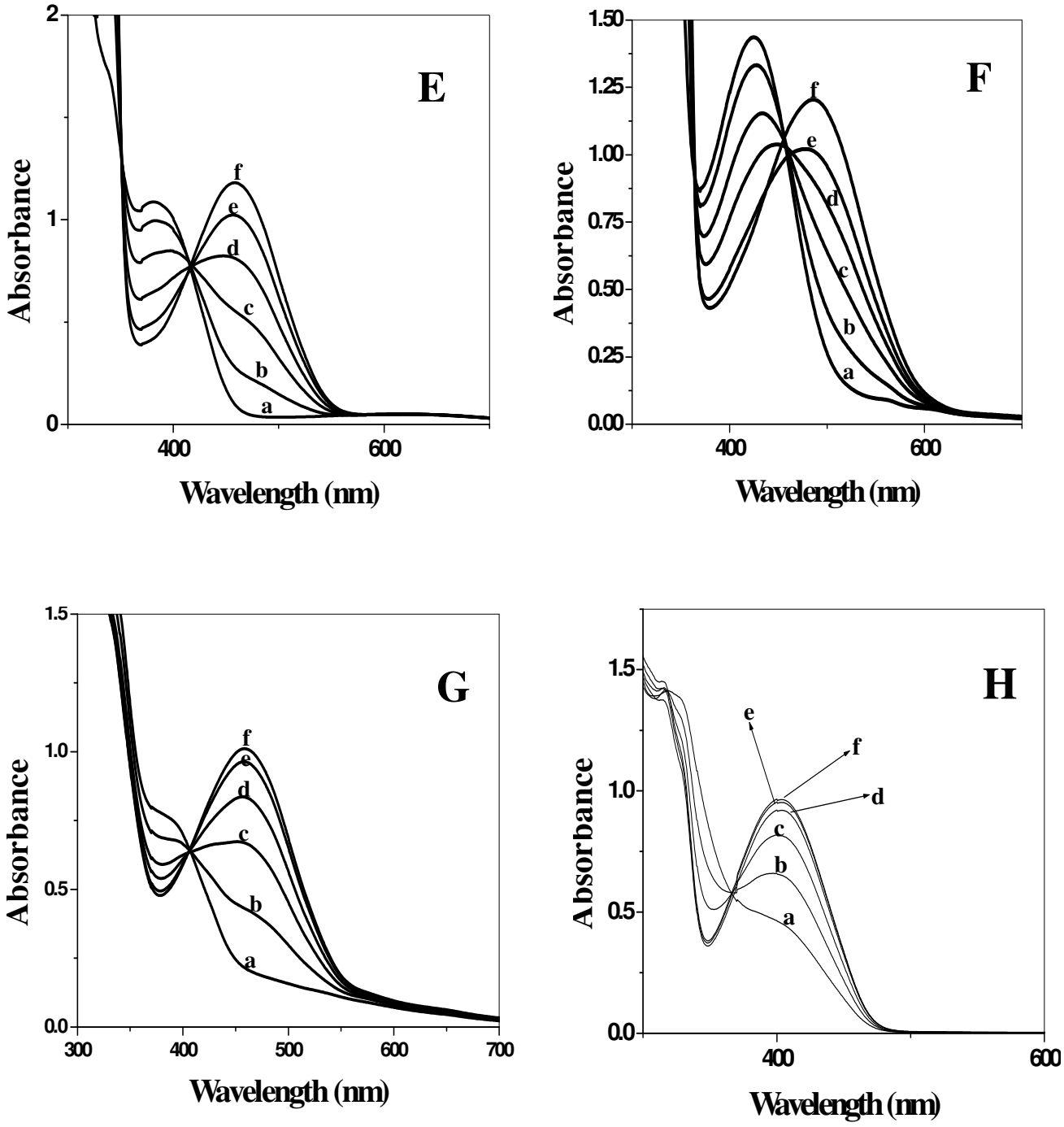


Figure S1. Change in UV-Vis spectra for {(A)- 2a, (B)-2b, (C)-2c, (D)-2d, (E) 2e, (F)-2f, (G)-2g. (H)-2h}(6.25×10^{-4} M) in DMSO with the addition of (1.25×10^{-6} - 0.625×10^{-5}M) of fluoride ion.

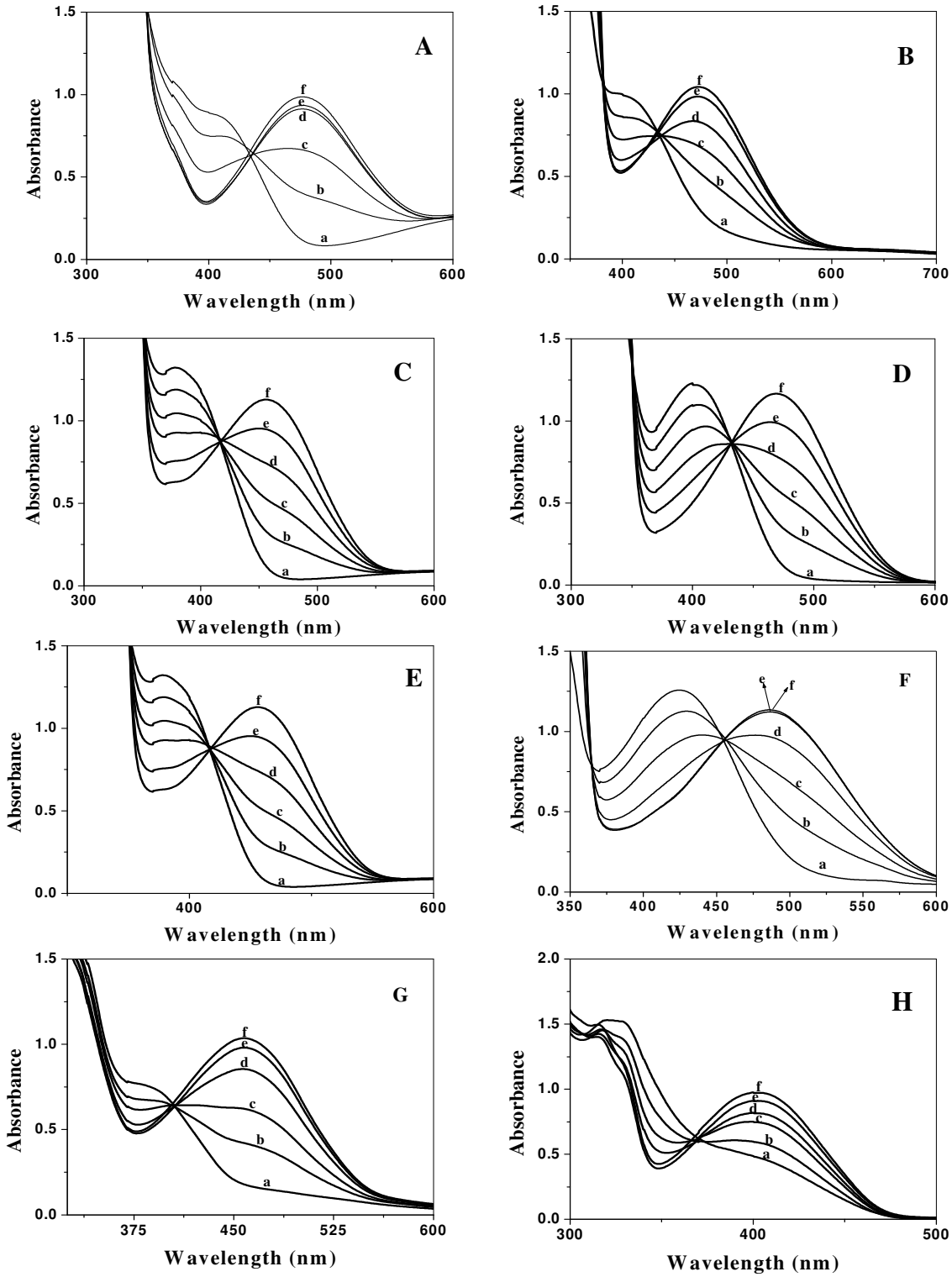


Figure S2. Change in UV-Vis spectra for {(A)- 2a, (B)-2b, (C)-2c, (D)-2d, (E) 2e, (F)-2f, (G)-2g. (H)-2h}(6.25×10^{-4} M) in DMSO with the addition of (1.25×10^{-6} - 0.625×10^{-5}M) of Cyanide ion.

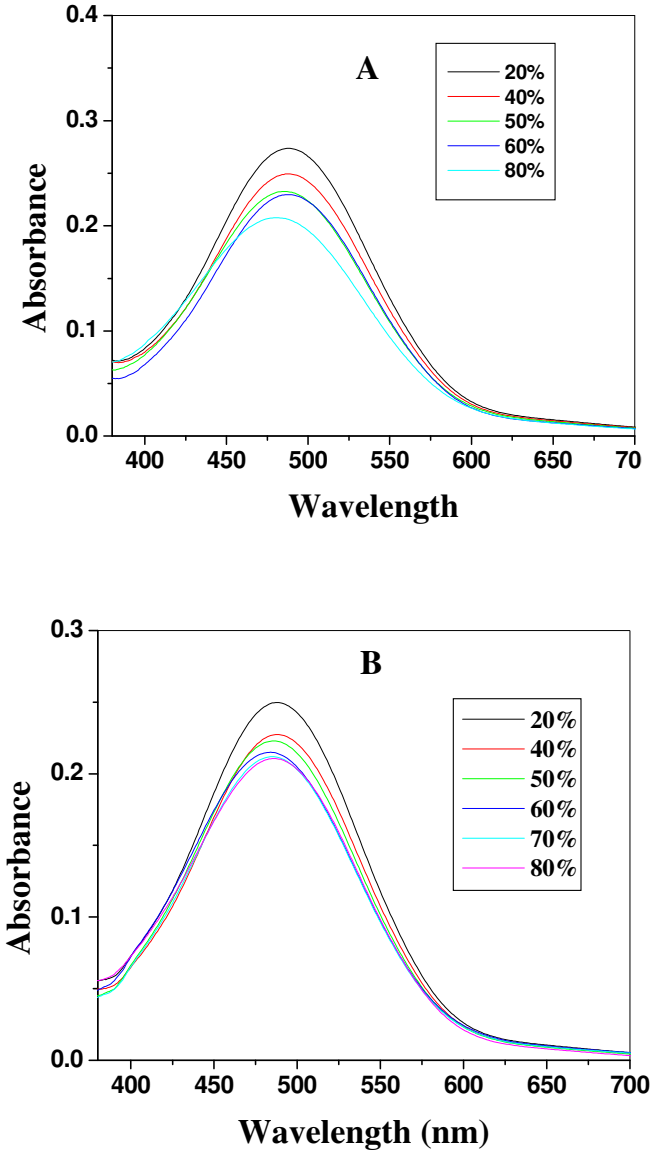
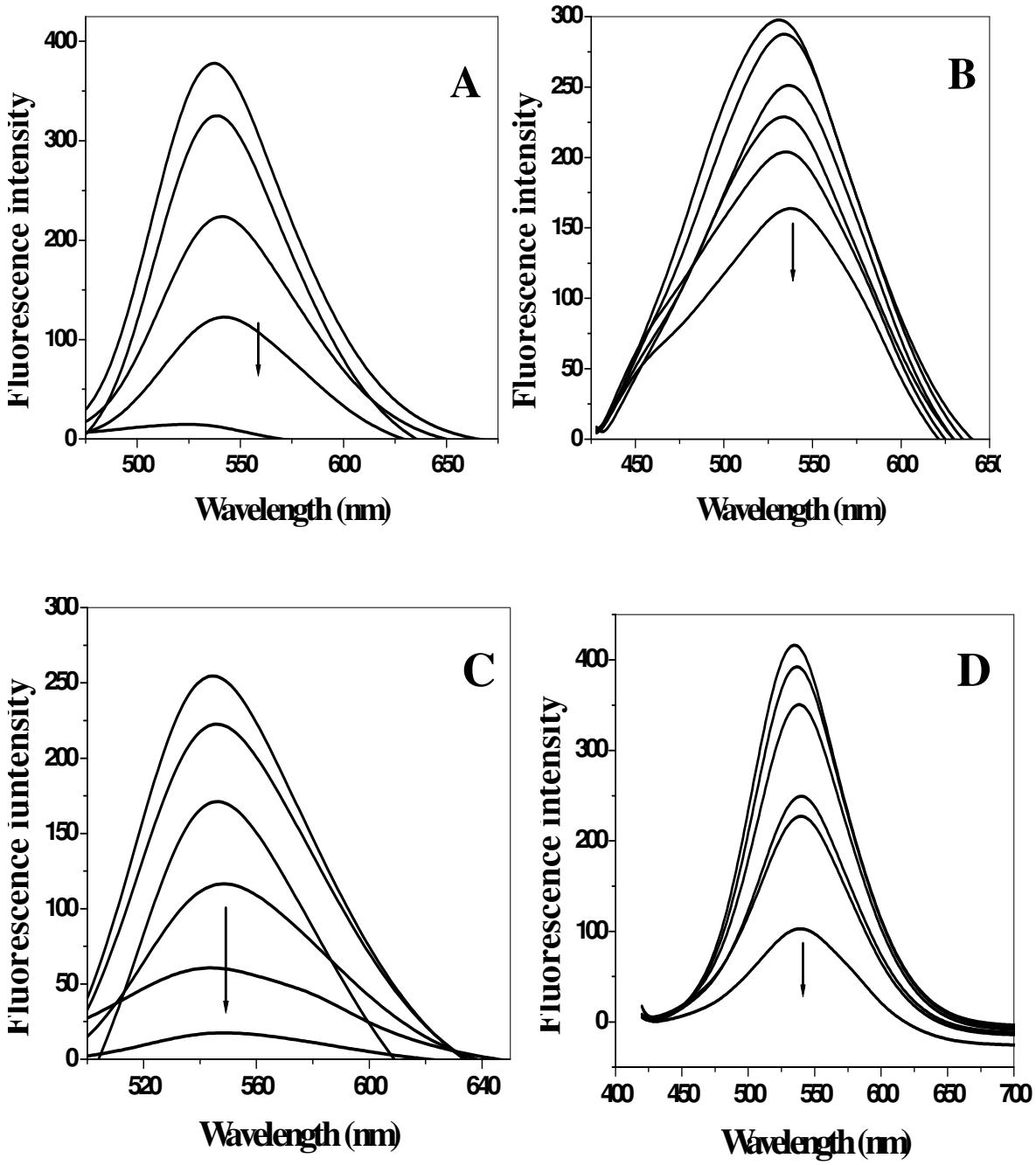


Figure S3. UV-Vis spectra of mixture of 2f (1.25 x 10^{-4} M) and fluoride and cyanide (1.25 x 10^{-4} M) ions in DMSO-water mixtures of varying composition.



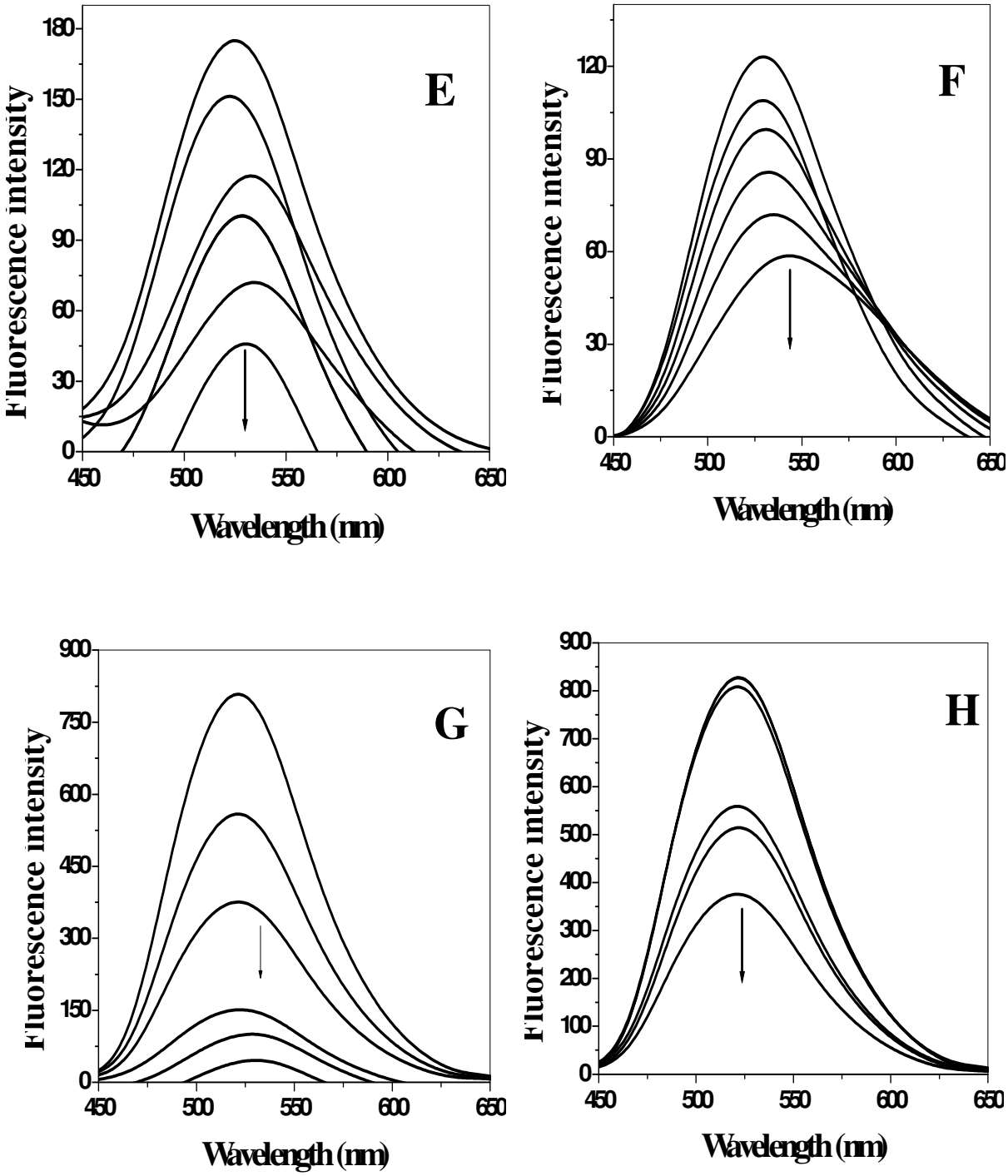
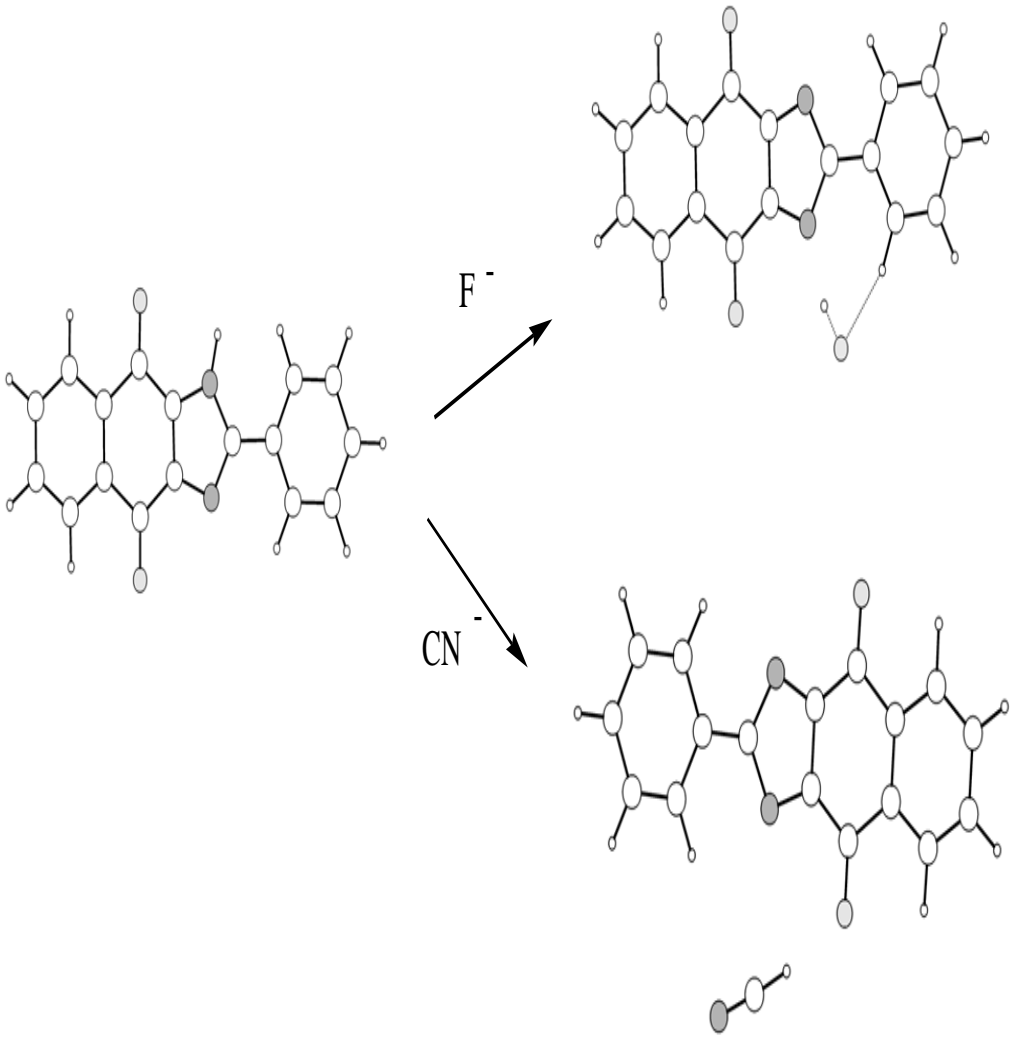
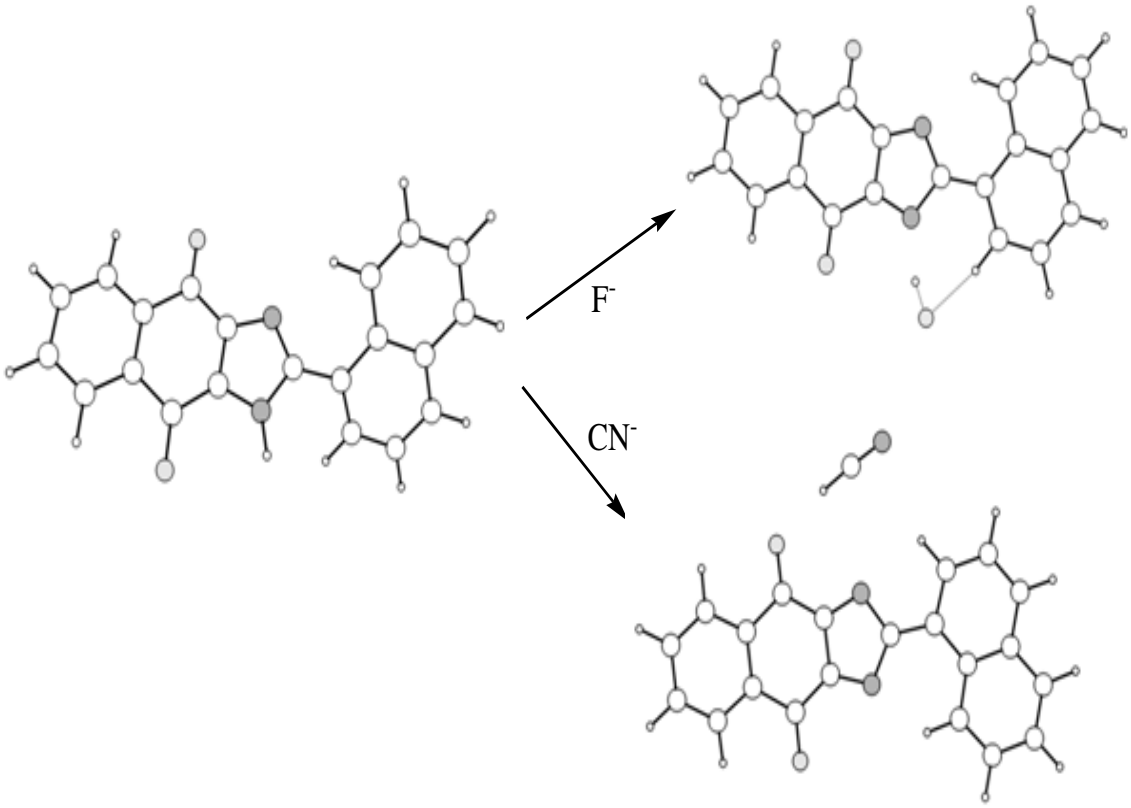


Figure S4. Change in fluorescence emission spectra for {(A)- 2a, (B)-2b, (C)-2c, (D)-2d, (E) 2e, (F)-2f, (G)-2g. (H)-2h}(6.25×10^{-4} M) in DMSO with the addition of (1.25×10^{-6} – 6.25×10^{-4} M) of Cyanide ion.



Optimized structure for 2a, 2a-F and 2a-CN



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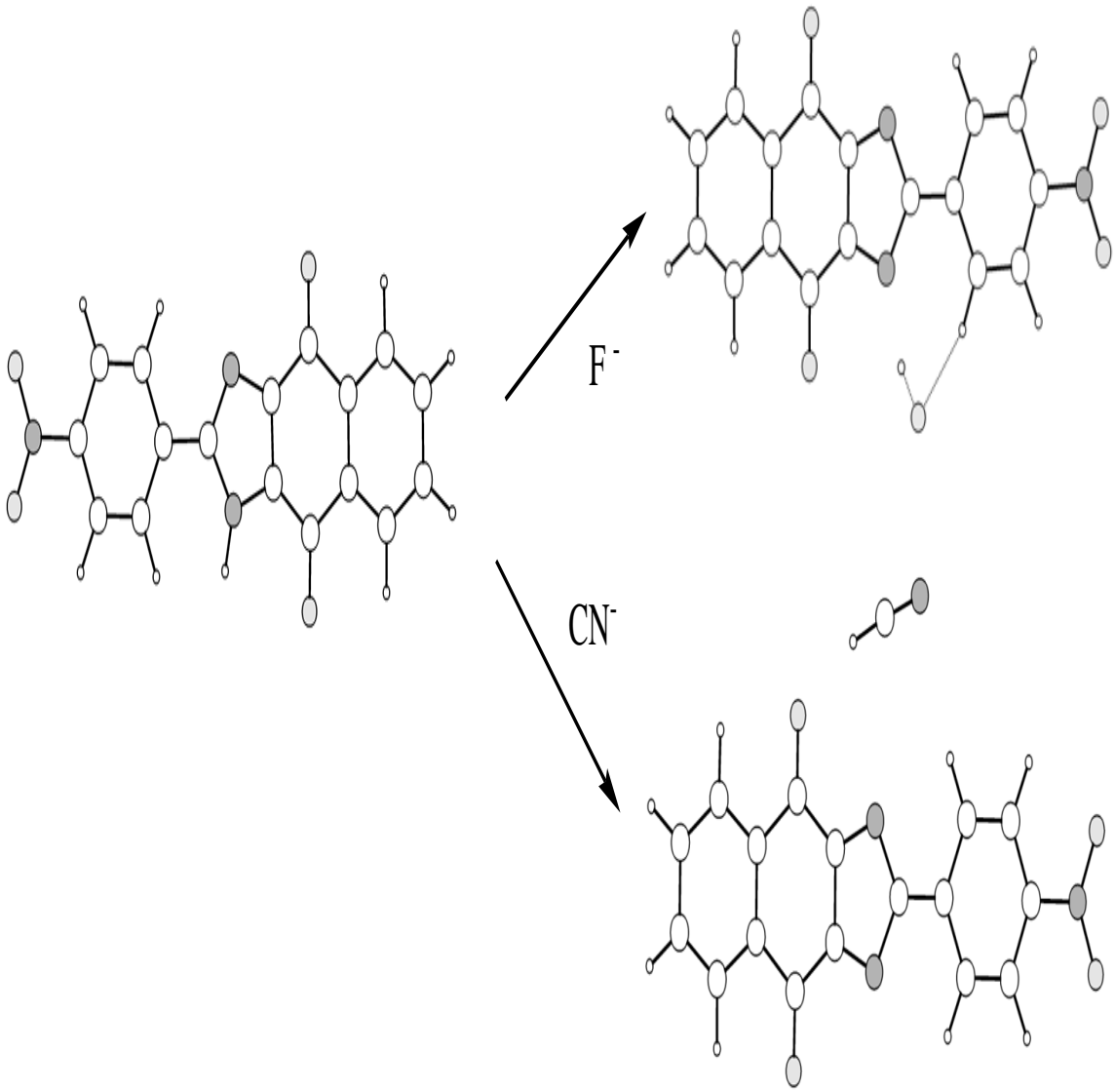
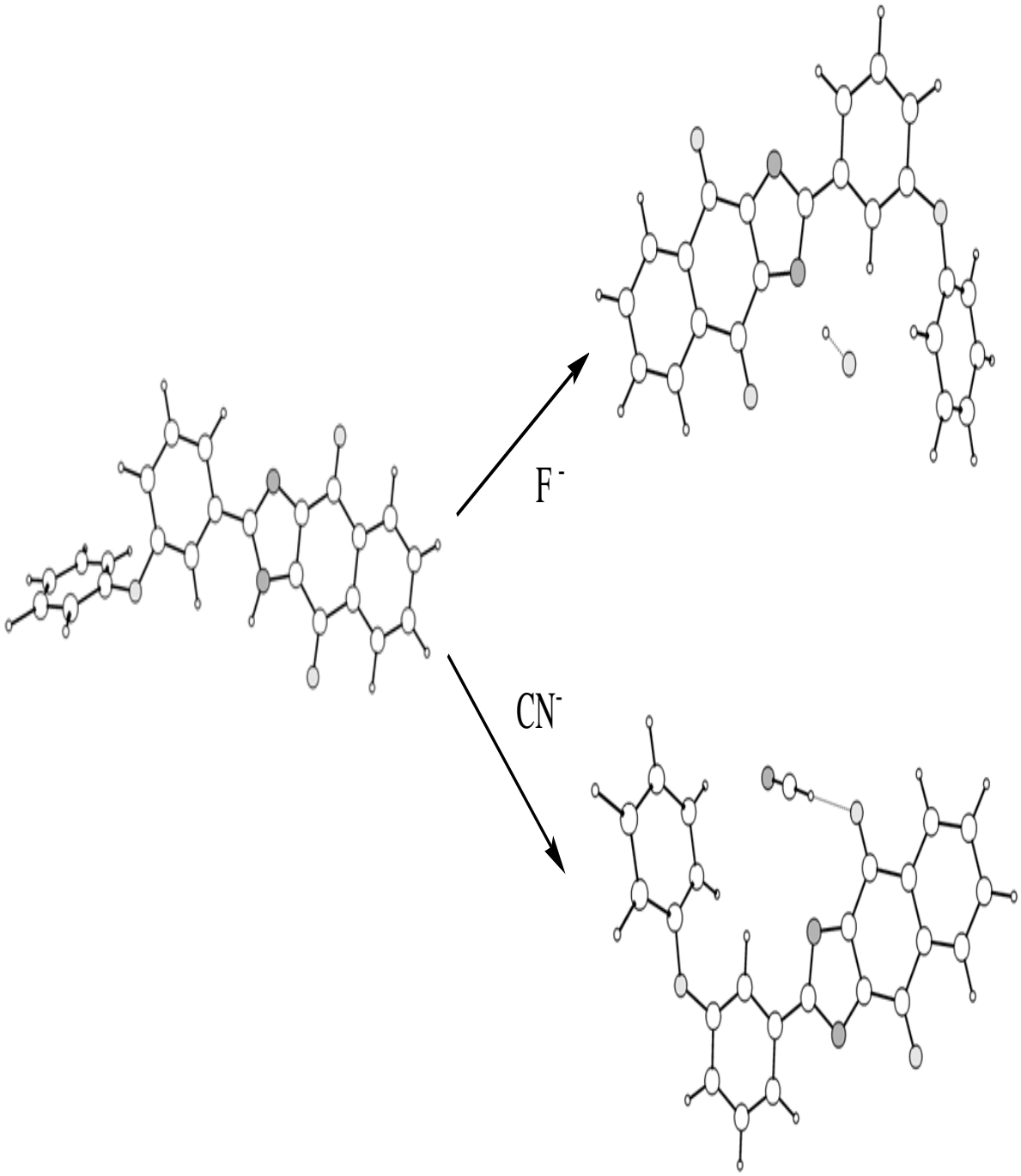
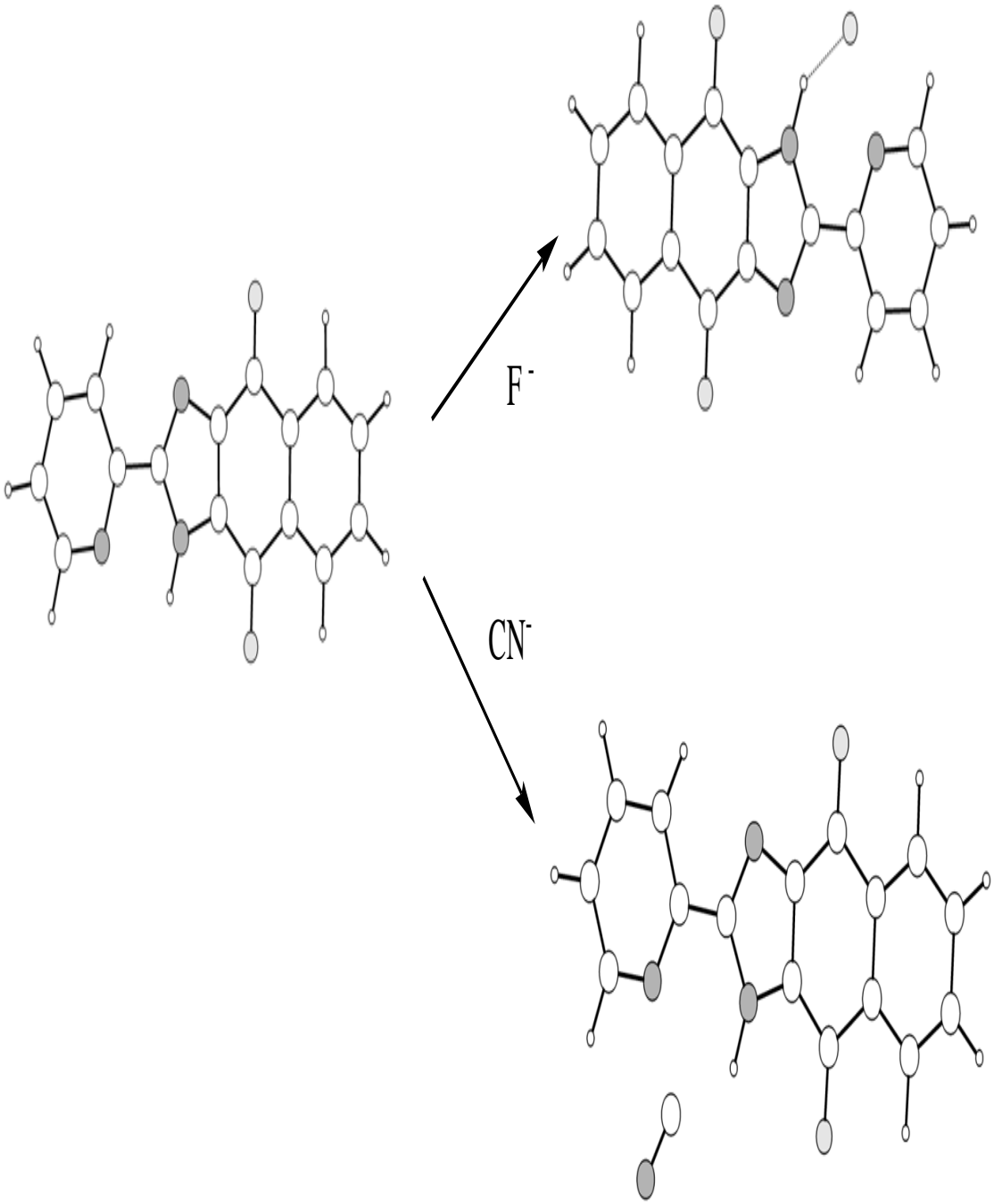


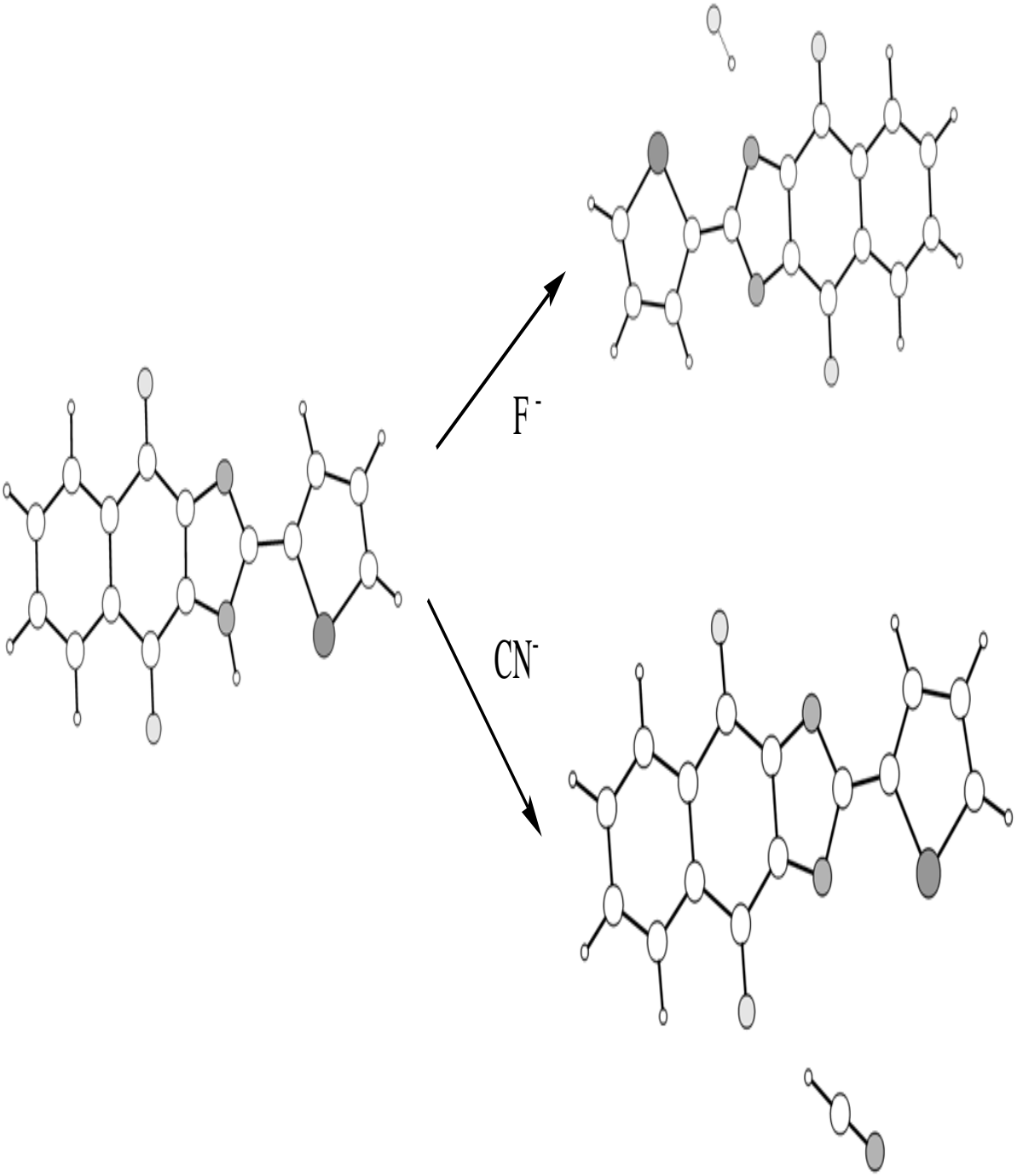
Optimized structure for 2c, 2c-F and 2c-CN



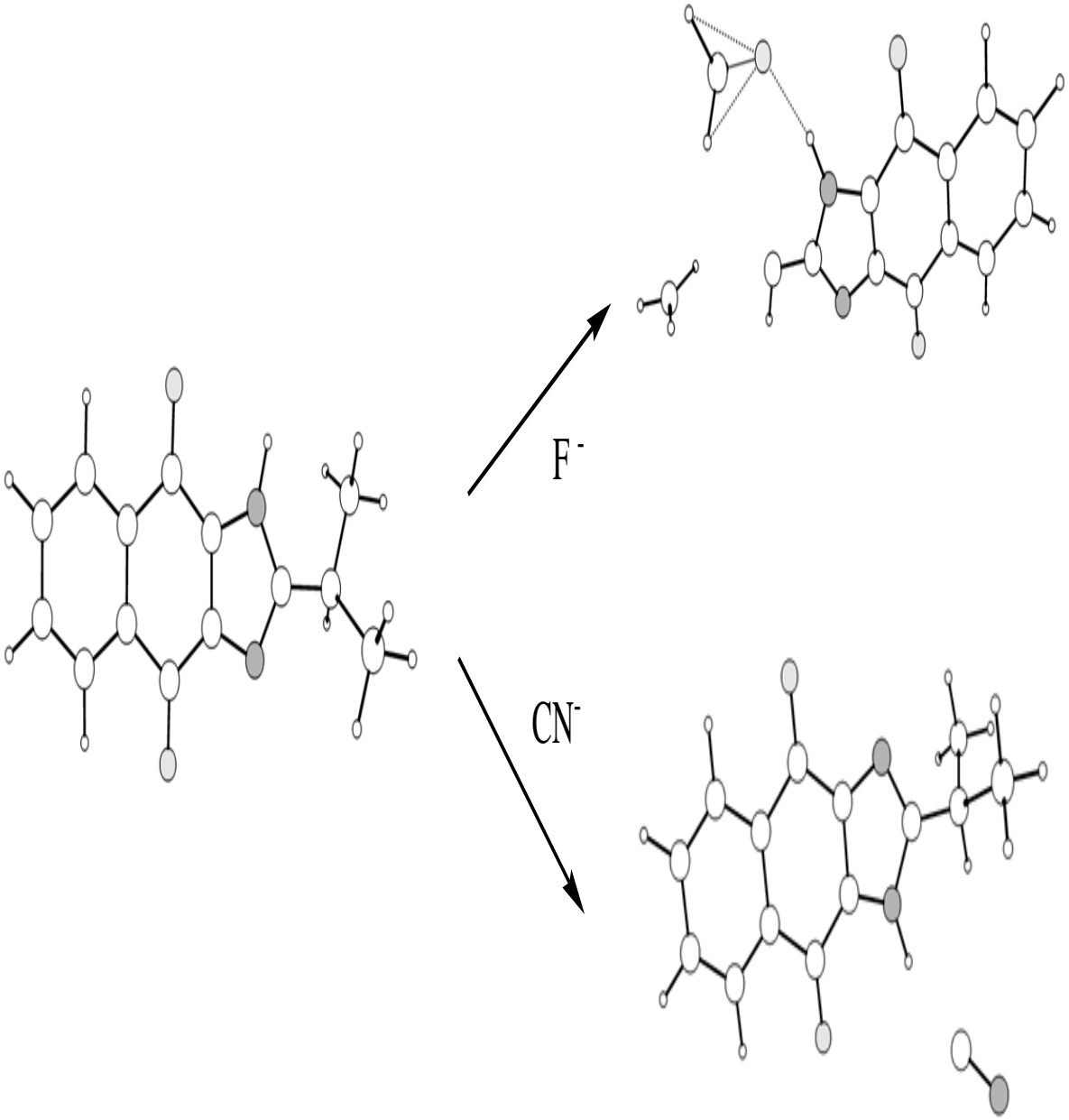
Optimized structure for 2d, 2d-F and 2d-CN



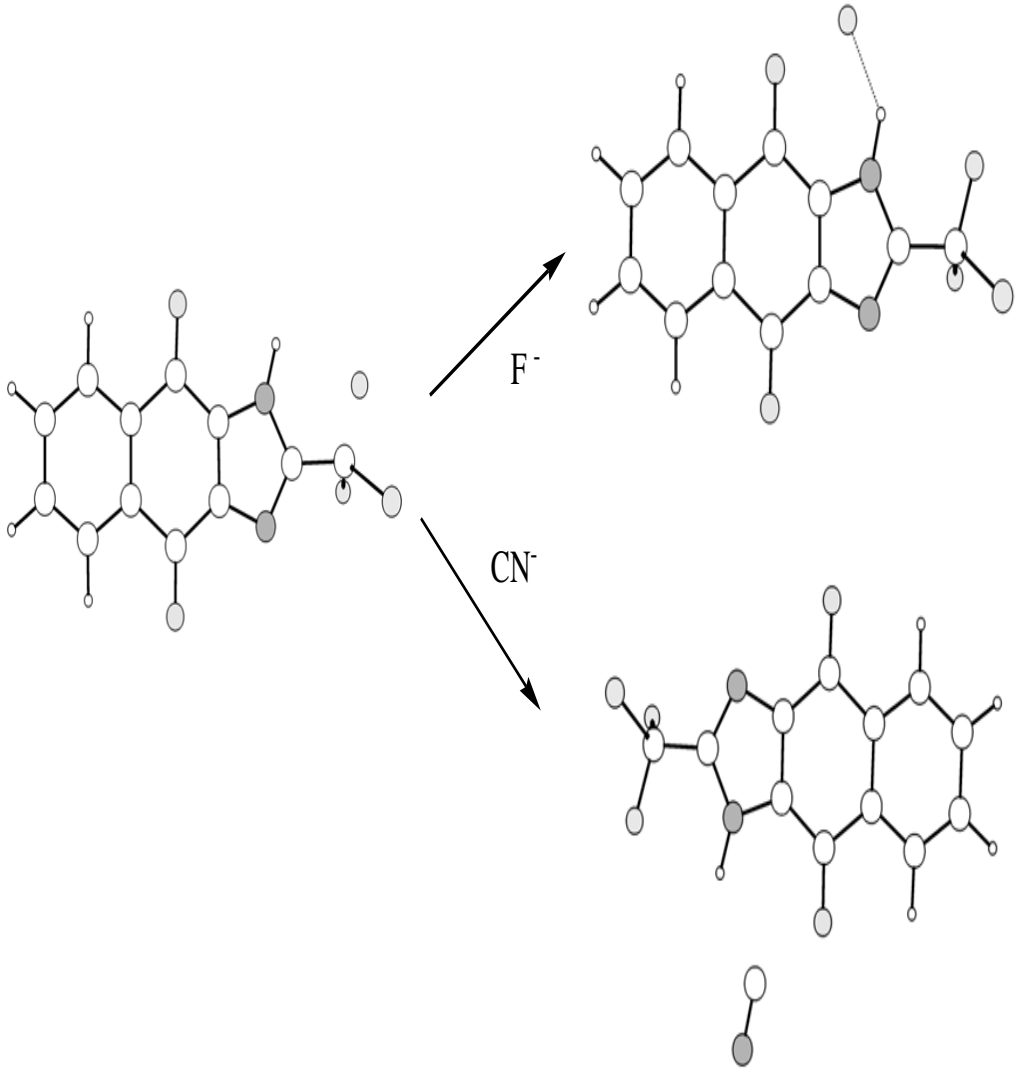
Optimized structure for 2e, 2e-F and 2e-CN



Optimized structure for 2f, 2f-F and 2f-CN



Optimized structure for 2g, 2g-F and 2g-CN



Optimized structure for 2h, 2h-F and 2h-CN

Figure S4. Optimized structure for (2a-h)f, and their F^- and CN^- complexes.

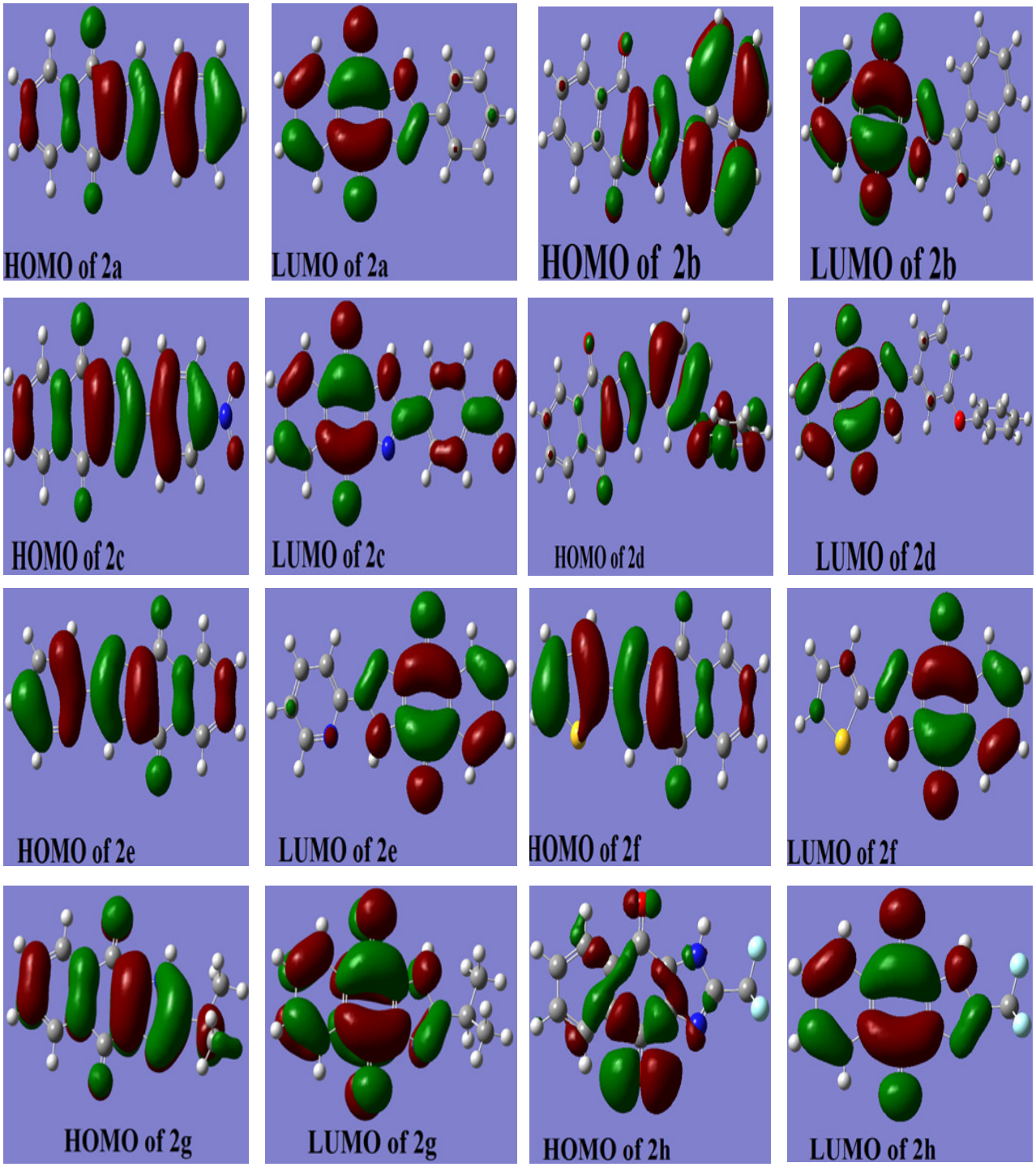


Figure S5. HOMO –LUMO for 2a-h.

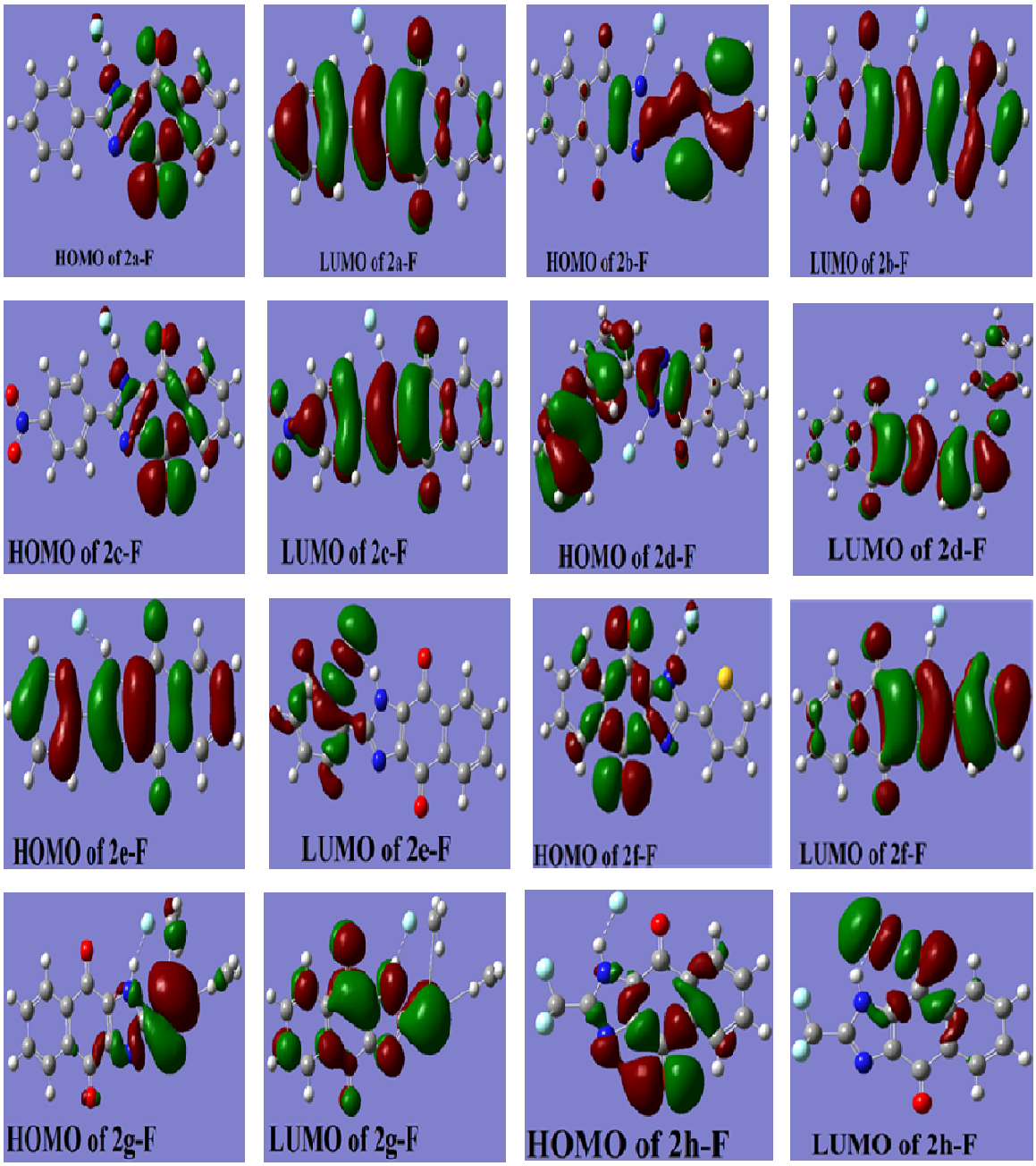


Figure S6. HOMO- LUMO for (2a-h)-F^- complexes.

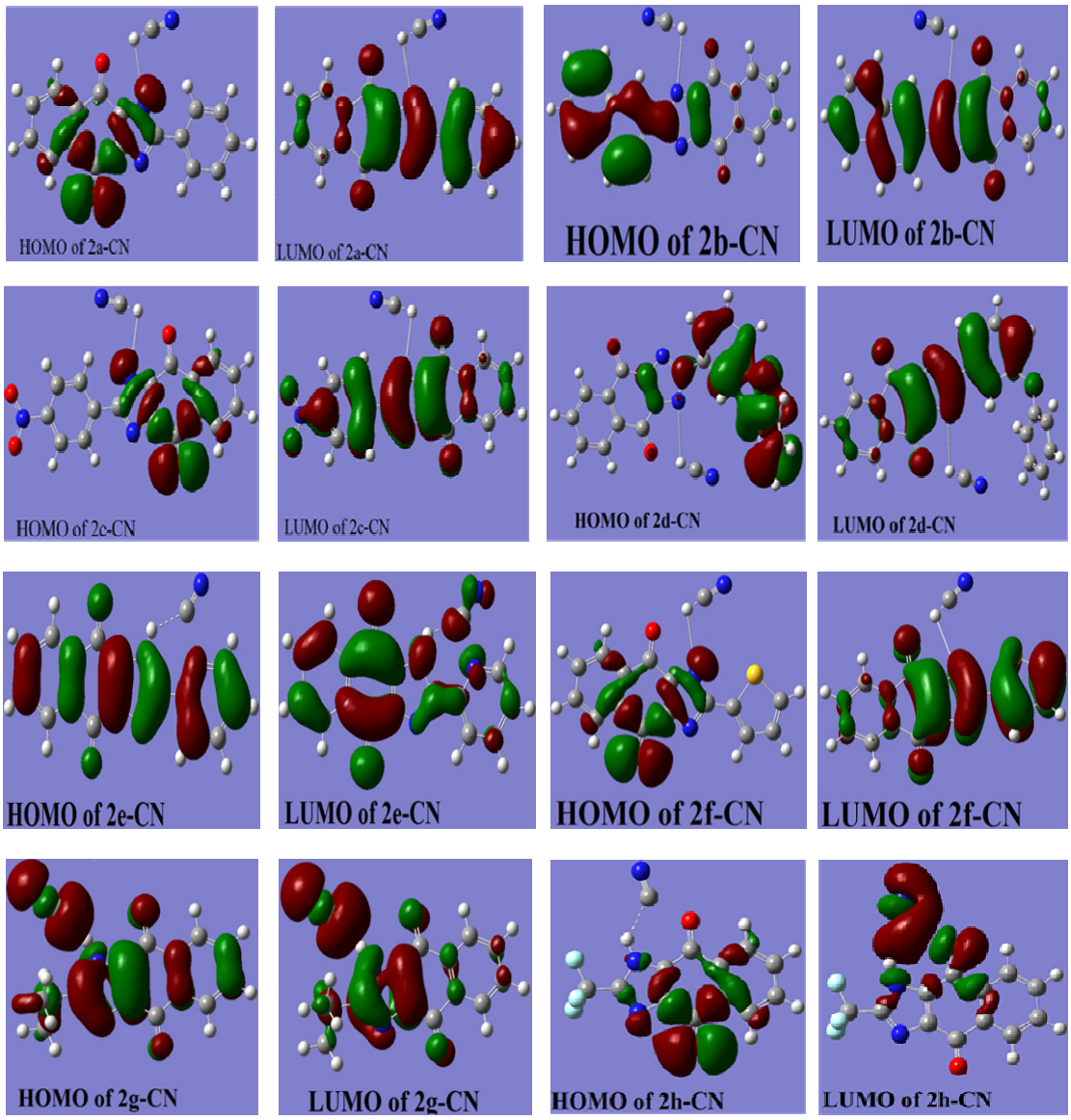
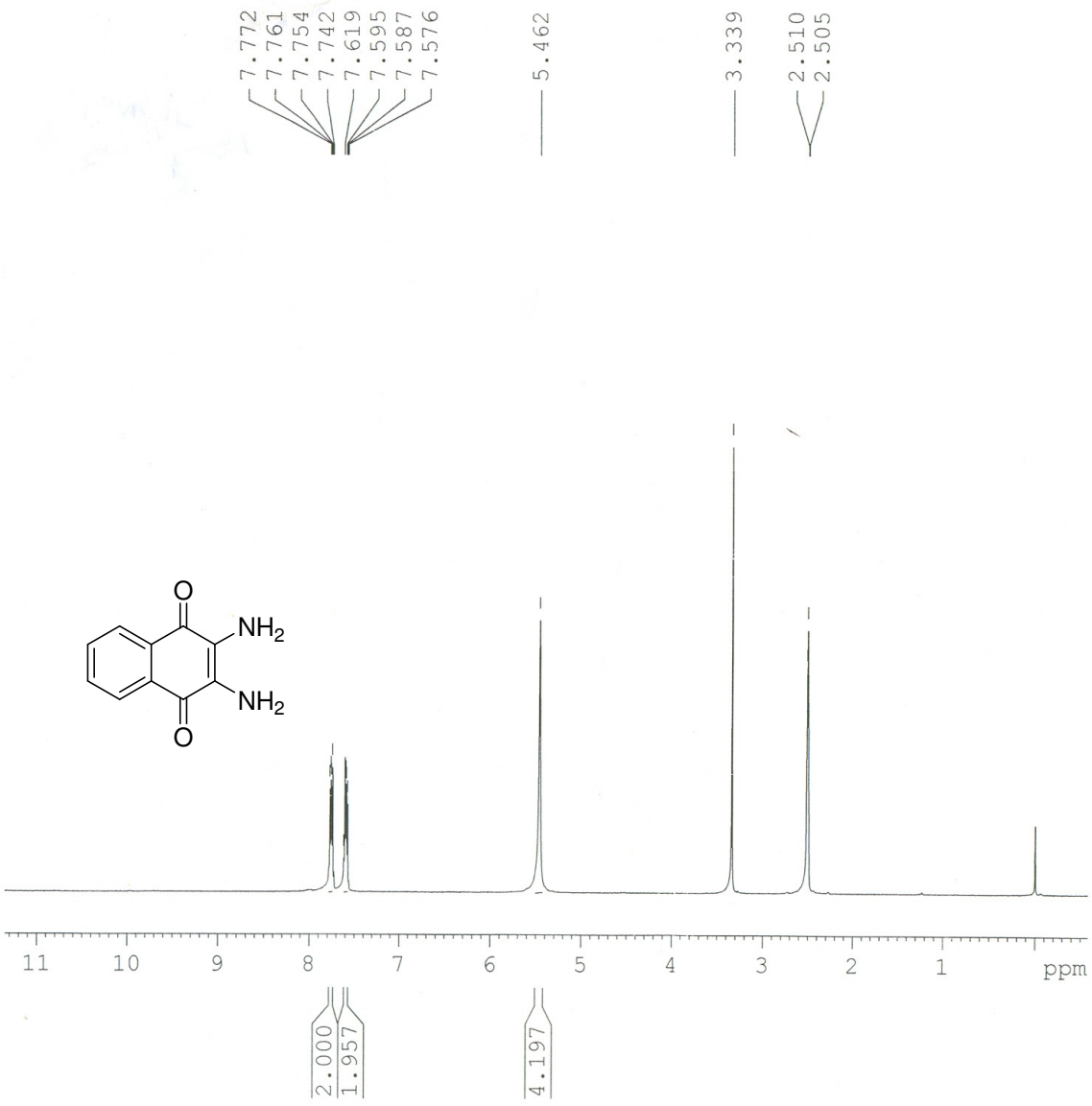
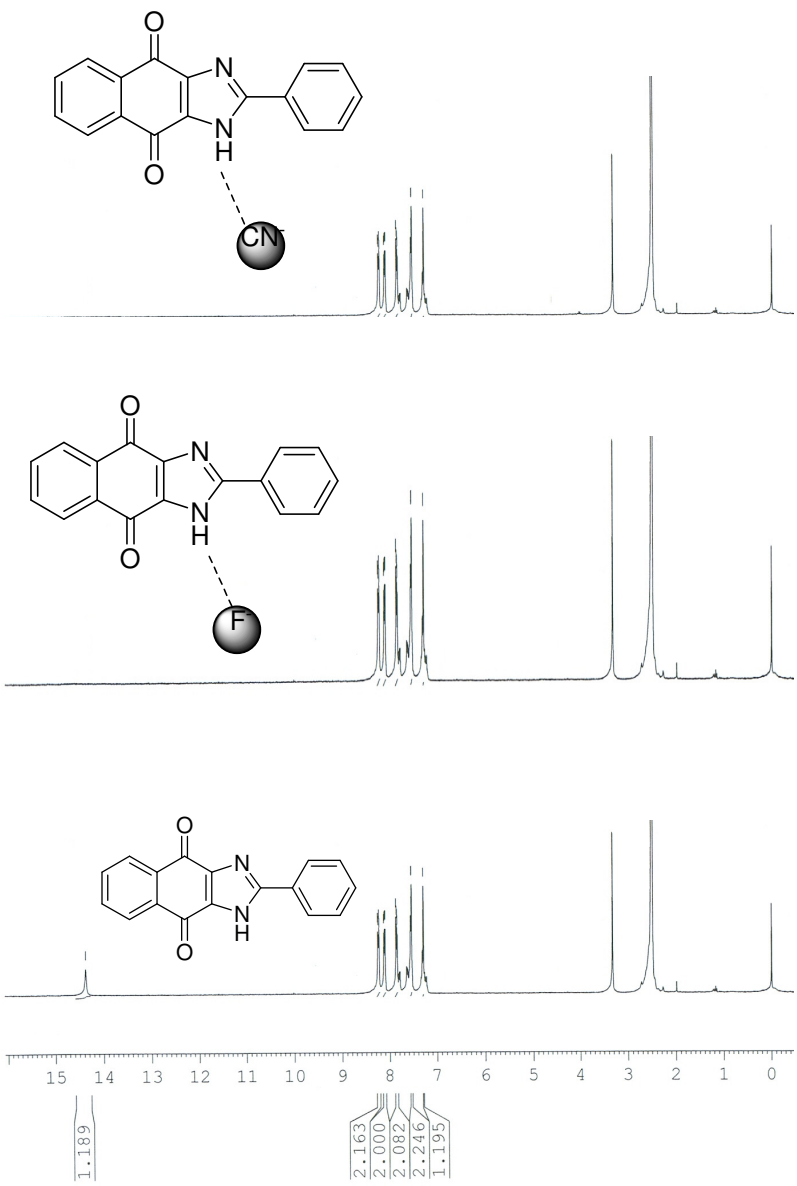


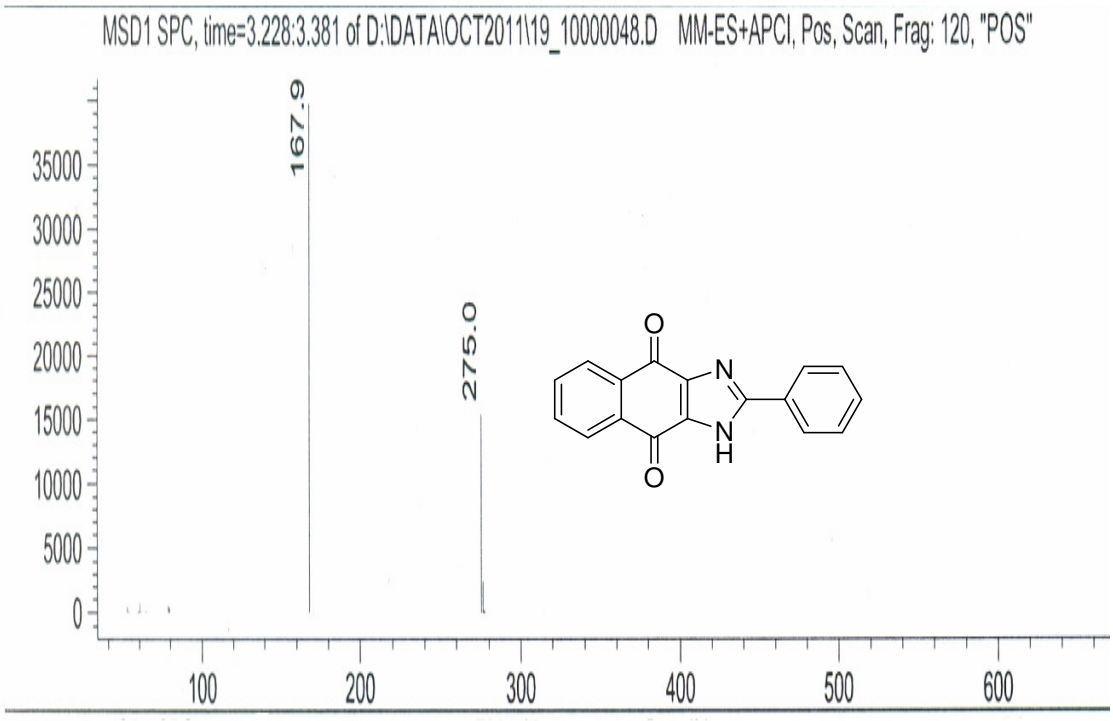
Figure S7. HOMO- LUMO for (2a-h)-CN^- complexes.



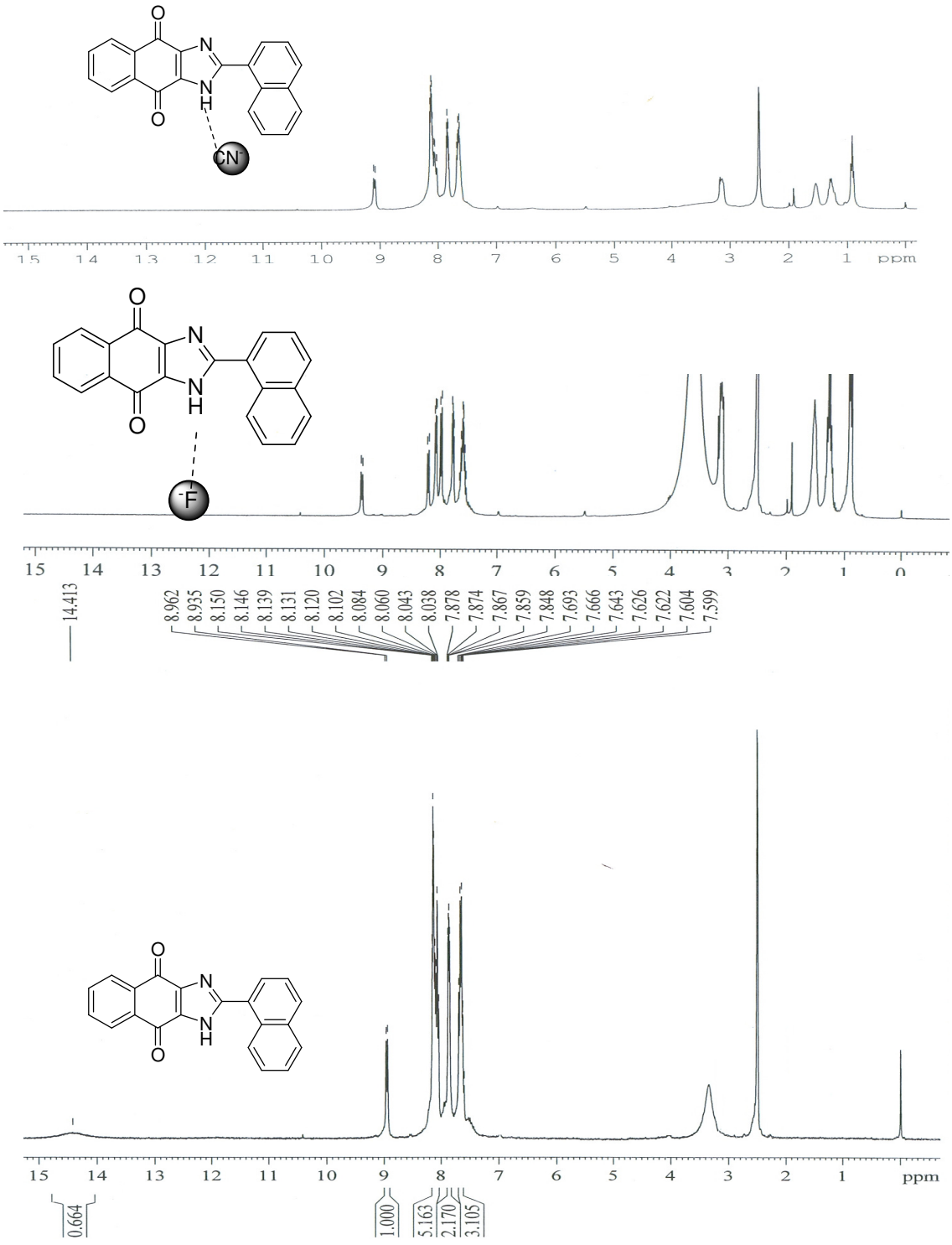
^{1}H NMR for**1**



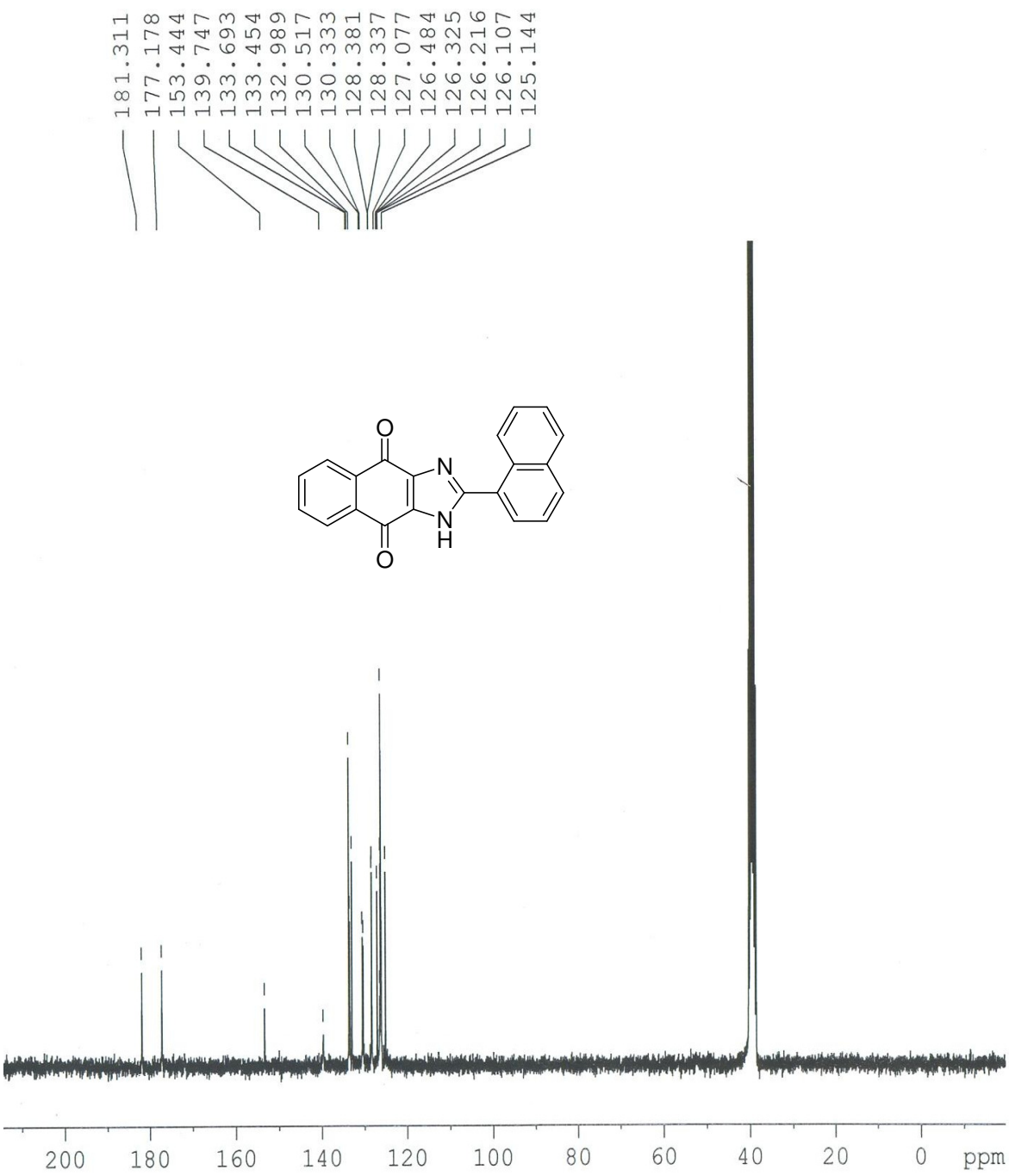
^{1}H NMR for 2a, 2a-F^{-} and 2a -CN^{-}



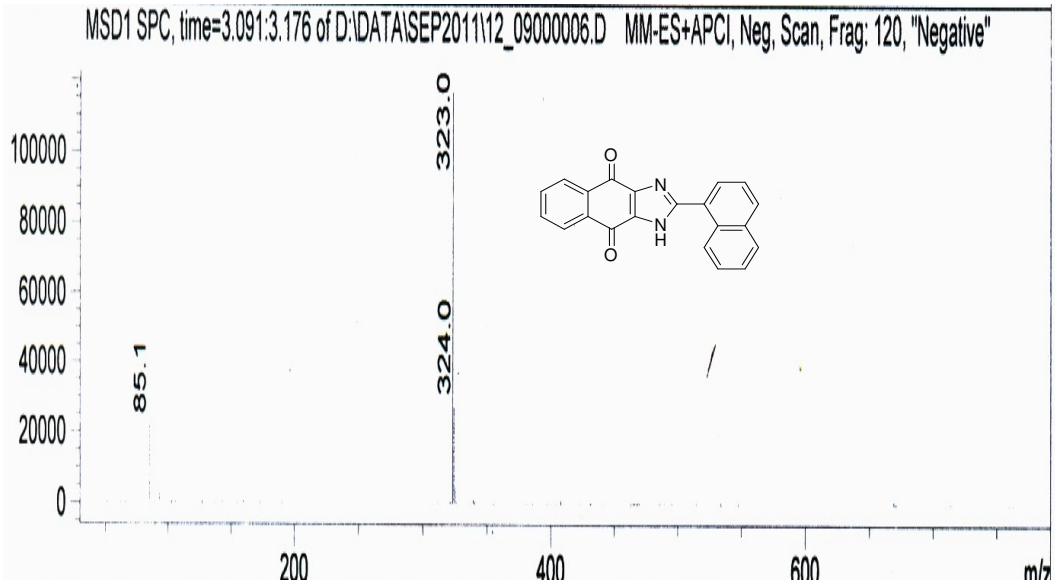
LCMS for 2a



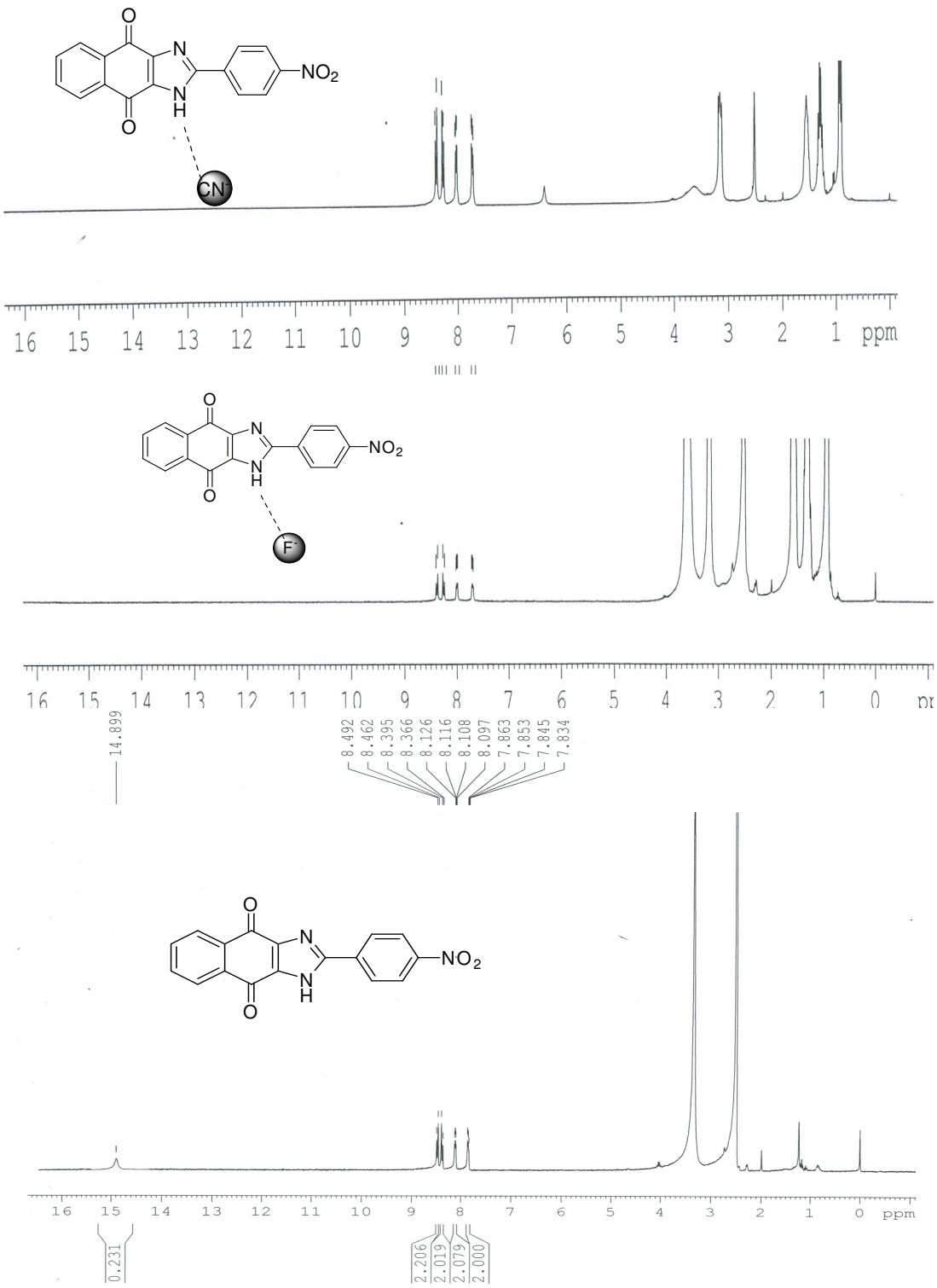
^{1}H NMR for 2b, 2b-F^{-} and 2b -CN^{-}



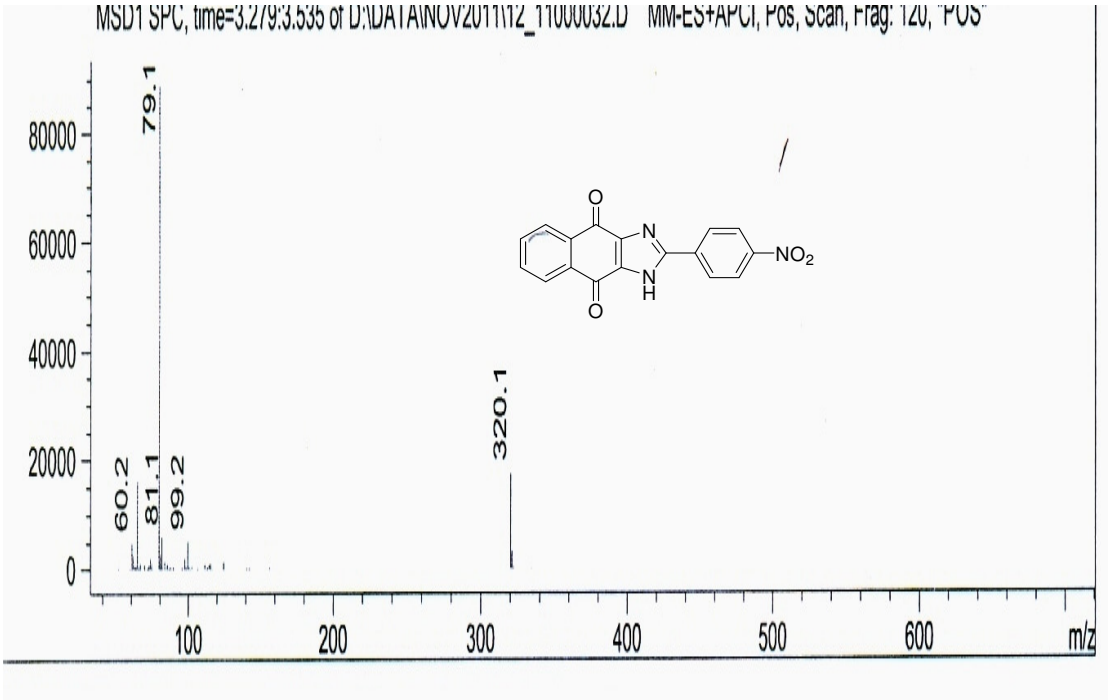
^{13}C NMR for2b



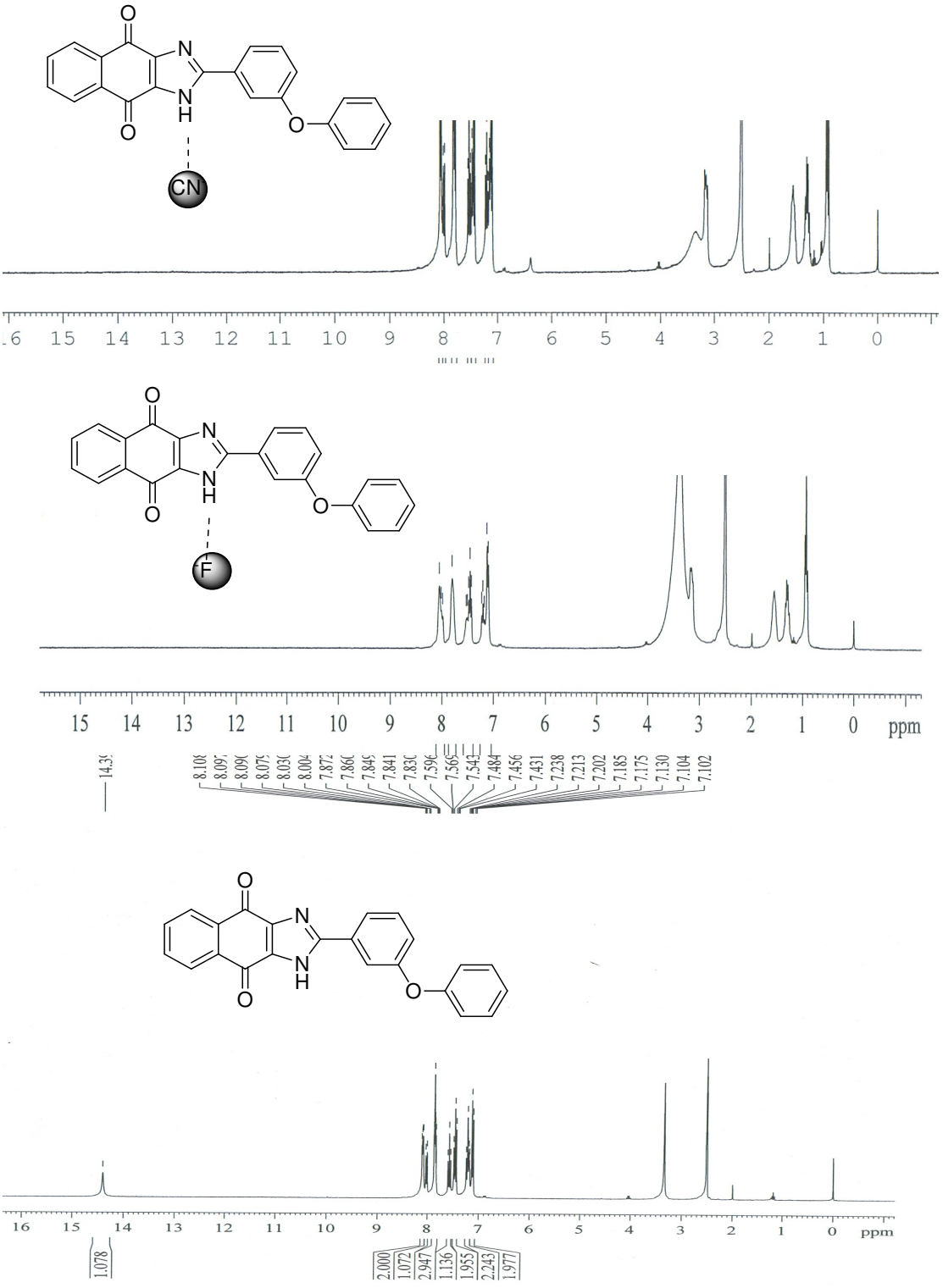
LCMS for 2b



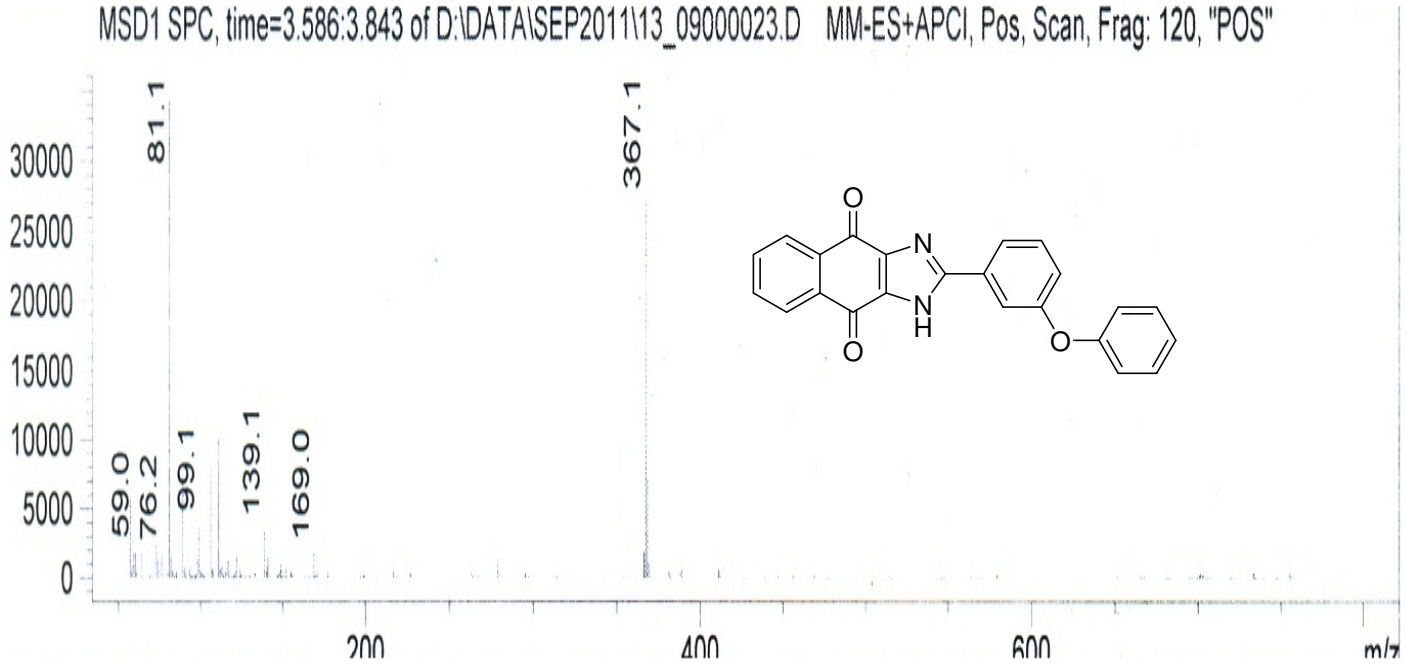
^{1}H NMR for 2c, 2c-F^{-} and 2c -CN^{-}



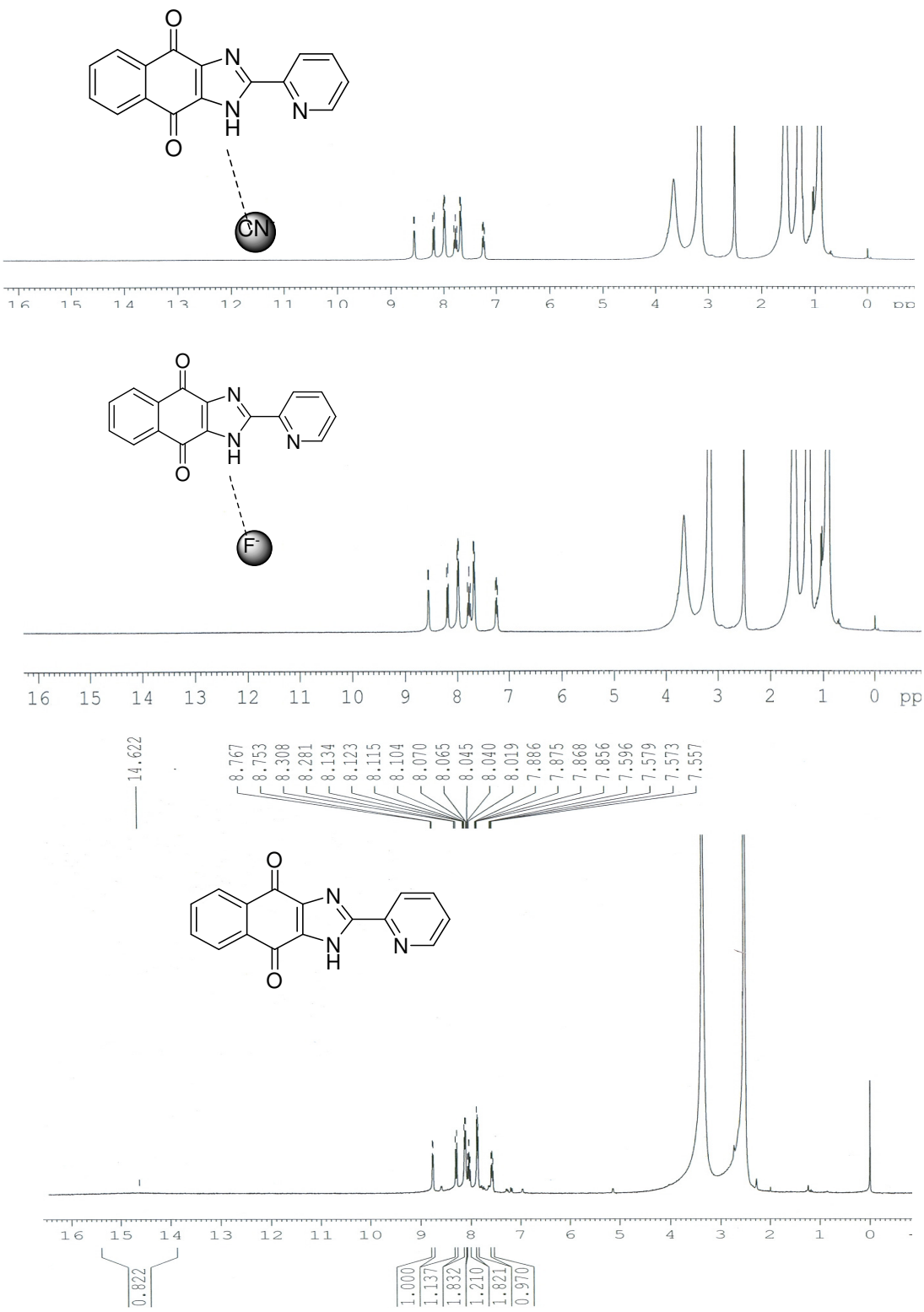
LCMS for 2c



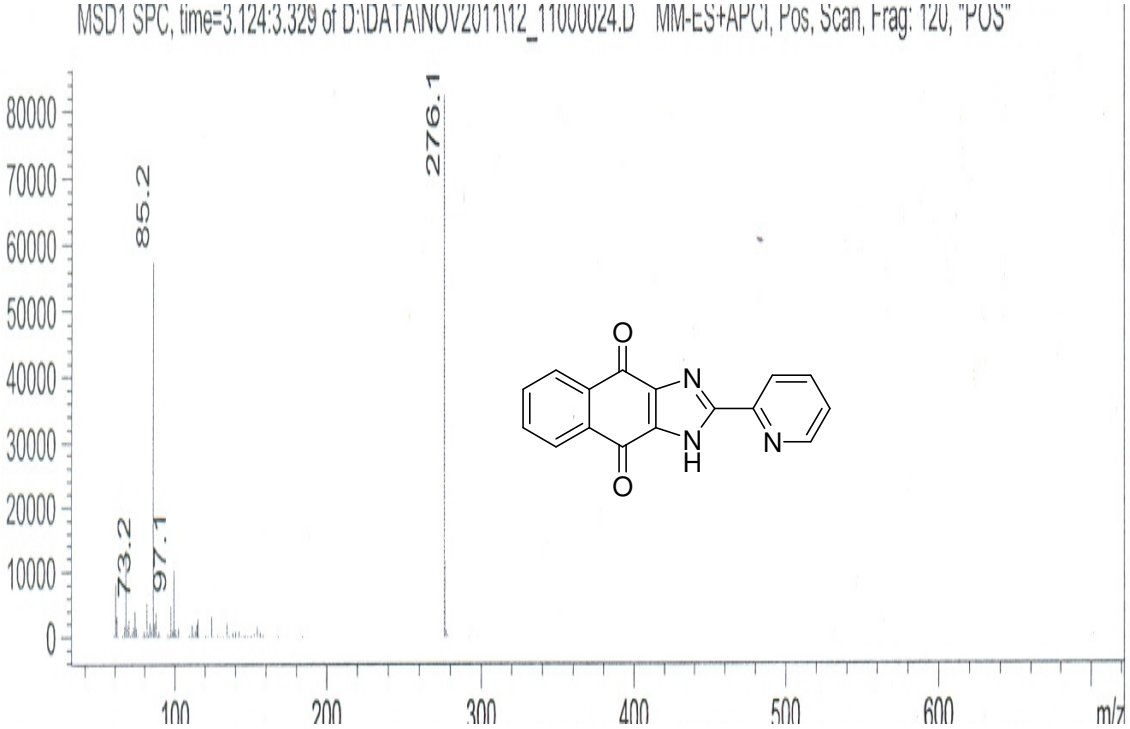
^{1}H NMR for 2d, 2d-F^{-} and 2d -CN^{-}



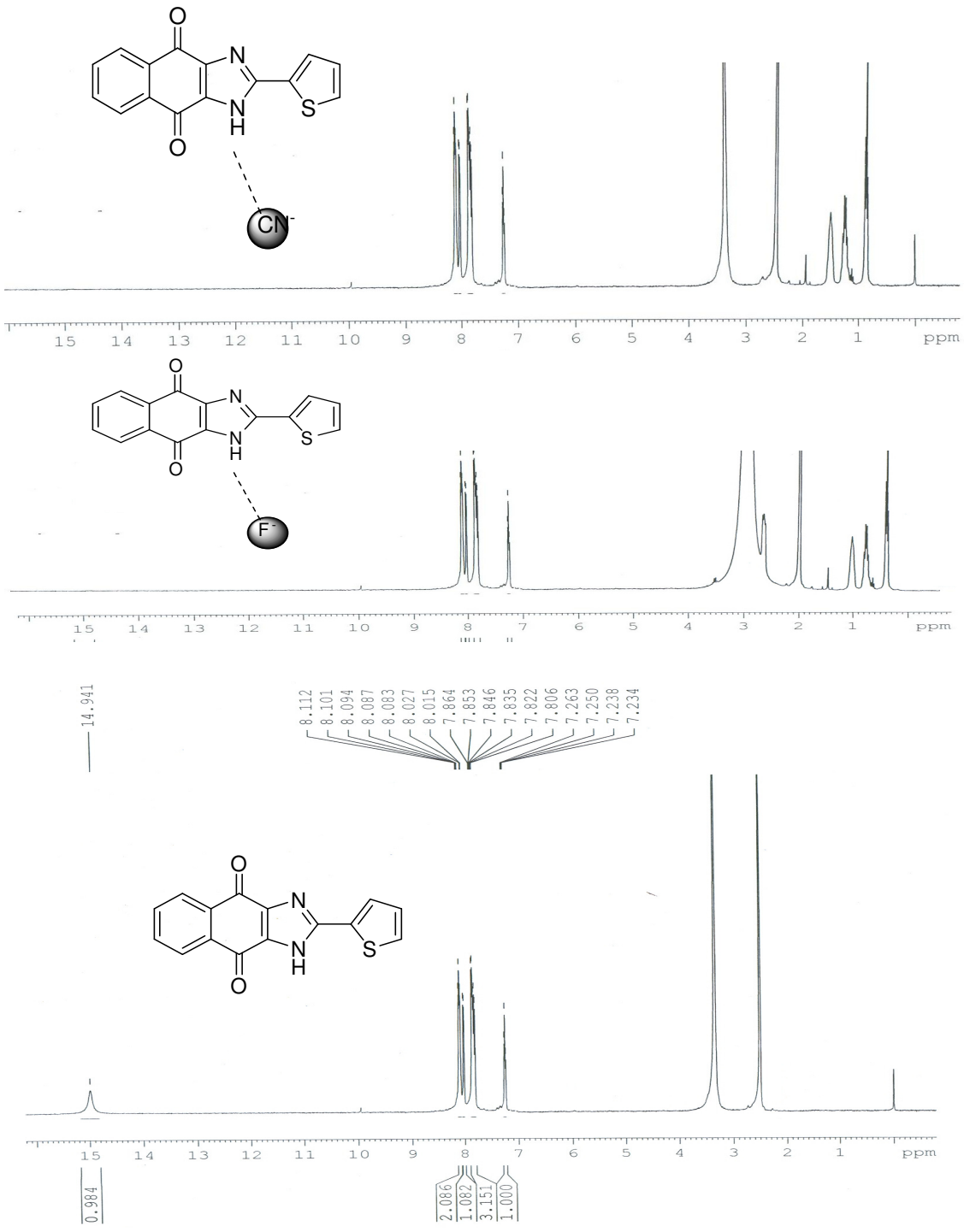
LCMS for 2d



^{1}H NMR for 2e, 2e-F^{-} and 2e -CN^{-}

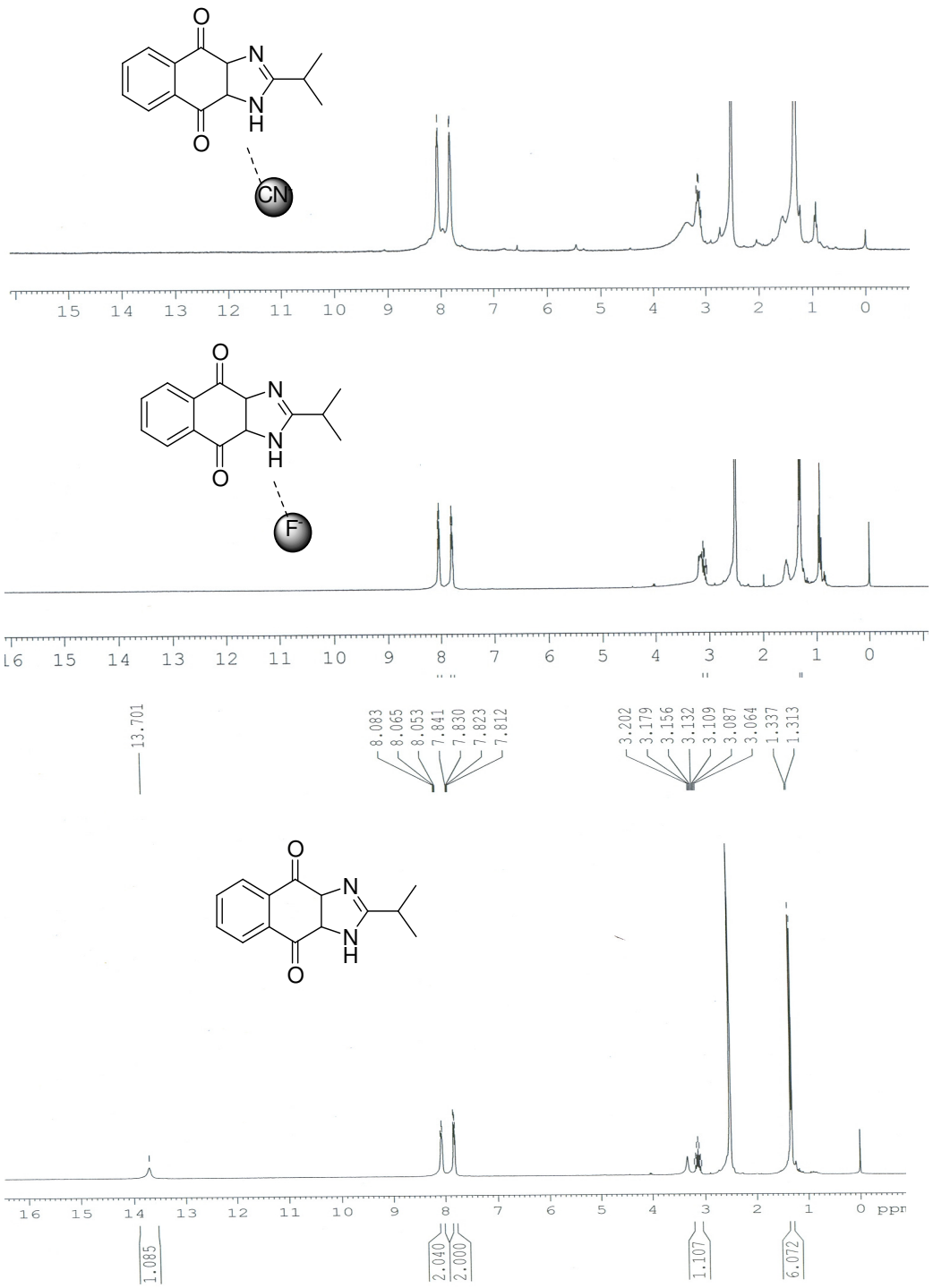


LCMS for 2e

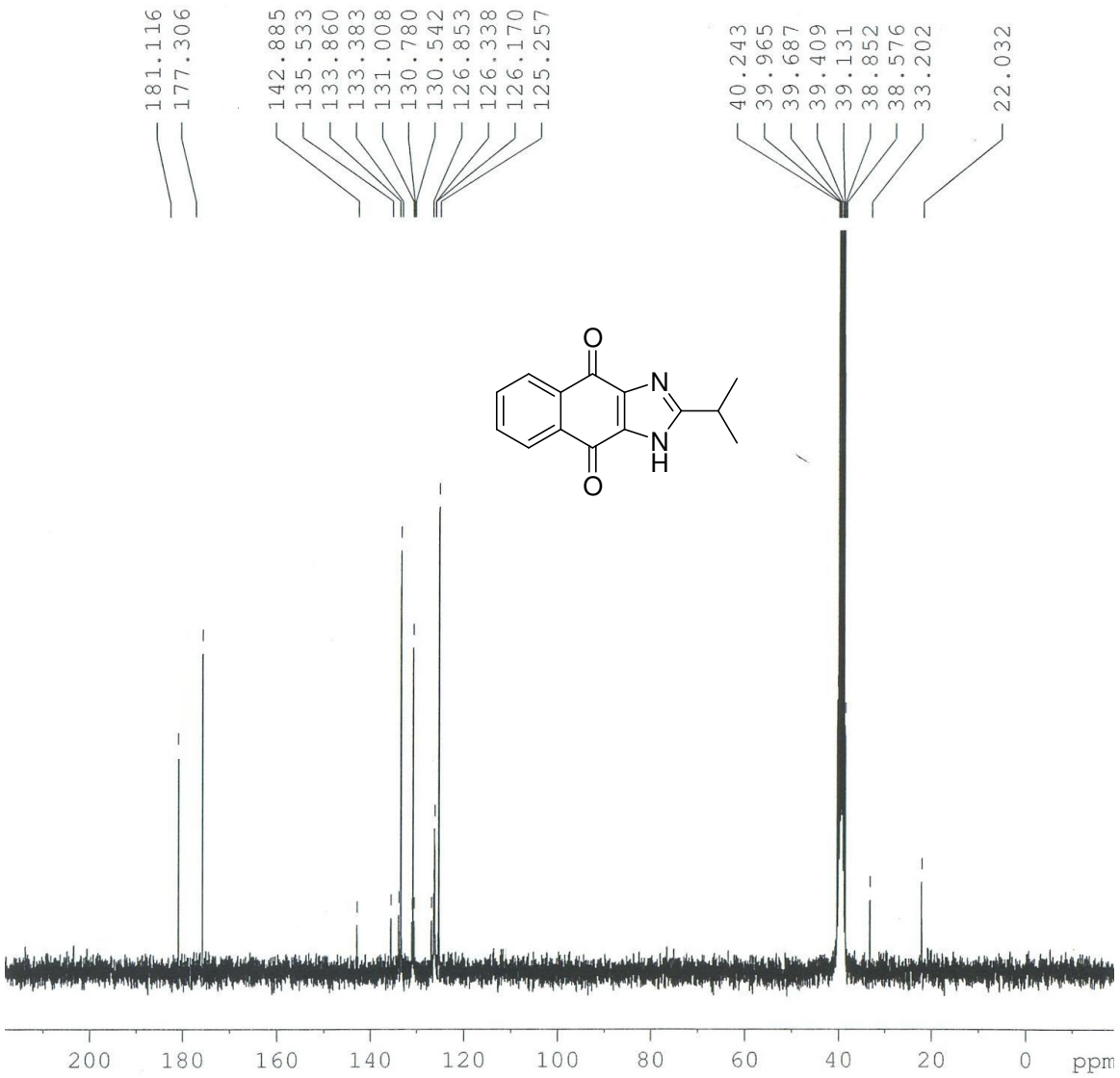


^{1}H NMR for 2f, 2f-F^{-} and 2f -CN^{-}

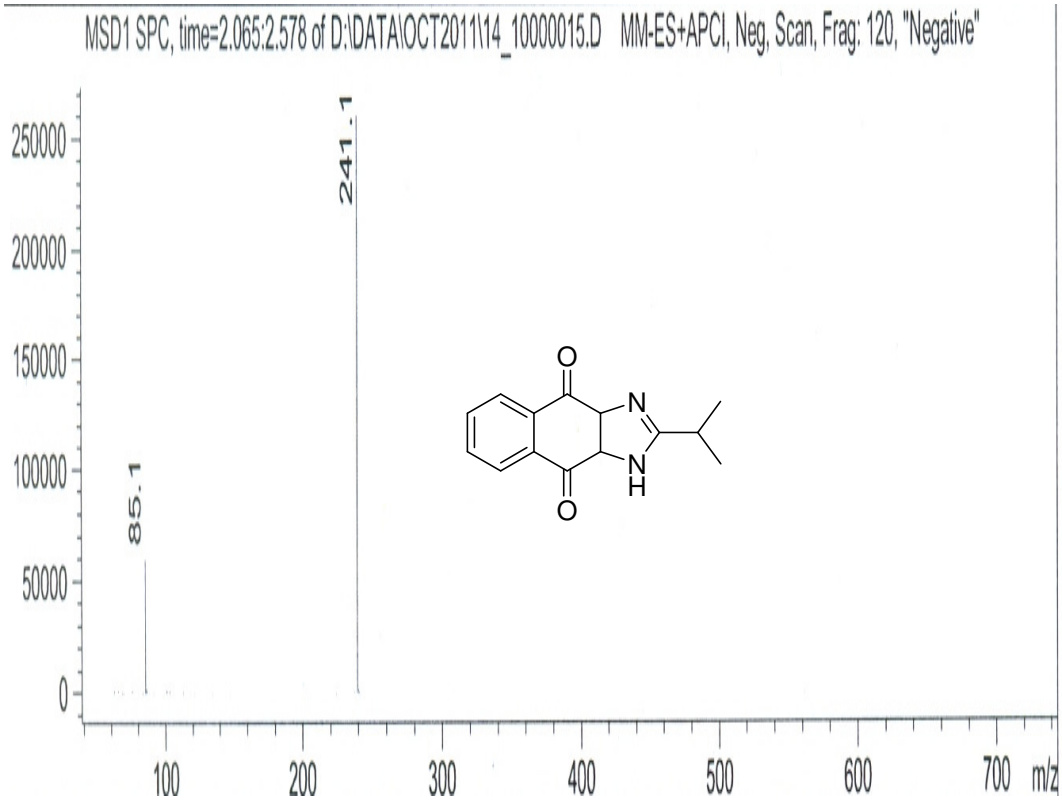
LCMS for 2f



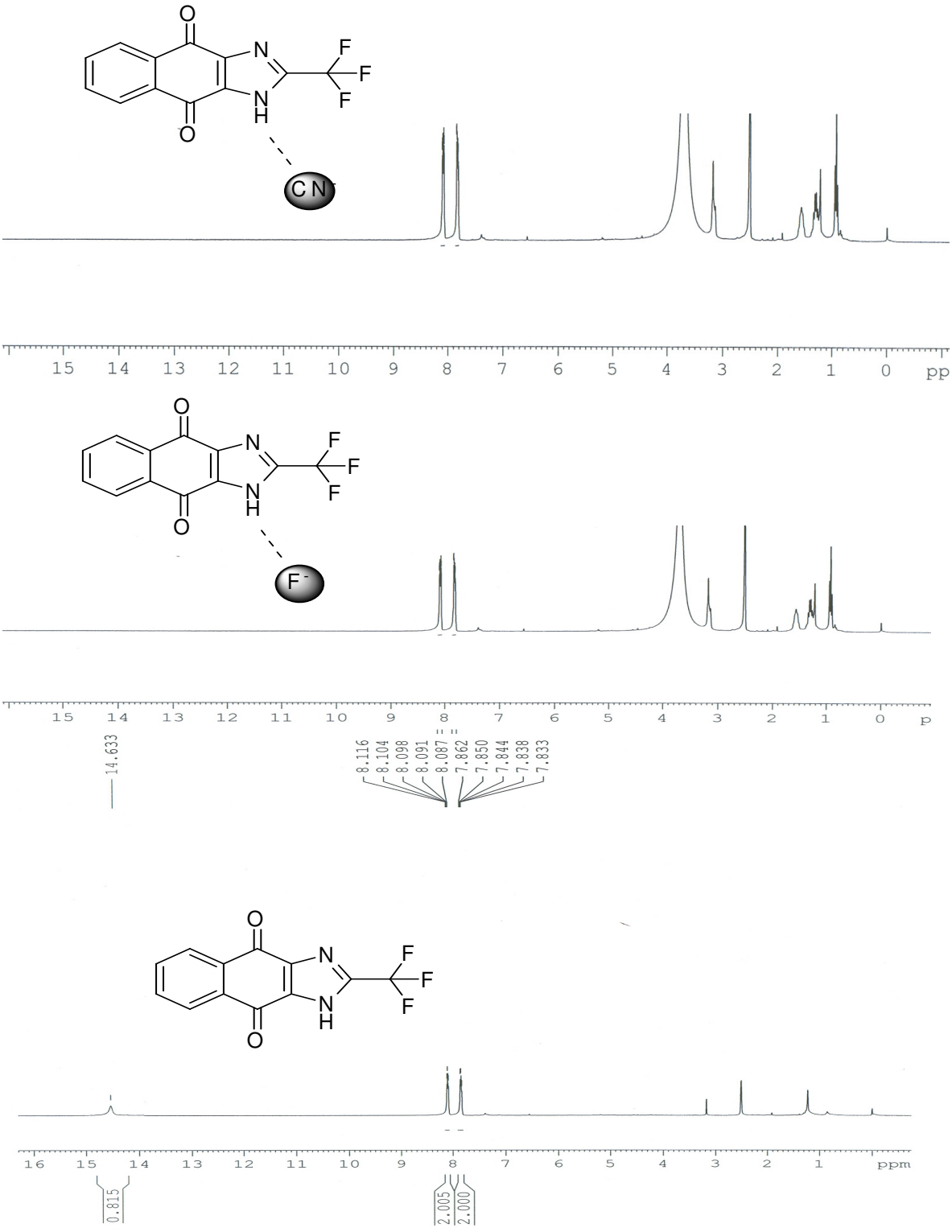
^{1}H NMR for 2g, 2g-F^{-} and 2g -CN^{-}



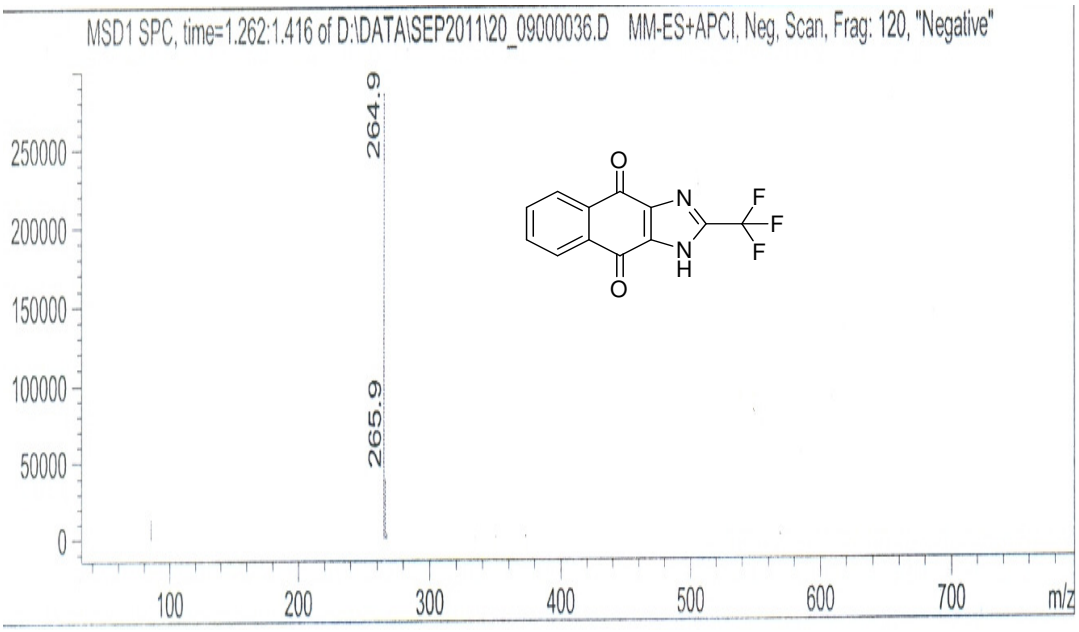
^{13}C NMR for 2g



LCMS for 2g



^{1}H NMR for 2h, 2h-F^{-} and 2h -CN^{-}



LCMS for 2h

Synthesis of 2-phenyl-1H-naphtho[2,3-d]imidazole-4,9-dione (2a).[41]

A mixture of compound **1** (0.5 g, 2.65 mmol) and benzaldehyde (0.280g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 6 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a yellow solid (0.626 g, yield =85%).

Synthesis of 2-(naphthalen-1-yl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2b).

A mixture of compound **1** (0.5 g, 2.65 mmol) and 1-naphthaldehyde (0.4134 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 6 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a yellow solid (0.7916 g, yield =91%).

Synthesis of 2-(4-nitrophenyl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2c).

A mixture of compound **1** (0.5 g, 2.65 mmol) and 4-nitro benzaldehyde (0.4015 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 8 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a greenish yellow solid (0.6926 g, yield = 81%).

Synthesis of 2-(3-phenoxyphenyl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2d).

A mixture of compound **1** (0.5 g, 2.65 mmol) and 3-phenoxybenzaldehyde (0.5247 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 12 h. After cooling to room temperature, the precipitate obtained from the reaction mixture was filtered through

a filter paper and washed with cold ethanol to get the pure product as a brown solid (0.8012 g, yield =82%).

Synthesis of 2-(pyridin-2-yl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2e).

A mixture of compound **1** (0.5 g, 2.65 mmol) and pyridine 2-carbaldehyde (0.2836 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 4 h. After colling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a yellow solid (0.6210 g, yield =85%).

Synthesis of 2-(thiophen-2-yl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2f).

A mixture of compound **1** (0.5 g, 2.65mmol) and thiophene-2-carbaldehyde (0.2968 g, 2.65 mmol) in DMSO (5 mL) was heated at 90º C with stirring for 5 h. After colling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a dark redish brown solid (0.6175 g, yield =83%).

Synthesis of 2-isopropyl-1H-naphtho[2,3-d]imidazole-4,9-dione (2g).

A mixture of compound 1 (0.5 g, 2.65 mmol) and isobutyraldehyde (0.1909 g, 2.65mmol) in DMSO (5 mL) was heated at 70º C with stirring for 12 h. After colling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a dark redish brown solid (0.410 g, yield =64%).

Synthesis of 2-(trifluoromethyl)-1H-naphtho[2,3-d]imidazole-4,9-dione (2h).

A mixture of compound 1 (0.5 g, 2.65mmol) in trifluoro aceticacid (2mL) was heated at

100º C with stirring for 12 h. After colling to room temperature, the precipitate obtained from the reaction mixture was filtered through a filter paper and washed with cold ethanol to get the pure product as a dark brown solid (0.5039 g, yield =71%).