

# Estimating Orientation Factors in the FRET Theory of Fluorescent Proteins: the TagRFP-KFP Pair and Beyond

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## Supporting Materials

**Table S1.** Cartesian coordinates (Å) of the TagRFP chromophore in the ground  $S_0$  state optimized in the QM(PBE0/cc-pVDZ)/MM(AMBER) calculations.

N -10.9220 -38.5530 23.4360  
H -10.0180 -38.8090 23.8200  
C -12.0720 -38.3710 24.2910  
H -12.9480 -38.4840 23.6370  
C -12.1340 -39.4140 25.3580  
H -11.4130 -39.1850 26.1470  
H -13.1240 -39.3710 25.8250  
C -11.8930 -40.8450 24.9110  
C -10.6120 -41.4100 25.0480  
H -9.8000 -40.8310 25.4590  
C -10.3790 -42.7370 24.6530  
H -9.3950 -43.1670 24.7740  
C -11.4180 -43.5050 24.1050  
H -11.2330 -44.5260 23.8010  
C -12.9410 -41.6280 24.3910  
H -13.9370 -41.2270 24.3120  
C -12.7020 -42.9500 23.9770  
H -13.5090 -43.5460 23.5740  
C -12.2100 -36.9490 24.8680  
O -13.1650 -36.6420 25.5520  
N -11.2690 -36.0180 24.4430  
C -10.2060 -35.7350 25.1140  
C -9.2560 -34.7660 24.5910  
N -8.0900 -34.5630 25.1640  
N -9.3540 -34.0350 23.4140  
C -8.1570 -33.3480 23.2200  
O -7.9780 -32.5690 22.2520  
C -7.3460 -33.7510 24.3420

C -5.9850 -33.6020 24.7040  
H -5.7930 -34.0550 25.6820  
C -4.8650 -33.1080 24.0710  
C -3.6040 -33.2090 24.7630  
H -3.5940 -33.6840 25.7490  
C -4.8610 -32.5120 22.7630  
H -5.8070 -32.4600 22.2270  
C -2.4510 -32.7300 24.2360  
H -1.4970 -32.7850 24.7730  
C -3.7200 -32.0200 22.2180  
H -3.7130 -31.5340 21.2400  
C -2.4580 -32.0700 22.9420  
O -1.4270 -31.5490 22.4750  
C -9.8180 -36.3830 26.4170  
H -10.1580 -37.4260 26.4080  
H -8.7260 -36.3790 26.5040  
C -10.4150 -35.6870 27.6020  
H -9.9780 -34.6880 27.6970  
H -11.4920 -35.5620 27.4330  
S -10.2130 -36.5660 29.1710  
C -8.4210 -36.5560 29.3290  
H -7.9530 -37.0910 28.5070  
H -8.0810 -35.5330 29.2910  
H -8.1280 -36.9980 30.2800  
C -10.3980 -34.0560 22.4250  
H -10.0270 -33.4760 21.5650  
H -10.6180 -35.0780 22.0950  
C -11.7070 -33.4450 22.8870  
O -12.7590 -33.6740 22.2970

**Table S2.** Cartesian coordinates (Å) of the TagRFP chromophore in the excited  $S_1$  state optimized in the QC CASSCF(6/6)/cc-pVDZ calculations.

C -11.1370 -38.3310 22.2310  
O -11.9140 -37.5490 21.7820  
N -11.0780 -38.7040 23.5300  
H -10.5300 -39.5110 23.7410  
C -12.1690 -38.3900 24.4150  
H -13.1330 -38.5960 23.9480  
C -12.2510 -36.9570 24.9370  
O -13.1400 -36.6520 25.6590  
N -11.2840 -36.0580 24.4960  
C -10.2590 -35.7810 25.1740  
C -9.2520 -34.8710 24.6070  
N -8.1030 -34.7100 25.1770  
N -9.3340 -34.1800 23.4080  
C -8.1330 -33.5470 23.1990  
O -7.9170 -32.7970 22.2420  
C -7.3020 -33.9690 24.3340  
C -5.9230 -33.8760 24.6890  
H -5.7150 -34.3760 25.6240

C -4.7800 -33.3690 23.9900  
 C -3.4770 -33.4810 24.6180  
 H -3.4010 -34.0250 25.5520  
 C -4.8230 -32.7220 22.7230  
 H -5.7700 -32.6600 22.2240  
 C -2.3770 -32.8950 24.1010  
 H -1.4330 -32.9360 24.6240  
 C -3.7020 -32.1250 22.1780  
 H -3.7410 -31.5770 21.2480  
 C -2.4430 -32.0990 22.8880  
 O -1.4910 -31.4060 22.4990  
 C -9.8940 -36.3900 26.5070  
 H -10.6920 -37.0300 26.8710  
 H -8.9720 -36.9630 26.4120  
 C -10.4340 -34.1000 22.4550  
 H -10.0250 -33.7180 21.5260  
 H -10.8510 -35.0860 22.2820  
 C -11.6060 -33.1910 22.8000  
 O -12.4490 -33.0260 21.9690  
 N -11.6520 -32.6500 24.0340  
 H -10.8300 -32.5410 24.5920  
 H -10.3610 -38.8110 21.6160  
 H -12.0960 -39.0240 25.2970  
 H -9.7200 -35.6130 27.2500  
 H -12.4210 -32.0360 24.2120

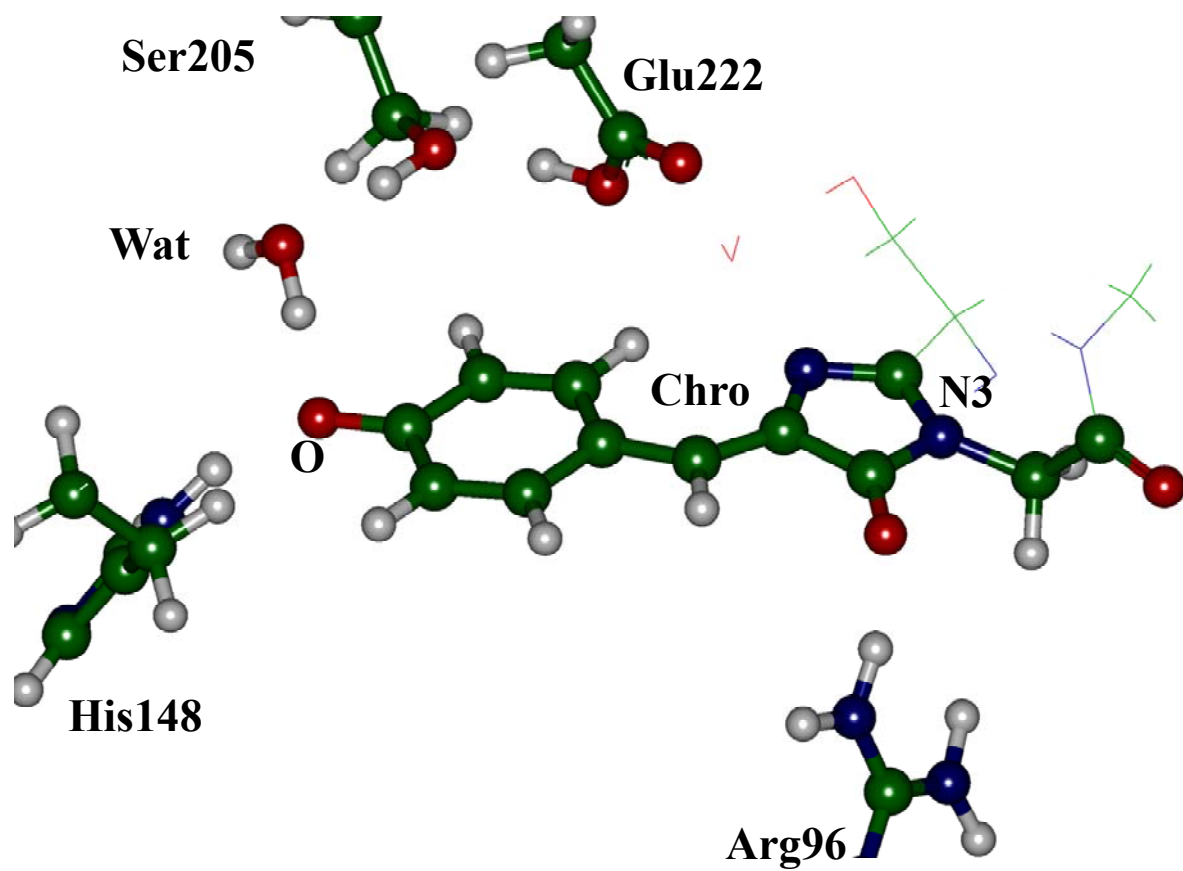
**Table S3.** Cartesian coordinates (Å) of the KFP chromophore in the ground  $S_0$  state optimized in the QM(PBE0/cc-pVDZ)/MM(AMBER) calculations.

C 58.8120 71.7570 -1.2300  
 N 58.2300 72.7920 -0.6630  
 N 58.0190 71.2120 -2.2300  
 C 56.8590 71.9640 -2.3280  
 O 55.9470 71.6870 -3.1250  
 C 57.0390 73.0110 -1.3340  
 C 56.3650 74.2300 -1.1350  
 H 56.8460 74.8190 -0.3500  
 C 55.3220 74.8800 -1.8040  
 C 55.1170 76.2800 -1.5500  
 H 55.7200 76.7610 -0.7760  
 C 54.4840 74.2810 -2.8010  
 H 54.5880 73.2110 -2.9780  
 C 54.2360 77.0370 -2.2670  
 H 54.1120 78.1070 -2.0850  
 C 53.5900 75.0210 -3.5140  
 H 52.9460 74.5780 -4.2730  
 C 53.4450 76.4440 -3.3220  
 O 52.6610 77.1180 -4.0470  
 O 60.6430 70.4190 -1.7150  
 C 60.1710 71.2710 -0.9600

C 60.9520 71.8280 0.1900  
H 61.9940 71.9140 -0.1460  
H 60.5830 72.8200 0.4740  
C 60.9010 70.9240 1.3860  
H 59.8580 70.8210 1.7000  
H 61.2700 69.9320 1.1070  
S 61.8520 71.5120 2.8100  
C 63.4980 70.9220 2.3600  
H 63.4950 69.8340 2.3060  
H 63.7990 71.3280 1.3940  
H 64.2120 71.2360 3.1210  
C 58.2880 70.1330 -3.1470  
H 57.4400 70.1130 -3.8490  
H 59.2080 70.3100 -3.7130  
C 58.3980 68.7610 -2.5080  
O 58.9100 67.8280 -3.1110

**Table S4.** Cartesian coordinates (Å) of the GFP chromophore in the ground  $S_0$  state optimized in the QM(PBE0/6-31G\*)/MM(AMBER) calculations.

C 25.1520 26.6260 36.4550  
C 25.9820 27.0850 37.6110  
N 27.2210 27.4630 37.5280  
C 27.6300 27.7280 38.8320  
C 28.7850 28.2990 39.2850  
H 28.8120 28.3760 40.3730  
C 29.9090 28.8900 38.6190  
C 30.0890 28.9620 37.2190  
H 29.3710 28.4700 36.5710  
C 30.8930 29.5230 39.4150  
H 30.7740 29.4870 40.4940  
C 31.1740 29.6210 36.6700  
H 31.2980 29.6370 35.5900  
C 31.9730 30.1820 38.8760  
H 32.7210 30.6340 39.5210  
C 32.1750 30.2520 37.4710  
O 33.2340 30.8190 36.9700  
C 26.5120 27.4500 39.7380  
O 26.3960 27.5710 40.9630  
N 25.4940 27.0520 38.9090  
C 24.1340 26.9580 39.3910  
H 23.9440 27.7550 40.1000  
H 23.4330 27.0920 38.5770  
C 23.8020 25.6450 40.0500  
O 22.9580 25.5520 40.9440  
N 24.4760 24.6220 39.5180



**Figure S1.** A part of the model system for the chromophore containing pocket of GFP.