

Supporting Information for Conical Intersection Dynamics in Solution: The Chromophore of Green Fluorescent Protein

A. Toniolo, S. Olsen, L. Manohar, and T. J. Martínez
Department of Chemistry
University of Illinois
Urbana, IL 61801

This document contains detailed information about the calculations reported in the accompanying paper. Unless otherwise specified, all *ab initio* calculations used the 6-31G basis set,¹ a SA-2-CAS(2/2) electronic wave function and the MOLPRO 2000.1 program.² The SA-2-CAS(2/2) wave function refers to a state-averaged CASSCF, equally weighting S_0 and S_1 .^{3,4} Semiempirical R-AM1-FOMO-CASCI(12/8) calculations were carried out using a development version of the MOPAC 2000 program.⁵ Coordinates are in Å unless otherwise specified.

References

- (1) Hehre, W. J., R. Ditchfield, R., Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257.
- (2) MOLPRO is a package of *ab initio* programs written by H.-J. Werner and P. J. Knowles, with contributions from R. D. Amos, A. Bernhardsson, A. Berning, P. Celani, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, C. Hampel, G. Hetzer, T. Korona, R. Lindh, A. W. Lloyd, S. J. McNicholas, F. R. Manby, W. Meyer, M. E. Mura, A. Nicklass, P. Palmieri, R. Pitzer, G. Rauhut, M. Schütz, H. Stoll, A. J. Stone, R. Tarroni, and T. Thorsteinsson.
- (3) Knowles, P. J.; Werner, H. J. *Chem. Phys. Lett.* **1985**, *115*, 259.
- (4) Werner, H. J.; Knowles, P. J. *J. Chem. Phys.* **1985**, *82*, 5053.
- (5) Stewart, J. J. P. MOPAC 2000; Fujitsu Limited: Tokyo, Japan, 1999.

I. Cartesian coordinates of structures along coordinate driving path in Figure 2a (neutral protonation state). In all cases, the I- and P-bond dihedral angles are fixed at the stated values and all other coordinates are optimized to minimize the energy on S₁.

R-AMI-FOMO-CAS(12/8)

I=0°

1	H	0.0000	0.0000	0.0000
2	C	1.1302	0.0000	0.0000
3	C	1.6505	1.3017	0.0000
4	C	1.7334	-1.2304	0.0000
5	C	3.1324	-1.4505	0.0000
6	C	3.6560	-2.7074	0.0000
7	C	2.8198	-3.8185	0.0000
8	O	3.2791	-5.1394	0.0000
9	C	1.4379	-3.6507	0.0000
10	C	0.9105	-2.3976	0.0000
11	H	3.8355	-0.5810	0.0000
12	H	4.7664	-2.8519	0.0000
13	H	0.7743	-4.5524	0.0000
14	H	-0.2017	-2.2641	0.0000
15	N	2.9807	1.6842	0.0000
16	C	3.0323	3.0248	0.0000
17	H	3.9805	3.6236	0.0000
18	N	1.7817	3.5837	0.0000
19	H	1.5580	4.5325	0.0000
20	C	0.8249	2.4975	0.0000
21	O	-0.4185	2.6911	0.0000
22	H	4.2734	-5.0324	0.0000

I=5°

1	H	0.0000	0.0000	0.0000
2	C	1.1302	0.0000	0.0000
3	C	1.6532	1.3005	0.0000
4	C	1.7344	-1.2296	-0.0301
5	C	3.1325	-1.4506	-0.0046
6	C	3.6606	-2.7041	-0.0747
7	C	2.8264	-3.8133	-0.1669
8	O	3.2882	-5.1312	-0.2440
9	C	1.4448	-3.6464	-0.1782
10	C	0.9146	-2.3966	-0.1058
11	H	3.8327	-0.5829	0.0820
12	H	4.7709	-2.8470	-0.0523
13	H	0.7829	-4.5469	-0.2450
14	H	-0.1978	-2.2653	-0.1130
15	N	2.9781	1.6809	-0.1276
16	C	3.0415	3.0179	-0.0417
17	H	3.9904	3.6133	-0.0944
18	N	1.8019	3.5783	0.1189
19	H	1.5878	4.5253	0.2063
20	C	0.8429	2.4950	0.1659
21	O	-0.3931	2.6906	0.3008
22	H	4.2821	-5.0233	-0.2234

I=10°

1	H	0.0000	0.0000	0.0000
2	C	1.1301	0.0000	0.0000
3	C	1.6597	1.2982	0.0000
4	C	1.7366	-1.2283	-0.0552
5	C	3.1345	-1.4434	-0.0113
6	C	3.6714	-2.6886	-0.1423
7	C	2.8455	-3.7946	-0.3082
8	O	3.3156	-5.1044	-0.4505
9	C	1.4627	-3.6347	-0.3246
10	C	0.9242	-2.3932	-0.1918
11	H	3.8265	-0.5788	0.1459
12	H	4.7819	-2.8270	-0.1064
13	H	0.8069	-4.5341	-0.4449
14	H	-0.1889	-2.2672	-0.2023
15	N	2.9688	1.6753	-0.2485
16	C	3.0612	3.0035	-0.0896
17	H	4.0096	3.5919	-0.1969
18	N	1.8506	3.5646	0.2227
19	H	1.6606	4.5064	0.3877
20	C	0.8890	2.4870	0.3174
21	O	-0.3257	2.6843	0.5822
22	H	4.3086	-4.9925	-0.4151

I=20°

1	H	0.0000	0.0000	0.0000
2	C	1.1302	0.0000	0.0000
3	C	1.6792	1.2921	0.0000
4	C	1.7414	-1.2246	-0.0981
5	C	3.1422	-1.4211	-0.0492
6	C	3.6996	-2.6494	-0.2534
7	C	2.8933	-3.7510	-0.4967
8	O	3.3805	-5.0437	-0.7192
9	C	1.5070	-3.6106	-0.5106
10	C	0.9498	-2.3871	-0.3034
11	H	3.8153	-0.5577	0.1804
12	H	4.8120	-2.7727	-0.2123
13	H	0.8656	-4.5106	-0.6886
14	H	-0.1655	-2.2781	-0.3112
15	N	2.9266	1.6679	-0.4750
16	C	3.1064	2.9672	-0.2012
17	H	4.0419	3.5418	-0.4262
18	N	2.0019	3.5168	0.3999
19	H	1.8912	4.4368	0.7018
20	C	1.0424	2.4515	0.5893
21	O	-0.0888	2.6398	1.1114
22	H	4.3720	-4.9225	-0.6731

I=30°

1	H	0.0000	0.0000	0.0000
2	C	1.1310	0.0000	0.0000
3	C	1.7039	1.2867	0.0000
4	C	1.7421	-1.2196	-0.1592
5	C	3.1478	-1.3944	-0.1631
6	C	3.7155	-2.6037	-0.4427
7	C	2.9186	-3.7027	-0.7114
8	O	3.4123	-4.9768	-1.0103
9	C	1.5280	-3.5824	-0.6758
10	C	0.9625	-2.3789	-0.3940
11	H	3.8105	-0.5286	0.0887
12	H	4.8307	-2.7103	-0.4436
13	H	0.8949	-4.4835	-0.8755
14	H	-0.1544	-2.2855	-0.3617
15	N	2.8386	1.6820	-0.6989
16	C	3.1473	2.9276	-0.3205
17	H	4.0482	3.4948	-0.6676
18	N	2.2398	3.4219	0.5874
19	H	2.2626	4.2908	1.0277
20	C	1.2963	2.3659	0.8656
21	O	0.3282	2.5040	1.6637
22	H	4.4039	-4.8466	-0.9904

I=45°

1	H	0.0000	0.0000	0.0000
2	C	1.1359	0.0000	0.0000
3	C	1.7354	1.2761	0.0000
4	C	1.7124	-1.2131	-0.3247
5	C	3.1007	-1.3593	-0.5328
6	C	3.6263	-2.5246	-1.0134
7	C	2.7980	-3.6002	-1.2903
8	O	3.2460	-4.8246	-1.7889
9	C	1.4252	-3.5023	-1.0606
10	C	0.9031	-2.3440	-0.5750
11	H	3.7804	-0.5021	-0.2906
12	H	4.7305	-2.6130	-1.1800
13	H	0.7693	-4.3844	-1.2730
14	H	-0.1990	-2.2673	-0.3810
15	N	2.5627	1.7901	-1.0132
16	C	3.1850	2.8543	-0.5238
17	H	3.9487	3.4542	-1.0791
18	N	2.8438	3.0951	0.7944
19	H	3.1964	3.7921	1.3744
20	C	1.9564	2.0407	1.1957
21	O	1.4682	1.9437	2.3610
22	H	4.2332	-4.6888	-1.8824

I=60°

1	H	0.0000	0.0000	0.0000
2	C	1.1392	0.0000	0.0000
3	C	1.7607	1.2477	0.0000
4	C	1.6873	-1.2435	-0.3238
5	C	3.0277	-1.3839	-0.7150
6	C	3.5055	-2.5655	-1.2089
7	C	2.6555	-3.6627	-1.3125
8	O	3.2226	-4.8269	-1.8296
9	C	1.3309	-3.5608	-0.9098
10	C	0.8601	-2.3802	-0.4155
11	H	3.7135	-0.5012	-0.6197
12	H	4.5735	-2.6636	-1.5299
13	H	2.4653	-5.4819	-1.8186
14	H	0.6522	-4.4486	-0.9864
15	H	-0.2076	-2.2998	-0.0812
16	N	2.3560	1.8644	-1.1368
17	C	3.1358	2.8278	-0.6877
18	H	3.7682	3.4830	-1.3370
19	N	3.1500	2.8989	0.6981
20	H	3.6605	3.5167	1.2483
21	C	2.3295	1.8306	1.1782
22	O	2.1486	1.5732	2.4077

I=75°

1	H	0.0000	0.0000	0.0000
2	C	1.1392	0.0000	0.0000
3	C	1.7903	1.2211	0.0000
4	C	1.7015	-1.2701	-0.2022
5	C	3.0736	-1.4335	-0.4402
6	C	3.6026	-2.6562	-0.7469
7	C	2.7693	-3.7684	-0.8148
8	O	3.3864	-4.9756	-1.1350
9	C	1.4079	-3.6374	-0.5694
10	C	0.8880	-2.4141	-0.2626
11	H	3.7385	-0.5309	-0.3775
12	H	4.6985	-2.7751	-0.9424
13	H	2.6322	-5.6347	-1.1298
14	H	0.7406	-4.5355	-0.6198
15	H	-0.2101	-2.3075	-0.0579
16	N	2.2441	1.8709	-1.1953
17	C	2.9700	2.8954	-0.8018
18	H	3.4899	3.6031	-1.4943
19	N	3.0698	2.9845	0.5815
20	H	3.5538	3.6567	1.0899
21	C	2.3527	1.8754	1.1288
22	O	2.2675	1.6218	2.3705

I=90°

1	H	0.0000	0.0000	0.0000
2	C	1.1392	0.0000	0.0000
3	C	1.8039	1.2094	0.0000
4	C	1.7136	-1.2825	-0.0094
5	C	3.1050	-1.4542	-0.0203
6	C	3.6670	-2.7007	-0.0443
7	C	2.8469	-3.8245	-0.0552
8	O	3.4975	-5.0555	-0.0800
9	C	1.4641	-3.6815	-0.0419
10	C	0.9115	-2.4346	-0.0164
11	H	3.7551	-0.5382	-0.0077
12	H	4.7791	-2.8292	-0.0524
13	H	2.7474	-5.7194	-0.0783
14	H	0.8069	-4.5883	-0.0492
15	H	-0.2044	-2.3158	-0.0031
16	N	2.1705	1.8974	-1.2077
17	C	2.7360	3.0206	-0.8235
18	H	3.1439	3.7930	-1.5217
19	N	2.7894	3.1519	0.5601
20	H	3.1572	3.8994	1.0606
21	C	2.1944	1.9800	1.1222
22	O	2.0915	1.7546	2.3683

SA-2-CAS(2/2)/6-31G

I=0°

H	0.28100	0.00000	-2.53000
C	0.28100	0.00000	-1.46700
N	1.35900	0.00000	-0.69900
N	-0.84100	0.00000	-0.69800
C	-0.47300	0.00000	0.64800
O	-1.26100	0.00000	1.62500
C	0.93600	0.00000	0.58900
H	-1.78100	0.00000	-1.01100
C	1.77000	0.00000	1.80900
H	1.18600	0.00000	2.71100
C	3.13200	0.00000	1.91200
C	4.00600	0.00000	0.76600
H	3.56800	0.00000	-0.20900
C	3.75600	0.00000	3.21600
H	3.12600	0.00000	4.08500
C	5.36900	0.00000	0.92900
H	6.01200	0.00000	0.06900
C	5.10500	0.00000	3.35700
H	5.57900	0.00000	4.31700
C	5.92300	0.00000	2.20800
O	7.26200	0.00000	2.42600
H	7.80800	0.00000	1.64800

I=15°

H	0.28000	0.03300	-2.52900
C	0.28000	0.03300	-1.46600
N	1.35800	0.03300	-0.69900
N	-0.84100	0.00500	-0.69700
C	-0.47200	-0.02700	0.64900
O	-1.26100	-0.04800	1.62600
C	0.93500	0.00600	0.58900
H	-1.78100	-0.01000	-1.01000
C	1.78200	-0.04900	1.80300
H	1.26500	0.23900	2.70000
C	3.10900	-0.36200	1.89000
C	3.89600	-0.75000	0.74900
H	3.42400	-0.78400	-0.20900
C	3.78000	-0.31200	3.16700
H	3.21300	-0.02900	4.03300
C	5.23000	-1.04500	0.88800
H	5.81000	-1.32900	0.03100
C	5.10000	-0.60700	3.28700
H	5.60900	-0.57000	4.22800
C	5.83400	-0.97600	2.14300
O	7.14600	-1.25500	2.33800
H	7.63900	-1.50100	1.56300

I=30°

H	0.28200	0.08500	-2.52600
C	0.28200	0.08500	-1.46200
N	1.35800	0.08500	-0.70400
N	-0.84200	0.01500	-0.69800
C	-0.47100	-0.06700	0.64800
O	-1.25900	-0.17200	1.61900
C	0.93200	0.05500	0.59500
H	-1.78000	-0.02800	-1.01200
C	1.79900	-0.21900	1.77200
H	1.64200	0.41000	2.63200
C	2.92100	-1.01000	1.78100
C	3.31300	-1.79800	0.65200
H	2.71200	-1.76500	-0.22900
C	3.76200	-1.05800	2.94600
H	3.48200	-0.48000	3.80700
C	4.46200	-2.55200	0.68800
H	4.75300	-3.13300	-0.16500
C	4.89800	-1.80400	2.97000
H	5.53800	-1.84300	3.82600
C	5.25200	-2.55700	1.83600
O	6.39700	-3.27300	1.92900
H	6.63700	-3.77900	1.15900

I=45°

H	0.29500	0.11700	-2.52000
C	0.29500	0.11700	-1.45500
N	1.35900	0.11700	-0.71100
N	-0.84500	0.02900	-0.69600
C	-0.47700	-0.09000	0.64300
O	-1.26100	-0.28000	1.60100
C	0.93100	0.10800	0.61800
H	-1.78000	-0.01700	-1.01800
C	1.74300	-0.41000	1.72900
H	2.06900	0.29600	2.48000
C	2.45800	-1.59900	1.72300
C	2.34900	-2.52600	0.65200
H	1.69200	-2.30100	-0.16000
C	3.36400	-1.90100	2.78300
H	3.45000	-1.21400	3.60300
C	3.11100	-3.67000	0.63500
H	3.03600	-4.36100	-0.18300
C	4.12300	-3.03300	2.76200
H	4.81600	-3.27300	3.54000
C	3.99300	-3.92200	1.68400
O	4.77700	-5.02100	1.72100
H	4.69000	-5.62600	0.99200

I=60°

H	0.31100	0.09700	-2.52100
C	0.31100	0.09700	-1.45600
N	1.36900	0.09700	-0.71200
N	-0.83500	0.02700	-0.69800
C	-0.48300	-0.07500	0.64800
O	-1.28500	-0.24400	1.59900
C	0.92300	0.09600	0.62000
H	-1.77000	0.00400	-1.02100
C	1.76500	-0.35800	1.71200
H	2.20900	0.38300	2.36600
C	2.30900	-1.62900	1.84000
C	1.99900	-2.65400	0.90900
H	1.32800	-2.43100	0.10700
C	3.22900	-1.92300	2.88900
H	3.46500	-1.15700	3.60200
C	2.57800	-3.89400	1.01400
H	2.35200	-4.66500	0.30400
C	3.80800	-3.15200	2.99400
H	4.50400	-3.39600	3.76800
C	3.47800	-4.14100	2.05400
O	4.08700	-5.33200	2.20700
H	3.86300	-6.00900	1.57700

I=75°

H	0.32500	0.05600	-2.52400
C	0.32500	0.05600	-1.45900
N	1.37900	0.05600	-0.71100
N	-0.82500	0.01600	-0.70000
C	-0.48700	-0.04000	0.65400
O	-1.30700	-0.14500	1.60400
C	0.91400	0.05800	0.61200
H	-1.76000	0.01200	-1.02400
C	1.80000	-0.18500	1.72500
H	2.21300	0.65800	2.26700
C	2.31400	-1.41900	2.09200
C	1.94800	-2.59700	1.38900
H	1.26600	-2.50600	0.57000
C	3.23300	-1.53200	3.17500
H	3.51300	-0.64700	3.71400
C	2.47000	-3.81400	1.74500
H	2.19700	-4.70400	1.21300
C	3.75600	-2.73900	3.53000
H	4.45000	-2.85300	4.33700
C	3.36900	-3.88300	2.81300
O	3.92100	-5.04300	3.20800
H	3.65900	-5.82500	2.73400

I=90°

H	0.33100	0.00900	-2.52500
C	0.33100	0.00900	-1.46000
N	1.38400	0.00900	-0.71000
N	-0.82000	0.00000	-0.70200
C	-0.48900	-0.00100	0.65400
O	-1.31600	-0.01900	1.60700
C	0.91100	0.00400	0.60900
H	-1.75500	0.00900	-1.02800
C	1.79900	0.04100	1.74100
H	2.10500	1.00000	2.14600
C	2.33500	-1.06200	2.38500
C	2.00800	-2.37800	1.96100
H	1.34300	-2.48600	1.13000
C	3.21400	-0.90500	3.49700
H	3.46000	0.08600	3.82800
C	2.53200	-3.46900	2.60200
H	2.28500	-4.46300	2.28500
C	3.73800	-1.98700	4.13700
H	4.39900	-1.90000	4.97200
C	3.39400	-3.27300	3.68700
O	3.94000	-4.29900	4.35900
H	3.70500	-5.17500	4.06900

II. Cartesian coordinates of structures along coordinate driving path in Figure 2b (anion protonation state, driving the I-bond torsional angle). In all cases, the I-bond dihedral angle is fixed at the stated values, the P-bond dihedral is fixed at 0°, and all other coordinates are optimized to minimize the energy on S₁.

R-AMI-FOMO-CAS(12/8)

I=0°

1	H	0.0000	0.0000	0.0000
2	C	1.1261	0.0000	0.0000
3	C	1.6722	1.2441	0.0000
4	C	1.7169	-1.3029	-0.0001
5	C	3.0833	-1.5480	-0.0001
6	C	3.5908	-2.8256	-0.0005
7	C	2.7458	-3.9654	0.0025
8	O	3.2133	-5.1717	0.0048
9	C	1.3513	-3.6989	0.0024
10	C	0.8731	-2.4149	0.0008
11	H	3.8124	-0.6998	-0.0009
12	H	4.6976	-2.9808	-0.0017
13	H	0.6390	-4.5599	0.0037
14	H	-0.2369	-2.2570	0.0009
15	N	3.0312	1.6074	-0.0001
16	C	3.1132	2.9231	-0.0001
17	H	4.0612	3.5118	-0.0005
18	N	1.8586	3.5326	-0.0005
19	H	1.6785	4.4848	-0.0009
20	C	0.8876	2.4884	-0.0002
21	O	-0.3569	2.7372	0.0002

I=15°

1	H	0.0000	0.0000	0.0000
2	C	1.1262	0.0000	0.0000
3	C	1.6727	1.2456	0.0000
4	C	1.7151	-1.2953	0.1461
5	C	3.0722	-1.5242	0.3301
6	C	3.5823	-2.7935	0.4597
7	C	2.7488	-3.9415	0.4210
8	O	3.2178	-5.1399	0.5457
9	C	1.3629	-3.6910	0.2362
10	C	0.8829	-2.4149	0.1034
11	H	3.7894	-0.6672	0.3799
12	H	4.6823	-2.9364	0.5960
13	H	0.6602	-4.5590	0.1987
14	H	-0.2192	-2.2692	-0.0425
15	N	3.0253	1.6071	-0.1372
16	C	3.1075	2.9224	-0.1567
17	H	4.0523	3.5102	-0.2415
18	N	1.8587	3.5334	-0.0417
19	H	1.6794	4.4856	-0.0374
20	C	0.8914	2.4898	0.0557
21	O	-0.3479	2.7399	0.1648

I=30°

1	H	0.0000	0.0000	0.0000
2	C	1.1289	0.0000	0.0000
3	C	1.6562	1.3349	0.0000
4	C	1.7394	-1.1906	-0.2248
5	C	3.1187	-1.3569	-0.5254
6	C	3.6641	-2.5577	-0.8074
7	C	2.9035	-3.7652	-0.8179
8	O	3.4113	-4.9086	-1.0874
9	C	1.5119	-3.5989	-0.4964
10	C	0.9841	-2.3959	-0.2163
11	H	3.7813	-0.4548	-0.5226
12	H	4.7550	-2.6294	-1.0444
13	H	0.8678	-4.5128	-0.4861
14	H	-0.1095	-2.3208	0.0274
15	N	2.7107	1.8187	-0.7385
16	C	3.0659	3.0119	-0.2624
17	H	3.9411	3.6061	-0.6195
18	N	2.2899	3.3821	0.8218
19	H	2.3848	4.1841	1.3593
20	C	1.3718	2.3003	1.0621
21	O	0.5064	2.3696	1.9834

I=45°

1	H	0.0000	0.0000	0.0000
2	C	1.1317	0.0000	0.0000
3	C	1.6503	1.3264	0.0000
4	C	1.7131	-1.1626	-0.4089
5	C	3.0221	-1.2596	-0.9405
6	C	3.5417	-2.4133	-1.4041
7	C	2.8089	-3.6407	-1.3913
8	O	3.2933	-4.7422	-1.8303
9	C	1.4850	-3.5410	-0.8484
10	C	0.9856	-2.3820	-0.3874
11	H	3.6528	-0.3332	-0.9713
12	H	4.5781	-2.4303	-1.8233
13	H	0.8655	-4.4716	-0.8176
14	H	-0.0575	-2.3585	0.0266
15	N	2.3406	1.9622	-1.0162
16	C	2.9897	3.0102	-0.5297
17	H	3.6800	3.6679	-1.1148
18	N	2.7998	3.1541	0.8331
19	H	3.2018	3.8230	1.4112
20	C	1.9783	2.0462	1.2522
21	O	1.5979	1.9440	2.4491

I=60°

1	H	0.0000	0.0000	0.0000
2	C	1.1281	0.0000	0.0000
3	C	1.6581	1.3102	0.0000
4	C	1.7357	-1.1645	-0.3749
5	C	3.0655	-1.2430	-0.8482
6	C	3.6317	-2.3949	-1.2577
7	C	2.9281	-3.6386	-1.2434
8	O	3.4578	-4.7412	-1.6315
9	C	1.5819	-3.5562	-0.7643
10	C	1.0346	-2.3962	-0.3572
11	H	3.6687	-0.2980	-0.8820
12	H	4.6854	-2.3967	-1.6315
13	H	0.9812	-4.4989	-0.7356
14	H	-0.0264	-2.3882	0.0088
15	N	2.1399	2.0188	-1.0880
16	C	2.8402	3.0614	-0.6711
17	H	3.4016	3.7693	-1.3334
18	N	2.8933	3.1413	0.7097
19	H	3.3773	3.7974	1.2371
20	C	2.1685	2.0033	1.2170
21	O	2.0056	1.8452	2.4525

I=75°

1	H	0.0000	0.0000	0.0000
2	C	1.1242	0.0000	0.0000
3	C	1.6729	1.2969	0.0000
4	C	1.7704	-1.1830	-0.2154
5	C	3.1559	-1.2769	-0.4831
6	C	3.7813	-2.4492	-0.7123
7	C	3.0890	-3.6964	-0.7037
8	O	3.6743	-4.8197	-0.9227
9	C	1.6871	-3.5985	-0.4340
10	C	1.0803	-2.4187	-0.2050
11	H	3.7497	-0.3253	-0.5065
12	H	4.8792	-2.4625	-0.9235
13	H	1.0928	-4.5454	-0.4177
14	H	-0.0229	-2.4002	0.0012
15	N	2.0582	2.0355	-1.1051
16	C	2.6853	3.1339	-0.7156
17	H	3.1461	3.8954	-1.3959
18	N	2.7716	3.2298	0.6626
19	H	3.2081	3.9316	1.1720
20	C	2.1375	2.0523	1.2014
21	O	2.0276	1.8950	2.4411

I=90°

1	H	0.0000	0.0000	0.0000
2	C	1.1230	0.0000	0.0000
3	C	1.6742	1.2938	0.0000
4	C	1.7841	-1.1930	-0.0179
5	C	3.1957	-1.2969	-0.0401
6	C	3.8435	-2.4802	-0.0574
7	C	3.1530	-3.7262	-0.0547
8	O	3.7590	-4.8606	-0.0736
9	C	1.7255	-3.6181	-0.0302
10	C	1.0961	-2.4281	-0.0114
11	H	3.7890	-0.3450	-0.0475
12	H	4.9614	-2.5013	-0.0755
13	H	1.1318	-4.5655	-0.0277
14	H	-0.0260	-2.4024	0.0086
15	N	1.9807	2.0604	-1.1102
16	C	2.4803	3.2250	-0.7278
17	H	2.8316	4.0386	-1.4122
18	N	2.5403	3.3457	0.6495
19	H	2.8835	4.1001	1.1548
20	C	2.0155	2.1194	1.1974
21	O	1.9212	1.9624	2.4380

SA-2-CAS(2/2)/6-3IG

I=0°

N	.000000	.000000	.000000
H	.000000	.000000	.988544
C	.000000	1.102465	-.839431
H	.000062	2.103225	-.474608
N	.000308	.753670	-2.088464
C	-.000220	-.651381	-2.141498
C	-.000223	-1.153492	-.764207
O	-.000397	-2.315071	-.314779
C	-.000322	-1.455788	-3.239859
H	-.000728	-2.513879	-3.063577
C	.000118	-1.018422	-4.684396
C	-.000151	.325704	-5.104103
H	-.000762	1.092846	-4.359608
C	.000211	.655610	-6.440855
H	.000163	1.683599	-6.749315
C	.001047	-.335376	-7.473988
C	.001499	-1.698102	-7.017651
H	.002168	-2.467312	-7.766089
C	.000964	-2.009219	-5.678236
H	.001260	-3.042270	-5.378548
O	.002291	-.044243	-8.711890

I=15°

N	.000000	.000000	.000000
H	.000000	.000000	.988780
C	.000000	1.082803	-.835481
H	.009449	2.093135	-.502551
N	-.029097	.692534	-2.095147
C	-.066641	-.665890	-2.115426
C	-.066894	-1.159690	-.771906
O	-.082359	-2.326860	-.315672
C	-.150477	-1.556992	-3.306455
H	.129505	-2.573903	-3.108059
C	-.487787	-1.198308	-4.582032
C	-.831098	.143695	-5.009258
H	-.796163	.923765	-4.279154
C	-1.170250	.422023	-6.295641
H	-1.416516	1.425009	-6.589831
C	-1.212839	-.580624	-7.330675
C	-.859615	-1.923900	-6.902666
H	-.876151	-2.688174	-7.656808
C	-.524759	-2.208218	-5.627208
H	-.270703	-3.216567	-5.350701
O	-1.524395	-.325658	-8.525006

I=30°

N	.000000	.000000	.000000
H	.000000	.000000	.989103
C	.000000	1.071741	-.846813
H	.068474	2.084054	-.525544
N	-.120724	.679213	-2.097539
C	-.245870	-.678649	-2.106378
C	-.223225	-1.157484	-.754539
O	-.300248	-2.308693	-.276339
C	-.569164	-1.542429	-3.280609
H	-.000376	-2.452987	-3.348188
C	-1.332953	-1.176095	-4.362932
C	-1.951799	.115146	-4.540915
H	-1.785355	.858466	-3.790226
C	-2.698846	.412379	-5.637454
H	-3.138774	1.385172	-5.751981
C	-2.927225	-.528498	-6.705143
C	-2.289325	-1.820579	-6.532450
H	-2.429445	-2.535929	-7.320928
C	-1.550679	-2.117785	-5.441334
H	-1.096021	-3.088994	-5.350922
O	-3.615391	-.257044	-7.725414

I=45°

N	.000000	.000000	.000000
H	.000000	.000000	.989219
C	.000000	1.062214	-.864943
H	.069053	2.075185	-.541561
N	-.124786	.688193	-2.104909
C	-.256493	-.694470	-2.127123
C	-.239987	-1.161173	-.745303
O	-.322328	-2.290369	-.257636
C	-.726298	-1.497233	-3.253439
H	.046837	-1.926735	-3.874126
C	-1.975111	-1.316967	-3.879599
C	-2.932860	-.334267	-3.495799
H	-2.691694	.325731	-2.685207
C	-4.123223	-.181393	-4.144569
H	-4.816881	.581811	-3.845228
C	-4.501241	-.997400	-5.267342
C	-3.518166	-1.979165	-5.660484
H	-3.759302	-2.595052	-6.506591
C	-2.338013	-2.123229	-5.002718
H	-1.637324	-2.873083	-5.329263
O	-5.600269	-.858144	-5.878247

I=60°

N	.000000	.000000	.000000
H	.000000	.000000	.989202
C	.000000	1.064400	-.862276
H	.066842	2.076301	-.534893
N	-.116698	.695042	-2.104062
C	-.244616	-.688201	-2.131310
C	-.227718	-1.160912	-.749635
O	-.303934	-2.291324	-.266926
C	-.683193	-1.486063	-3.269763
H	.104298	-1.883736	-3.892692
C	-1.943203	-1.344696	-3.888701
C	-2.937229	-.410682	-3.480752
H	-2.719777	.242268	-2.657255
C	-4.137498	-.293910	-4.119913
H	-4.860247	.433391	-3.800512
C	-4.488594	-1.101644	-5.256758
C	-3.468927	-2.033607	-5.673648
H	-3.689280	-2.642882	-6.530202
C	-2.279100	-2.142150	-5.024448
H	-1.550896	-2.856745	-5.369634
O	-5.597124	-.995144	-5.858990

I=75°

N	.000000	.000000	.000000
H	.000000	.000000	.989033
C	.000000	1.077118	-.845600
H	.032829	2.083765	-.496892
N	-.054207	.729458	-2.097646
C	-.123576	-.656470	-2.152579
C	-.107147	-1.160266	-.776264
O	-.124410	-2.300437	-.320887
C	-.336110	-1.443309	-3.350499
H	.547282	-1.745867	-3.887277
C	-1.583348	-1.571161	-4.005844
C	-2.779889	-.942763	-3.568183
H	-2.744814	-.319183	-2.693213
C	-3.967297	-1.084320	-4.229556
H	-4.852554	-.588095	-3.877709
C	-4.096853	-1.874967	-5.422194
C	-2.876640	-2.497876	-5.863645
H	-2.929332	-3.091128	-6.757561
C	-1.700042	-2.350608	-5.190852
H	-.815712	-2.841877	-5.561597
O	-5.195644	-2.006415	-6.044359

I=90°

N	.000000	.000000	.000000
H	.000000	.000000	.988981
C	.000000	1.086600	-.833992
H	.002501	2.089079	-.471703
N	-.004033	.753619	-2.090416
C	-.015133	-.633414	-2.163518
C	.003222	-1.154481	-.791424
O	.035952	-2.299531	-.352172
C	-.019437	-1.401357	-3.389231
H	.942595	-1.665129	-3.792842
C	-1.180798	-1.821814	-4.077077
C	-2.504287	-1.539509	-3.645647
H	-2.643187	-.968050	-2.744892
C	-3.606993	-1.959693	-4.335026
H	-4.594547	-1.728216	-3.981578
C	-3.513742	-2.720241	-5.550228
C	-2.169623	-3.001918	-5.977569
H	-2.055888	-3.569636	-6.882366
C	-1.078231	-2.576269	-5.278226
H	-.092865	-2.815042	-5.643063
O	-4.534383	-3.112412	-6.197276

III. Cartesian coordinates of structures along coordinate driving path in Figure 2c (anion protonation state, driving the P-bond torsional angle). In all cases, the P-bond dihedral angle is fixed at the stated values, the I-bond dihedral is fixed at 0°, and all other coordinates are optimized to minimize the energy on S₁.

R-AMI-FOMO-CAS(12/8)

P=0°

1	H	0.0000	0.0000	0.0000
2	C	1.1261	0.0000	0.0000
3	C	1.6728	1.2437	0.0000
4	C	1.7172	-1.3028	0.0001
5	C	3.0838	-1.5477	0.0003
6	C	3.5911	-2.8254	-0.0012
7	C	2.7461	-3.9652	-0.0001
8	O	3.2136	-5.1714	0.0004
9	C	1.3514	-3.6989	-0.0001
10	C	0.8734	-2.4148	-0.0003
11	H	3.8131	-0.6997	0.0006
12	H	4.6978	-2.9808	-0.0020
13	H	0.6393	-4.5599	0.0000
14	H	-0.2366	-2.2570	-0.0007
15	N	3.0320	1.6062	0.0002
16	C	3.1148	2.9218	0.0005
17	H	4.0631	3.5101	0.0005
18	N	1.8606	3.5321	0.0003
19	H	1.6810	4.4844	0.0005
20	C	0.8889	2.4884	0.0001
21	O	-0.3555	2.7380	0.0003

P=15°

1	H	0.0000	0.0000	0.0000
2	C	1.1252	0.0000	0.0000
3	C	1.6822	1.2374	0.0000
4	C	1.7190	-1.3046	0.0078
5	C	3.0486	-1.5570	0.3140
6	C	3.5687	-2.8289	0.2856
7	C	2.7722	-3.9549	-0.0498
8	O	3.2506	-5.1557	-0.0753
9	C	1.4122	-3.6800	-0.3543
10	C	0.9256	-2.3992	-0.3351
11	H	3.7317	-0.7197	0.6040
12	H	4.6488	-2.9904	0.5230
13	H	0.7356	-4.5313	-0.6113
14	H	-0.1528	-2.2314	-0.5914
15	N	3.0468	1.5824	0.0080
16	C	3.1463	2.8968	-0.0040
17	H	4.1011	3.4733	0.0145
18	N	1.8998	3.5226	-0.0160
19	H	1.7323	4.4767	-0.0268
20	C	0.9150	2.4916	-0.0191
21	O	-0.3265	2.7584	-0.0325

P=30°

1	H	0.0000	0.0000	0.0000
2	C	1.1232	0.0000	0.0000
3	C	1.7060	1.2225	0.0000
4	C	1.7248	-1.3052	0.0707
5	C	2.9194	-1.5639	0.7261
6	C	3.4853	-2.8143	0.7278
7	C	2.8571	-3.9174	0.0870
8	O	3.3664	-5.1023	0.0988
9	C	1.6264	-3.6333	-0.5713
10	C	1.1126	-2.3644	-0.5934
11	H	3.4466	-0.7411	1.2723
12	H	4.4696	-2.9791	1.2306
13	H	1.0803	-4.4696	-1.0721
14	H	0.1521	-2.1812	-1.1416
15	N	3.0826	1.5197	0.0714
16	C	3.2249	2.8300	0.0335
17	H	4.1934	3.3776	0.0925
18	N	2.0027	3.4946	-0.0549
19	H	1.8689	4.4522	-0.0997
20	C	0.9849	2.4969	-0.0891
21	O	-0.2454	2.8086	-0.1703

P=45°

1	H	0.0000	0.0000	0.0000
2	C	1.1228	0.0000	0.0000
3	C	1.7265	1.2130	0.0000
4	C	1.7248	-1.2841	0.2478
5	C	2.6158	-1.5071	1.3007
6	C	3.2502	-2.7082	1.4608
7	C	2.9929	-3.8055	0.5953
8	O	3.5502	-4.9523	0.7472
9	C	2.0672	-3.5563	-0.4769
10	C	1.5074	-2.3265	-0.6420
11	H	2.8406	-0.6732	2.0126
12	H	4.0072	-2.8378	2.2736
13	H	1.8207	-4.3959	-1.1710
14	H	0.8185	-2.1616	-1.5124
15	N	3.0930	1.4711	0.2472
16	C	3.2832	2.7732	0.1655
17	H	4.2623	3.2918	0.2738
18	N	2.1122	3.4628	-0.1399
19	H	2.0197	4.4189	-0.2536
20	C	1.0733	2.4911	-0.2649
21	O	-0.1270	2.8408	-0.5121

P=60°

1	H	0.0000	0.0000	0.0000
2	C	1.1228	0.0000	0.0000
3	C	1.7390	1.2097	0.0000
4	C	1.7216	-1.2614	0.3152
5	C	2.3023	-1.5192	1.5672
6	C	2.9463	-2.6856	1.8315
7	C	3.0284	-3.7295	0.8597
8	O	3.5955	-4.8516	1.1020
9	C	2.4339	-3.4420	-0.4209
10	C	1.8448	-2.2485	-0.6636
11	H	2.2618	-0.7236	2.3540
12	H	3.4468	-2.8447	2.8194
13	H	2.4781	-4.2329	-1.2098
14	H	1.4177	-2.0511	-1.6818
15	N	3.0975	1.4413	0.3150
16	C	3.3214	2.7366	0.2176
17	H	4.3094	3.2324	0.3646
18	N	2.1841	3.4444	-0.1637
19	H	2.1173	4.4003	-0.3027
20	C	1.1296	2.4893	-0.3199
21	O	-0.0508	2.8611	-0.6340

P=75°

1	H	0.0000	0.0000	0.0000
2	C	1.1212	0.0000	0.0000
3	C	1.7498	1.2034	0.0000
4	C	1.7239	-1.2758	0.1978
5	C	2.1362	-1.7113	1.4691
6	C	2.7410	-2.9082	1.6562
7	C	2.9741	-3.8065	0.5633
8	O	3.5199	-4.9520	0.7260
9	C	2.5532	-3.3414	-0.7316
10	C	1.9753	-2.1295	-0.8854
11	H	1.9750	-1.0356	2.3477
12	H	3.0868	-3.2196	2.6738
13	H	2.7227	-4.0128	-1.6100
14	H	1.6749	-1.7957	-1.9125
15	N	3.1359	1.4023	0.1999
16	C	3.3684	2.6988	0.1362
17	H	4.3702	3.1782	0.2362
18	N	2.2116	3.4359	-0.1021
19	H	2.1459	4.3980	-0.1885
20	C	1.1325	2.4996	-0.1998
21	O	-0.0663	2.8982	-0.3977

P=90°

1	H	0.0000	0.0000	0.0000
2	C	1.1203	0.0000	0.0000
3	C	1.7557	1.1992	0.0000
4	C	1.7242	-1.2877	0.0093
5	C	2.0266	-1.9463	1.2133
6	C	2.5762	-3.1811	1.2386
7	C	2.8797	-3.8892	0.0259
8	O	3.3899	-5.0619	0.0339
9	C	2.5685	-3.2011	-1.1966
10	C	2.0192	-1.9660	-1.1855
11	H	1.8072	-1.4254	2.1806
12	H	2.8126	-3.6828	2.2104
13	H	2.7970	-3.7183	-2.1620
14	H	1.7929	-1.4604	-2.1594
15	N	3.1586	1.3801	0.0094
16	C	3.3950	2.6776	0.0066
17	H	4.4064	3.1472	0.0107
18	N	2.2252	3.4320	-0.0044
19	H	2.1589	4.3979	-0.0083
20	C	1.1321	2.5069	-0.0089
21	O	-0.0785	2.9212	-0.0171

SA-2-CAS(2/2)/6-31G

P=0°

N	.000000	.000000	.000000
H	.000000	.000000	.988544
C	.000000	1.102465	-.839431
H	.000062	2.103225	-.474608
N	.000308	.753670	-2.088464
C	-.000220	-.651381	-2.141498
C	-.000223	-1.153492	-.764207
O	-.000397	-2.315071	-.314779
C	-.000322	-1.455788	-3.239859
H	-.000728	-2.513879	-3.063577
C	.000118	-1.018422	-4.684396
C	-.000151	.325704	-5.104103
H	-.000762	1.092846	-4.359608
C	.000211	.655610	-6.440855
H	.000163	1.683599	-6.749315
C	.001047	-.335376	-7.473988
C	.001499	-1.698102	-7.017651
H	.002168	-2.467312	-7.766089
C	.000964	-2.009219	-5.678236
H	.001260	-3.042270	-5.378548
O	.002291	-.044243	-8.711890

P=15°

N	.000000	.000000	.000000
H	.000000	.000000	.988594
C	.000000	1.104063	-.837661
H	-.095231	2.101103	-.474804
N	.111749	.761225	-2.082318
C	.202934	-.641268	-2.134182
C	.129046	-1.148500	-.762922
O	.173660	-2.309296	-.312348
C	.373524	-1.432886	-3.229861
H	.356123	-2.493751	-3.070071
C	.505193	-.967758	-4.662112
C	.171358	.326528	-5.104023
H	-.201355	1.029298	-4.389789
C	.341718	.698986	-6.417515
H	.101072	1.694036	-6.739574
C	.853533	-.201541	-7.407249
C	1.202306	-1.510448	-6.926092
H	1.594977	-2.208401	-7.640549
C	1.047315	-1.855931	-5.604914
H	1.336687	-2.839468	-5.279998
O	1.004469	.126022	-8.625381

P=30°

N	.000000	.000000	.000000
H	.000000	.000000	.988921
C	.000000	1.116272	-.823791
H	-.233031	2.093003	-.467319
N	.286895	.809380	-2.046363
C	.509208	-.579274	-2.098875
C	.321633	-1.118353	-.758033
O	.428898	-2.277110	-.309852
C	.939793	-1.310296	-3.173043
H	.866958	-2.379850	-3.093862
C	1.262831	-.737585	-4.535581
C	.634695	.405386	-5.072047
H	-.147217	.867641	-4.507216
C	1.030779	.948066	-6.267275
H	.568573	1.838582	-6.647633
C	2.091678	.376526	-7.049775
C	2.748588	-.761839	-6.461003
H	3.558850	-1.199888	-7.011633
C	2.369171	-1.253475	-5.239033
H	2.908048	-2.077723	-4.808318
O	2.445827	.848779	-8.168774

P=45°

N	.000000	.000000	.000000
H	.000000	.000000	.989319
C	.000000	1.131679	-.805308
H	-.321710	2.085548	-.454941
N	.404489	.866574	-2.000573
C	.705086	-.508179	-2.055245
C	.451478	-1.082842	-.753345
O	.599446	-2.240342	-.306526
C	1.302258	-1.169759	-3.114391
H	1.128846	-2.233635	-3.163965
C	1.716146	-.476936	-4.377280
C	.892906	.459514	-5.056619
H	-.112318	.587104	-4.709815
C	1.356927	1.214451	-6.090972
H	.735990	1.950599	-6.563447
C	2.713373	1.095752	-6.571238
C	3.562884	.200520	-5.818905
H	4.587511	.124293	-6.127977
C	3.088475	-.488363	-4.742735
H	3.753478	-1.102468	-4.165052
O	3.139090	1.748537	-7.556968

P=60°

N	.000000	.000000	.000000
H	.000000	.000000	.988853
C	.000000	1.119154	-.818087
H	-.267198	2.090054	-.468064
N	.339370	.819223	-2.025976
C	.584580	-.565396	-2.065923
C	.379466	-1.110418	-.758090
O	.501501	-2.270242	-.291497
C	1.084620	-1.260262	-3.172797
H	.840138	-2.310431	-3.221701
C	1.411868	-.578943	-4.444441
C	.439558	.139047	-5.206104
H	-.581269	.083069	-4.884455
C	.777613	.901751	-6.273782
H	.044949	1.470963	-6.811772
C	2.153261	1.020097	-6.717125
C	3.141453	.351068	-5.893808
H	4.168958	.462935	-6.180607
C	2.778265	-.355288	-4.794138
H	3.525066	-.804729	-4.168613
O	2.470249	1.677124	-7.731915

P=75°

N	.000000	.000000	.000000
H	.000000	.000000	.988295
C	.000000	1.101236	-.836482
H	-.154243	2.096184	-.485764
N	.198634	.753804	-2.064864
C	.341670	-.643298	-2.088946
C	.221500	-1.149680	-.763894
O	.290391	-2.312551	-.279069
C	.635914	-1.392517	-3.238571
H	.469889	-2.454957	-3.197543
C	.826443	-.770048	-4.556425
C	-.272445	-.278789	-5.331261
H	-1.256767	-.411296	-4.928041
C	-.094382	.351781	-6.514683
H	-.919631	.737686	-7.080492
C	1.232340	.557423	-7.069981
C	2.343673	.095800	-6.257417
H	3.329329	.266431	-6.644074
C	2.137592	-.504740	-5.061644
H	2.967093	-.818248	-4.458842
O	1.406461	1.105972	-8.176120

P=90°

N	.000000	.000000	.000000
H	.000000	.000000	.988047
C	.000000	1.092339	-.845715
H	-.000717	2.099052	-.494584
N	.000023	.721907	-2.084297
C	.000805	-.681786	-2.102078
C	.001444	-1.169021	-.766580
O	.001810	-2.332960	-.274406
C	.001914	-1.458756	-3.269442
H	-.006389	-2.528805	-3.172099
C	-.011009	-.879103	-4.616893
C	-1.236514	-.594286	-5.299584
H	-2.148536	-.782208	-4.768300
C	-1.262842	-.103450	-6.559998
H	-2.183682	.108371	-7.067231
C	-.036401	.166708	-7.290664
C	1.203662	-.105475	-6.584200
H	2.114716	.104311	-7.109612
C	1.201225	-.595003	-5.322970
H	2.123034	-.784311	-4.809381
O	-.047466	.605143	-8.457271

IV. Twisted MECI geometries for neutral protonation state of GFP chromophore, as depicted in Figure 3. The R-AM1-FOMO-CASCI(12/8) structure labeled S_0/S_1 MECI in Figure 6 is the same as this one.

R-AM1-FOMO-CASCI(12/8)

N	0.628	1.797	3.443
N	0.846	2.224	1.231
H	0.514	1.984	4.390
H	0.515	3.829	2.581
H	2.394	-0.001	0.062
H	-1.352	-0.023	0.583
H	-2.913	-0.969	-1.149
H	0.479	-1.838	-3.731
H	2.029	-0.916	-1.981
H	-3.007	-1.934	-3.184
C	0.659	2.730	2.428
C	0.947	0.753	1.519
C	0.828	0.492	2.855
C	1.289	0.122	0.380
C	0.421	-0.432	-0.604
C	-0.963	-0.440	-0.386
C	-1.808	-0.953	-1.332
C	-1.296	-1.457	-2.522
C	0.085	-1.438	-2.762
C	0.917	-0.938	-1.811
O	0.852	-0.588	3.522
O	-2.068	-2.000	-3.531

SA-2-CAS(2/2)/6-31G

N	0.713	1.692	3.447
N	0.747	2.418	1.377
H	0.713	1.692	4.436
H	0.675	3.798	2.952
H	2.238	0.157	0.076
H	-1.375	0.246	0.391
H	-2.920	-0.878	-1.265
H	0.494	-2.127	-3.556
H	2.009	-1.021	-1.916
H	-2.945	-2.152	-3.276
C	0.713	2.792	2.606
C	0.704	0.993	1.434
C	0.806	0.510	2.703
C	1.169	0.280	0.273
C	0.386	-0.301	-0.667
C	-1.037	-0.268	-0.485
C	-1.856	-0.877	-1.381
C	-1.265	-1.539	-2.480
C	0.139	-1.598	-2.698
C	0.943	-0.993	-1.800
O	0.937	-0.678	3.209
O	-1.997	-2.154	-3.380

V. Energy difference gradient (g) and nonadiabatic coupling (h) vectors at MECI geometry given in IV. Atom ordering follows that given in the MECI geometries in IV. R-AMI vectors have been rotated in the g-h plane to achieve maximal coincidence with the SA-2-CAS g and h vectors (only the plane spanned by the g and h vectors has chemical significance).

R-AMI-FOMO-CASCI(12/8)

Nonadiabatic Coupling (h)

0.106596	0.022126	-0.019506
0.464388	0.106976	0.011457
-0.003783	-0.000110	-0.003207
-0.066685	-0.012013	-0.017262
0.009794	0.353455	-0.213960
0.003841	-0.003827	0.010814
-0.001402	0.001562	0.000538
0.000455	-0.000329	-0.001293
0.005996	-0.009385	0.007072
-0.004426	-0.001674	-0.000232
0.041069	-0.015008	0.019018
-0.120323	-0.218908	0.153360
-0.408120	-0.025914	-0.203903
-0.089214	0.201287	0.115752
0.009506	-0.433623	0.152395
-0.027953	0.018932	-0.007940
0.003474	0.017203	0.010567
-0.037626	-0.030278	-0.033522
0.030536	0.030321	-0.006199
-0.008104	0.003187	-0.016614
0.066609	-0.022124	0.013703
0.025372	0.018119	0.028970

Energy difference gradient (g)

0.049138	0.002162	0.059662
0.200160	-0.220888	0.175514
-0.003991	-0.005983	0.008217
-0.030912	0.007688	0.026858
-0.059043	0.201961	-0.024066
-0.007355	-0.011985	-0.017464
0.003000	-0.000037	-0.003148
-0.000882	0.001274	0.003761
-0.012121	-0.007655	-0.004151
0.012204	0.001875	0.002172
0.000080	0.075858	-0.011201
-0.022154	0.409482	-0.299300
-0.238194	-0.112418	0.307001
0.025890	-0.324751	-0.423752
0.050184	-0.105315	0.214503
0.040670	0.001007	-0.020615
-0.004908	-0.012564	-0.034298
0.098488	0.050468	0.096528
-0.087408	-0.005163	-0.017771
0.025776	0.027248	0.043733
0.027463	0.069290	-0.003473
-0.066063	-0.041496	-0.078743

SA-2-CAS(2/2)/6-31G

Nonadiabatic Coupling (h)

0.100	0.063	-0.073
0.446	-0.023	0.019
-0.003	-0.014	-0.005
-0.067	0.000	-0.001
0.021	0.319	-0.244
0.018	0.053	-0.018
0.005	0.005	-0.002
-0.002	0.004	0.001
-0.001	0.000	-0.002
-0.014	-0.005	-0.002
0.012	0.029	0.032
-0.216	-0.039	0.200
-0.402	-0.022	-0.274
-0.081	0.070	-0.061
0.117	-0.252	0.280
-0.088	0.010	-0.007
-0.017	-0.003	0.080
-0.067	-0.081	-0.057
0.092	0.011	-0.011
-0.002	-0.047	-0.064
0.064	-0.164	0.132
0.083	0.086	0.080

Energy difference gradient (g)

0.087	0.066	0.087
0.189	-0.141	-0.012
-0.001	0.008	0.009
-0.031	0.000	0.008
-0.029	0.241	-0.067
-0.034	0.022	-0.030
-0.009	0.002	-0.004
0.002	-0.001	-0.005
0.002	0.003	0.003
0.023	0.005	0.007
-0.013	-0.077	0.124
0.105	0.126	-0.355
-0.276	-0.306	0.349
0.157	0.046	-0.016
-0.168	-0.279	0.004
0.139	0.027	0.003
0.033	-0.084	-0.084
0.105	0.072	0.140
-0.144	0.003	0.009
0.007	0.067	0.098
-0.006	0.293	-0.107
-0.138	-0.093	-0.163

VI. Twisted (about I-bond) MECI geometries for anionic protonation state of GFP chromophore, as depicted in Figure 4.

R-AMI-FOMO-CASCI(12/8)

H	-2.153	-0.375	-0.174
C	-1.064	-0.342	0.075
C	-0.429	0.876	0.126
C	0.964	1.051	0.059
C	1.557	2.265	0.063
C	0.810	3.474	0.144
O	1.371	4.644	0.118
C	-0.593	3.293	0.249
C	-1.168	2.071	0.242
H	1.611	0.139	-0.021
H	2.668	2.338	-0.013
H	-1.236	4.205	0.331
H	-2.283	1.994	0.323
C	-0.510	-1.589	-0.226
N	-0.197	-2.171	-1.374
C	0.232	-3.445	-1.237
H	0.489	-4.123	-2.086
N	0.182	-3.878	0.059
H	0.414	-4.762	0.383
C	-0.271	-2.752	0.865
O	-0.395	-2.913	2.082

SA-2-CAS(2/2)/6-3IG

H	-2.330	-0.378	0.100
C	-1.276	-0.418	0.309
C	-0.523	0.838	0.211
C	0.875	0.922	0.232
C	1.549	2.123	0.168
C	0.879	3.379	0.079
O	1.502	4.502	0.016
C	-0.543	3.275	0.066
C	-1.198	2.065	0.126
H	1.464	0.022	0.309
H	2.625	2.142	0.186
H	-1.102	4.191	0.002
H	-2.277	2.057	0.109
C	-0.664	-1.672	-0.089
N	-0.431	-2.106	-1.380
C	0.160	-3.265	-1.318
H	0.464	-3.824	-2.174
N	0.362	-3.713	-0.047
H	0.800	-4.554	0.233
C	-0.157	-2.747	0.826
O	-0.177	-2.837	2.031

VII. Energy difference gradient (g) and nonadiabatic coupling (h) vectors at MECI geometry given in **VI**. Atom ordering follows that given in the MECI geometries in **VI**. R-AM1 vectors have been rotated in the g-h plane to achieve maximal coincidence with the SA-2-CAS g and h vectors (only the plane spanned by the g and h vectors has chemical significance).

R-AM1-FOMO-CASCI(12/8)

Nonadiabatic Coupling (h)

0.080866	-0.036927	-0.088955
-0.105605	-0.030559	0.138663
0.072464	0.081431	-0.010746
-0.102070	-0.050449	0.000434
-0.001404	0.098809	0.006372
-0.101260	-0.164927	0.006757
0.067675	0.129527	-0.003500
0.108020	0.065441	-0.005049
-0.001436	-0.120181	-0.002452
0.003498	0.008358	-0.000923
-0.001056	-0.002546	0.000290
-0.000143	-0.002655	-0.000738
0.005040	0.004011	-0.000766
-0.035500	0.279960	-0.505485
-0.128687	0.159412	0.283254
-0.011203	-0.158463	0.077021
0.037250	-0.018838	-0.012556
0.027451	-0.092021	-0.106113
0.013080	-0.011156	-0.002808
0.042098	-0.111996	0.484901
0.030930	-0.026230	-0.257615

Energy difference gradient (g)

0.042779	0.094823	-0.397191
-0.114529	-0.063465	-0.098544
-0.011139	-0.053393	0.342571
0.019331	0.005015	-0.005899
-0.002101	-0.010134	-0.004224
-0.008285	-0.005126	0.013961
0.004972	0.009964	-0.002215
0.000299	-0.002195	-0.018640
-0.009945	0.014469	0.023793
0.000805	0.001852	0.005394
-0.000105	0.000011	-0.006132
-0.000924	0.000479	-0.006430
0.001969	0.000067	0.007337
0.184433	0.009641	0.142283
-0.411050	-0.136503	-0.033688
-0.099951	-0.039119	-0.024289
0.087980	0.043948	0.024865
-0.169107	-0.048297	-0.016063
0.027794	0.022623	0.000774
0.573178	0.195278	0.045181
-0.116392	-0.039935	0.007154

SA-2-CAS(2/2)/6-31G

Nonadiabatic Coupling (h)

0.035	-0.044	-0.090
-0.227	-0.250	0.276
0.241	0.327	-0.072
-0.223	-0.063	-0.002
-0.008	0.154	-0.008
-0.110	-0.170	0.012
0.097	0.162	-0.011
0.159	0.067	0.002
0.035	-0.224	-0.006
0.024	-0.007	0.001
0.008	0.003	-0.000
-0.001	0.006	0.002
-0.009	-0.002	-0.002
-0.125	0.273	-0.234
-0.035	0.009	0.028
0.015	-0.028	0.130
0.004	-0.000	0.003
0.032	-0.074	-0.047
0.007	-0.007	-0.004
0.094	-0.167	0.307
-0.011	0.032	-0.286

Energy difference gradient (g)

0.060	0.087	-0.398
-0.055	-0.116	-0.162
0.047	0.063	0.370
0.016	0.015	0.004
-0.006	-0.016	0.014
-0.020	0.015	0.036
0.003	-0.002	-0.010
0.021	0.006	-0.022
-0.015	-0.031	0.053
-0.000	0.001	-0.025
-0.000	-0.002	-0.015
-0.000	-0.002	-0.015
0.001	-0.000	0.005
0.112	-0.002	0.147
-0.503	-0.191	0.010
-0.000	-0.027	0.019
0.071	0.037	0.000
-0.112	-0.059	-0.027
0.009	0.004	0.000
0.449	0.272	-0.006
-0.074	-0.053	0.021

VIII. Coordinates of R-AM1-FOMO-CASCI(12/8) S_0/S_1 MECI of neutral GFP chromophore in a microsolvated environment, as depicted in Figure 5.

Atoms treated with QM method (Chromophore + 1 Water molecule)

H	-0.379080724	-0.000394787	-2.029975276
C	-0.364611459	-0.058216078	-0.902523287
C	0.864600393	-0.127126089	-0.296997826
C	1.067042611	-0.118283054	1.094999819
C	2.321396928	-0.077896280	1.634031567
C	3.427953362	-0.040554938	0.795740621
O	4.687110299	0.049078940	1.412023344
C	3.274771285	-0.073765722	-0.576958905
C	2.022266183	-0.137254035	-1.107440722
H	0.175152290	-0.136004539	1.771342273
H	2.466519310	-0.073646551	2.741505925
H	5.312811992	0.198245800	0.640816835
H	4.174960864	-0.064803538	-1.245414179
H	1.906419317	-0.190637086	-2.214670550
C	-1.668784846	-0.000488831	-0.375598189
N	-2.375170655	1.162392702	-0.110077791
C	-3.648696445	0.872649076	0.167548252
H	-4.447456239	1.637899078	0.383275436
N	-3.870108284	-0.480759350	0.135148452
H	-4.708908892	-0.950332273	0.340499201
C	-2.639248573	-1.103167421	-0.221194656
O	-2.532390386	-2.355847328	-0.435639683
O	6.398926449	0.703119385	-1.102823998
H	7.203160448	0.943783561	-0.567036735
H	6.760956298	-0.127022625	-1.529932589

Atoms treated with MM force field (50 water molecules)

O	-1.730567576	2.764509291	1.840549702
H	-1.895575202	2.199097672	0.976054218
H	-1.859135113	1.944005508	2.438784051
O	2.097757250	2.158224939	4.207268872
H	3.071871315	2.356337166	3.940641592
H	1.683555532	2.739927648	3.476552497
O	0.719071202	3.709144978	2.370648399
H	-0.250152448	3.385480571	2.253562452
H	0.593400476	4.613434282	2.793006919
O	-2.226125861	-2.745933079	-2.998290055
H	-2.266191216	-2.620161736	-1.977760393
H	-1.459096480	-3.414053997	-2.924943676
O	-6.498326458	0.536832903	-1.462306092
H	-6.805928398	0.692007644	-0.497740897
H	-6.884566037	-0.402481887	-1.608489702
O	-4.856962261	-3.454126787	-2.794907318
H	-3.880112444	-3.249353560	-3.026617649
H	-5.274564306	-3.283694609	-3.709446653
O	-0.137419648	-4.285929031	-1.985475374
H	0.406170631	-3.588485571	-2.523574380
H	0.506089453	-5.047282901	-2.121435289
O	1.227383969	-2.540861156	-3.395644308
H	2.037645247	-2.727689568	-2.792103735
H	1.455980959	-1.672731653	-3.867231410

O	3.065943735	-3.338941023	-1.587098414
H	3.362464934	-3.476903469	-0.622328022
H	3.948476298	-2.975082966	-1.974635499
O	-7.100843465	-2.062345443	-2.099619379
H	-6.256662326	-2.642360356	-2.132126560
H	-7.208085202	-2.142616230	-3.109820979
O	4.115127578	-0.110815073	-4.039216039
H	4.116186344	0.901934659	-3.957310512
H	3.168398140	-0.198152236	-4.401772394
O	-8.266096288	-2.474646317	0.303966009
H	-8.977663682	-3.173113361	0.193664475
H	-7.897019484	-2.372824681	-0.646638416
O	-4.268718344	3.868715309	1.878643591
H	-3.260260842	3.739778139	1.979942621
H	-4.518631790	3.097755079	2.507196962
O	-4.826603601	1.498611107	3.098360193
H	-3.889854426	1.086150934	3.206323003
H	-5.202710448	0.818589285	3.776408082
O	1.338230088	0.093176072	-4.562238499
H	0.343400637	-0.132295713	-4.671253617
H	1.197781736	0.936913371	-4.010921419
O	1.099054259	2.407763019	-2.913798822
H	1.389590703	2.591946042	-1.950715576
H	0.137340694	2.646287052	-2.677140075
O	-1.288691340	2.969393674	-1.507072879
H	-2.026382808	3.640441004	-1.252371459
H	-1.715944757	2.212808184	-0.886374931
O	-2.358470178	0.439713984	3.121372680
H	-2.115632028	-0.557471460	3.074076136
H	-1.600927284	0.622647046	3.805621614
O	-1.615831668	-2.177872230	2.894783176
H	-2.563299467	-2.577639909	2.843903800
H	-1.170212476	-2.781672687	2.203397585
O	-0.513960961	-3.504606194	0.625498613
H	-1.334756818	-3.055981866	0.183887165
H	-0.256547490	-3.919768811	-0.273084030
O	-1.355819484	-0.378318226	-4.344271173
H	-2.095609952	0.251154719	-4.054473256
H	-1.667918619	-1.286615886	-4.004003153
O	-6.356170702	-2.287013491	-4.805923282
H	-6.479259968	-2.214416792	-5.800065518
H	-5.896636064	-1.388523036	-4.588950735
O	1.234094743	3.232141732	-0.270999889
H	1.106528805	3.397829534	0.732515394
H	0.258511955	3.260837523	-0.561059607
O	-3.524735178	4.249234857	-0.779140367
H	-3.885251802	4.330925638	0.168198629
H	-4.323712515	3.891235755	-1.301797340
O	-5.395773396	2.883798178	-2.243294636
H	-5.903013553	2.050300112	-1.924283267
H	-6.137684942	3.373742204	-2.716410999
O	-4.554170625	-3.857281998	-0.081325046
H	-3.695245952	-3.298545312	-0.234103206
H	-4.772615677	-4.004026877	-1.063377544
O	-4.175322710	-2.934226668	2.427191265
H	-4.333569411	-3.527519871	1.607374414
H	-5.056636498	-2.432593796	2.312133330

O	5.451483320	-2.189028208	2.570644231
H	5.081368144	-1.316897836	2.171450943
H	5.504048503	-1.797851394	3.505063595
O	5.239756986	-2.203599073	-2.625426894
H	6.218972296	-2.014174074	-2.409767676
H	4.946059578	-1.429898017	-3.229062734
O	3.932834231	-3.805914881	1.019875174
H	4.516987751	-3.221535818	1.630522735
H	4.439317606	-4.671828436	1.080728341
O	-6.420470434	-1.460684631	1.933981932
H	-6.770188528	-0.535242556	1.678846369
H	-7.147003789	-1.964284058	1.401769241
O	-6.798516947	1.152584599	1.209206107
H	-6.171874857	1.328564533	2.000218497
H	-7.051756768	2.146001114	1.127562268
O	-0.247475918	0.861826908	4.614133467
H	0.604216809	1.427924173	4.591064099
H	0.195115520	-0.060717301	4.653998536
O	-3.129433771	1.554401856	-3.189676494
H	-3.869631773	2.213555421	-2.946397538
H	-2.347824328	2.077710164	-2.802708206
O	3.019314737	-0.247334052	5.274752581
H	2.611065073	0.654844028	5.036432002
H	2.236944353	-0.872676567	5.087986481
O	1.572476455	-3.256795937	2.356899618
H	0.842138576	-3.416490322	1.658604959
H	2.405193437	-3.490028286	1.817271696
O	0.760563757	-1.634413171	4.331516752
H	-0.154690455	-1.934505186	3.998528891
H	1.221943319	-2.269651228	3.664519528
O	3.830090666	3.230755706	0.719685438
H	4.387785038	3.287556661	-0.131395269
H	2.906029199	3.248928519	0.293858013
O	4.575771911	2.536480538	3.238352909
H	5.557745453	2.768103211	3.034328387
H	4.285638401	2.796196374	2.285258705
O	-6.876367099	3.842819420	1.089748330
H	-5.916578333	4.030687368	1.390639348
H	-7.345216030	4.707436384	1.291059590
O	3.639636061	2.622342460	-3.814261302
H	2.657224159	2.565807648	-3.518711223
H	3.542800192	3.141924931	-4.670027233
O	5.234861285	3.093497885	-1.642316345
H	5.613645705	2.143807388	-1.606150036
H	4.666283232	2.995162783	-2.488048532
O	5.501555519	0.112152008	4.311303953
H	5.138503015	1.000443535	3.955116811
H	4.640782286	-0.095116792	4.835608310
O	7.649904111	-1.531207311	0.987246525
H	7.902312884	-0.857968019	1.714650480
H	6.930090470	-1.998376554	1.534117749
O	7.117578819	2.787152632	2.438092387
H	7.613228228	1.904264138	2.488736339
H	7.317446747	3.128220484	1.492616540
O	7.458470553	3.622771507	-0.127709724
H	6.602388364	3.551869504	-0.680778262
H	7.946418753	4.368424007	-0.586375841

O	-5.249456894	-0.041827672	-3.911624563
H	-5.702867374	0.221137787	-3.041189612
H	-4.381863724	0.484907279	-3.818458944
O	7.917433357	0.164045865	3.127317472
H	7.005638439	0.140743679	3.606973189
H	8.518918090	0.195924245	3.931995212
O	7.782123303	-1.729418486	-1.680155718
H	8.652012876	-2.205961965	-1.826866324
H	7.753144818	-1.698999039	-0.650149954
O	-5.664069321	-0.644426991	4.452505969
H	-6.033363455	-1.109825932	3.623461479
H	-5.348437188	-1.411404092	5.019033181

IX Structures corresponding to S_0 minimum of isolated neutral GFP chromophore using R-AM1-FOMO-CASCI(12/8), as shown in Figure 6.

C	0.3943	-0.1861	-3.1259
C	0.4829	-0.0778	-1.6395
N	1.8445	0.2121	-1.3277
C	2.5102	0.2789	-2.4480
N	1.7198	0.0514	-3.5807
C	-0.5490	-0.2100	-0.8074
C	-0.6281	-0.1215	0.6135
C	0.4589	-0.3224	1.4598
C	0.3301	-0.2231	2.8227
C	-0.8983	0.0828	3.3780
C	-1.9973	0.2773	2.5612
C	-1.8557	0.1704	1.2018
O	-0.9404	0.1731	4.7801
O	-0.5717	-0.4238	-3.8841
H	-1.5415	-0.4034	-1.3134
H	1.4622	-0.5854	1.0367
H	1.2143	-0.3896	3.4896
H	-1.9021	0.3763	4.9596
H	-2.9965	0.5186	3.0051
H	-2.7544	0.3268	0.5488
H	3.6089	0.4952	-2.5310
H	2.0196	0.0555	-4.5055

X Structures corresponding to S_0 minimum of neutral GFP chromophore microsolvated with 51 water molecules using R-AM1-FOMO-CASCI(12/8) with QM/MM method. Microsolvated S_1 minimum and S_0/S_1 MECI coincide and are given in **VIII**.

Atoms treated with QM method (Chromophore + 1 Water molecule)

H	-0.561352592	0.014730618	-2.198168278
C	-0.552958843	-0.039823478	-1.069304223
C	0.748008257	-0.123039609	-0.501897813
C	1.041512014	-0.909654555	0.612230161
C	2.319350108	-1.029348588	1.086614293
C	3.345229410	-0.349368748	0.454225533
O	4.627260429	-0.488072714	1.002796962
C	3.082248235	0.424289642	-0.666456088
C	1.800764326	0.528005628	-1.131636951
H	0.220018099	-1.489608592	1.098503321
H	2.539333450	-1.677559979	1.972052518
H	5.191952468	0.072663940	0.396336231
H	3.921389232	0.949007165	-1.186854025
H	1.589634671	1.153824805	-2.036964840
C	-1.769257517	-0.018576432	-0.510307472
N	-2.147797246	0.040857477	0.859035558
C	-3.466569096	0.004898607	0.929317050
H	-4.072216346	0.046925386	1.877122834
N	-4.055383837	-0.072335111	-0.320536983
H	-5.021095223	-0.161827679	-0.494262031
C	-3.026163063	-0.063448281	-1.276874666
O	-3.223651373	-0.091486557	-2.540951018
O	6.848887680	0.874847655	-0.970183507
H	6.272749268	1.649111488	-0.704412377
H	6.253697084	0.485583368	-1.672663769

Atoms treated with MM force field (50 water molecules)

O	-1.208919555	-0.742560407	3.048137607
H	-1.542799467	-0.386319156	2.092477759
H	-1.256038089	-1.707366579	2.711588574
O	1.513665234	-2.893033532	4.631659525
H	2.472239212	-2.770689972	4.918697783
H	1.247793111	-1.908262495	4.633163549
O	1.118836902	-0.203935906	4.286676064
H	0.213682225	-0.380075423	3.830174786
H	1.104834670	0.812398086	4.177397244
O	-2.725549859	2.096561064	-3.774568651
H	-2.911001442	1.181930507	-3.324955810
H	-1.984383616	1.694705877	-4.369399220
O	-6.640497838	1.352978434	0.280403005
H	-7.385715049	0.673471654	0.363258353
H	-6.779623921	1.534252352	-0.717171532
O	-5.109528780	3.310718721	-3.193791659
H	-4.283482169	2.809016363	-3.535930417
H	-4.708873000	4.242013212	-3.301115800
O	-0.604652486	0.969503719	-4.929937167
H	0.089619684	1.713559431	-5.054479093
H	0.101885405	0.254442130	-4.759504805
O	1.458670459	2.688180063	-4.771443301
H	2.297860843	2.135317244	-4.608624458
H	1.365467624	3.215023546	-3.904634040

O	3.550563281	1.111284829	-3.895350202
H	4.264999956	0.437152900	-3.598262678
H	3.812714745	1.886937771	-3.287051508
O	-6.945839576	1.434293314	-2.430890737
H	-6.409046187	2.217483467	-2.817790052
H	-6.455598761	0.739459727	-3.018221041
O	3.859484521	3.431976794	-2.364606966
H	4.126218813	4.258740060	-2.872798542
H	2.848555498	3.620924644	-2.296892622
O	-8.423432385	-0.432281047	-1.107198548
H	-9.340649653	-0.545881605	-1.498861464
H	-7.999080463	0.257993400	-1.734758597
O	-3.531264852	-0.264537209	4.393943835
H	-2.551537336	-0.333924133	4.105570475
H	-3.698665701	-1.254017785	4.191797360
O	-3.839315591	-2.814601001	3.417472741
H	-3.011914687	-3.017745969	2.838626788
H	-3.934809570	-3.715107743	3.856693327
O	1.218927490	3.892627077	-2.289684105
H	0.226362554	4.125702222	-2.409943529
H	1.144145763	3.711900973	-1.276471329
O	1.157017072	3.275399214	0.314684803
H	1.947701465	3.033055851	0.911101920
H	0.406836996	2.820436009	0.833895500
O	-0.853470464	2.085657394	1.788286588
H	-1.643414997	2.192952305	2.449462976
H	-1.272365242	1.195963487	1.407093857
O	-1.591072241	-3.239770337	1.988552456
H	-1.572086495	-3.351620470	0.969741483
H	-0.693171493	-3.707241198	2.167924712
O	-1.396926150	-3.491218537	-0.748569252
H	-2.416133223	-3.543842369	-0.911245339
H	-1.191746254	-3.149137571	-1.690172735
O	-0.530034389	-2.548536727	-3.224687607
H	0.426681149	-2.819809681	-2.996567137
H	-0.189492913	-1.784114228	-3.801523477
O	-1.497204657	4.139065154	-2.490530615
H	-1.839491195	3.804067311	-1.575362949
H	-1.902071817	3.375177356	-3.044962199
O	-3.715942022	5.685335842	-2.798289980
H	-2.799834160	5.236544050	-2.692589274
H	-3.459310859	6.563460393	-3.212673669
O	-2.989071917	2.290510927	3.314073722
H	-3.381502387	1.546651886	3.883919815
H	-3.775972872	2.619978607	2.743971570
O	-4.765000531	2.931980418	1.355653679
H	-5.545753341	2.326679153	1.063662276
H	-5.075937812	3.683557798	0.723796298
O	-3.255565791	-2.339335831	-3.812002455
H	-3.136854592	-1.413085937	-3.377894534
H	-2.272953438	-2.598432325	-3.840864201
O	-3.980649160	-3.312652348	-1.337140971
H	-3.988061424	-3.130904825	-2.339949127
H	-4.908701832	-2.951944996	-1.083757189
O	4.725015566	-2.940117080	-1.568189462
H	5.394296097	-2.900875606	-0.782994733
H	4.446331843	-3.886950195	-1.284153454

O	5.059079126	2.957741004	0.077440075
H	4.255452408	2.855322772	0.702565290
H	4.589661092	3.166820764	-0.806746783
O	5.332130782	-0.730898580	-3.003567377
H	5.057315162	-1.537738345	-2.429126904
H	5.928148585	-1.211189289	-3.654464037
O	-6.272727224	-2.076733225	-0.606555113
H	-6.275181635	-2.024231618	0.420067064
H	-7.150211936	-1.594923300	-0.805914903
O	-5.994351661	-1.735949655	2.038948703
H	-5.282774740	-2.240574057	2.564705619
H	-6.271412830	-1.077288307	2.774150527
O	0.932343389	-4.159019064	2.355051418
H	1.066937230	-3.746361770	3.290377184
H	1.936542571	-4.396415633	2.336408081
O	-2.423219665	3.231246857	-0.180799881
H	-1.772112633	2.955283454	0.548528879
H	-3.294463305	3.247005425	0.345267543
O	8.108301675	-0.742101267	0.811142948
H	9.024379535	-0.738979650	0.394842923
H	7.621307234	-0.098914801	0.176235872
O	1.425481632	-0.702170023	-4.153781145
H	2.209038287	-0.047804984	-4.171571665
H	1.831545347	-1.407349012	-3.534999244
O	2.114685199	-2.700222116	-2.398279883
H	1.813028328	-3.248826445	-1.587381148
H	3.111227634	-2.724368364	-2.170018251
O	3.177086417	2.519572060	2.067386400
H	3.876290065	2.013342577	2.618788417
H	2.451377281	2.519000340	2.789003525
O	3.563583217	-4.512204913	2.113755886
H	3.942514774	-4.773365145	1.210761296
H	4.302895031	-3.929339843	2.511892589
O	3.733812520	-0.936788702	4.328766370
H	4.188609537	-0.043656200	4.135147070
H	2.763707825	-0.610458215	4.329026949
O	5.181898530	1.264330403	3.497798644
H	5.896974110	0.532283733	3.477150417
H	5.826530212	1.959780008	3.101924866
O	5.367661365	-2.673169032	3.068910009
H	6.086536285	-1.987368525	3.304288346
H	4.655240682	-2.115386840	3.556937713
O	7.173542062	-0.622319414	3.348249487
H	7.559344119	-0.628676709	2.395955935
H	8.004550348	-0.533727341	3.907382286
O	1.173866396	-4.243853010	-0.348480710
H	1.086068938	-4.215777776	0.674033685
H	0.171680547	-4.094132132	-0.509802597
O	3.667399936	-5.247038690	-0.639329592
H	2.685034823	-4.963719611	-0.535426237
H	3.576565861	-6.227241402	-0.841944847
O	-6.218581843	0.015648439	4.089537971
H	-5.236703935	0.012286289	4.372123179
H	-6.659919193	0.671774953	4.706033150
O	-5.466444574	-0.351296510	-3.705498509
H	-4.559919590	-0.214790657	-3.221186270
H	-5.208504401	-1.187751899	-4.207143913

O	-5.289232863	4.556474144	-0.709301802
H	-4.740862115	5.238103297	-1.223218740
H	-5.471988958	3.979941921	-1.526048716
O	6.376268251	-2.909428977	0.521230814
H	7.095091585	-2.204532492	0.660031242
H	5.967819715	-2.900853181	1.458205108
O	6.811925019	2.899183209	2.115017604
H	7.356038965	3.736881319	2.029648750
H	6.214550487	2.955668387	1.280975189
O	0.991260150	2.453467066	3.704938195
H	0.279233290	2.334992993	2.972723126
H	0.573318064	3.175046486	4.269152257