Electronic Supplementary Information

Molecular Modelling of the pH Influence in the Geometry and the Absorbance Spectrum of near-Infrared TagRFP675 Fluorescent Protein.

Carlos Randino[1], Ricard Gelabert[1], Miquel Moreno[1]*, José M. Lluch[1,2] and Kiryl D. Piatkevich[3]

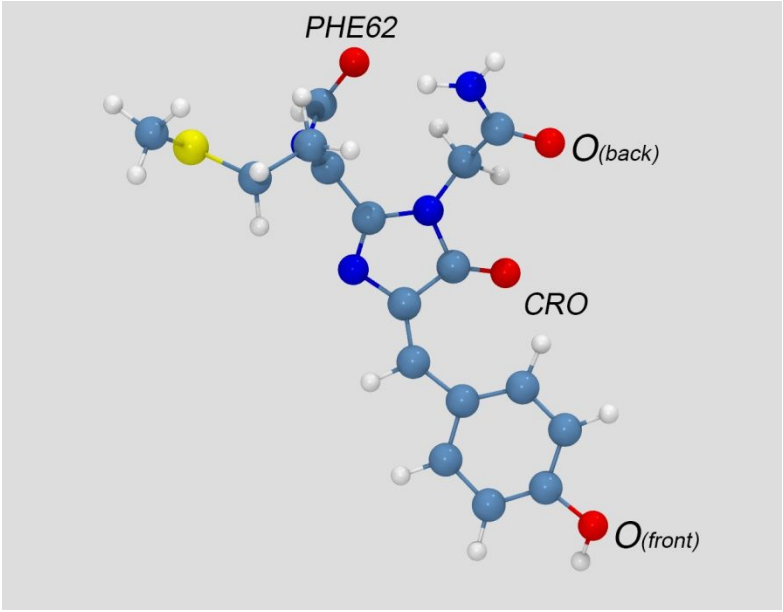
[1]Departament de Química, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona (Spain)

[2] Institut de Biotecnologia i de Biomedicina, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona (Spain)

[3] Massachusetts Institute of Technology Media Lab, Massachusetts Institute of Technology, Cambridge, MA 02139

[*] Corresponding author at Universitat Autònoma de Barcelona

Tel: +34935812174; E-mail address: miquel.moreno@uab.cat



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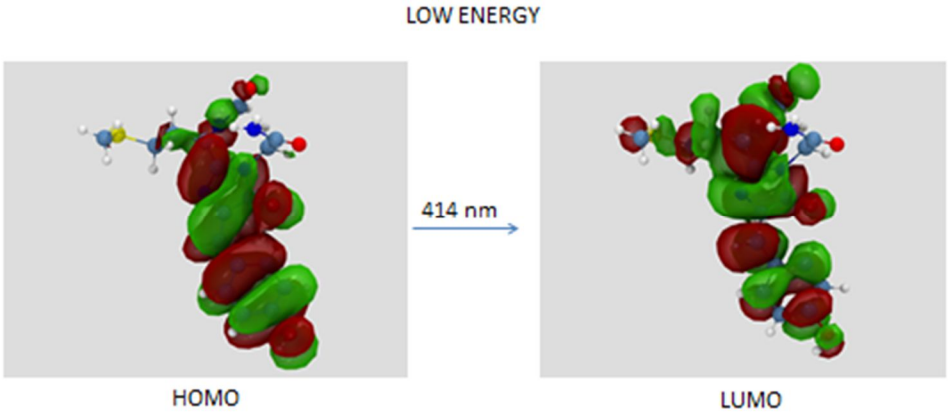

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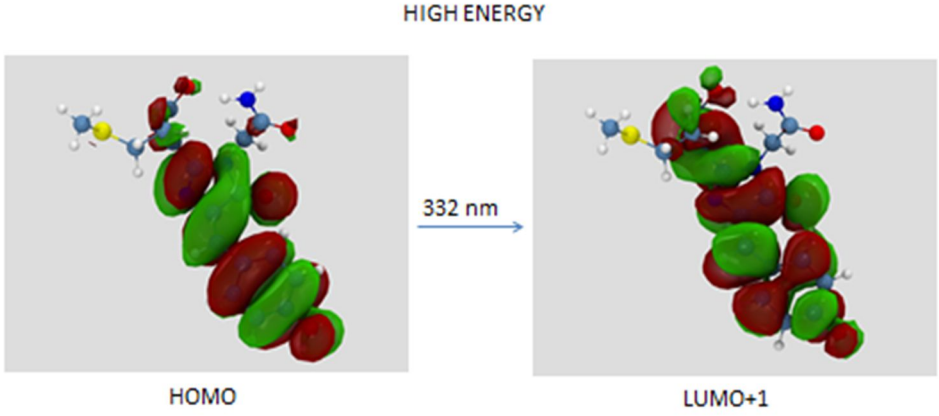
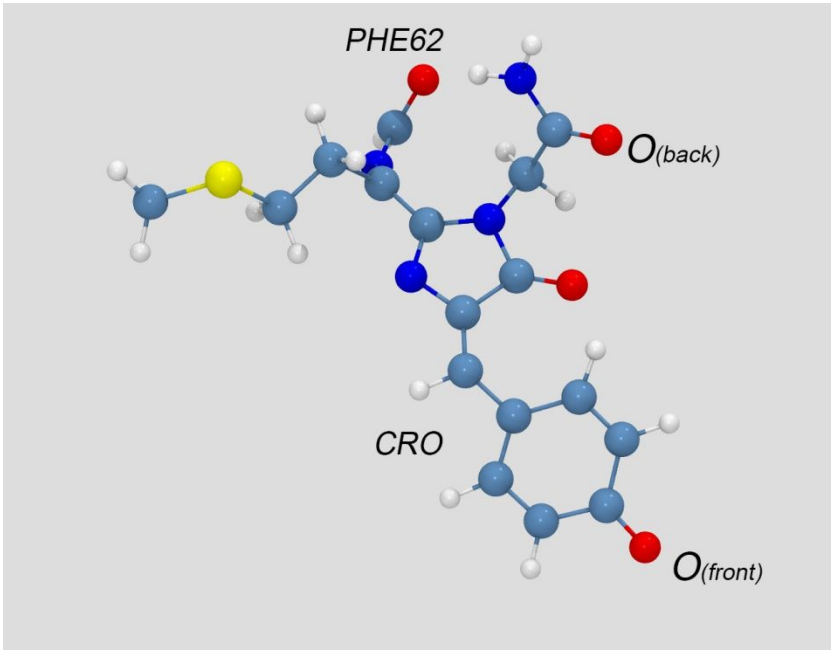


(c)

Figure S1: Shape of the molecular orbitals involved in the relevant electronic transitions of the TagRFP675 protein as obtained from the simulation of the *trans* neutral chromophore. (a) Geometry of the chromophore. (b) Molecular orbitals mainly involved in the low energy absorption band of the absorption spectrum. (c) Molecular orbitals mainly involved in the high energy absorption band of the absorption spectrum.



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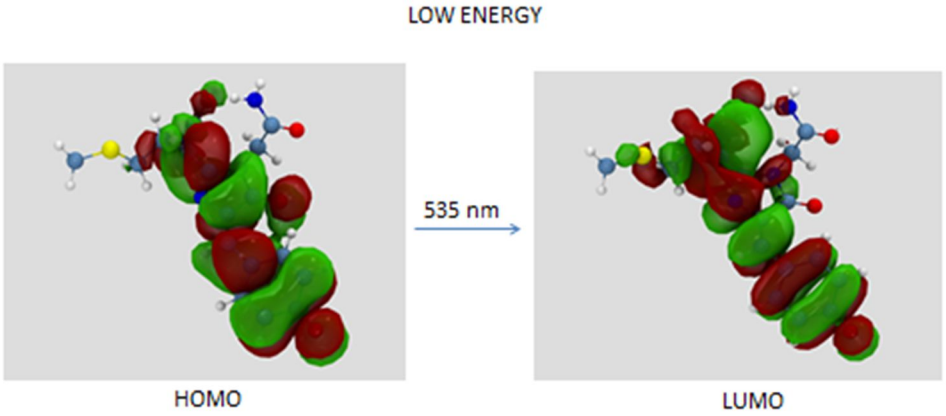

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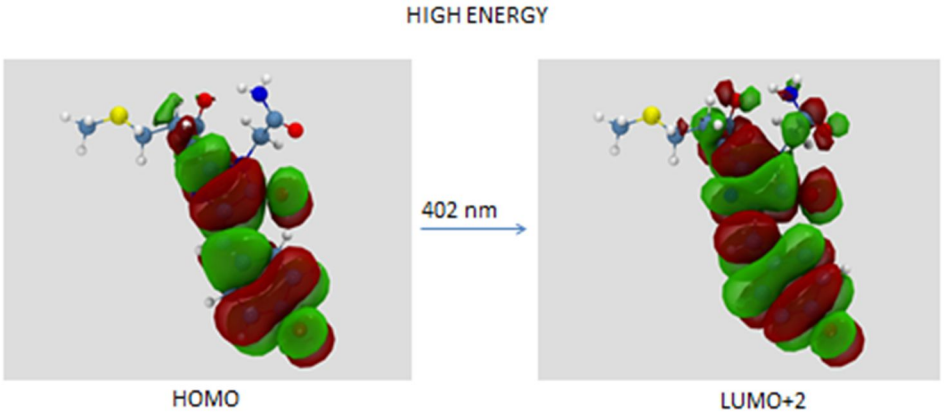
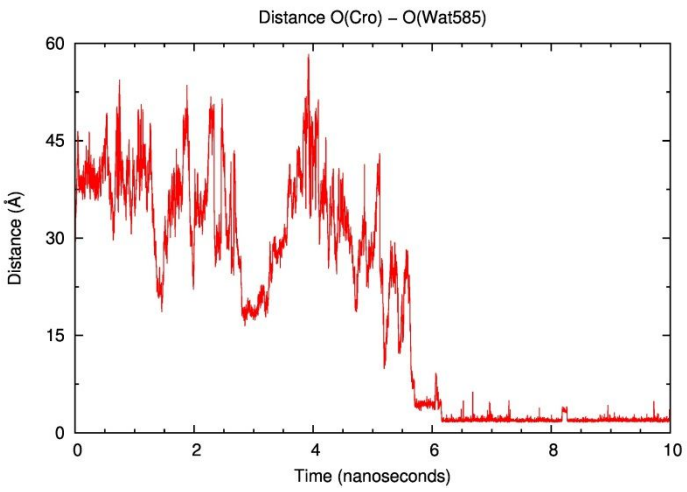


(c)

Figure S2: Shape of the molecular orbitals involved in the relevant electronic transitions of the TagRFP675 protein as obtained from the simulation of the *trans* anionic chromophore. (a) Geometry of the chromophore. (b) Molecular orbitals mainly involved in the low energy absorption band of the absorption spectrum. (c) Molecular orbitals mainly involved in the high energy absorption band of the absorption spectrum.



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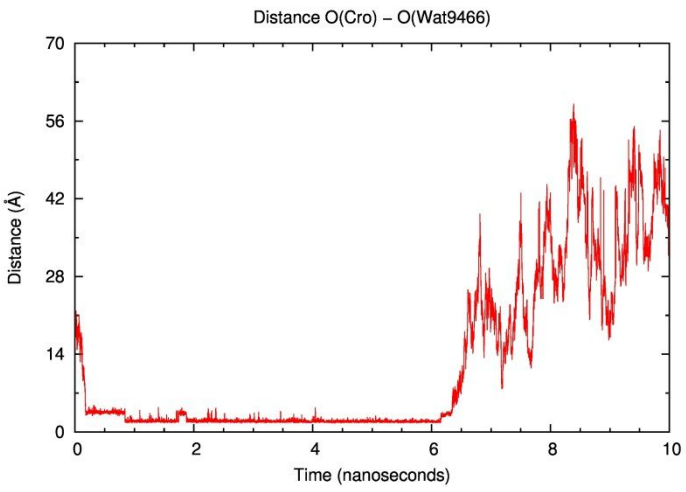

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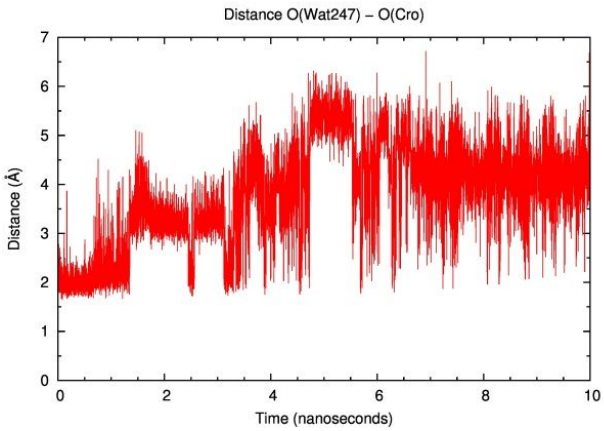
Figure S3: H-Bond interactions of the O-H phenolic group ($O_{(front)}$) of the neutral *cis* chromophore with solvent water molecules at pH=4.5.



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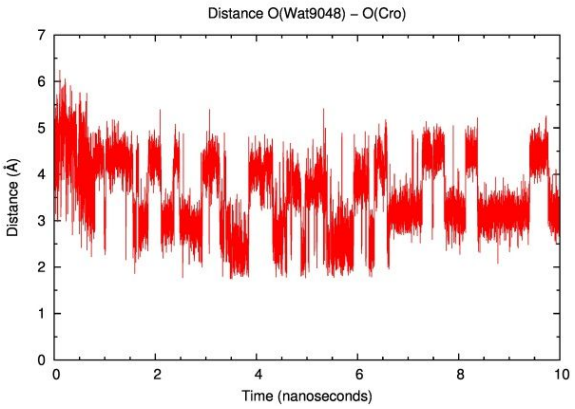

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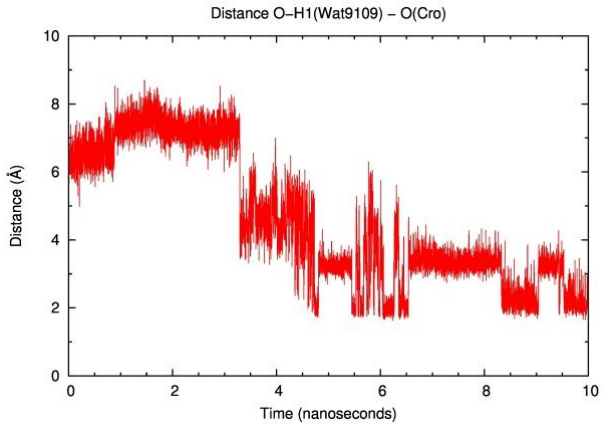

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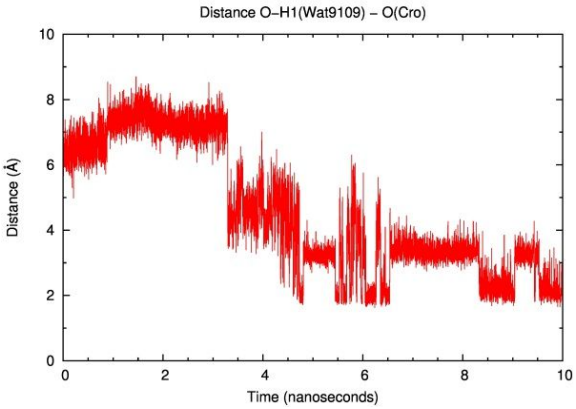
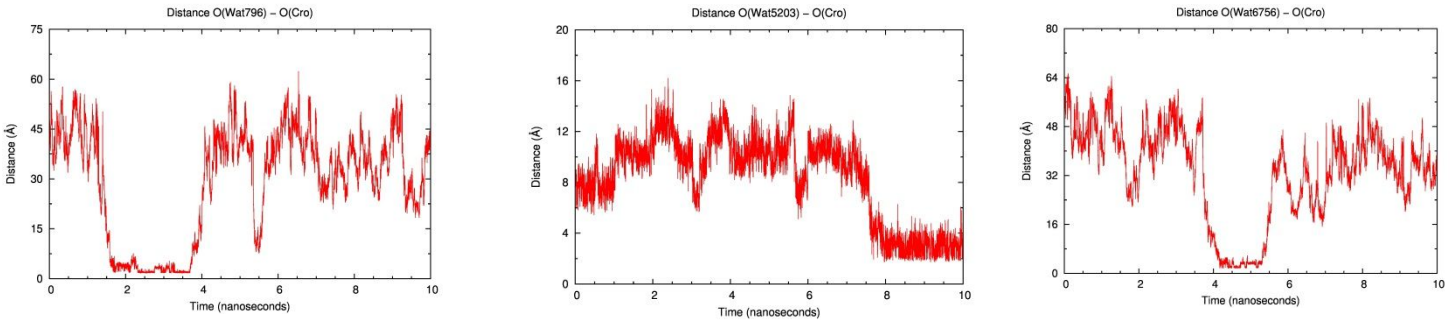


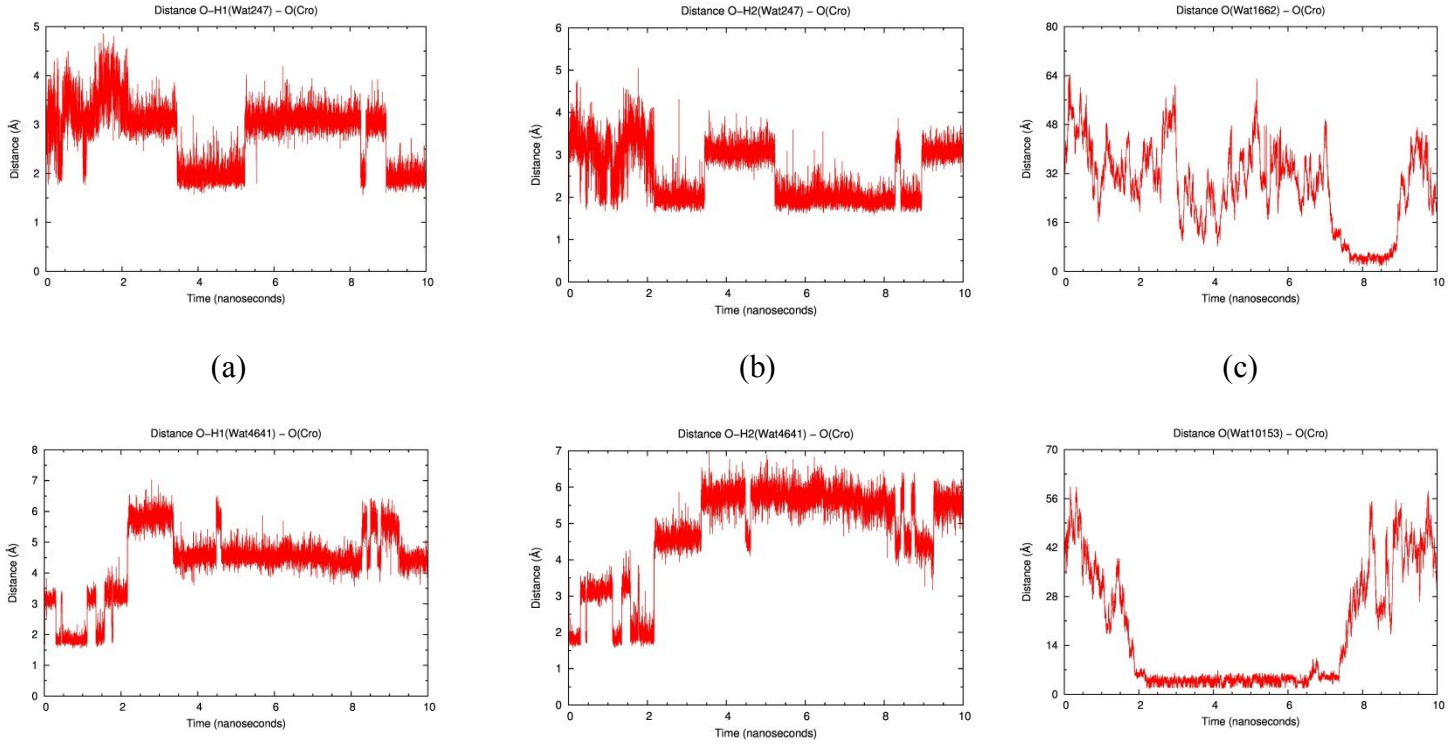
(d)

Figure S4: H-Bond interactions of the O-H phenolic group ($O_{(front)}$) of the neutral *trans* chromophore with solvent water molecules at pH=4.5.



(a) (b) (c)

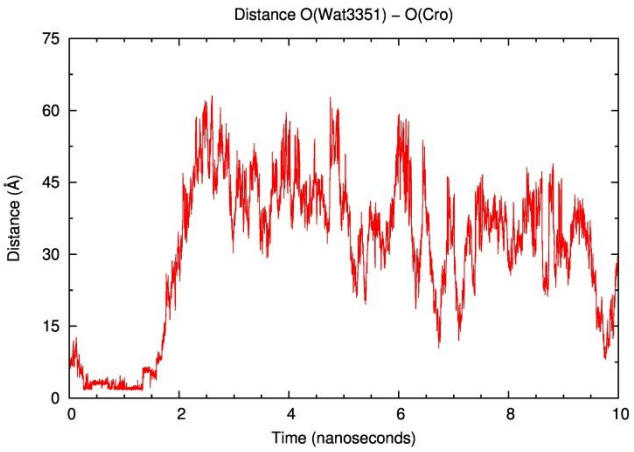
Figure S5: H-Bond interactions of the phenolic oxygen atom ($O_{(front)}$) of the anionic *cis* chromophore with solvent water molecules at pH=4.5.



(a) (b) (c)

(d) (e) (f)

Figure S6: H-Bond interactions of the phenolic oxygen atom ($O_{(front)}$) of the anionic *trans* chromophore with solvent water molecules at pH=4.5.



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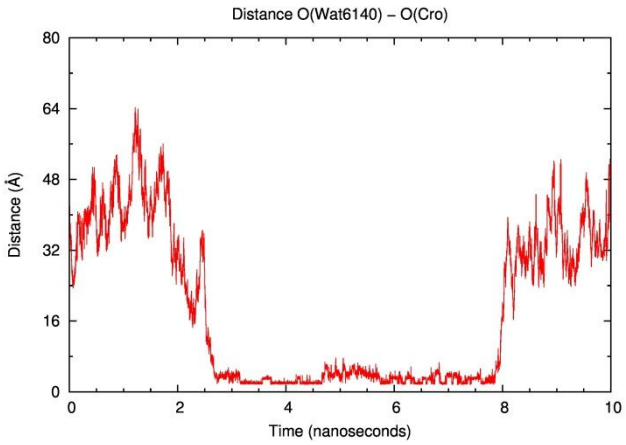

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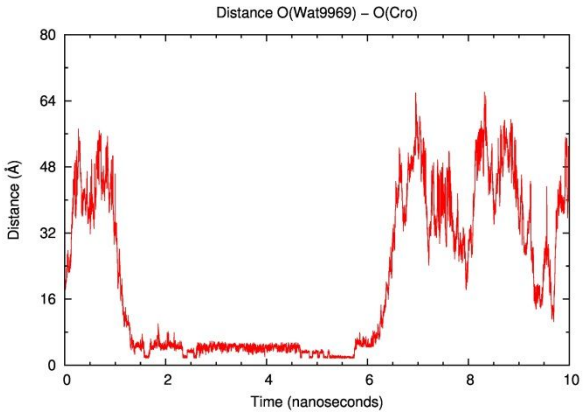

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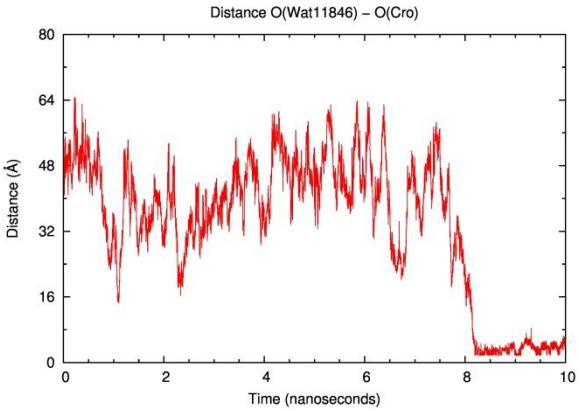

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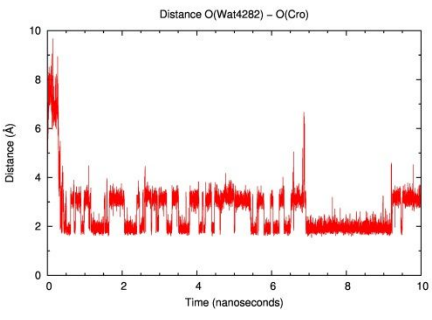
Figure S7: H-Bond interactions of the phenolic oxygen atom ($O_{(front)}$) of the anionic *cis* chromophore with solvent water molecules at pH=7.5.



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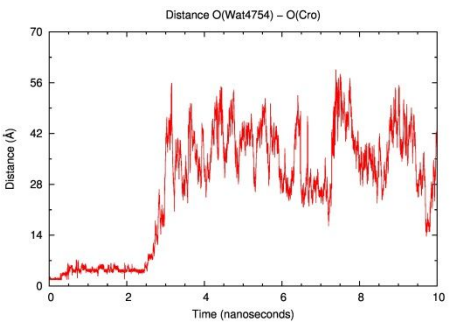

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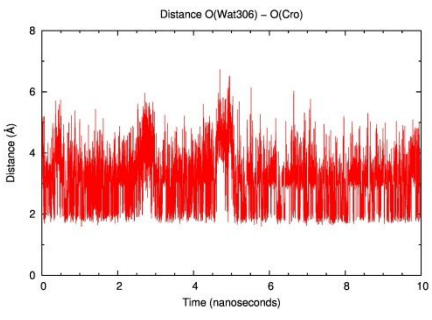

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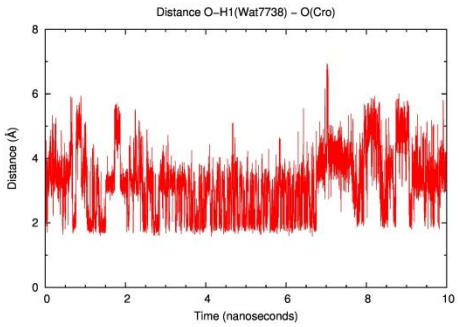
Figure S8: H-Bond interactions of the phenolic oxygen atom ($O_{(front)}$) of the anionic *cis* chromophore with solvent water molecules at pH=10.



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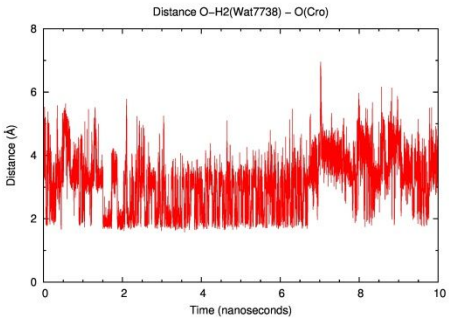

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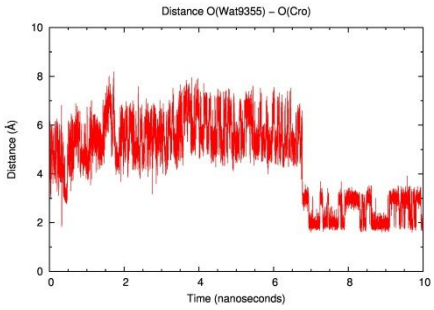

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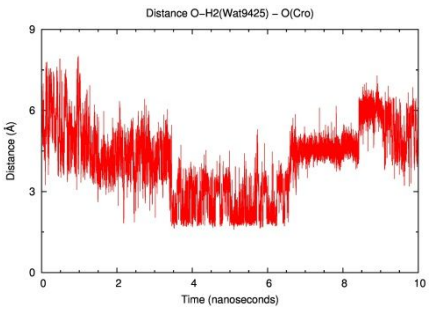

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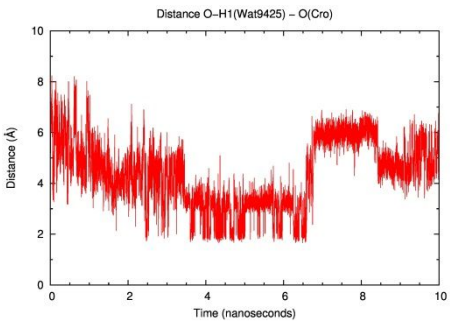

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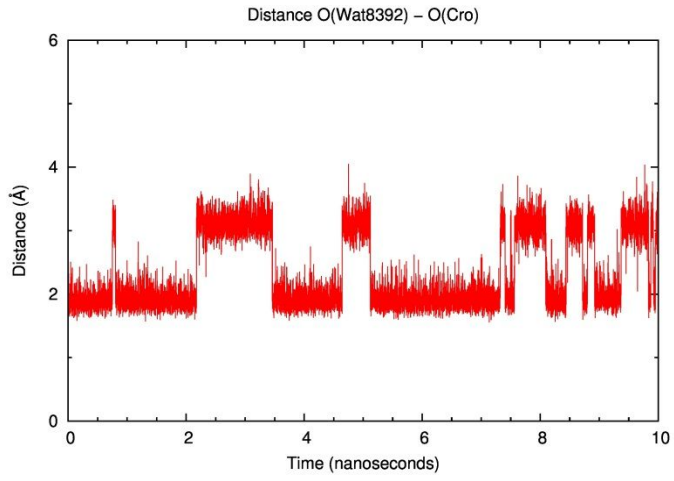
Figure S9: H-Bond interactions of the phenolic oxygen atom ($O_{(front)}$) of the anionic *trans* chromophore with solvent water molecules at pH=7.5.



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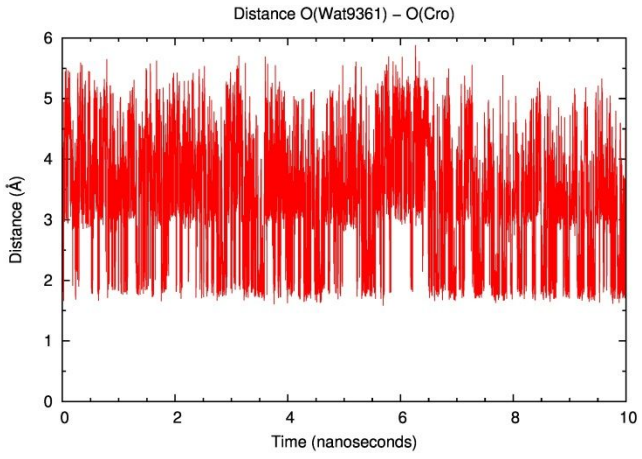

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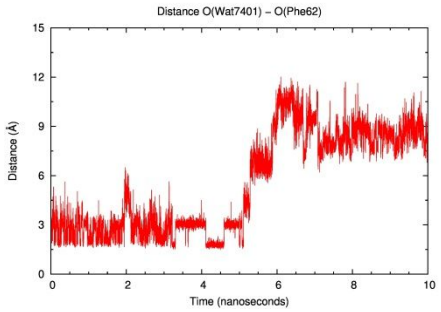

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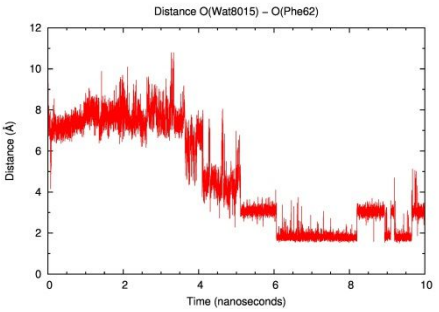

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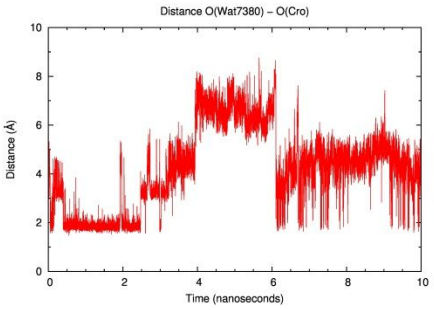

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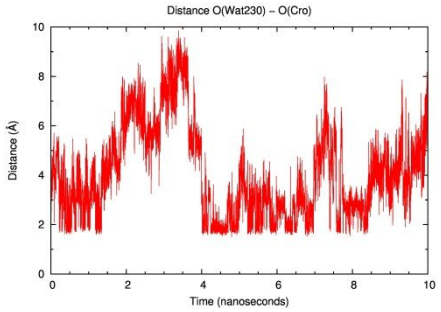

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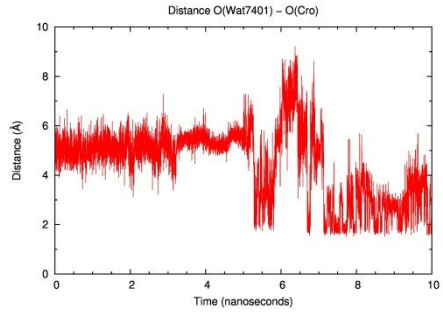

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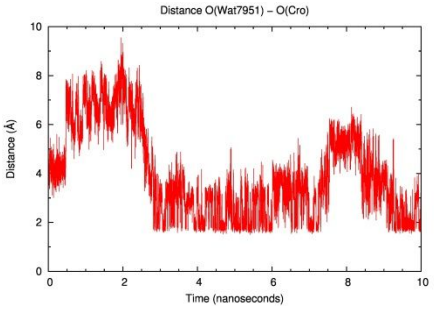

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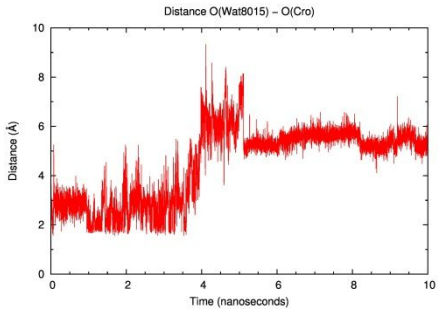
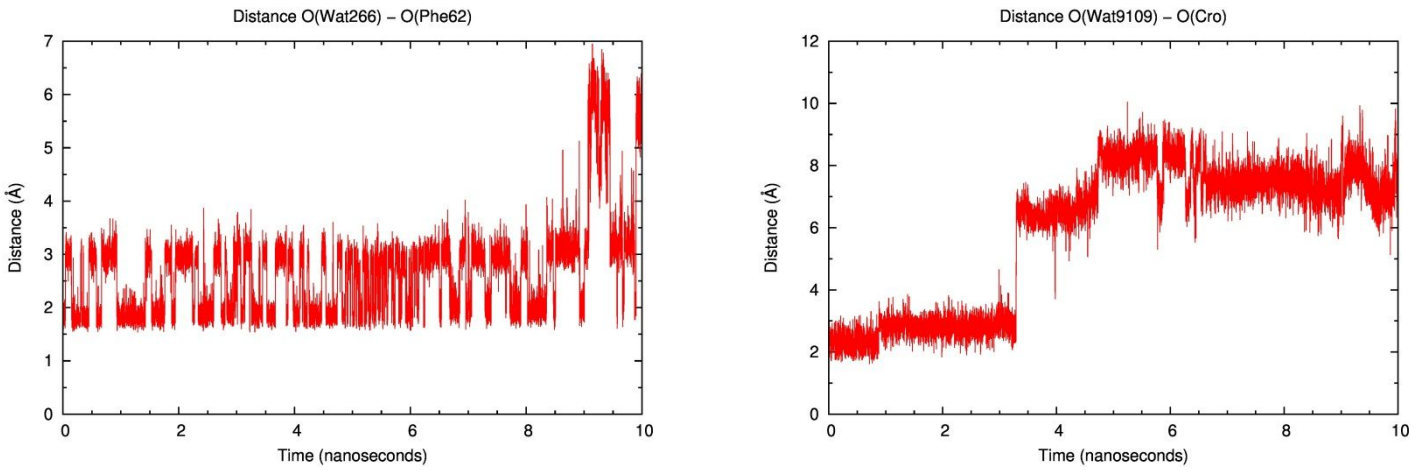


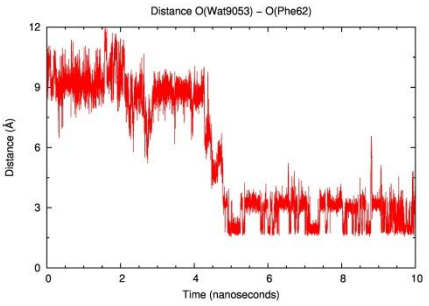
(g)

Figure S11: H-Bond interactions found in the imidazolinone ring region of the neutral *cis* chromophore ($O_{(back)}$ and Phe62) with solvent water molecules at pH=4.5.



(a) (b)

Figure S12: H-Bond interactions found in the imidazolinone ring region of the neutral *trans* chromophore ($O_{(back)}$ and Phe62) with solvent water molecules at pH=4.5.



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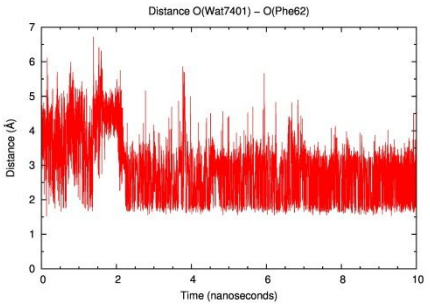

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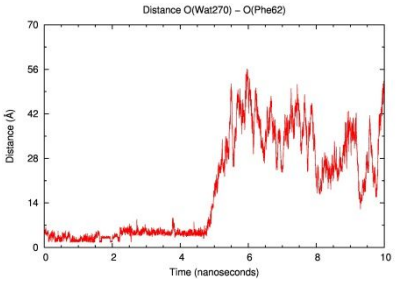

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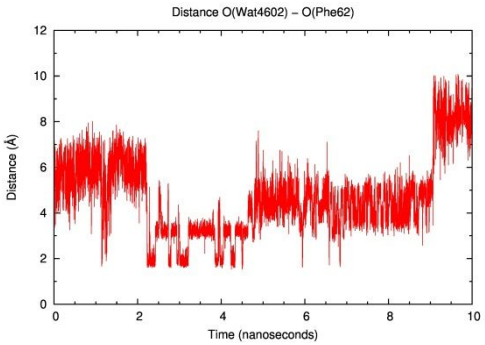

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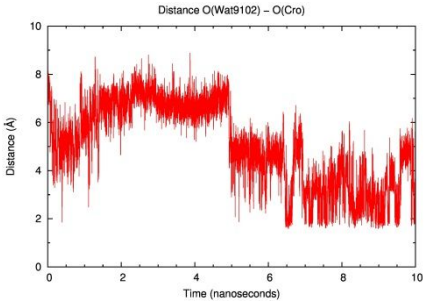

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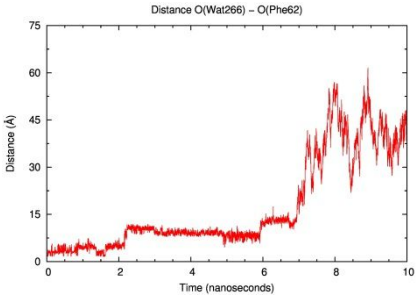

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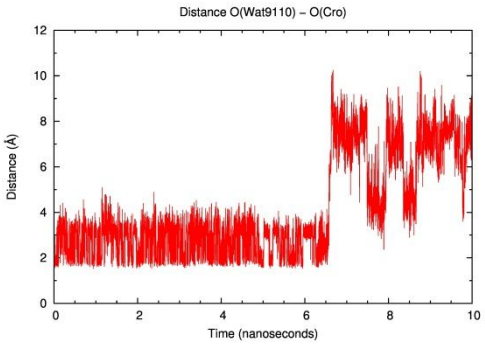

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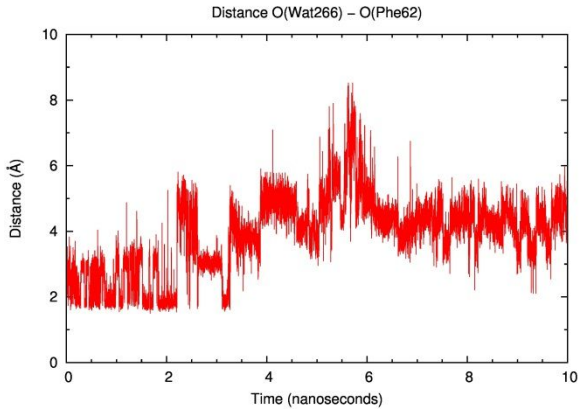
Figure S13: H-Bond interactions found in the imidazolinone ring region of the anionic *cis* chromophore ($O_{(back)}$ and Phe62) with solvent water molecules at pH=4.5.



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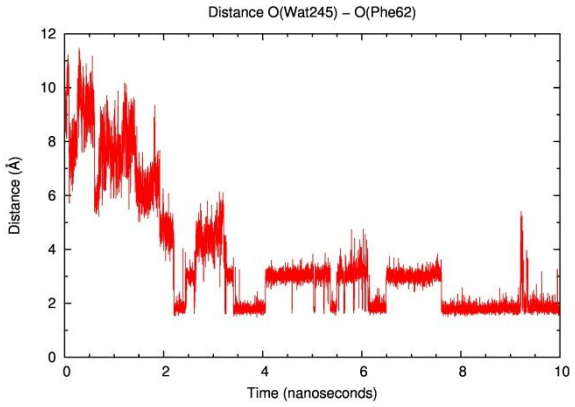

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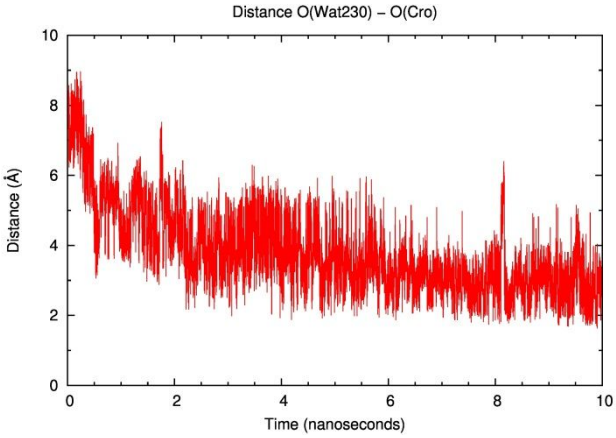

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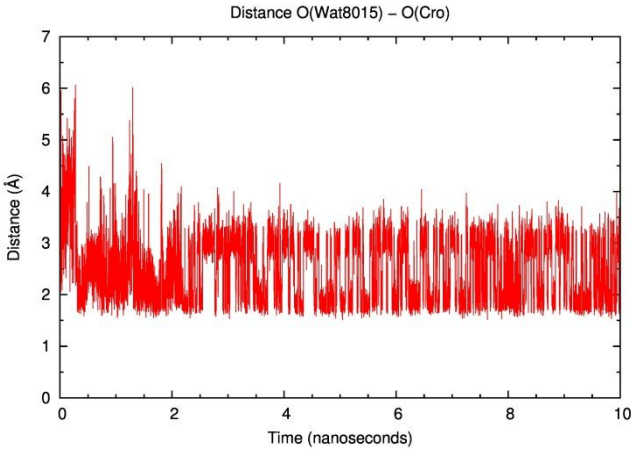

(d)

Figure S14: H-Bond interactions found in the imidazolinone ring region of the anionic *trans* chromophore ($O_{(back)}$ and Phe62) with solvent water molecules at pH=4.5.