

Pyrrolylamidourea based anion receptors

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Supplementary information

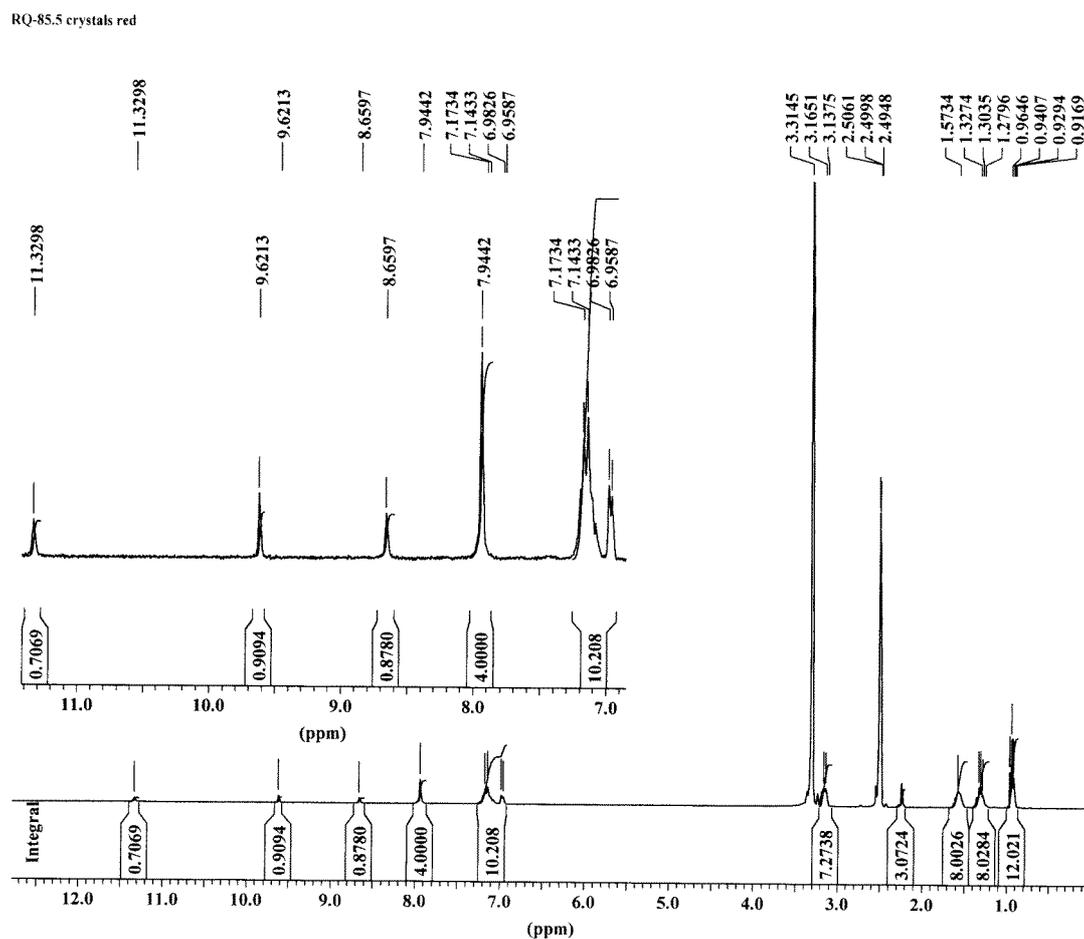


Figure S1 ^1H NMR spectra of the TBA salt of deprotonated compound 4 in $\text{DMSO-}d_6$.

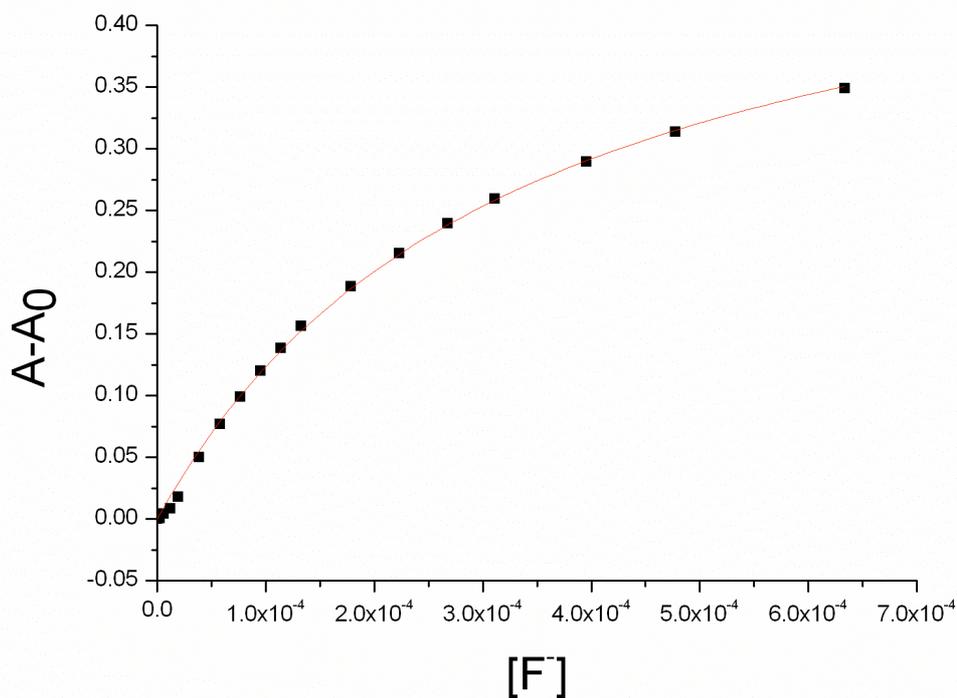
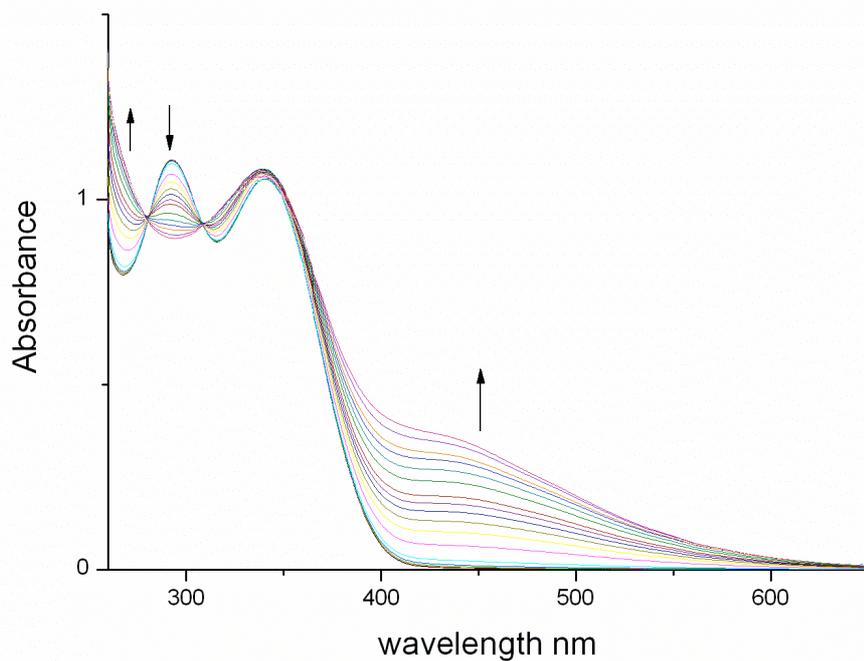


Figure S2 a) UV-vis absorption spectrophotometric titration of compound **2** with TBA fluoride in DMSO at 25 °C. b) Variation of absorbance at 390 nm versus concentration of anion. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B\times[G^-]/(1+(K\times[G^-]))$.

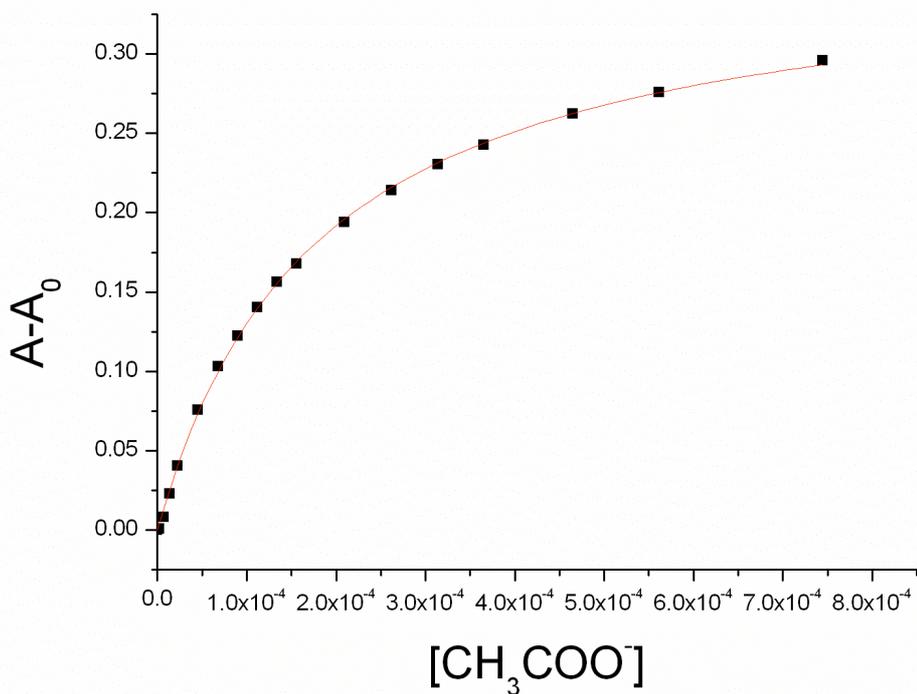
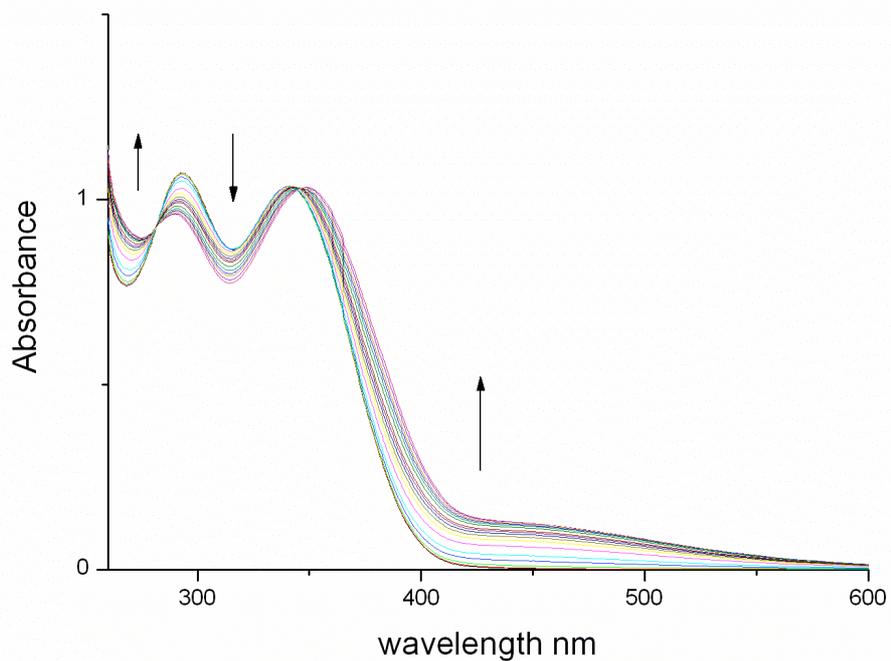


Figure S3 a) UV-vis absorption spectrophotometric titration of compound **2** with TBA acetate in DMSO at 25 °C. b) Variation of absorbance at 390 nm versus concentration of anion. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B\times[G^-]/(1+(K\times[G^-]))$

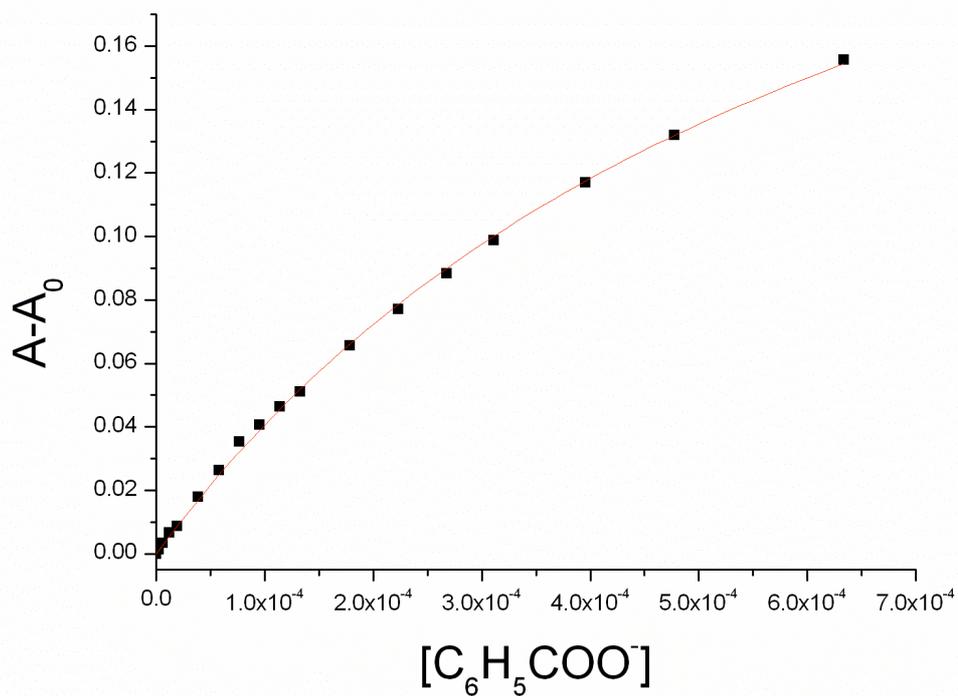
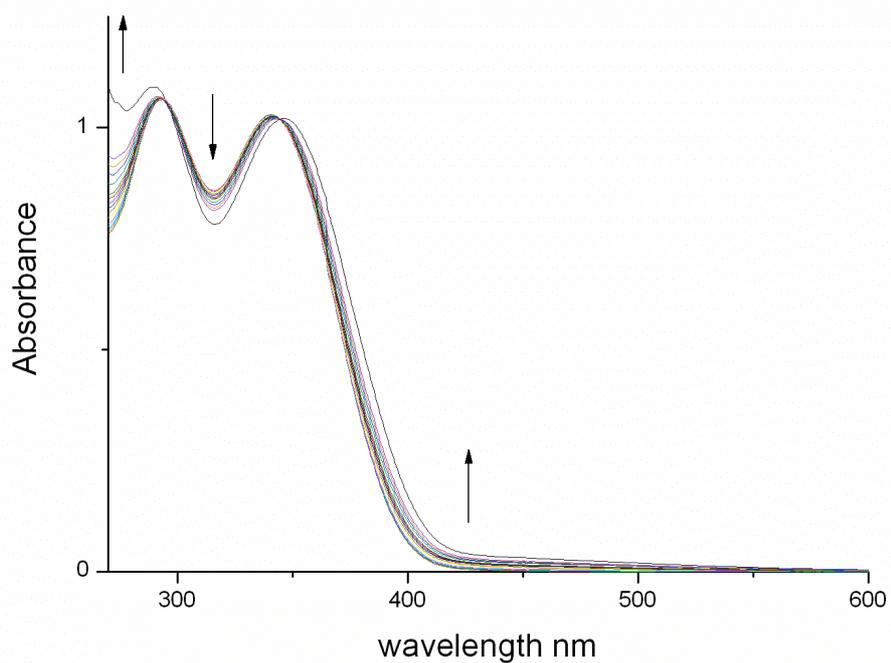


Figure S4 a) UV-vis absorption spectrophotometric titration of compound **2** with TBA benzoate in DMSO at 25 °C. b) Variation of absorbance at 390 nm versus concentration of anion. The trend line is the result of the non linear least-square fit of the experimental data according to $A - A_0 = B \times [G^-] / (1 + (K \times [G^-]))$

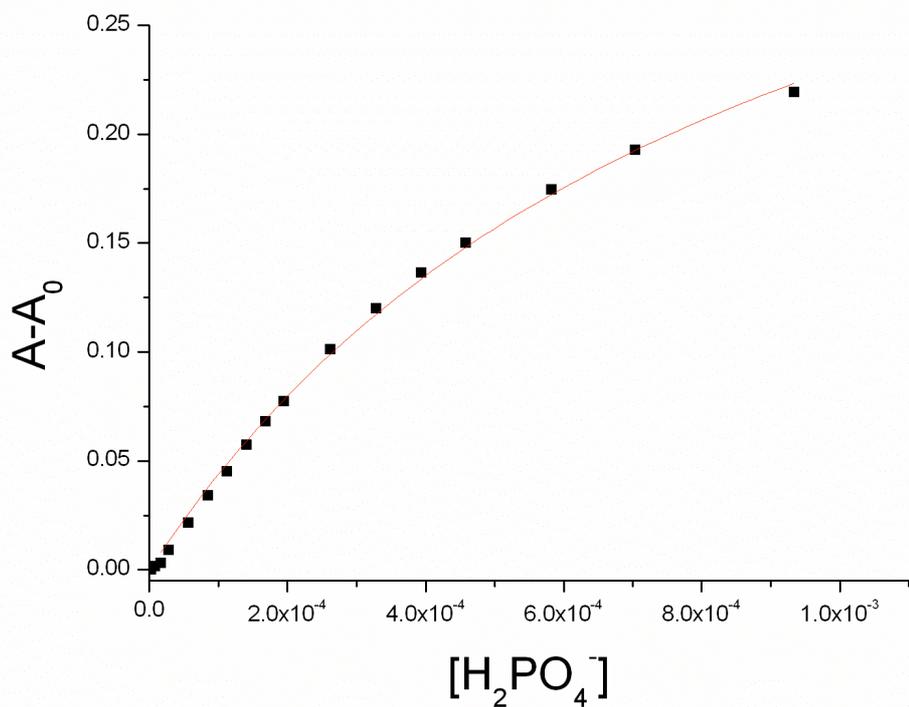
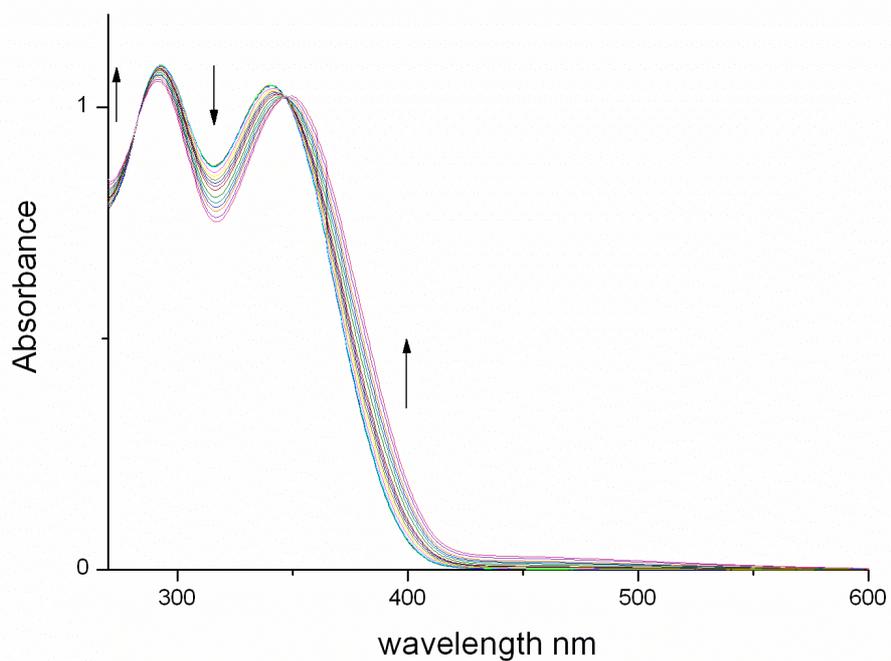


Figure S5 a) UV-vis absorption spectrophotometric titration of compound **2** with TBA dihydrogenphosphate in DMSO at 25 °C. b) Variation of absorbance at 390 nm versus concentration of anion. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B\times[G^-]/(1+(K\times[G^-]))$

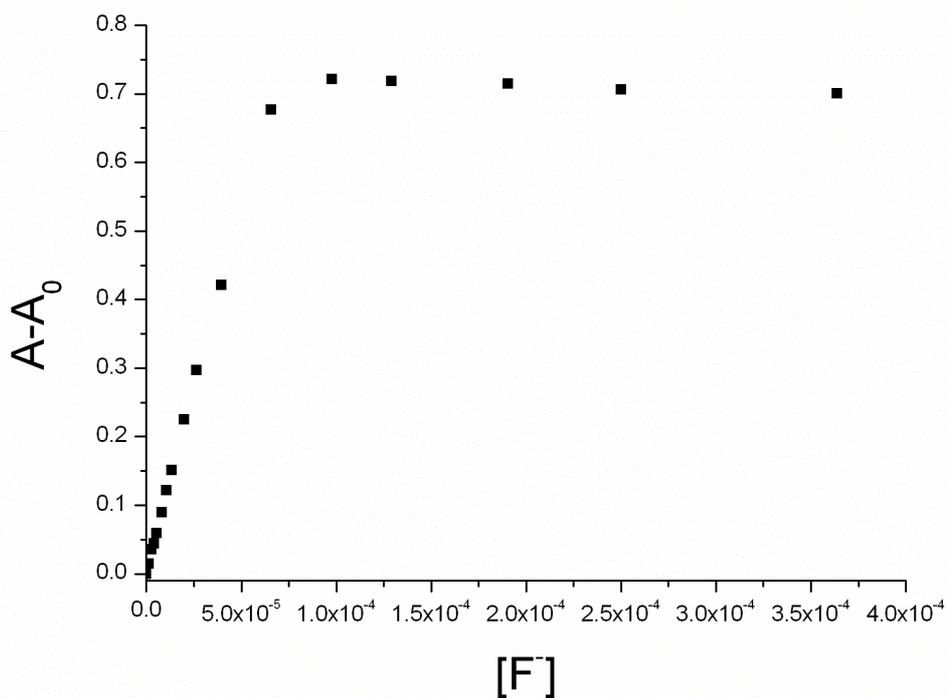
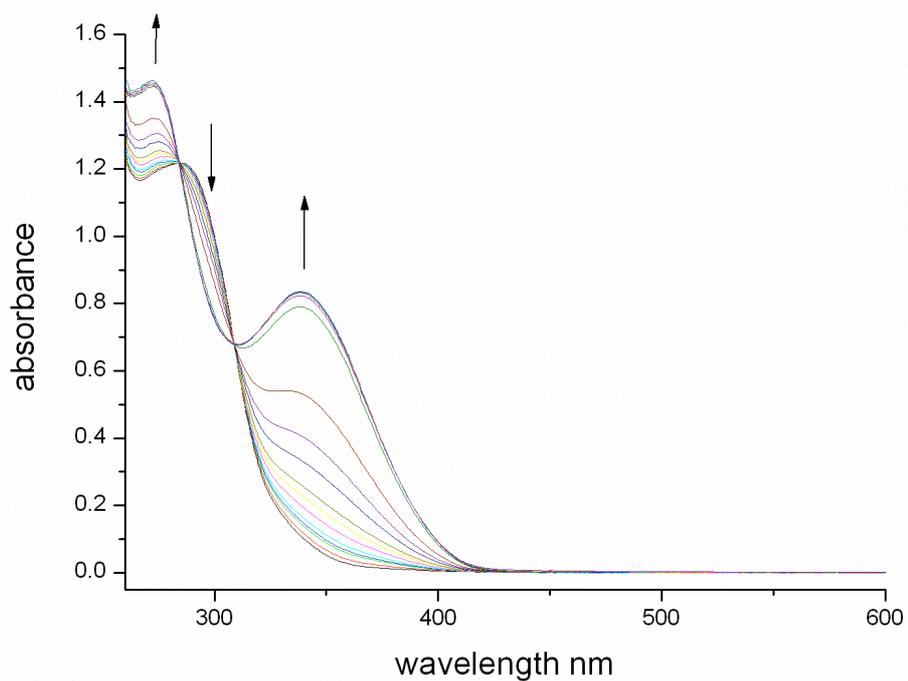


Figure S6 a) UV-vis absorption spectrophotometric titration of compound **3** with TBA fluoride in DMSO at 25 °C. b) Variation of absorbance at 360 nm versus concentration of anion.

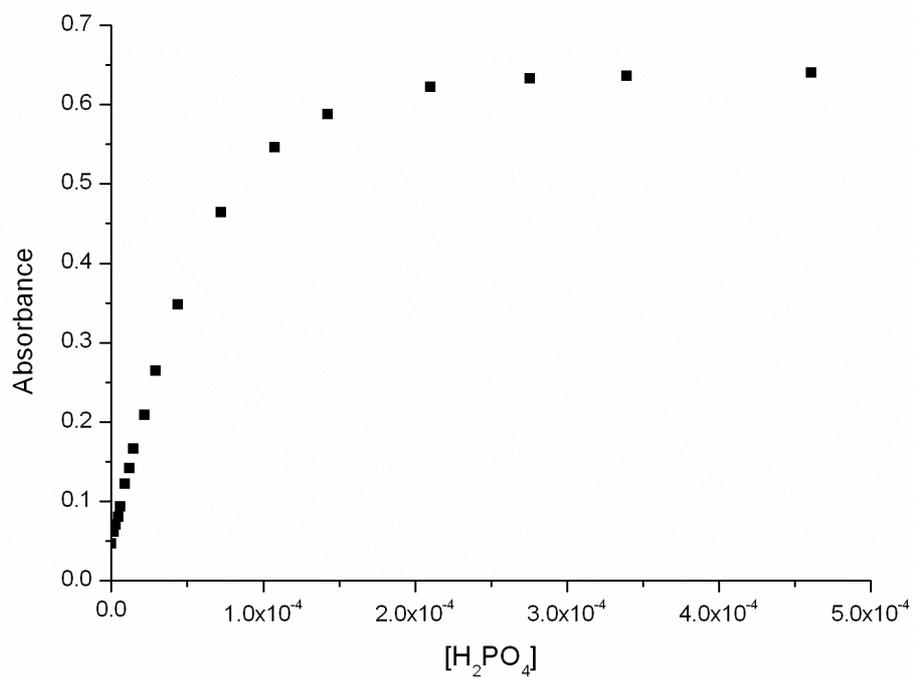
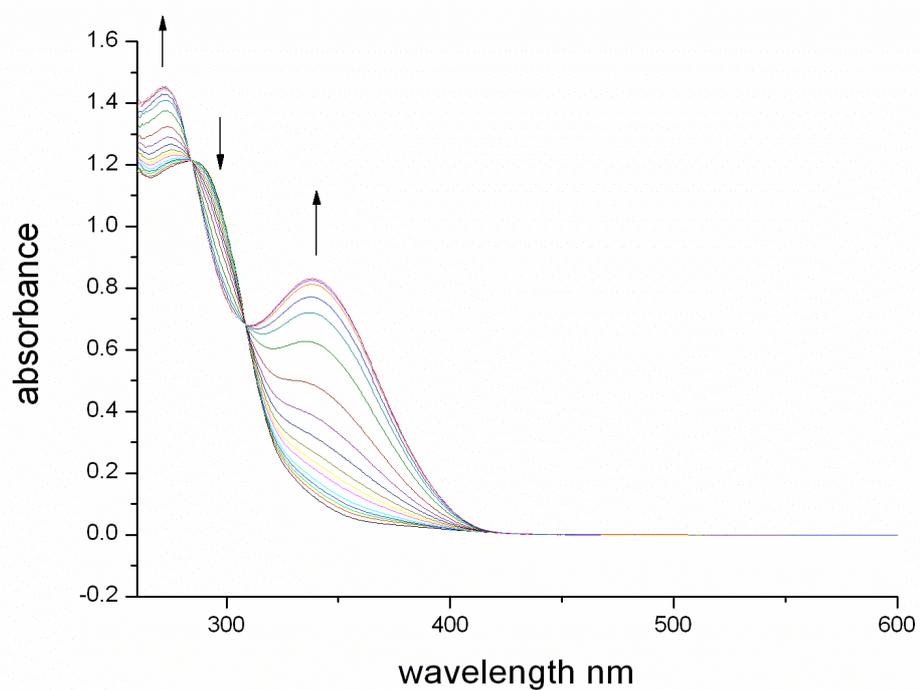


Figure S7 a) UV-vis absorption spectrophotometric titration of compound **3** with TBA dihydrogenphosphate in DMSO at 25 °C. b) Variation of absorbance at 360 nm versus concentration of anion.

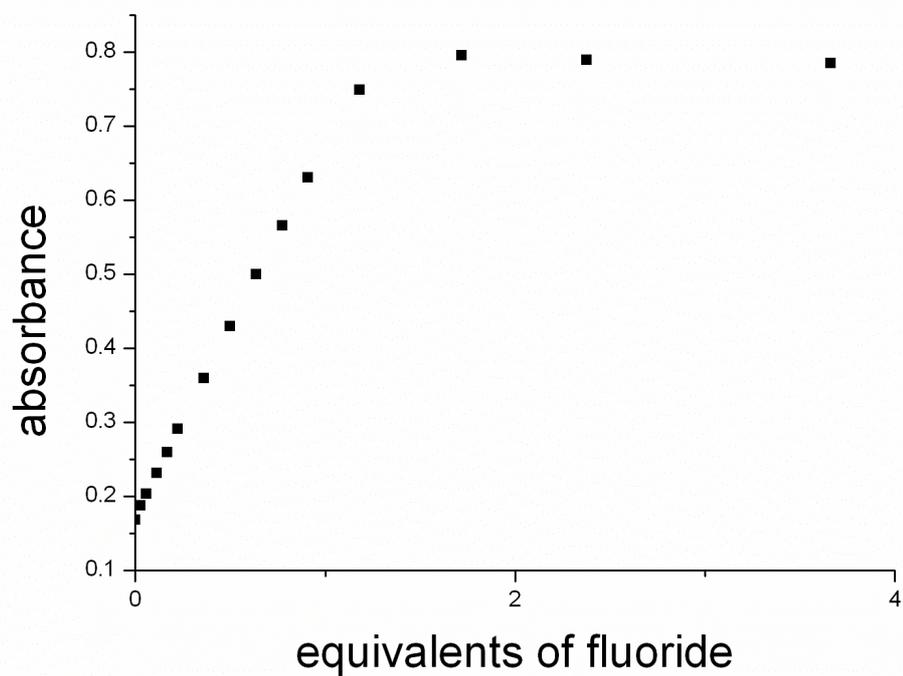
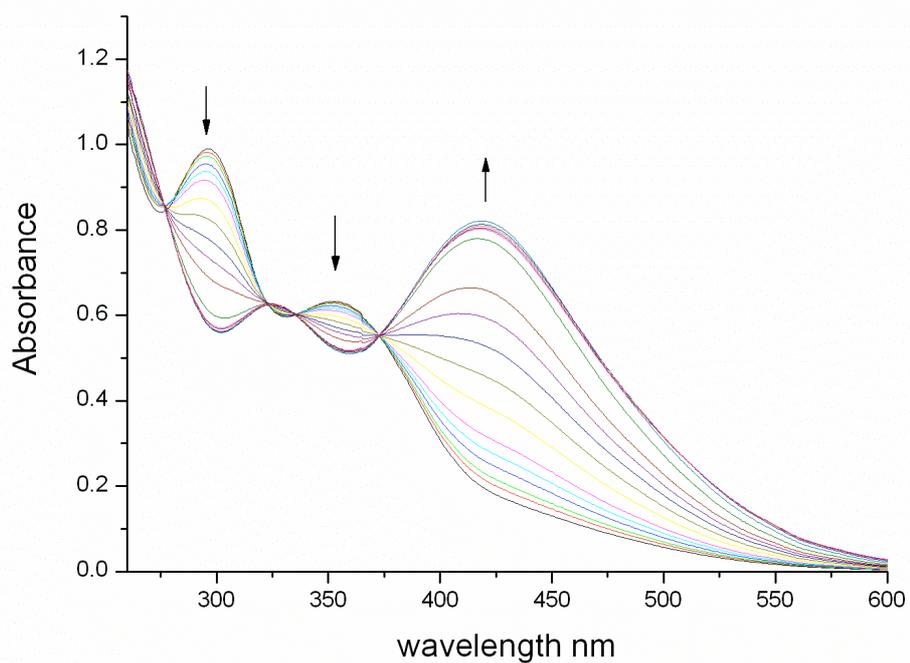


Figure S8 a) UV-vis absorption spectrophotometric titration of compound **4** with TBA fluoride in DMSO at 25 °C. b) Variation of absorbance at 360 nm versus equivalents of fluoride.

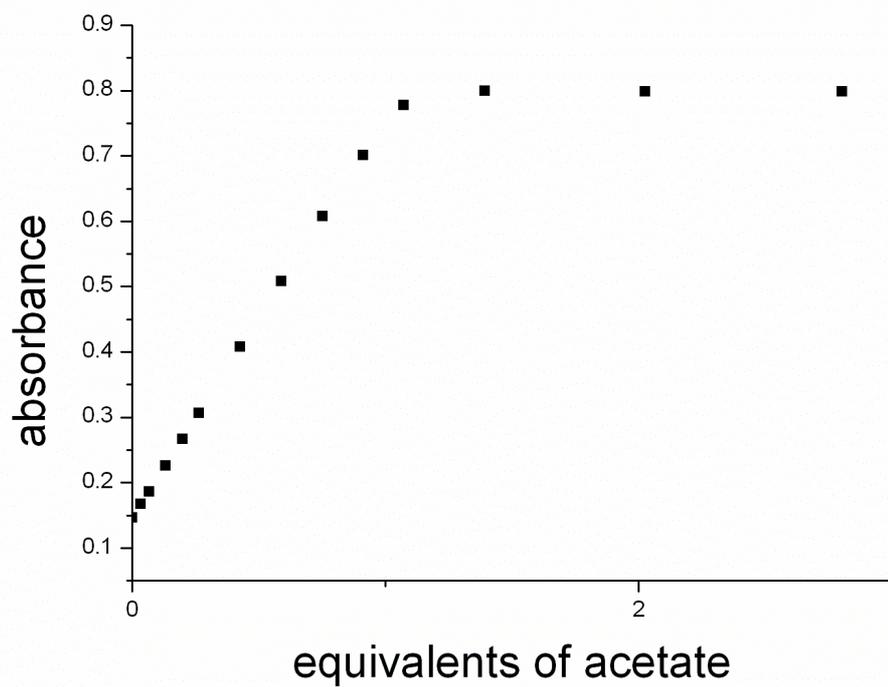
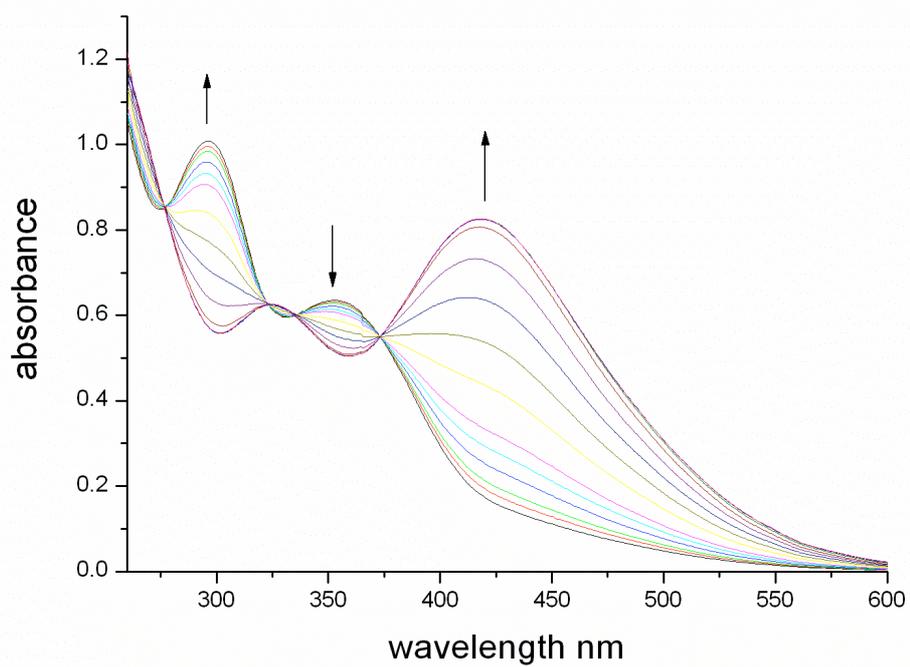


Figure S9 a) UV-vis absorption spectrophotometric titration of compound **4** with TBA acetate in DMSO at 25 °C. b) Variation of absorbance at 450 nm versus equivalents of acetate.

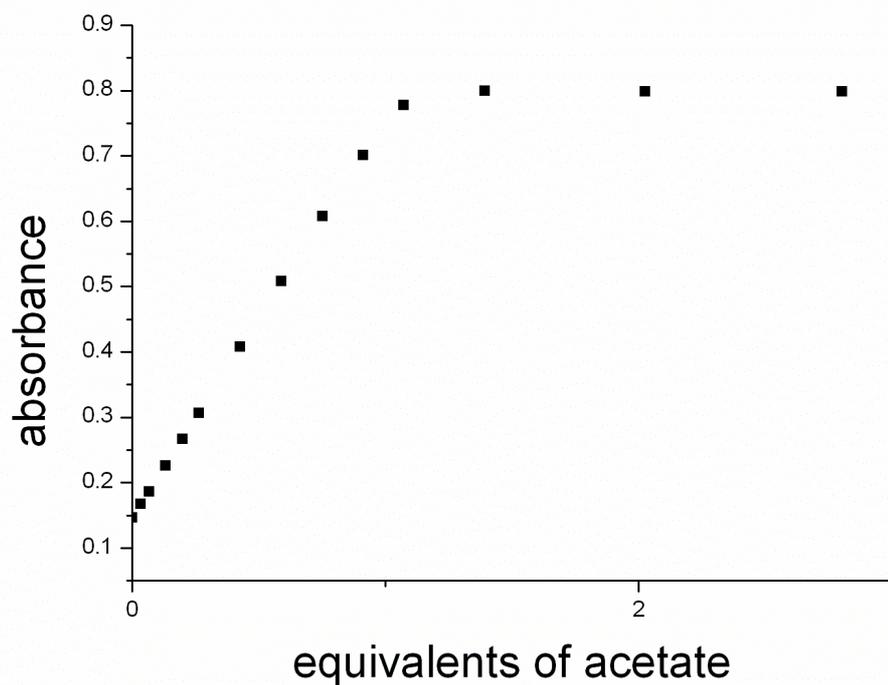
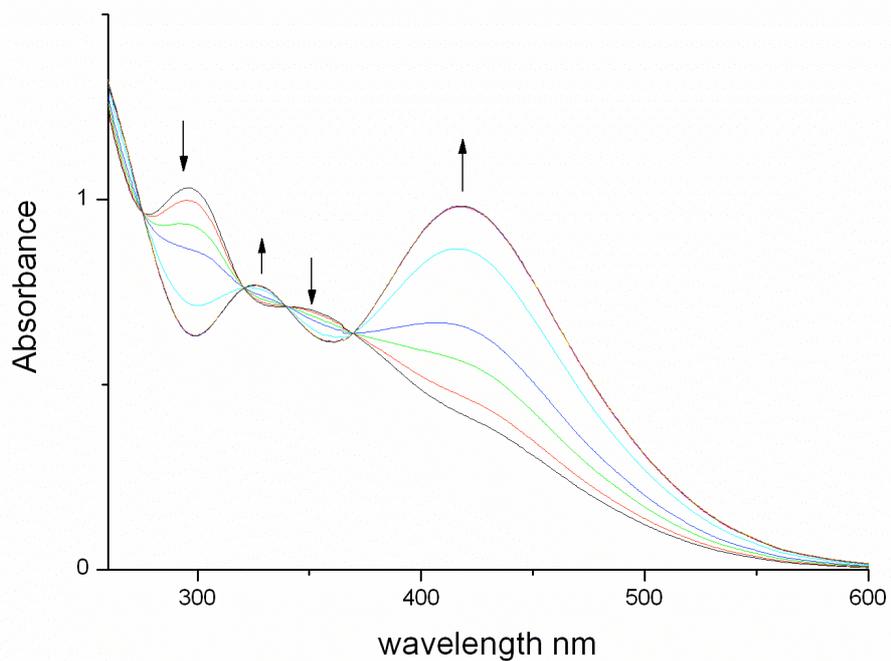


Figure S10 a) UV-vis absorption spectrophotometric titration of compound **4** with TBA acetate in DMSO/ water 9:1 at 25 °C. b) Variation of absorbance at 450 nm versus equivalents of acetate.

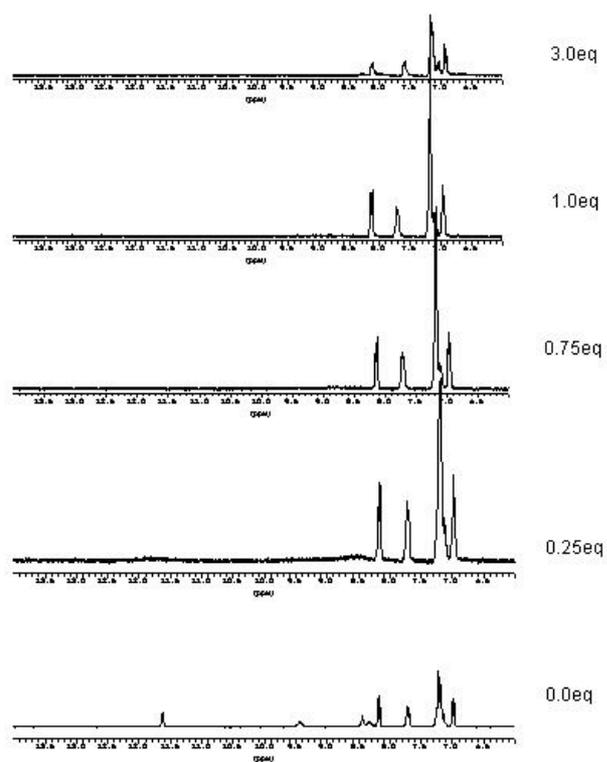


Figure S11 Stack plot of ^1H NMR spectra of compound **2** in the presence of increasing amounts of TBAF recorded in $\text{DMSO-}d_6$.

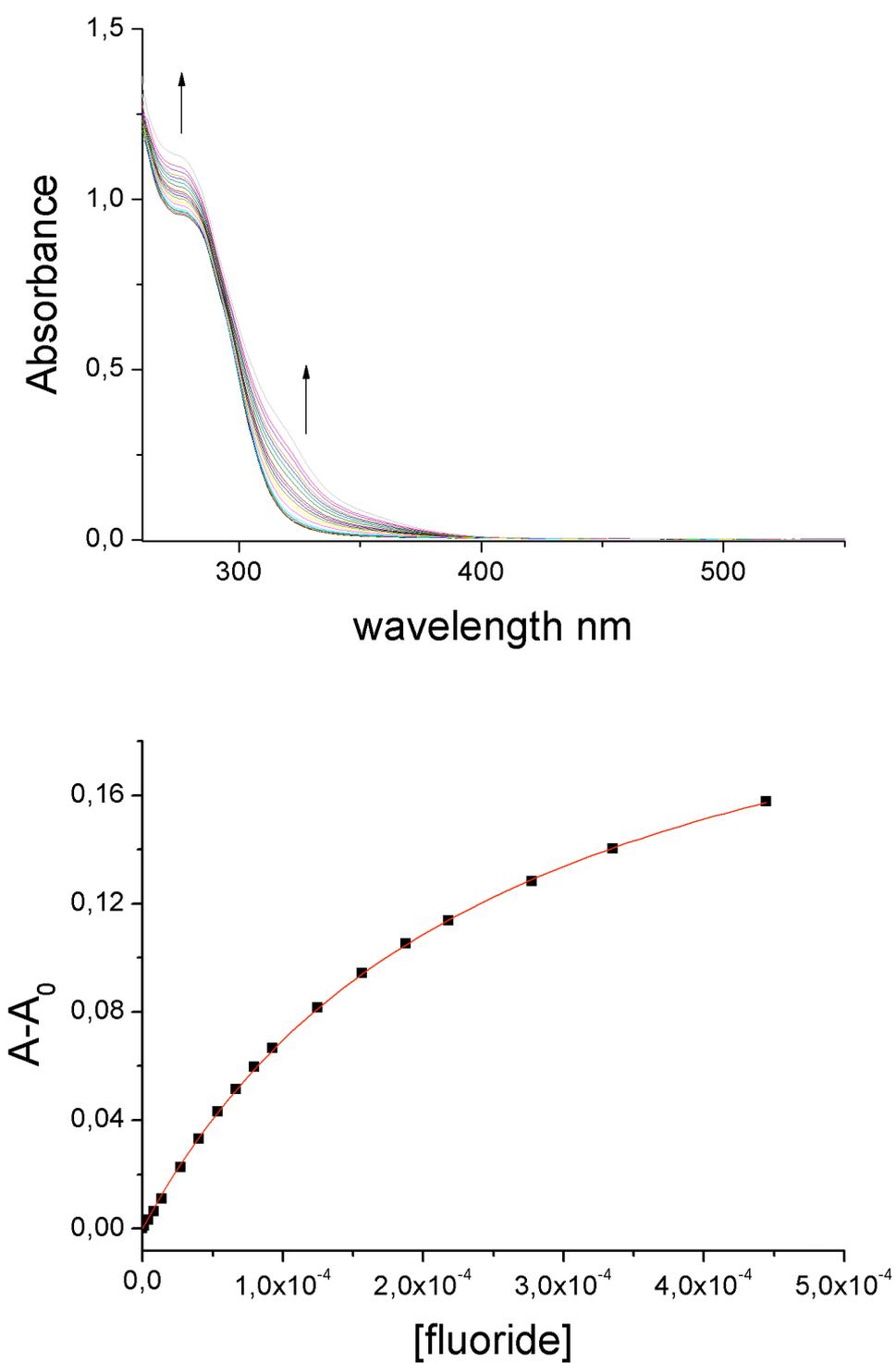


Figure S12 a) UV-vis absorption spectrophotometric titration of compound **5** with TBA fluoride in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of fluoride. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B \times [G^-]/(1+(K \times [G^-]))$.

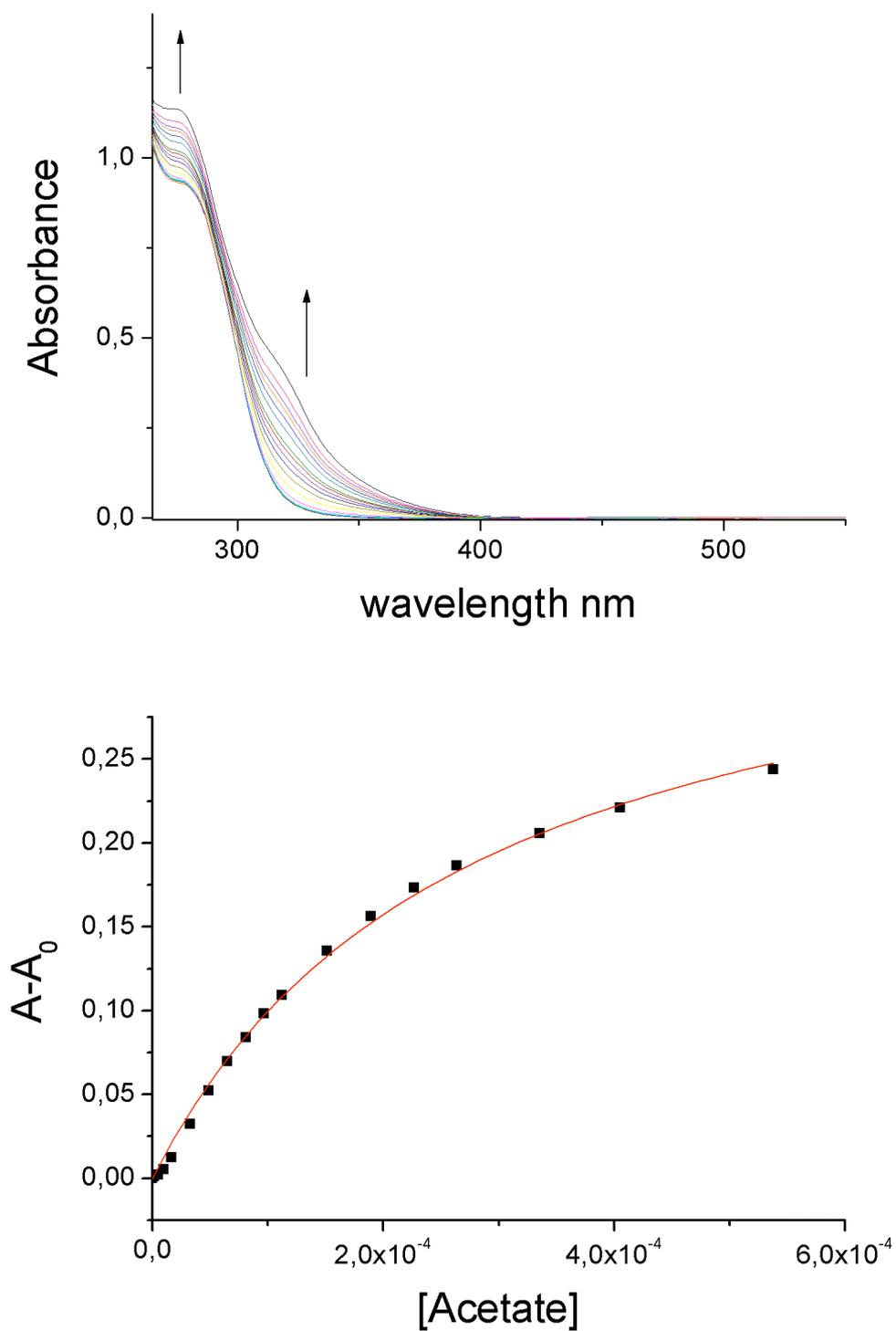


Figure S13 a) UV-vis absorption spectrophotometric titration of compound **5** with TBA acetate in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of acetate. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B \times [G]/(1+(K \times [G]))$.

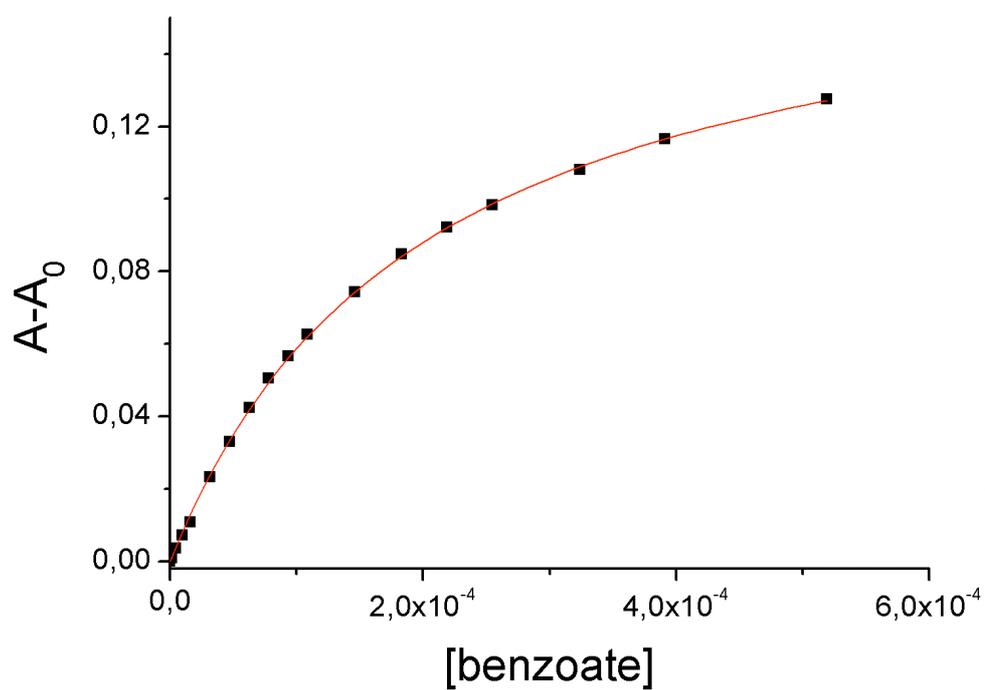
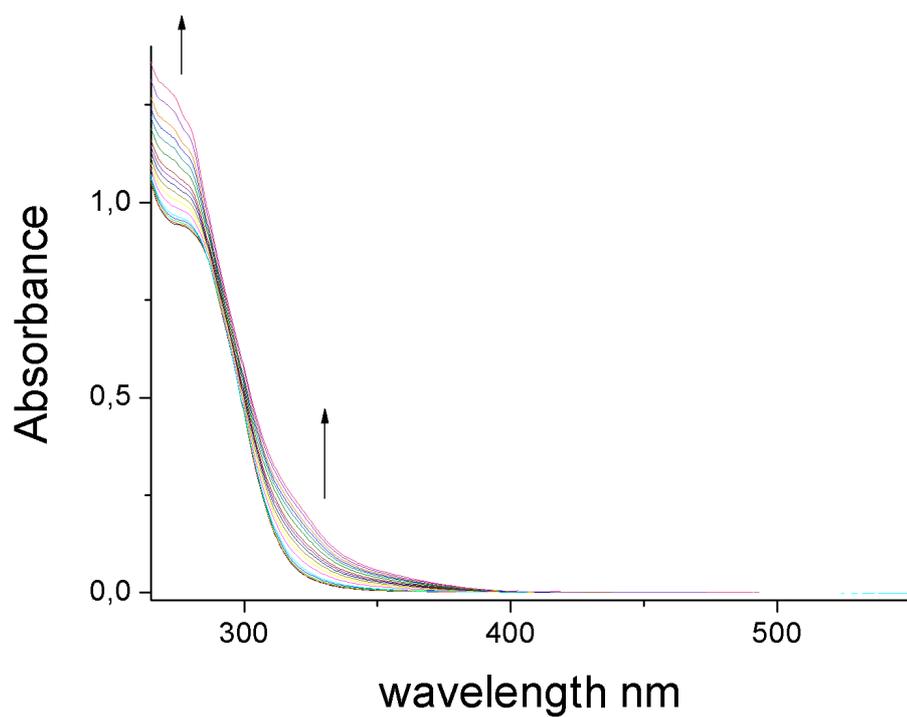


Figure S14 a) UV-vis absorption spectrophotometric titration of compound **5** with TBA benzoate in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of benzoate. The trend line is the result of the non linear least-square fit of the experimental data according to $A - A_0 = B \times [G^-] / (1 + (K \times [G^-]))$.

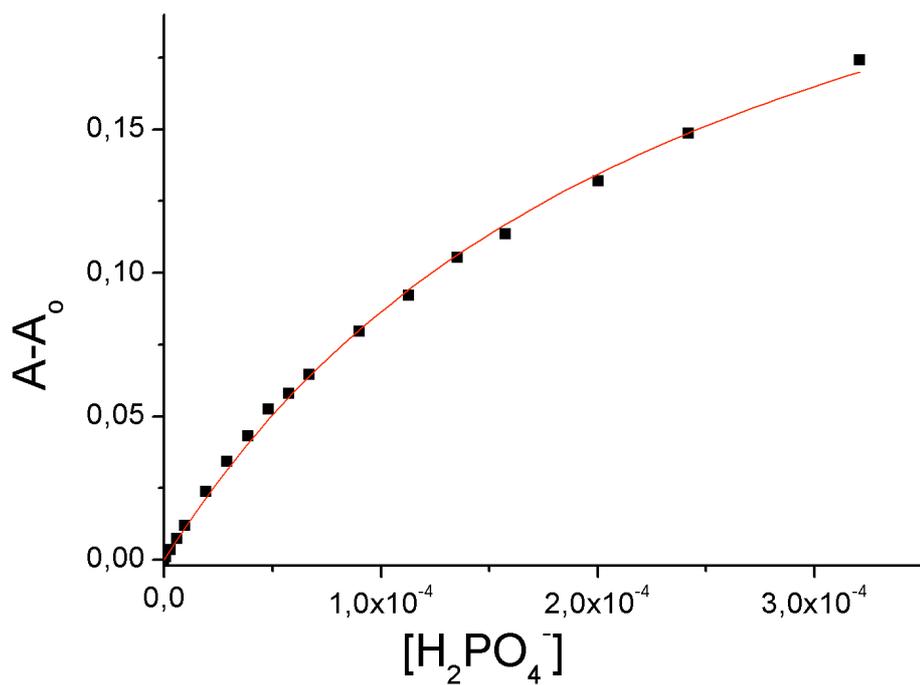
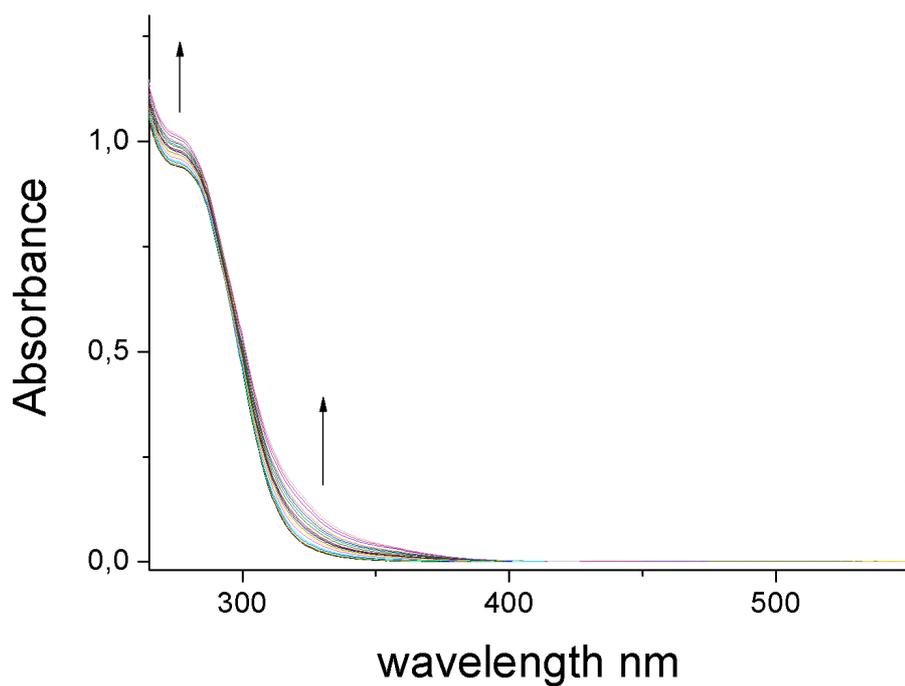


Figure S15 a) UV-vis absorption spectrophotometric titration of compound **5** with TBA dihydrogenphosphate in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of dihydrogenphosphate. The trend line is the result of the non linear least-square fit of the experimental data according to $A - A_0 = B \times [G^-] / (1 + (K \times [G^-]))$.

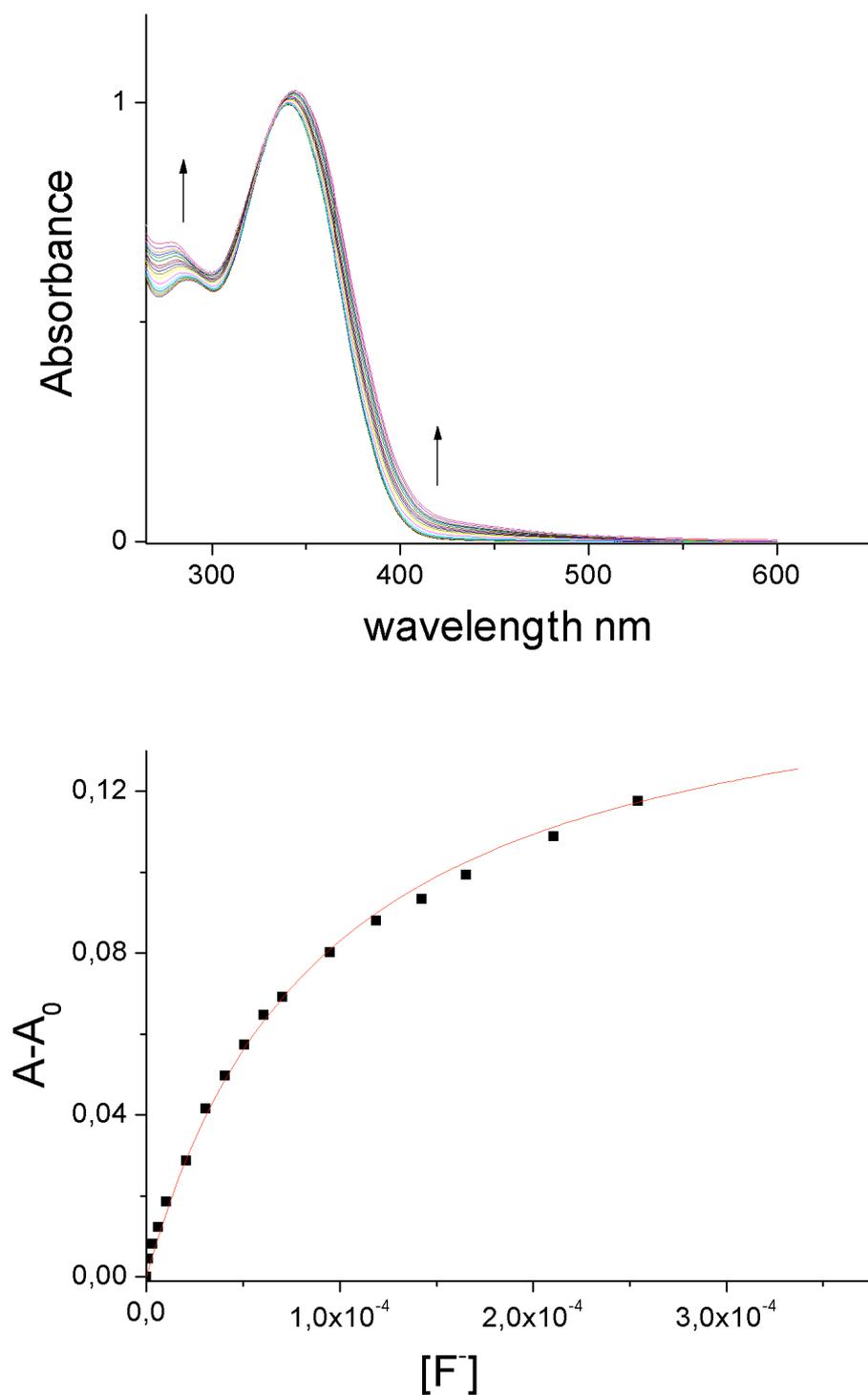


Figure S16 a) UV-vis absorption spectrophotometric titration of compound **6** with TBA fluoride in DMSO at 25 °C. b) Variation of absorbance at 400 nm versus concentration of fluoride. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B \times [G^-]/(1+(K \times [G^-]))$.

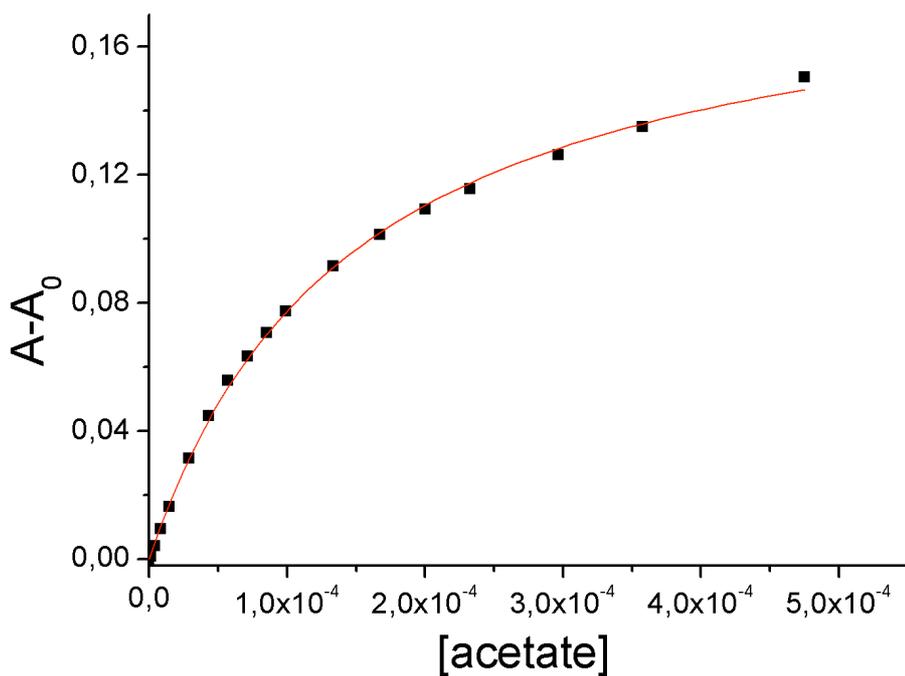
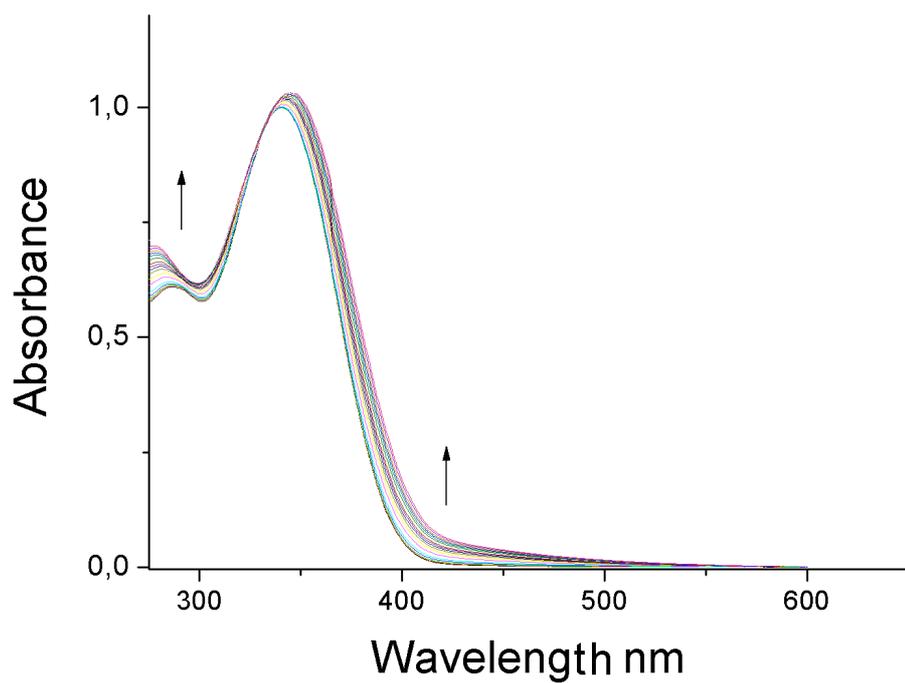


Figure S17 a) UV-vis absorption spectrophotometric titration of compound **6** with TBA acetate in DMSO at 25 °C. b) Variation of absorbance at 400 nm versus concentration of acetate. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B\times[G]/(1+(K\times[G]))$.

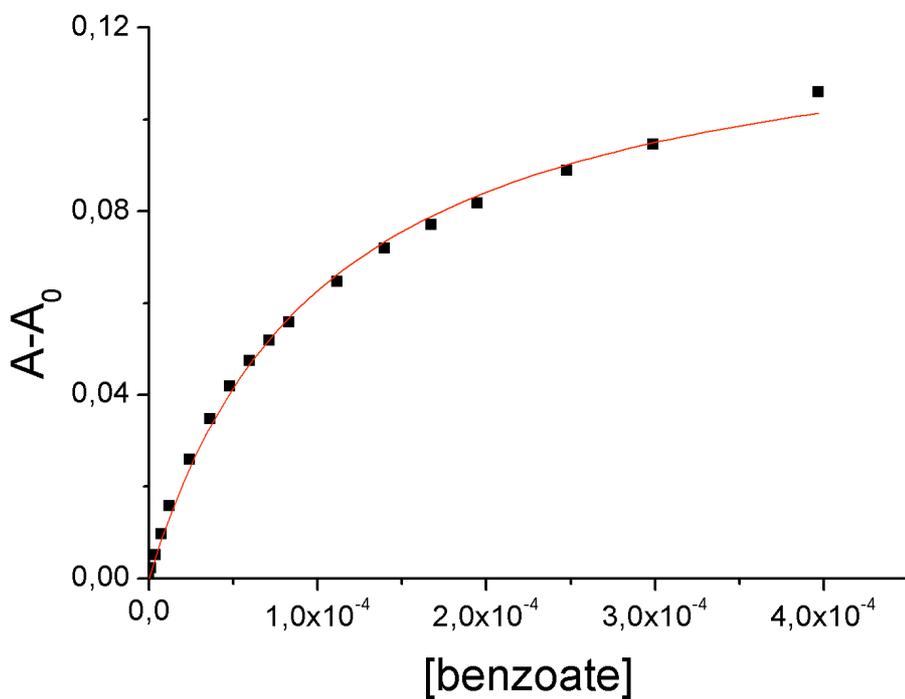
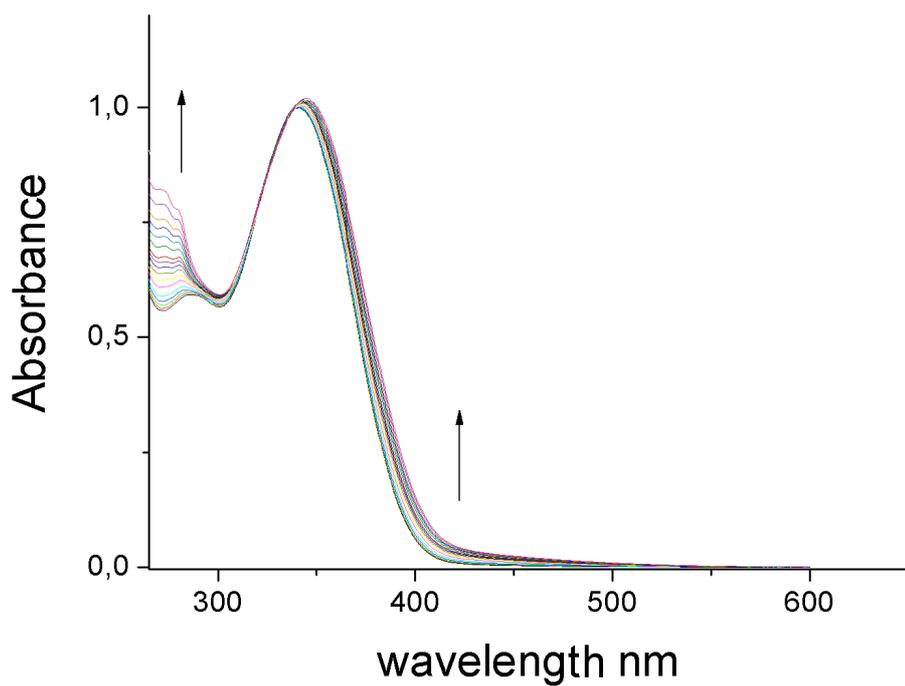


Figure S18 a) UV-vis absorption spectrophotometric titration of compound **6** with TBA benzoate in DMSO at 25 °C. b) Variation of absorbance at 400 nm versus concentration of benzoate. The trend line is the result of the non linear least-square fit of the experimental data according to $A - A_0 = B \times [G^-] / (1 + (K \times [G^-]))$.

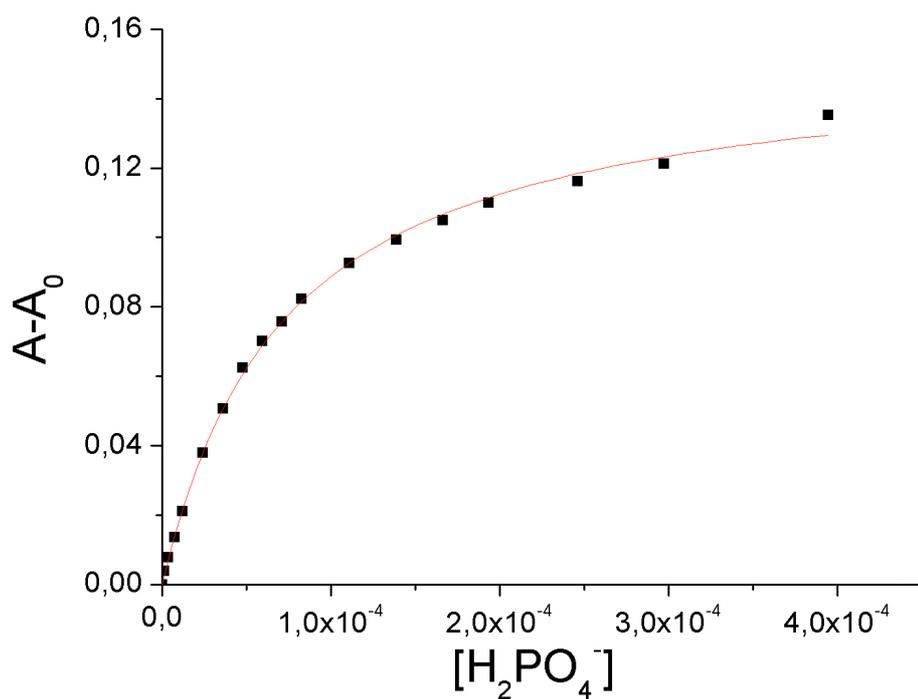
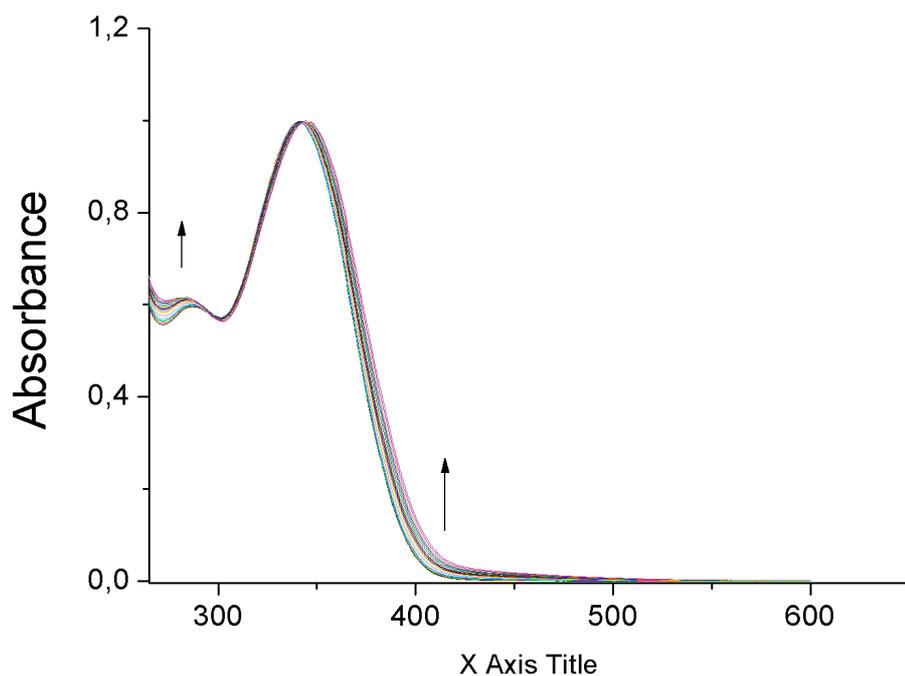


Figure S19 a) UV-vis absorption spectrophotometric titration of compound **6** with TBA dihydrogenphosphate in DMSO at 25 °C. b) Variation of absorbance at 400 nm versus concentration of dihydrogenphosphate. The trend line is the result of the non linear least-square fit of the experimental data according to $A - A_0 = B \times [G^-] / (1 + (K \times [G^-]))$.

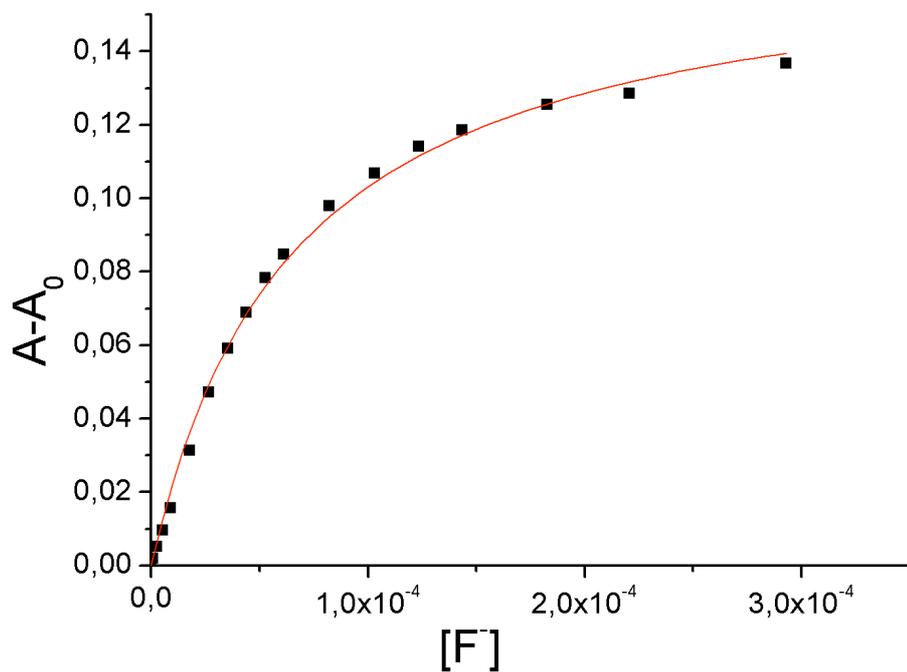
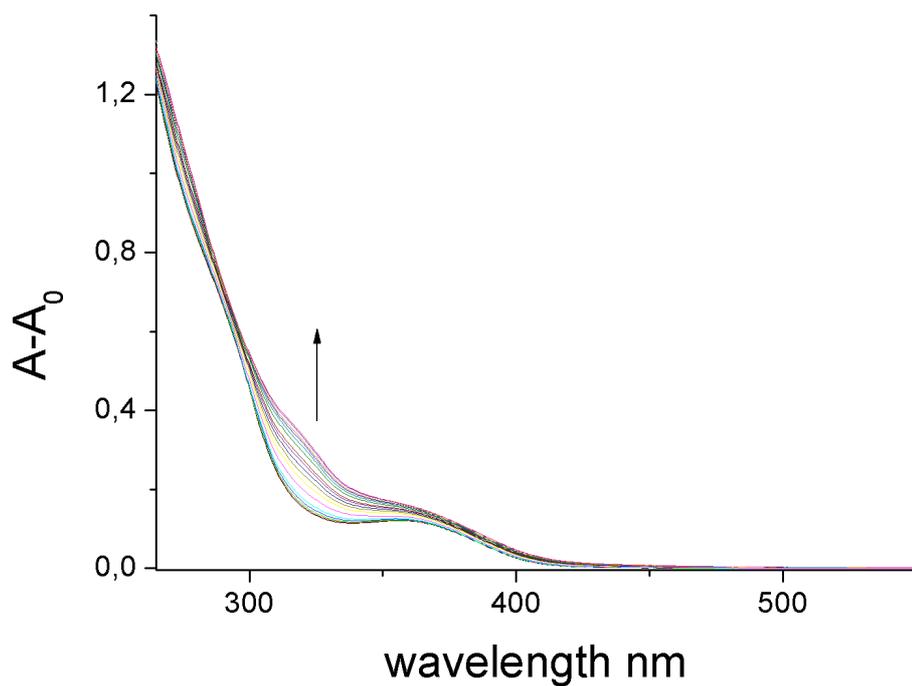


Figure S20 a) UV-vis absorption spectrophotometric titration of compound **7** with TBA fluoride in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of fluoride. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B \times [G^-]/(1+(K \times [G^-]))$.

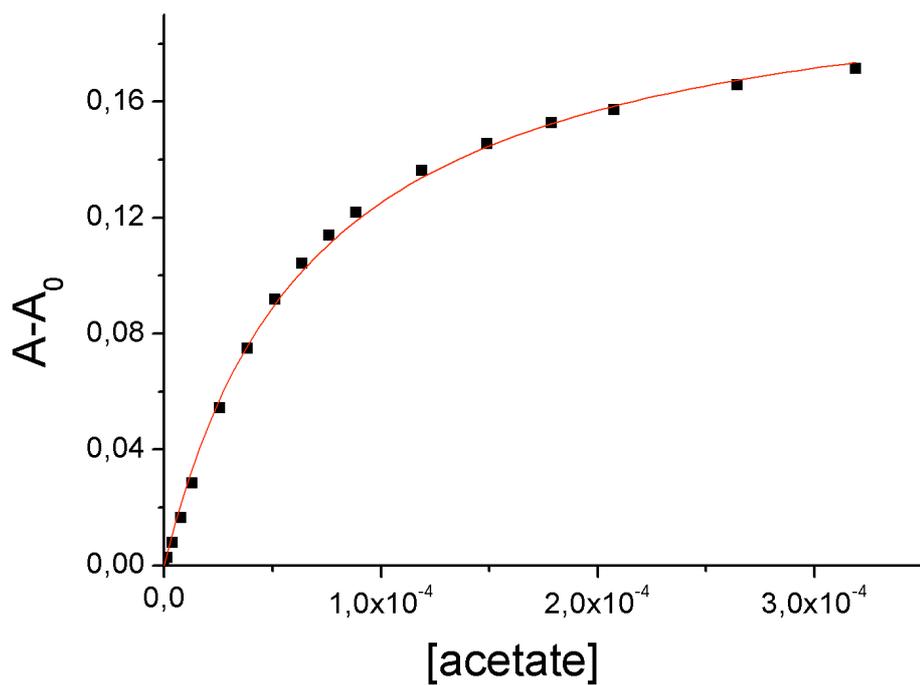
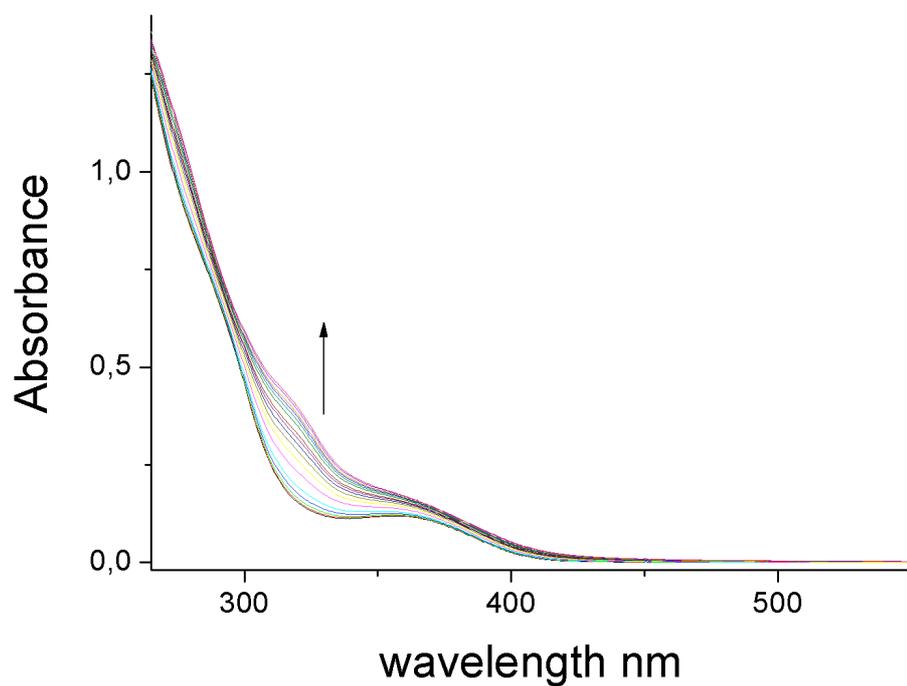


Figure S21 a) UV-vis absorption spectrophotometric titration of compound **7** with TBA acetate in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of acetate. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B\times[G]/(1+(K\times[G]))$.

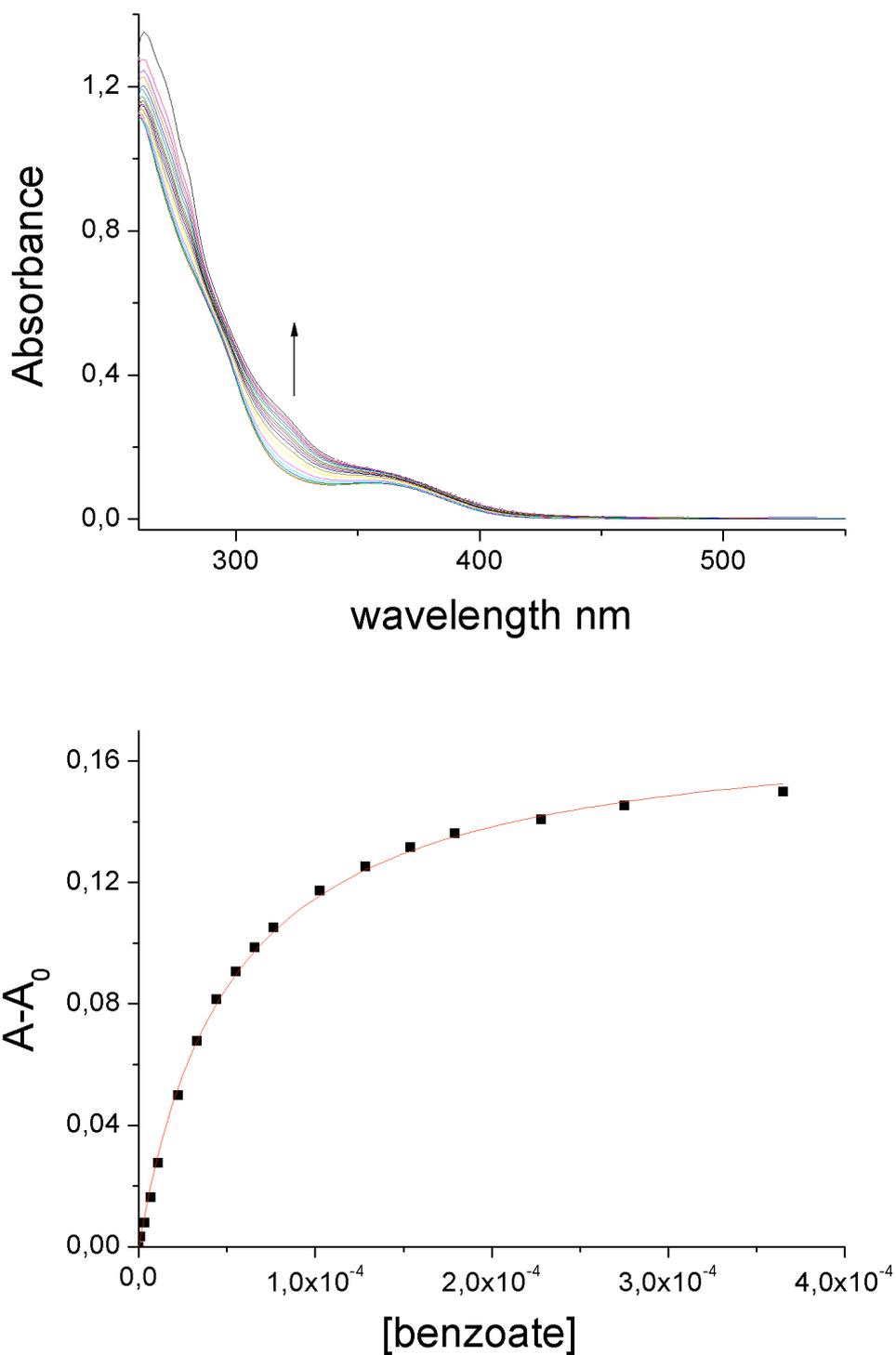


Figure S22 a) UV-vis absorption spectrophotometric titration of compound **7** with TBA benzoate in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of benzoate. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B \times [G^-]/(1+(K \times [G^-]))$.

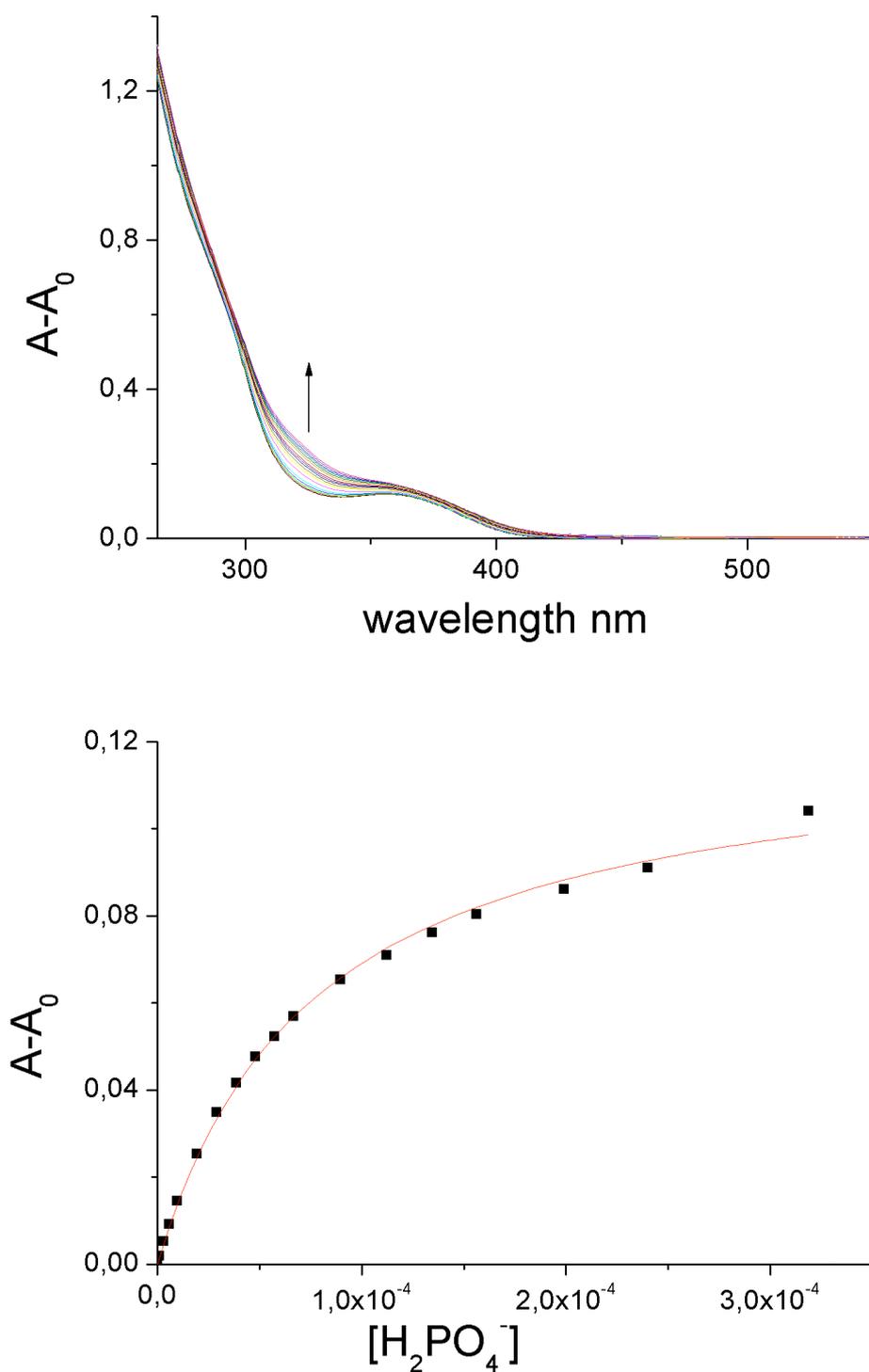


Figure S23 a) UV-vis absorption spectrophotometric titration of compound **7** with TBA dihydrogenphosphate in DMSO at 25 °C. b) Variation of absorbance at 330 nm versus concentration of dihydrogenphosphate. The trend line is the result of the non linear least-square fit of the experimental data according to $A-A_0=B \times [G^-]/(1+(K \times [G^-]))$.